CHEMISTRY
A European Journal

Supporting Information

Exploring the Potential of Fulvalene Dimetals as Platforms for Molecular Solar Thermal Energy Storage: Computations, Syntheses, Structures, Kinetics, and Catalysis

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1. Solvent Solubility Screens of 1b and 2b

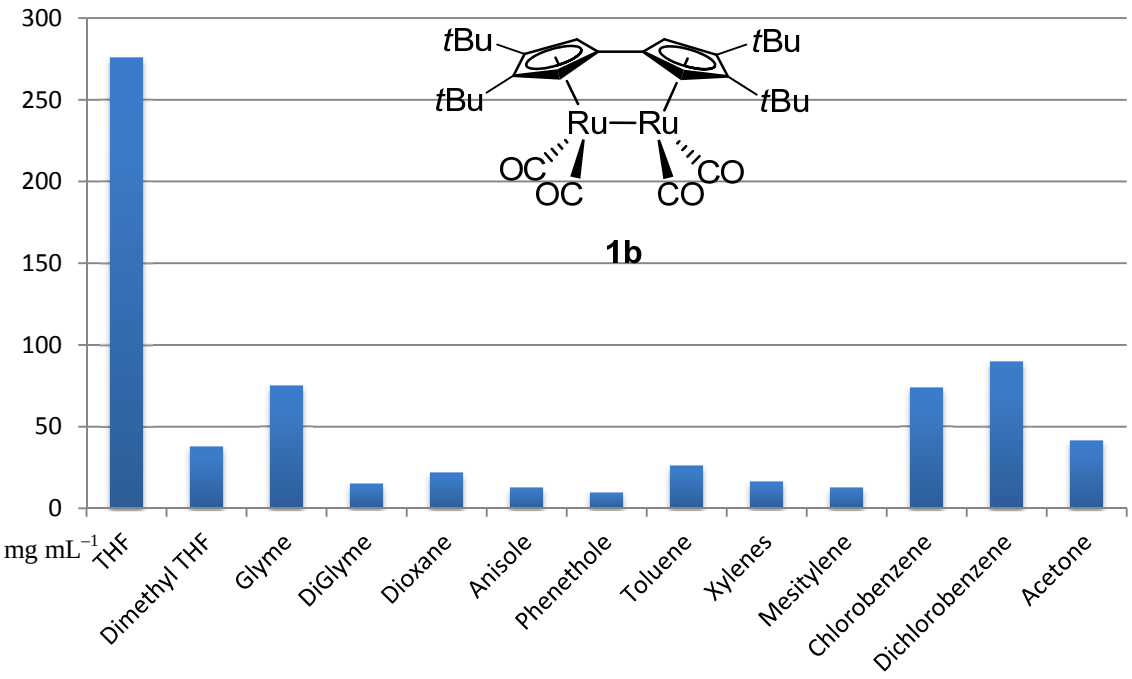


Figure S1. Solvent screen of **1b**. A 2 mL vial was loaded with a microstir bar and weighed. The vial was then charged with **1b** and the mass of the vial, stir bar, and sample was recorded. While stirring, the solvent to be analyzed was added via a microliter syringe until **1b** had completely dissolved. After weighing the total, using the density of the solvent, the mass per volume was determined for each of the respective solvents.

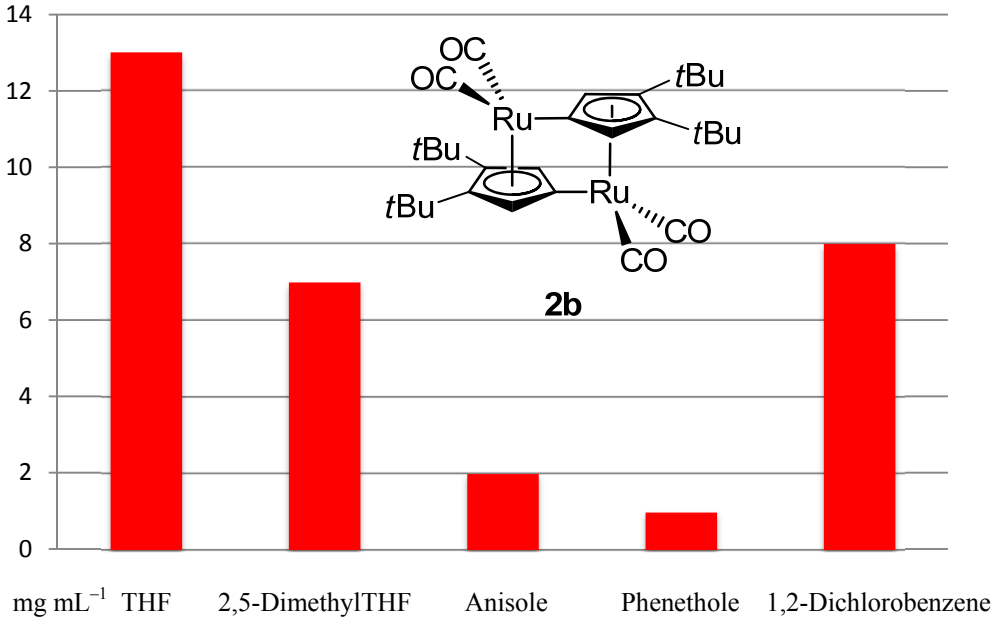


Figure S2. Solvent screen of **2b**. The procedure was the same as that in Figure S1.

2. Synthetic Procedures

(1,1',3,3'-Tetra-*tert*-butylfulvalene)tetracarbonyldiruthenium (4): See main text.

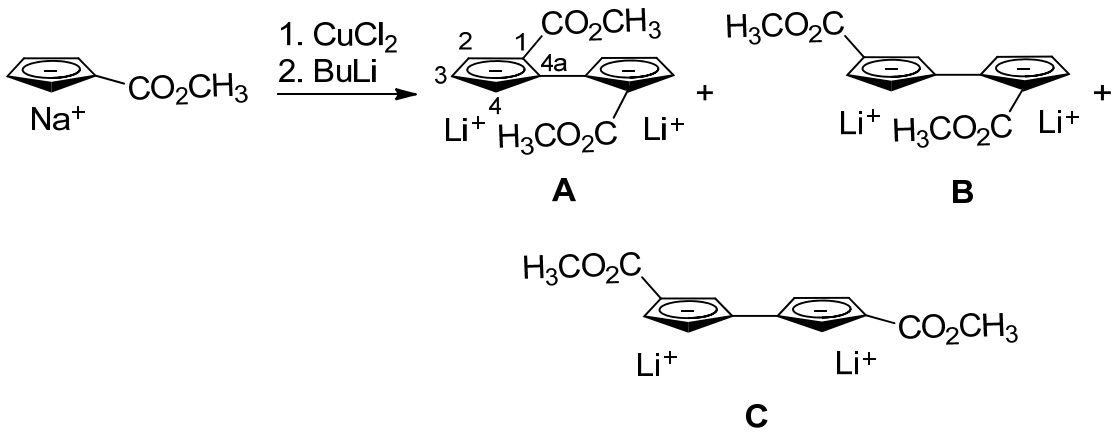
(1,1',3,3'-Tetra-*tert*-butylfulvalene)tetracarbonyldiruthenium dichloride (5): See main text.

(1,1',3,3'-Tetra-*tert*-butylfulvalene)tetracarbonyldiruthenium diiodide (6): See main text.

Iodonium salt 7: See main text.

(1,2,2',3'-Tetraphenylfulvalene)tetracarbonyldiruthenium (9): See main text.

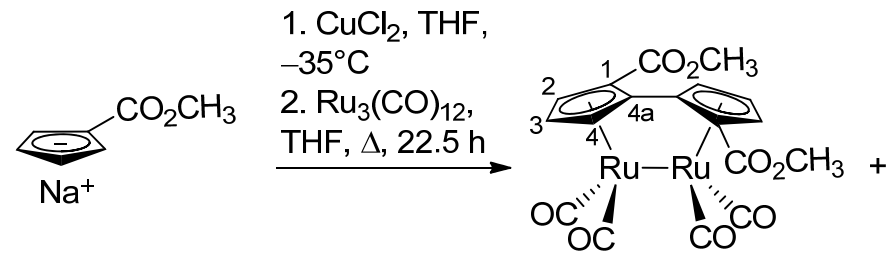
Dimethyl dilithium fulvalene dianion dicarboxylates A, B, and C:



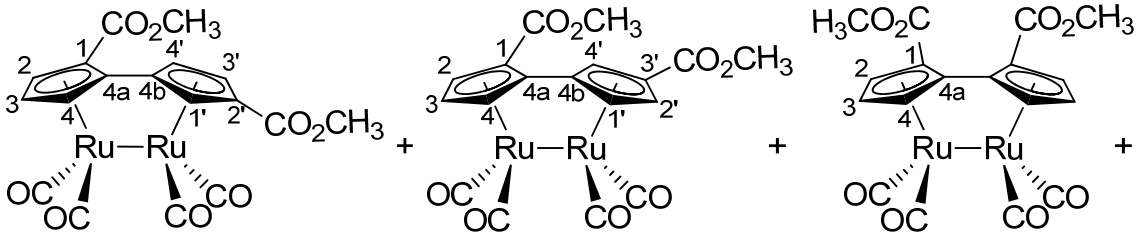
Methyl sodium cyclopentadienyl anion carboxylate[1] (1.60 g, 10.95 mmol) in THF (20 mL) was added dropwise within 60 min to a slurry of dry $CuCl_2$ (1.53 g, 11.38 mmol) in THF (20 mL) at –35°C. Stirring for an additional 5 min, followed by addition of pentane (150 mL) and filtration at –78°C gave a pale green solution of dimethyl dihydrofulvalenedicarboxylate, stored as such until further use.
Treatment with BuLi in hexanes (2.5 M, 4.40 mL, 11 mmol) at –78°C and warming to RT was followed by evaporation of solvent and the addition of pentane/Et_2O (2:1, 100 mL). The green precipitate was collected on a frit and washed with pentane (3x20 mL) to give a mixture of isomers **A**–**C** (1.20 g, 85%) contaminated with other complexes, in which **A** predominated. **A** (major isomer): ^{1}H NMR (500 MHz, [D_8]THF; see structure for numbering scheme): δ=6.41 (dd, $J_{2,3}$=4.08, $J_{2,4}$=2.67 Hz, 2H; H2), 5.74 (dd, $J_{2,3}$=4.09, $J_{3,4}$=2.26 Hz, 2H; H3), 5.65 (dd, $J_{2,4}$=2.66, $J_{3,4}$=2.27 Hz, 2H; H4), 3.49 (s, 6H; CH_3) ppm; ^{13}C NMR ([D_8]THF): δ=169.8 (OCO), 128.3 (C1), 112.1 (C2), 111.9 (C4), 108.9 (C3), 104.8 (C4a), 50.1 (CH_3) ppm; IR (KBr): $\tilde{\nu}$=2952, 2873, 1575, 1469, 1341, 1198, 1107, 750 cm^{-1}.

[1] W. P. Hart, D. Shihua, M. D. Rausch, *J. Organomet. Chem*. **1985**, *282*, 111.

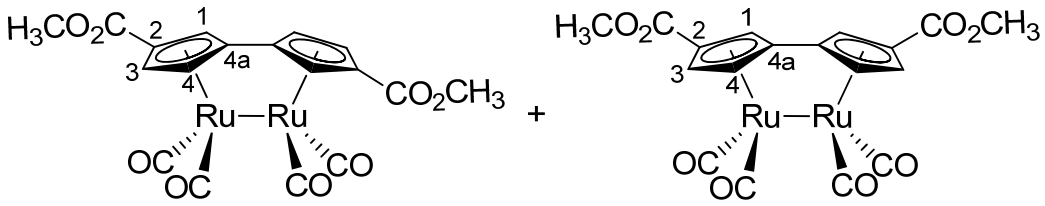
(Dimethyl fulvalenedicarboxylate)tetracarbonyldiruthenium (10) and its isomers:



10



D **E** **F**



G **H**

A solution of dimethyl dihydrofulvalenedicarboxylate (250 mL), prepared as above from methyl sodium cyclopentadienyl anion carboxylate (5.42 g, 37.1 mmol) and $CuCl_2$ (5.21 g, 38.8 mmol), was added in aliquots (20 mL) at 12 min intervals to boiling $Ru_3(CO)_{12}$ (4.12 g, 6.44 mmol) in THF (350 mL). Reflux was maintained for another 20 h, the mixture filtered through alumina (400 g), the solvent removed, and the residue chromatographed on alumina (2.65 kg) to separate eleven yellow fractions. Pure hexanes eluted a band of traces of recovered $Ru_3(CO)_{12}$, and gradient EtOAc-hexanes (0.1–0.5%) produced fractions 2–6, containing mixtures of small amounts of uncharacterizable compounds. Gradient EtOAc-hexanes (5–30%) furnished successively all six possible (dimethyl fulvalenedicarboxylate)tetracarbonyldiruthenium isomers **10** and **D**–**H** in five yellow fractions. None contained pure material, but showed partial enrichment of the respective complex (combined yield 1.45 g, 30%, ratio **10**:**D**:**E**:**F**:**G**:**H**=40:10:13:1:2:3). To obtain sufficient purity for unambiguous NMR measurements, these fractions were subjected individually to further column and preparative thin layer chromatography (alumina or silica, EtOAc/hexanes). Only **10** (0.96 g, 20%) could be sequestered pure

from fraction 6 by crystallization from EtOAc/hexanes, allowing for complete characterization and X-ray analysis.

10: See main text.

D: ^{1}H NMR (500 MHz, [D$_8$]THF; see structure for numbering scheme): δ=6.46 (dd, $J_{2,3}$=3.01, $J_{2,4}$=1.95 Hz, 1H; H2), 6.35 (dd, $J_{3',4'}$=3.10, $J_{1',3'}$=1.75 Hz, 1H; H3'), 5.91 (t, $J_{2,3=3,4}$=3.01 Hz, 1H; H3), 5.21 (dd, $J_{3',4'}$=3.10, $J_{1',4'}$=2.06 Hz, 1H; H4'), 4.94 (dd, $J_{1',4'}$=2.06, $J_{1',3'}$=1.75 Hz, 1H; H1'), 4.60 (dd, $J_{3,4}$=3.01, $J_{2,4}$=1.95 Hz, 1H; H4), 3.80 (s, 3H; β-CH$_3$), 3.60 (s, 3H, α-CH$_3$) ppm; ^{13}C NMR ([D$_8$]THF): δ=205.5, 205.3, 205.0, 204.9 (RuCO), 166.0, 165.2 (OCO), 96.4 (C$_{quat}$), 95.5 (C$_{quat}$), 93.7 (C$_{quat}$), 92.7, 91.5, 91.1 (C2, C3, C3'), 89.0 (C$_{quat}$), 84.6, 83.0, 82.3 (C4, C4', C1'), 52.9 (β-CH$_3$), 52.85 (α-CH$_3$) ppm.

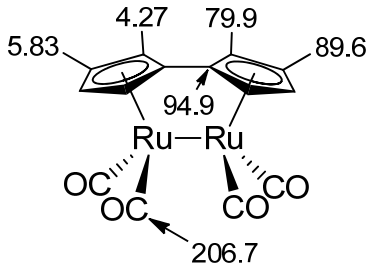
E: ^{1}H NMR (500 MHz, [D$_8$]THF; see structure for numbering scheme): δ=6.44 (dd, $J_{2,3}$=3.04, $J_{2,4}$=1.94 Hz, 1H; H2), 6.32 (dd, $J_{1',2'}$=3.11, $J_{2',4'}$=1.68 Hz, 1H; H2'), 5.96 (t, $J_{2,3=3,4}$=3.02 Hz, 1H; H3), 5.81 (dd, $J_{1',4'}$=2.04, $J_{2',4'}$=1.68 Hz, 1H; H4'), 4.53 (dd, $J_{3,4}$=3.01, $J_{2,4}$=1.95 Hz, 1H; H4), 4.43 (dd, $J_{1',2'}$=3.13, $J_{1',4'}$=2.04 Hz, 1H; H1'), 3.76 (s, 3H; β-CH$_3$) 3.58 (s, 3H, α-CH$_3$) ppm; ^{13}C NMR ([D$_8$]THF): δ=205.8, 205.7, 205.0, 203.8 (RuCO), 165.9, 165.5 (OCO), 95.2 (C$_{quat}$), 94.8 (C$_{quat}$), 93.9 (C$_{quat}$), 93.1, 93.0, 91.1 (C2, C3, C2'), 88.1 (C$_{quat}$), 85.0, 83.8, 82.6 (C4, C4', C1'), 52.89 (β-CH$_3$), 52.82 (α-CH$_3$) ppm.

F: ^{1}H NMR (400 MHz, [D$_8$]THF; see structure for numbering scheme): δ=6.35 (dd, $J_{2,3}$=2.98, $J_{2,4}$=1.98 Hz, 2H; H2), 5.82 (t, $J_{2,3=3,4}$=3.00 Hz, 2H; H3), 4.31 (dd, $J_{3,4}$=3.02, $J_{2,4}$=1.98 Hz, 2H; H4), 3.51 (s, 6H; CH$_3$) ppm; ^{13}C NMR ([D$_8$]THF): δ=205.8, 205.4 (RuCO), 165.8 (OCO), 94.2 (C$_{quat}$), 92.2 (C3), 91.5 (C$_{quat}$), 90.2, 83.4 (C3, C4), 52.9 (CH$_3$) ppm.

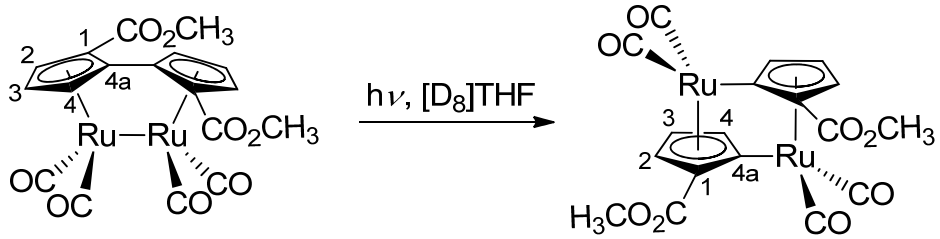
G: ^{1}H NMR (500 MHz, [D$_8$]THF; see structure for numbering scheme): δ=6.36 (dd, $J_{3,4}$=3.03, $J_{1,3}$=1.65 Hz, 2H; H3), 5.01 (dd, $J_{1,4}$=2.00, $J_{1,3}$=1.67 Hz, 2H; H1), 4.60 (dd, $J_{3,4}$=3.03, $J_{1,4}$=2.03 Hz, 2H; H4), 3.80 (s, 6H, CH$_3$) ppm; ^{13}C NMR ([D$_8$]THF): δ=92.6, 81.7, 81.5 (C3, C1, C4) ppm.

H: ^{1}H NMR (500 MHz, [D$_8$]THF; see structure for numbering scheme): δ=6.37 (dd, $J_{3,4}$=3.01, $J_{1,3}$=1.67 Hz, 2H; H3), 5.08 (dd, $J_{1,4}$=2.00, $J_{1,3}$=1.67 Hz, 2H; H1), 4.49 (dd, J$_{3,4}$=3.02, $J_{1,4}$=2.02 Hz, 2H; H4), 3.80 (s, 6H; CH$_3$) ppm; ^{13}C NMR ([D$_8$]THF): δ=92.2, 81.50, 81.45 (C2, C4, C1) ppm.
C$_{quat}$ of **G** and **H** (not assignable to the individual isomers): δ=205.4, 205.1, 204.7, 204.3 (RuCO), 165.39, 165.33 (OCO), 96.35, 96.31, 96.08, 95.8, 52.8, 52.7 (CH$_3$) ppm.

For comparison, NMR assignments of $FvRu_2(CO)_4$ in $[D_8]$THF (ppm):



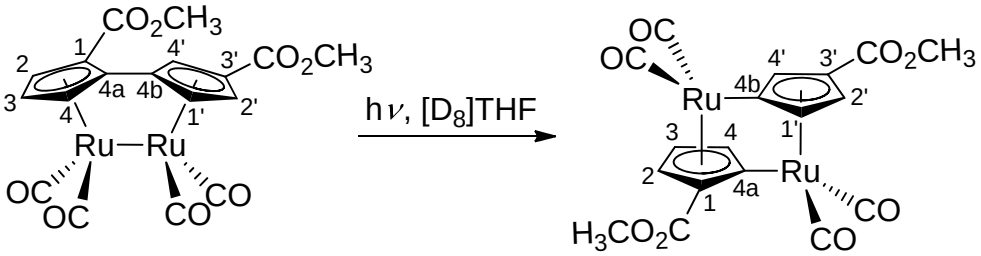
Photoisomerizations of (dimethyl fulvalenedicarboxylate)tetracarbonyldiruthenium isomers: Qualitative NMR experiments with various enriched fractions of dimethyl fulvalenedicarboxylate)tetracarbonyldiruthenium isomers (see preceding) showed that all appeared to undergo photoisomerization (to varying degrees). Semiquantitative experiments were executed with **10** and **E**, respectively.



10 **11**

11: See main text.

I:

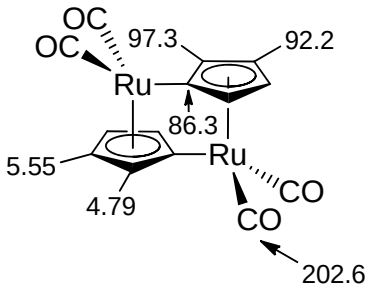


E **I**

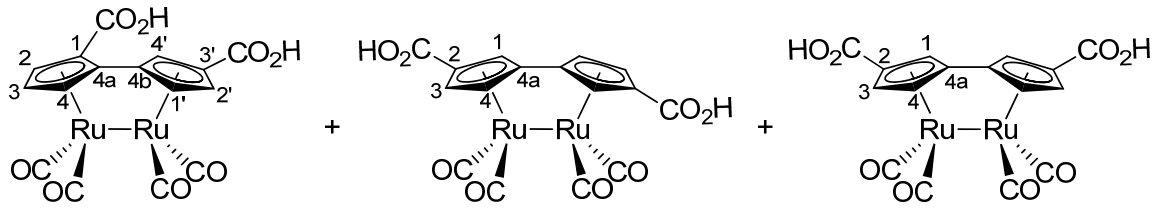
Prepared from **E** as described in the synthesis of **11** from **10** above. **I**: ^{1}H NMR (500 MHz, $[D_8]$THF; see structure for numbering scheme): δ=6.28 (dd, $J_{1',2'}$=2.64, $J_{2',4'}$=1.59 Hz, 1H; H2'), 6.15 (dd, $J_{2,3}$=3.15, $J_{2,4}$=1.87 Hz, 1H; H2), 5.76 (dd, $J_{2,3}$=3.14, $J_{3,4}$=2.39 Hz, 1H; H3), 5.34 (t, $J_{1',4'=2',4'}$=1.76 Hz, 1H; H4'), 5.06 (dd, $J_{3,4}$=2.36, $J_{2,4}$=1.90 Hz, 1H;

H4), 4.62 (dd, $J_{1',3'}$=2.64, $J_{1',4'}$=1.90 Hz, 1H; H1'), 3.74 (s, 3H; CH_3), 3.72 (s, 3H; CH_3) ppm.

For comparison, NMR assignments of (μ_2-η^1:η^5-cyclopentadienyl)$_2$Ru$_2$(CO)$_4$ in [D_8]THF (ppm):



Hydrolysis of C–F mixture to J–L:

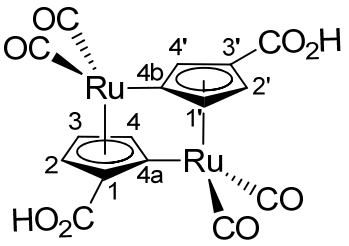


J **K** **L**

A mixture of diesters **E–H** (fraction 4 of the chromatographic work-up of their synthesis above; 108 mg, 0.193 mmol) in the ratio 65:2:10:15 in THF (3 mL) at –30°C was added to a solution of KOH (45 mg, 0.80 mmol) in EtOH (20 mL). Slow warming to RT and stirring overnight caused the bright yellow color to change to opaque beige. The solvent was removed by rotary evaporation, the remaining creamy solid redissolved in degassed H_2O (100 mL), filtered through celite, and treated at 0°C with aqueous HCl (4%; 700 µL). The pH of the solution changed from 10 to 4, during which precipitation occurred. After 3 h, the supernatant liquid was removed by syringe, the resulting orange yellow solid washed with water (2x40 mL), redissolved in Et_2O (70 mL), the solution washed again with water (2x50 mL), dried with $MgSO_4$, and filtered. Evaporation of the solvent produced a yellow powder of a mixture of diacids (48 mg, 47%) in the ratio **J**:**K**:**L**=6:2:1 (^{1}H NMR spectroscopy; signals due to hydrolyzed **F** could not be detected). **J**: ^{1}H NMR (400 MHz, [D_8]THF; see structure for numbering scheme): δ=11.4 (br s, 1H; OH), 6.42 (dd, $J_{2,3}$=3.00, $J_{2,4}$=1.96 Hz, 1H; H2), 6.26 (dd, $J_{1',2'}$=3.08, $J_{2',4'}$=1.68 Hz, 1H; H2'), 5.92 (t, $J_{2,3=3,4}$=3.00 Hz, 1H; H3), 5.87 (dd, $J_{1',4'}$=2.03, $J_{2',4'}$=1.68 Hz, 1H; H4'), 4.46 (dd, $J_{3,4}$=2.99, $J_{2,4}$=1.96 Hz, 1H; H4), 4.37 (dd, $J_{1',2'}$=3.09, $J_{1',4'}$=2.04 Hz, 1H; H1') ppm; ^{13}C NMR ([D_8]THF): δ=206.0, 205.95, 205.4, 204.1 (RuCO), 166.4, 166.0, (OCO), 96.0 (C_{quat}), 95.0 (C_{quat}), 93.8 (C_{quat}), 93.4, 93.0, 90.7 (C2, C2', C3), 89.0 (C_{quat}), 84.7, 84.4, 82.3 (C4, C4', C1') ppm; MS (FAB) of mixture: *m/z* 532 [M^+].
K: ^{1}H NMR (400 MHz, [D_8]THF; see structure for numbering scheme): δ=11.4 (br s, OH), 6.31 (dd, $J_{3,4}$=3.00, $J_{1,3}$=1.65 Hz, 2H; H3), 4.94 (dd, $J_{1,4}$=2.01, $J_{1,3}$=1.66 Hz, 2H;

H1), 4.56 (dd, $J_{3,4}$=3.00, $J_{1,4}$=2.01 Hz, 2H; H4); ^{13}C NMR ([D$_8$]THF; partial): δ=165.8 (OCO), 92.6, 81.8, 81.3 (C3, C1, C4) ppm.
L: ^{1}H NMR (400 MHz, [D$_8$]THF; see structure for numbering scheme): δ=11.4 (br s, OH), 6.32 (dd, $J_{3,4}$=2.96, $J_{1,3}$=1.66 Hz, 2H; H3), 5.03 (dd, $J_{1,4}$=2.08, $J_{1,3}$=1.62 Hz, 2H; H1), 4.44 (dd, $J_{3,4}$=2.97, $J_{1,4}$=2.04 Hz, 2H; H4) ppm.

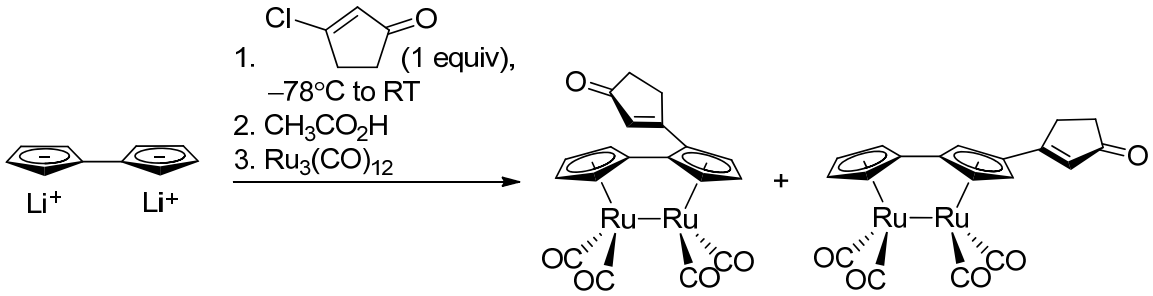
Photoisomerization of J–L mixture:



M

In an NMR tube, a sample of the mixture **J**–**L** (5 mg) in [D$_8$]THF was irradiated for 16 h using a Sylvania ELH 300 W slide projector lamp causing 50% conversion. Only **M** (derived from **J**) could be identified clearly: ^{1}H NMR (400 MHz, [D$_8$]THF; see structure for numbering scheme): δ=6.22 (dd, $J_{1',2'}$=2.59, $J_{2',4'}$=1.57 Hz, 1H; H2'), 6.14 (dd, $J_{2,3}$=3.10, $J_{2,4}$=1.87 Hz, 1H; H2), 5.74 (dd, $J_{2,3}$=3.10, $J_{3,4}$=2.39 Hz, 1H; H3), 5.29 (t, $J_{1',4'=2',4'}$=1.7 Hz, 1H; H4'), 5.03 (t, $J_{3,4=2,4}$=2.1 Hz, 1H; H4), 4.64 (dd, $J_{1',2'}$=2.58, $J_{1',4'}$=1.92 Hz, 1H; H1') ppm.

[1- And 2-(3-oxo-1-cyclopentenyl)fulvalene]tetracarbonyldiruthenium (12) and (13):



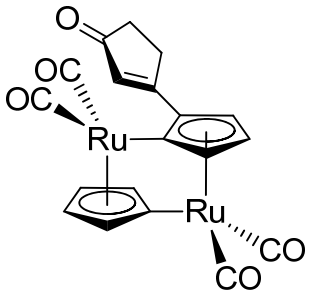
12 **13**

Dilithiofulvalene dianion [derived from Na(DME)Cp (6.25 g, 35.1 mmol)],[2] in THF (250 mL) was cooled to –78°C and treated with 3-chloro-2-cyclopentenone (2.05 g, 17.6 mmol) neat via syringe. The deep brown-black mixture was stirred for 15 min and then allowed to warm to RT. After renewed cooling to –78°C, AcOH (1.06 g, 17.6 mmol) was added by syringe, and the solution stirred for 5 min and then allowed to warm to RT over a 5 min period. Degassed heptane (450 mL) was introduced against an N_2 purge and the mixture stirred for 30 s, followed by extraction with 1% aqueous $Na_2S_2O_3$ (400 mL). The organic phase was dried over anhydrous Na_2SO_4, decanted into a 1 L Erlenmeyer flask,

[2] J. C. Smart, C. J. Curtis, *Inorg. Chem.* **1977**, *16*, 1788.

cooled to –78°C, and purged with N_2 for 15 min. This solution was then added via cannula in 10 mL aliquots over a period of 4 h to a 1 L round-bottom flask fitted with a septum-capped reflux condenser and magnetic stirrer bar, containing $Ru_3(CO)_{12}$ (5.00 g, 7.82 mmol) and dry, degassed, and boiling DME (400 mL). The mixture was heated to reflux for another 12 h, cooled to RT, the solvents removed, and the residue chromatographed on silica gel (50g). Et_2O-hexane (2:8) eluted a yellow-orange band, the contents of which were not identified. Et_2O-THF (8:2) produced a mixture of **12** and **13**, along with $FvRu_2(CO)_4$ (**1a**) and $[CpRu(CO)_2]_2$. This fraction was rechromatographed on silica gel (250 g), eluting with Et_2O-hexane (8:2), to furnish (in order of elution) a broad-yellow band of $FvRu_2(CO)_4$ (**1a**) and $[CpRu(CO)_2]_2$ (~1% combined yield), followed by **12** (625 mg, 10.2%) as an orange-yellow powder. M.p. 249–250°C (dec.; from CH_2Cl_2-hexane). ^{1}H NMR (300 MHz, [D$_8$]THF): δ=6.35 (t, J=1.8 Hz, 1H), 6.34 (dd, J=2.9, 1.9 Hz, 1H), 5.94 (td, J=2.9, 1.6 Hz, 1H), 5.88 (t, J=2.9 Hz, 1H), 5.79 (td, J=2.8, 1.6 Hz, 1H), 4.54 (dt, J=2.8, 1.8 Hz, 1H), 4.48 (dt, J=2.8, 1.7 Hz, 1H), 4.38 (dd, J=3.0, 1.8 Hz, 1H), 2.88 (m, 1H), 2.20 (m, 3H) ppm; ^{13}C NMR ([D$_8$]THF): δ=206.6, 206.5, 206.13, 206.07, 205.8, 168.4, 134.6, 98.7, 94.9, 90.6, 89.9, 89.3, 88.4, 88.2, 81.8, 81.0, 78.1, 35.4, 32.2 ppm; IR (CH_2Cl_2): $\tilde{\nu}$=2021, 1960, 1710, 1608 cm^{-1}; UV/Vis (THF): λ_{max} (logε)=246 (4.30), 332 (3.79), 401sh nm (3.18); MS (70 eV): m/z (%): 524 [M^+] (44), 496 (21), 466 (61), 437 (54), 410 (46), 380 (100), 353 (44); elemental analysis calcd (%) for $C_{19}H_{12}O_5Ru_2$: C 43.68, H 2.32; found: C 43.44, H 2.47.
Further elution presented **13** (917 mg, 15.0%) as an orange-yellow powder. M.p. 244–245°C (dec.; from CH_2Cl_2-hexane). ^{1}H NMR (300 MHz, [D$_6$]acetone): δ=6.45 (dd, J=2.9, 1.7 Hz, 1H), 6.38 (t, J=1.7 Hz, 1H), 5.94 (m, 2H), 5.05 (t, J=1.8 Hz, 1H), 4.53 (m, 3H), 2.94 (m, 2H), 2.46 (apparent t, J=5.1 Hz, 2H) ppm; ^{13}C NMR ([D$_8$]THF): δ=207.0 (2C), 206.0 (2C), 205.5, 167.7, 128.4, 103.3, 95.6, 94.5, 89.7, 89.5, 89.0, 80.3, 80.0, 79.5, 78.2, 35.4, 29.6 ppm; IR (CH_2Cl_2): $\tilde{\nu}$=2019, 1958, 1709, 1607 cm^{-1}; UV/Vis (THF): λ_{max} (logε)=268 (4.57), 360 (4.26), 412sh nm (3.72); MS (70 eV): m/z (%): 524 [M^+] (73), 495 (38), 467 (90), 437 (73), 380 (100), 353 (29); elemental analysis calcd (%) for $C_{19}H_{12}O_5Ru_2$: C 43.68, H 2.32; found: C 43.86, H 2.33.

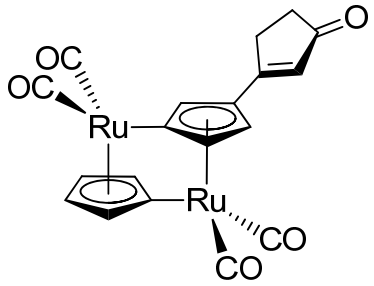
Photoisomerization of 12 to 14:



14

See main text.

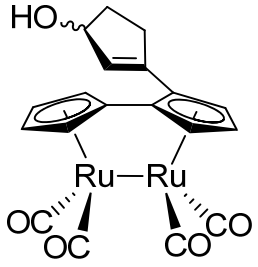
Photoisomerization of 13 to 15:



15

See main text.

[1-(3-Hydroxy-1-cyclopentenyl)fulvalene]tetracarbonyldiruthenium (N):



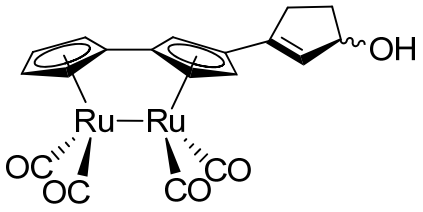
N

To **12** (200 mg, 0.383 mmol) in CH_2Cl_2 (50 mL) at 0°C was added *i*Bu_2AlH (1 M in CH_2Cl_2, 0.600 mL, 0.600 mmol). The mixture was stirred for 2 h at 0°C and subjected to standard aqueous workup to give the two diastereomeric alcohols **N** (185 mg, 92.1%) in the ratio 1.3:1. While not necessary, the isomers could be separated by silica gel chromatography (150 g), eluting with Et_2O-hexane (8:2), delivering first the minor isomer of **N** as yellow-orange crystals. M.p. 201–203°C (dec.; from hexane-THF). ^{1}H NMR (500 MHz, [D_8]THF): δ=5.90 (m, 2H), 5.80 (td, J=3.0, 1.7 Hz, 1H), 5.72 (td, J=3.0, 1.7 Hz, 1H), 5.65 (t, J=2.9 Hz, 1H), 4.79 (td, J=2.8, 1.7 Hz, 1H), 4.63 (m, 1H), 4.33 (td, J=2.8, 1.8 Hz, 1H), 4.07 (dd, J=3.1, 3.0 Hz, 1H), 3.86 (d, J=5.8 Hz, 1H), 2.33 (m, 1H), 2.12 (m, 2H), 1.58 (m, 1H) ppm; ^{13}C NMR ([D_8]THF): δ=206.8, 206.5, 206.4, 206.3, 138.5, 136.8, 100.9, 95.2, 90.9, 89.3, 88.2, 87.9, 87.1, 80.5, 79.5, 78.6, 77.4, 35.7, 34.6 ppm; IR (CH_2Cl_2): $\tilde{\nu}$=3608, 2017, 1955 cm^{-1}; MS (70 eV): *m/z* (%): 526 [M^+] (54), 496 (8), 466 (42), 438 (42), 409 (81), 394 (100); elemental analysis calcd (%) for $C_{19}H_{14}O_5Ru_2$: C 43.51, H 2.69; found: C 43.57, H 2.77.

A subsequent band contained the major diastereomer of **N** as yellow-orange crystals. M.p. 190–191°C (dec.; from hexane-THF). ^{1}H NMR (500 MHz, [D_8]THF): δ=5.95 (dd,

J=2.7, 1.9 Hz, 1H), 5.81 (td, *J*=2.9, 1.6 Hz, 1H), 5.75 (m, 1H), 5.72 (td, *J*=2.8, 1.6 Hz, 1H), 5.66 (t, *J*=1.9 Hz, 1H), 4.68 (m, 1H), 4.51 (td, *J*=2.9, 1.6 Hz, 1H), 4.34 (td, *J*=2.8, 1.8 Hz, 1H), 4.06 (dd, *J*=2.9, 2.0 Hz, 1H), 3.82 (d, *J*=6.1 Hz, 1H), 2.61 (m, 1H), 2.15 (m, 1H), 1.98 (m, 1H), 1.61 (m, 1H) ppm; ^{13}C NMR ([D_8]THF): δ=206.7, 206.4, 206.3, 206.2, 137.9, 137.6, 101.1, 95.2, 90.9, 89.4, 88.1, 88.0, 87.1, 80.5, 79.5, 78.2, 77.9, 36.1, 34.8 ppm; IR (CH_2Cl_2): $\tilde{\nu}$=3606, 2017, 1955 cm^{-1}; MS (FAB): *m/z* 526 [M^+]; elemental analysis calcd (%) for $C_{19}H_{14}O_5Ru_2$: C 43.51, H 2.69; found: C 43.05, H 2.62.

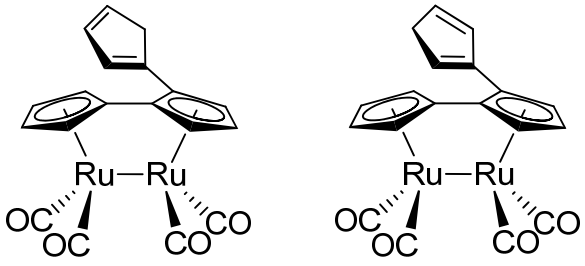
[2-(3-Hydroxy-1-cyclopentenyl)fulvalene]tetracarbonyldiruthenium (O):



O

Cyclopentenone **13** (110 mg, 0.21 mmol) was reduced in a manner identical to that of **12** to yield an inseparable mixture of diastereomers (1.3:1) of **O** (105 mg, 95%) as a canary yellow solid. M.p. 113–114°C (dec.; from hexane-acetone). ^{1}H NMR (300 MHz, [D_6]acetone): δ=6.14 (m, 4H), 5.89 (m, 4H), 4.85 (m, 2H), 4.71 (dd, *J*=4.2, 2.0 Hz, 2H), 4.45 (m, 2H), 4.38 (m, 4H), 3.93 (d, *J*=6.4 Hz, 0.87H), 3.89 (d, *J*=6.2 Hz, 1.13H), 2.63 (m, 2H), 2.38 (m, 4H), 1.75 (m, 2H) ppm; ^{13}C NMR ([D_8]THF): δ=206.5, 206.4, 206.3 (2C), 206.1 (2C), 206.0 (2C), 138.0, 137.8, 132.5, 132.2, 107.5, 107.3, 94.8, 94.7, 93.9, 93.8, 89.1 (2C), 87.1 (2C), 79.4, 79.3 (2C), 78.81, 78.77, 77.62, 77.55, 77.36, 77.25, 34.8, 34.7, 33.0, 32.9 ppm; IR (CH_2Cl_2): $\tilde{\nu}$=3682, 3680, 2015, 1952 cm^{-1}; UV/Vis (THF): λ_{max} (logε)=234 (4.26), 262sh (4.19), 341 (3.89), 391sh nm (3.34); MS (70 eV): *m/z* (%): 526 [M^+] (3), 508 (45), 480 (22), 452 (50), 424 (33), 394 (100); elemental analysis calcd (%) for $C_{19}H_{14}O_5Ru_2$: C 43.51, H 2.69; found: C 43.29, H 2.60.

[1-(Cyclopenta-1,3-dien-1-yl- and cyclopenta-1,4-dien-1-yl)fulvalene]tetracarbonyldiruthenium (P):

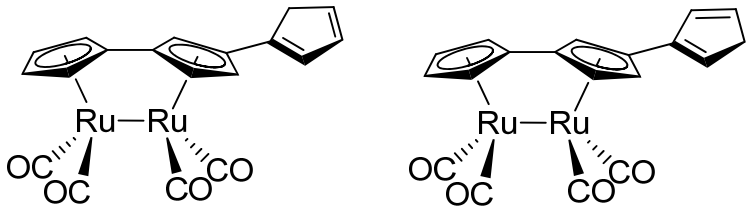


P

A solution of 4-methylbenzenesulfonic acid monohydrate (2.3 mg, 0.012 mmol) in C_6H_6 (15 mL) maintained at 60°C was added by cannula to **N** (63 mg, 0.12 mmol) in C_6H_6. The mixture was stirred for 2 min, neutralized with aqueous $NaHCO_3$, dried over K_2CO_3, filtered through silica gel (15 g), and subsequently subjected to chromatography on the

same support. Elution with Et_2O-hexane (1:1) gave a mixture (3:2) of the 1,3- and 1,4-diene isomers **P** (60 mg, 99%) as canary yellow crystals. M.p. 186–188°C (dec.; from Et_2O-hexane). ^1H NMR (300 MHz, [D_6]acetone): δ (major isomer)=6.02 (m, 2H), 5.86 (m, 2H), 5.74 (m, 2H), 4.47 (m, 2H), 4.20 (m, 2H), 3.23 (m, 1H), 2.81 (m, 1H); δ (minor isomer)=6.57 (m, 1H), 6.35 (m, 5H), 5.74 (m, 2H), 4.25 (m, 1H), 4.17 (m, 1H), 3.35 (m, 1H), 2.78 (m, 1H) ppm; ^{13}C NMR ([D_8]THF): δ (major isomer)=206.9, 206.5, 206.3, 206.2, 139.7, 134.9, 134.1, 133.0, 101.0, 95.4, 91.4, 89.3, 88.8, 87.8, 86.9, 80.4, 79.5, 78.0, 45.9; δ (minor isomer)=206.9, 206.5, 206.3, 206.2, 139.1, 135.4, 135.2, 133.5, 99.6, 95.2, 91.5, 89.6, 89.2, 88.0, 87.0, 80.3, 79.4, 79.0, 42.9 ppm; IR (CH_2Cl_2): $\tilde{\nu}$=2016, 1954 cm^{-1}; UV/Vis (THF): λ_{max} (logε)=240 (4.27), 273 (4.21), 329 (3.96), 399sh nm (3.22); MS (70 eV): *m/z* (%): 508 [M^+] (22), 480 (6), 452 (25), 424 (30.0), 396 (54), 78 (100); elemental analysis calcd (%) for $C_{19}H_{12}O_4Ru_2$: C 45.06, H 2.39; found: C 44.82, H 2.62.

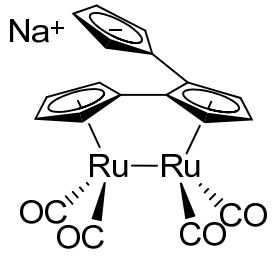
[2-(Cyclopenta-1,3-dien-1-yl- and cyclopenta-1,4-dien-1-yl)fulvalene]tetracarbonyldiruthenium (Q):



Q

Dehydration of **O** (55.5 mg, 0.106 mmol), executed in a manner identical to that employed for **N**, gave an inseparable mixture (3:1) of the 1,3- and1,4-diene isomers of **Q** (47.6 mg, 88.7%) as canary yellow crystals. M.p. 162–163°C (dec.; from Et_2O-hexane). ^1H NMR (300 MHz, [D_6]acetone): δ (major isomer)=6.84 (td, *J*=2.1, 1.4 Hz, 1H), 6.47 (m, 1H), 6.42 (m, 1H), 6.28 (dd, *J*=2.8, 1.7 Hz, 1H), 5.90 (m, 2H), 4.84 (dd, *J*=1.9, 1.8 Hz, 1H), 4.45 (m, 1H), 4.37 (m, 2H), 3.25 (dd, *J*=2.7, 1.4 Hz, 1H), 3.22 (dd, *J*=2.7, 1.4 Hz, 1H); δ (minor isomer)=6.67 (m, 1H) 6.48 (m, 1H), 6.42 (m, 1H), 6.30 (m, 1H), 6.28 (m, 1H), 5.87 (m, 2H), 4.88 (dd, *J*=1.9, 1.8 Hz, 1H), 4.40 (m, 1H), 4.38 (m, 1H), 3.14 (m, 2H) ppm; ^{13}C NMR ([D_8]THF): δ (major isomer)=206.9, 206.4, 206.3, 206.0, 140.1, 133.6, 133.4, 130.4, 108.3, 89.13 (2C), 89.09 (2C), 86.4, 79.3 (2C), 78.7, 76.4, 42.9, δ (minor isomer)=206.9, 206.4, 206.3, 206.0, 140.0, 135.2, 132.8, 129.0, 108.1, 94.8 (2C), 93.7 (2C), 87.1, 79.4, 79.3, 78.8, 77.2, 42.7 ppm; IR (CH_2Cl_2): $\tilde{\nu}$=2012, 1950 cm^{-1}; UV/Vis (THF): λ_{max} (logε)=236 (4.41), 274 (4.39), 345 (4.13), 396sh nm (3.65); MS (70 eV): *m/z* (%): 508 [M^+] (26), 480 (23), 452 (28), 424 (30), 396 (100); elemental analysis calcd (%) for $C_{19}H_{12}O_4Ru_2$: C 45.06, H 2.39; found: C 45.15, H 2.73.

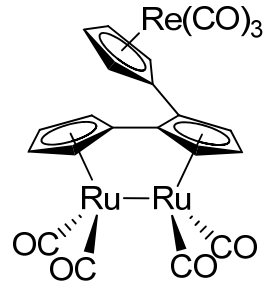
[1-(Cyclopentadienide-1-yl)fulvalene sodium]tetracarbonyldiruthenium (R):



R

In a glovebox, a solution of **P** (10 mg, 0.02 mmol) containing $NaNH_2$ (5 mg, 0.13 mmol) in THF (3 mL) was stirred for 5 min. The resulting orange-red mixture was filtered through glass wool and the filtrate, containing only **R** by ^{1}H NMR, used without further purification. ^{1}H NMR (400 MHz, [D$_8$]THF): δ=5.68 (t, J=2.7 Hz, 2H), 5.65 (td, J=2.8, 1.7 Hz, 1H), 5.62 (dd, J=2.7, 1.8 Hz, 1H), 5.60 (dd, J=2.7, 2.7 Hz, 2H), 5.40 (m, 2H), 4.36 (dt, J=2.8, 1.7 Hz, 1H), 4.14 (dt, J=2.8, 1.7 Hz, 1H), 3.75 (dd, J=2.9, 1.9 Hz, 1H) ppm; ^{13}C NMR ([D$_8$]THF): δ=112.5, 108.1, 107.5 (2C), 105.4 (2C), 97.5, 91.5, 87.4, 86.6, 84.4, 83.8, 79.8, 79.0, 76.1 ppm (RuCO not detected).

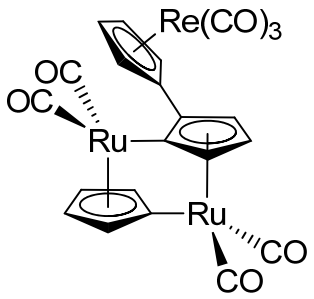
1-[Cyclopentadienylrhenium(tricarbonyl)fulvalene]tetracarbonyldiruthenium (16):



16

In a glovebox, a solution of **R** prepared from **P** (40 mg, 0.079 mmol) in THF (5 mL) was added to [Re(CO)$_3$(THF)Br]$_2$ (33.3 mg, 0.040 mmol) in THF (5 mL) and the mixture allowed to stir for l h. Chromatography on silica gel (60 g), eluting with hexane-THF (8:2), gave air-stable **16** (50 mg, 82%) as yellow crystals. M.p. 243–246°C (dec.; from hexane-acetone). ^{1}H NMR (400 MHz, [D$_8$]THF): δ=6.02 (dt, J=2.8, 1.7 Hz, 1H), 5.86 (td, J=2.8, 1.5 Hz, 1H), 5.82 (dd, J=2.8, 1.8 Hz, 1H), 5.80 (td, J=2.8, 1.6 Hz, 1H), 5.70 (t, J=2.9 Hz, 1H), 5.47 (td, J=2.8, 1.7 Hz, 1H), 5.36 (td, J=2.8, 1.7 Hz, 1H), 5.11 (dt, J=2.8, 1.7 Hz, 1H), 4.37 (dt, J=2.9, 1.8 Hz, 1H), 4.19 (dd, J=2.9, 1.8 Hz, 1H), 3.88 (dt, J=2.9, 1.6 Hz, 1H) ppm; ^{13}C NMR ([D$_8$]THF): δ=206.7, 206.00, 205.97, 205.9, 194.6, 99.8, 95.6, 94.2, 94.0, 93.8, 91.7, 90.8, 89.8, 88.8, 87.2, 85.6, 84.2, 80.7, 80.2, 79.7 ppm; IR (CH_2Cl_2): $\tilde{\nu}$=2018, 1958, 1935 cm^{-1}; UV/Vis (THF): λ_{max} (logε)=247 (4.08), 276 (4.05), 329 (3.83), 400sh nm (3.10); MS (70 eV): m/z (%): 776 [M^+] (39), 750 (8), 722 (15), 692 (33), 663 (70), 608 (60), 578 (100), 551 (39); elemental analysis calcd (%) for $C_{22}H_{11}O_7ReRu_2$: C 34.07, H 1.43; found: C 34.32, H 1.83.

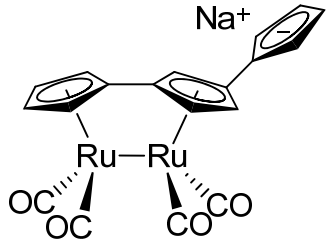
Photoisomerization of 16 to 18:



18

See main text.

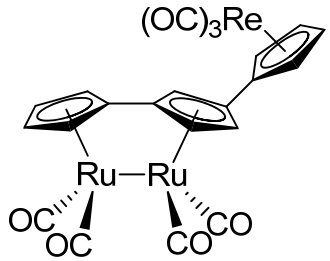
[2-(Cyclopentadienide-1-yl)fulvalene sodium]tetracarbonyldiruthenium (S):



S

In a glovebox, a solution of **Q** (10 mg, 0.02 mmol) containing $NaNH_2$ (5 mg, 0.13 mmol) in THF (3 mL) was stirred for 5 min. The resulting orange-red mixture was filtered through glass wool and the filtrate, containing only **S** by ^{1}H NMR, used without further purification. ^{1}H NMR (400 MHz, [D_8]THF): δ=6.11 (t, J=2.7 Hz, 2H), 6.00 (dd, J=2.7, 1.8 Hz, 1H), 5.77 (td, J=2.8, 1.6 Hz, 1H), 5.71 (t, J=2.8 Hz, 2H), 5.66 (td, J=2.8, 1.6 Hz, 1H), 4.52 (t, J=1.8 Hz, 1H), 4.25 (td, J=2.8, 1.7 Hz, 1H), 4.07 (t, J=2.3 Hz, 1H), 4.00 (td, J=2.8, 1.7 Hz, 1H) ppm; ^{13}C NMR ([D_8]THF): δ=210.1, 207.7, 207.5, 207.2, 124.5, 108.9, 107.4 (2C), 105.5 (2C), 95.7, 91.0, 88.3, 88.1, 81.1, 78.8, 78.4, 76.4, 71.3 ppm.

2-[Cyclopentadienylrhenium(tricarbonyl)fulvalene]tetracarbonyldiruthenium (17):

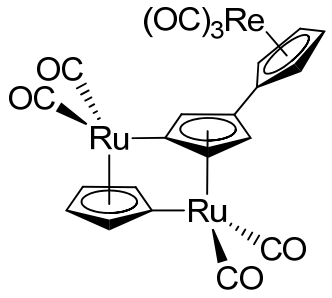


17

In a glovebox, a solution of **S** prepared from **Q** (50 mg, 0.099 mmol) in THF (5 mL) was added to [$Re(CO)_3(THF)Br]_2$ (46 mg, 0.050 mmol) in THF (5 mL) and the mixture allowed to stir for 30 min. Chromatography on silica gel (60 g), eluting with hexane-THF

(8:2), gave air-stable **17** (41 mg, 53%) as yellow crystals. M.p. 273–274°C (dec.; from hexane-acetone). ^{1}H NMR (400 MHz, [D$_8$]THF): δ=6.24 (dd, J=2.9, 1.8 Hz, 1H), 6.14 (dt, J=2.9, 1.8 Hz, 1H), 5.84 (td, J=2.8, 1.7 Hz, 1H), 5.82 (td, J=2.8, 1.7 Hz, 1H), 5.73 (dt, J=2.8, 1.7 Hz, 1H), 5.57 (td, J=2.8, 1.7 Hz, 1H), 5.51 (td, J=2.8, 1.7 Hz, 1H), 4.73 (t, J=1.9 Hz, 1H), 4.28 (m, 3H) ppm; ^{13}C NMR ([D$_8$]THF): δ=206.6, 206.1, 205.9, 205.6, 195.1, 102.8, 100.8, 94.4, 94.1, 89.4, 89.3, 87.6, 85.8, 85.4, 84.1, 83.7, 79.5, 79.3, 79.0, 77.4 ppm; IR (CH_2Cl_2): $\tilde{\nu}$=2026, 1962, 1937 cm^{-1}; UV/Vis (THF): λ_{max} (logε)=269 (4.14), 341 (3.86), 400sh nm (3.10); MS (70 eV): *m/z* (%): 778 [M^+] (30), 750 (17), 722 (27), 692 (53), 666 (78), 638 (42), 610 (32), 578 (100); elemental analysis calcd (%) for $C_{22}H_{11}O_7ReRu_2$: C 34.07, H 1.43; found: C 33.91, H 1.35.

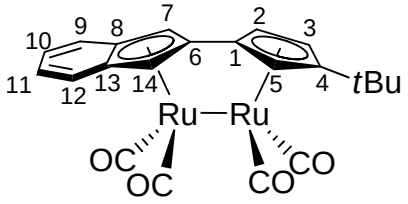
Photoisomerization of 17 to 19:



19

See main text.

(Benzo[3,4]-3'-*tert*-butylfulvalene)tetracarbonyldiruthenium (20):[3]



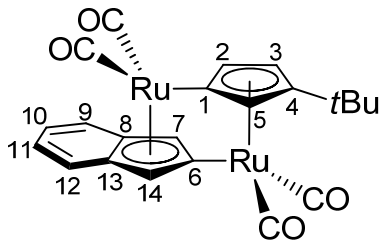
20

To $Ru_3(CO)_{12}$ (1.30 g, 2.0 mmol) in toluene (40 mL) was added 2-[4-(*tert*-butyl)cyclopenta-1,3- and 1,4-dien-1-yl]-1*H*-indene (0.74 g, 3.1 mmol)[4] and the mixture boiled for 6.5 h. After removal of solvent, the residue was chromatographed on alumina, eluting with petroleum ether-CH_2Cl_2 (3:1, then 1:1), to afford **20** (0.92 g, 56%) as an orange powder. ^{1}H NMR (500 MHz, $CDCl_3$; see structure for numbering scheme): δ=7.40 (AA'm, 2H), 7.25 (BB'm, 2H), 5.60 (t, J=2.1 Hz, 1H), 4.69 (s, 2H), 4.21 (t, J=2.1 Hz, 1H), 4.11 (t, J=2.0 Hz, 1H), 1.30 (s, 9H) ppm; ^{1}H NMR (500 MHz, [D$_8$]THF): δ=7.43 (m, 2H; H10, H11), 7.23 (m, 2H; H9, H12), 5.82 (dd, J=2.8, 2.0 Hz, 1H; H2), 5.03 (dd, J=2.0, 0.9 Hz, 1H; H7 or H14), 5.02 (dd, J=2.0, 0.9 Hz, 1H; H7 or H14), 4.60

[3] B. Li, X. Tan, S. Xu, H. Song, B. Wang, *J. Organomet. Chem.* **2009**, *694*, 1503.
[4] D. Tews, P. Escarpa Gaede, *Tetrahedron Lett.* **2004**, *45*, 9029.

(t, J=1.9 Hz, 1H; H5), 4.43 (dd, J=2.8, 2.0 Hz, 1H; H3), 1.30 (s, 9H; CH_3) ppm; ^{13}C NMR ([D_8]THF): δ=204.2, 203.1, 202.4, 202.2 (RuCO)**,** 128.2 (C4), 127.18 (C12), 127.13 (C9), 123.76 (C10), 123.73 (C11), 110.7 (2C; C8, C13), 96.7 (C6), 91.9 (C1), 86.8 (C2), 78.1 (C5), 77.3 (C3), 72.3 (C7), 72.2 (C14), 32.2 (CH_3), 31.9 (CCH_3) ppm; IR (crystal): $\tilde{\nu}$=2962, 2007, 1997, 1945, 1920, 1443, 1364, 1260 cm^{-1}; UV/Vis (hexane): λ_{max} (logε)= 241 (4.44), 299 (3.88), 381 (4.00), 450sh nm (3.22).

Photoisomerization of 20 to 21:

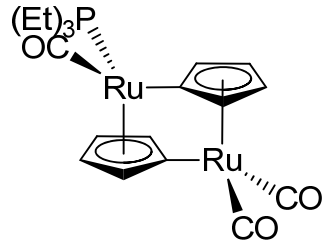


21

See main text.

Kinetics of thermal reversions of 2b, 14, 15, 18, 19, and 21. **2b**: A stock solution of **2b** (10.2 mg, 0.0152 mmol) in dried and degassed toluene (25 mL) was prepared inside a glovebox. Clean first order kinetics were recorded on a UV-Vis spectrometer by monitoring the rates of increase of the absorbance of **1b** at 395sh nm over the temperature range of 60–100°C, with data points collected in 5°C increments, $\Delta H^{\neq}$=25.0(±0.96) kcal mol^{-1} and $\Delta S^{\neq}$=–4.5(±2.7) e.u.
The experiment was repeated with diglyme as the solvent, $\Delta H^{\neq}$=24.1(±1.1) kcal mol^{-1}, $\Delta S^{\neq}$=–6.6(±3.6) e.u.
14, **15**, **18**, and **19**: In each case, a standard solution of the photoisomer (3.0 x 10^{-5} M) in diglyme was prepared in a glovebox and the rates of increase of the respective absorbances of **12 (**401sh nm), **13 (**412sh nm), **16** (400sh nm), and **17** (400sh nm) monitored by UV-Vis over greater than three half-lives at 65, 85, and 99°C, as above, $\Delta H^{\neq}$=25.4(± 0.1) kcal mol^{-1}, $\Delta S^{\neq}$=6.9(±0.2) e.u. for **14**, $\Delta H^{\neq}$=24.9(±1.2) kcal mol^{-1}, $\Delta S^{\neq}$=4.9(±3.5) e.u. for **15**, $\Delta H^{\neq}$=25.1(±0.3) kcal mol^{-1}, $\Delta S^{\neq}$=5.1(±0.9) e.u. for **18**, and $\Delta H^{\neq}$=22.3(±3.4) kcal mol^{-1}, $\Delta S^{\neq}$=–3.6(±9.5) e.u. for **19**.
21: In a glovebox, a stock solution of **21** (10.9 mg, 0.0198 mmol) was prepared in dried, degassed toluene (25 mL) and kinetic runs executed as above over the temperature range of 60–99 °C with data points collected in 10°C increments by monitoring the rates of increase of the absorbance of **20** at 450sh nm, $\Delta H^{\neq}$=22.6(±1) kcal mol^{-1}, $\Delta S^{\neq}$=–12.6(±3) e.u.

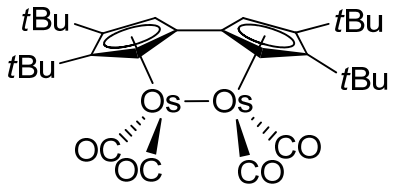
Photoisomerization of 22 to 23:



23

See main text.

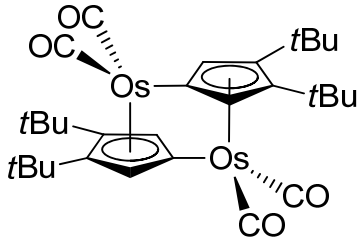
(2,2',3,3'-Tetra-*tert*-butylfulvalene)tetracarbonyldiosmium (24):[5]



24

A solution of 2,2',3,3'-tetra-*tert*-butyldihydrofulvalene (100 mg, 0.28 mmol) and $Os_3(CO)_{12}$ (210 mg, 0.23 mmol) in *o*-xylene (30 mL) under Ar was kept at reflux for 70 h. The mixture was cooled to RT, the dark brownish solution filtered through an Al_2O_3 plug, and the solvent evaporated. Column chromatography (Al_2O_3), eluting with CH_2Cl_2-petroleum ether (1:3), afforded **24** (100 mg, 42%) as a light yellow powder.

Photoisomerization of 24 to 25:[6]

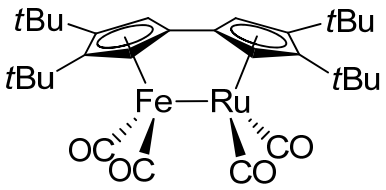


25

A pale yellow solution of **24** (20 mg, 0.024 mmol) in THF (15 mL) in a Pyrex vessel was irradiated with a projector lamp for 8 h. Removal of solvent and crystallization from CH_2Cl_2-hexanes (1:3) gave colorless **25** (18.6 mg, 93%).

(2,2',3,3'-Tetra-*tert*-butylfulvalene)tetracarbonyliron–ruthenium (27):

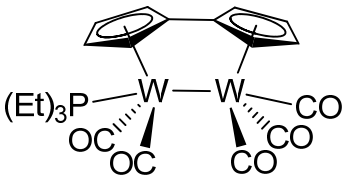
[5] Improving on B. Zhu, O. Š. Miljanić, K. P. C. Vollhardt, M. J. West, *Synthesis* **2005**, *19*, 3373.



27

See main text.

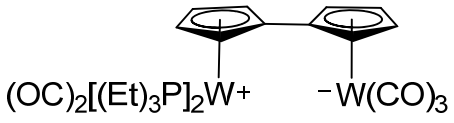
(Fulvalene)pentacarbonyl(triethylphosphine)ditungsten (S):



S

In a glove box, $FvW_2(CO)_6$ (100 mg, 0.15 mmol) in THF (6 mL), contained in a Pyrex bomb fitted with a Teflon stopcock, was treated with $P(Et)_3$ (44 μL, 35 mg, 0.3 mmol). The bomb was sealed, heated to 120°C for 16 h, cooled to RT, and the solvent evaporated. Crystallization from Et_2O-petroleum ether afforded **S** (75 mg, 66%) as a dark purple solid. M.p. 130–140°C (dec.; from Et_2O-petroleum ether); ^{1}H NMR (600 MHz, [D8]THF): δ=5.27 (t, J=1.8 Hz, 2H), 4.99 (quin, J=2.4 Hz, 2H), 4.70 (t, J=2.4 Hz, 2H), 4.67 (t, J=2.1 Hz, 2H), 2.06 (quin, J=7.8 Hz, 6H), 1.14 (dt, J=16.2, 7.2 Hz, 9H) ppm; ^{13}C NMR ([D8]THF): δ=88.8 (d, J=1.35 Hz), 87.7, 83.5, 83.4, 82.7, 81.3, 22.4 (d, J=31.1 Hz), 7.49 (d, J=2.6 Hz) ppm; ^{31}P NMR ([D8]THF): δ=14.98 (J_{P-W}=300 Hz) ppm; IR (crystal): $\tilde{\nu}$=1962, 1855, 1795, 1456, 1417, 1378, 1034, 982 cm^{-1}; UV/VIS (THF): λ_{max} (logε)=287 (4.14), 356 (4.40), 596 nm (3.23); MS (EI): *m/z* (%): 754 [M^+] (50), 726 (21), 670 (60), 640 (67)610 (61), 578 (71), 552 (77), 524 (37), 496 (11), 289 (100); HRMS (EI): *m/z* calcd for $C_{21}H_{23}O_5PW_2$: 754.0302; found: 754.0316.

(Fulvalene)pentacarbonylbis(triethylphosphine)ditungsten zwitterion (T) (structure tentative):[6]



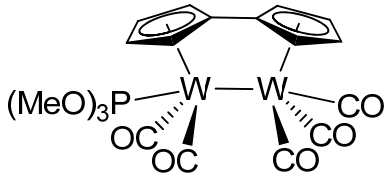
T

In a glove box, $FvW_2(CO)_6$ (100 mg, 0.15 mmol) in THF (6 mL), contained in a Pyrex bomb fitted with a Teflon stopcock, was treated with $P(Et)_3$ (295 μL, 230 mg, 2.0 mmol). The bomb was sealed, heated to 120°C for 16 h, cooled to RT, and the solvent evaporated. Crystallization from Et_2O-petroleum ether afforded **T** (55 mg, 42%) as a

[6] For related zwitterions of FvW complexes, see, e.g.: a) D. S. Brown, M.-H. Delville, K. P. C. Vollhardt, D. Astruc, *Organometallics* **1996**, *15*, 2360; b) M. Tilset, K. P. C. Vollhardt, R. Boese, *Organometallics* **1994**, *13*, 3146.

yellow brown powder. M.p. 80–100°C (dec.; from Et_2O-petroleum ether); ^{1}H NMR (600 MHz, [D8]THF): δ=5.98 (t, J=2.4 Hz, 2H), 5.68 (t, J=2.7 Hz, 2H), 5.06 (t, J=2.4 Hz, 2H), 4.98 (quin, J=2.4 Hz, 2H), 1.86 (quin, J=7.8 Hz, 12H), 1.05 (dt, J=15.6, 7.8 Hz, 18H) ppm; ^{13}C NMR ([D8]THF): δ=139.4, 112.7, 109.6, 104.3, 81.5, 72.5, 18.8 (m), 7.88 ppm; ^{31}P NMR ([D8]THF): δ=8.22 (J_{P-W}=229 Hz) ppm; IR (crystal): $\tilde{\nu}$=1922, 1821, 1519, 1454, 1347, 1031, 708, 666 cm^{-1}; UV/VIS (THF): λ_{max} (logε)=268 (3.77), 349 (3.53), 465 (3.30) nm; MS (EI): *m/z* (%): 844 [M^+–CO] (51), 816 (38), 760 (20), 726 (32), 670 (100); HRMS (EI): *m/z* calcd for $C_{26}H_{38}O_4P_2W_2$ [M^+–CO]: 844.1264; found: 844.1240.

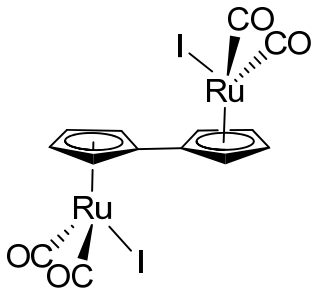
(Fulvalene)pentacarbonyl(trimethylphosphite)ditungsten (U):



U

In a glove box, $FvW_2(CO)_6$ (100 mg, 0.15 mmol) in THF (6 mL), contained in a Pyrex bomb fitted with a Teflon stopcock, was treated with $P(OMe)_3$ (0.30 mL, 315 mg, 2.5 mmol). The bomb was sealed, heated to 120°C for 36 h, cooled to RT, and the solvent evaporated. Crystallization from Et_2O-petroleum ether afforded **U** (100 mg, 88%) as dark purple crystals. M.p. 170–190°C (dec.; from Et_2O-petroleum ether); ^{1}H NMR (600 MHz, [D8]THF): δ=5.33 (t, J=2.2 Hz, 2H), 5.04 (quin, J=2.2 Hz, 2H), 4.72 (t, J=2.1 Hz, 2H), 4.67 (t, J=2.2 Hz, 2H), 3.68 (d, J=11.4 Hz, 9H) ppm; ^{13}C NMR ([D8]THF): δ=89.9 (d, J=2.0 Hz), 88.7, 84.0 (d, J=1.4 Hz), 83.5, 82.6, 81.2, 52.1 (d, J=5.4 Hz) ppm; ^{31}P NMR ([D8]THF): δ=155.8 (J_{P-W}=504 Hz) ppm; IR (crystal): $\tilde{\nu}$=3117, 2952, 1966, 1919, 1899, 1880, 1862, 1819, 1462, 1419, 1004, 837, 772, 738, 698 cm^{-1}; UV/VIS (THF): λ_{max} (logε)=344 (4.17), 573 (2.90) nm; MS (EI): *m/z* (%): 760 [M^+] (50), 732 (28), 676 (42), 648 (31), 605 (100), 573 (58), 525 (44); HRMS (EI): *m/z* calcd for $C_{18}H_{17}O_8PW_2$: 759.9680; found: 759.9694.

(Fulvalene)tetracarbonyldiruthenium diiodide (31):



31

From **2a** (or **1a**) and HI: A saturated solution of **2a** in [D6]acetone (2 mL, 80 mg, 0.18 mmol; see Figure S1) was prepared in a glovebox and transferred to a 10 mL flask fitted with a 14/20 outer joint connected via a Teflon vacuum valve to a vacuum line. After

thorough degassing, the solution was frozen with liquid N_2 and the valve opened briefly to allow the addition of concentrated HI (2 equiv). On melting, the evolution of gas was apparent and the initially colorless mixture turned bright orange. The solution was refrozen in liquid N_2 and the flask connected through the 14/20 joint to a mass spectrometer**.** H_2 was the only species detected among the volatiles. Thawing, followed by solvent evaporation, gave **31** (126 mg, 100%). A similarly processed solution of **1a** underwent no reaction with HI on the timescale of the experiment with **2a**. H_2 evolution occurred also on treatment of **2a** with other strong acids, such as HCl or HBF_4, but in these cases ^{1}H NMR monitoring revealed fulvalene product mixtures accompanied by considerable decomposition**.**

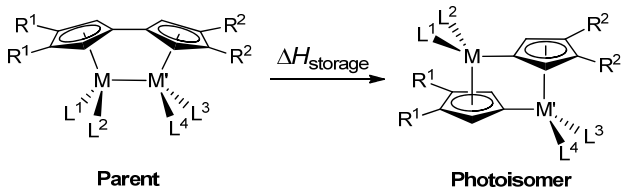
From **1a** (or **2a**) and I_2: A solution of **1a** (442 mg, 1.0 mmol) in THF (100 mL) was treated with I_2 (254 mg, 1 mmol) in THF (20 mL). After stirring at RT for 5 min, heptane (50 mL) was added, and the volume of the ensuing mixture reduced to ~ 30 mL on a rotary evaporator, resulting in the precipitation of large bright orange crystals. Recrystallization from toluene gave **31** (632 mg, 91%). The same procedure applied to **2a** (on a 0.1 mmolar scale) generated **31** in 88%. M.p. 258°C (dec.; from toluene); ^{1}H NMR (400 MHz, $CDCl_3$): δ=5.66 (t, J=1.9 Hz, 4 H), 5.40 (t, J=1.9 Hz,4 H) ppm; ^{1}H NMR (400 MHz, [D6]acetone): δ=6.13 (t, J=1.9 Hz, 4 H), 5.71 (t, J=1.9 Hz, 4 H) ppm; ^{13}C NMR ([D6]acetone): δ=196.4, 101.2, 87.0, 85.1 ppm; IR (KBr): $\tilde{\nu}$=2035, 1978 cm^{-1}; MS (EI): *m/z* (%): 612 [M^+–3CO] (12), 585 (62), 570 (70), 542 (30), 514 (10), 486 (16), 459 (100); elemental analysis calcd (%) for $C_{14}H_8I_2O_4Ru_2$: C 24.15, H 1.16; found: C 24.31, H 1.24.

1% $AgNO_3$-SiO_2: Under strict exclusion of light, to a solution of $AgNO_3$ (VWR-Alfa Aesar, 99.995%; 100 mg) in triply deionized H_2O (5mL) was added ultrapure SiO_2 (Fisher Scientific-Acros Organics, 10g) and the mixture shaken well. The volatiles were removed in vacuo and the residue calcined for 12 h at 150°C.

Cyclic voltammetry with 2a and b: Experiments were carried under an N_2 atmosphere inside a glovebox. Solutions were prepared in THF containing $Bu_4N^+PF_6^-$ (0.1 M) and **2** (1.0 mM). The working electrode was glassy carbon, and the reference and auxiliary electrodes consisted of platinum wires. Sweep rates were conducted at 100 mV s^{-1} and were subsequently increased to 1 and 10 V s^{-1} in an effort to attain quasi-reversible waves. Data collection proceeded first in the absence of ferrocene and was then repeated with ferrocene as an internal standard. Individual runs were started with either cathodic or anodic currents to probe potential reversibility.

3. Density Functional Theory Calculations
a. Table 1

Table 1. DFT estimates of $\Delta H_{storage}$ by the (2,2'-R^1_2-3,3'-R^2_2)FvM_2L_4 frame (M=Fe, Ru, Os).



Entry	R	M	L	$\Delta H_{storage}$ (kcal mol^{-1})
1 (cf. **1a→2a**)	$R^{1,2}$=H	M=M'=Ru	L^{1-4}=CO	20.8[a,7], 20.1[b]
2	$R^{1,2}$=OH	M=M'=Ru	L^{1-4}=CO	22.1[a], 21.8[b]
3 (cf. **1b→2b**)	$R^{1,2}$=*t*Bu	M=M'=Ru	L^{1-4}=CO	21.8[a], 21.0[b]
4	$R^{1,2}$=Me	M=M'=Ru	L^{1-4}=CO	21.7[a]
5 (cf. **8**)	$R^{1,2}$=C_6H_5	M=M'=Ru	L^{1-4}=CO	22.5[b]
6	$R^{1,2}$=Cl	M=M'=Ru	L^{1-4}=CO	20.1[a]
7	$R^{1,2}$=CF_3	M=M'=Ru	L^{1-4}=CO	19.4[a]
8	$R^{1,2}$=NO_2	M=M'=Ru	L^{1-4}=CO	18.5[a], 17.6[b]
9 (cf. **20→21**)	R^1=Benzo (indenyl ligand), one R^2=*t*Bu, second R^2=H	M=M'=Ru	L^{1-4}=CO	20.0[a], 19.0[b]
10	R^1=Benzo (indenyl ligand), R^2=H	M=M'=Ru	L^{1-4}=CO	19.3[a]
11	R^1=NMe_2, R^2=NO_2	M=M'=Ru	L^{1-4}=CO	22.0[a]
12	R^1=OH, R^2=CF_3	M=M'=Ru	L^{1-4}=CO	21.5[a]
13	R^1=OH, R^2=NO_2	M=M'=Ru	L^{1-4}=CO	21.5[a], 20.6[b]
14 (cf. **27**)	$R^{1,2}$=H	M=Ru, M'=Fe	L^{1-4}=CO	18.0[a]
15	$R^{1,2}$=H	M=M'=Fe	L^{1-4}=CO	15.9[a,7], 15.4[b]

[7] Y. Kanai, V. Srinivasan, S. K. Meier, K. P. C. Vollhardt, J. C. Grossman, *Angew. Chem.* **2010***, 122,* 9110; *Angew. Chem., Int. Ed.* **2010**, *49*, 8926

16	$R^{1,2}$=H	M=Ru, M'=Os	L^{1-4}=CO	12.1[a]
17	$R^{1,2}$=H	M=Fe, M'=Os	L^{1-4}=CO	11.0[a]
18 (cf. **24**→**25**)	$R^{1,2}$=H	M=M'=Os	L^{1-4}=CO	10.2[a,7]
19	$R^{1,2}$=H	M=M'=Ru	L^{1-4}=CS	20.7[a]
20	$R^{1,2}$=H	M=M'=Ru	L^{1-4}=H_2	20.3[a]
21	$R^{1,2}$=H	M=M'=Ru	L^{1-4}=2,2'-bipy (bidentate)	16.3[a]
22	$R^{1,2}$=H	M=M'=Ru	L^{1-4}=$P(OH)_3$	17.3[a]
23	$R^{1,2}$=H	M=M'=Ru	L^{1-4}=PF_3	15.2[a]
24	$R^{1,2}$=H	M=M'=Ru	L^{1-4}=PH_3	10.9[a]
25	$R^{1,2}$=H	M=M'=Ru	L^{1-4}=AsH_3	9.3[a]
26	$R^{1,2}$=H	M=M'=Ru	L^{1-4}=NH_3	–1.2[a], –3.5[b]
27	$R^{1,2}$=H	M=M'=Ru	$L^{1,2}$=2,2'-bipy (bidentate), $L^{3,4}$=CO	18.7[b]
28	$R^{1,2}$=H	M=M'=Ru	$L^{1,2}$=PEt_3, $L^{3,4}$=CO	18.6[b]
29 (cf. **22**→**23**)	$R^{1,2}$=H	M=M'=Ru	L^{1}=PEt_3, L^{2-4}=CO	17.3[b]
30	$R^{1,2}$=H	M=M'=Ru	$L^{1,2}$=PH_3, $L^{3,4}$=CO	17.2[b]
31	$R^{1,2}$=H	M=M'=Fe	$L^{1,2}$=PEt_3, $L^{3,4}$=CO	16.5[b]
32	$R^{1,2}$=H	M=M'=Fe	$L^{1,2}$=2,2'-bipy (bidentate), $L^{3,4}$=CO	14.6[b]
33	$R^{1,2}$=H	M=M'=Fe	$L^{1,2}$=PH_3, $L^{3,4}$=CO	14.0[b]

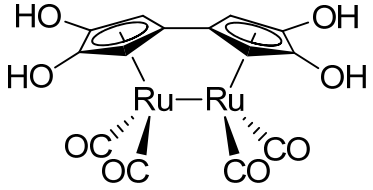
34	$R^{1,2}$=H	M=M'=Fe	L^1=PEt_3, L^{2-4}=CO	12.4[b]
35	$R^{1,2}$=OH	M=M'=Fe	L^{1-4}=CO	16.0[b]
36	R^1=OH, R^2=NO_2	M=M'=Fe	L^{1-4}=CO	15.8[b]
37	$R^{1,2}$=NO_2	M=M'=Fe	L^{1-4}=CO	13.9[b]

[a] Method: DFT-PBE with plane-wave basis (PBE/PW). PBE=Functional of Perdew, Burke, and Ernzerhof. [b] Method: BP86/Lanl2dz&631+g(d,p).

Method A: DFT-PBE with plane-wave basis (PBE/PW)

All calculations are performed using Quantum-Espresso code using PBE functional with the planewave basis set with ultrasoft pseudopotentials with the same set of parameters as in the previous work.[7]

Entry 2
Parent



Energy: -525.4151057253
Molecular coordinates

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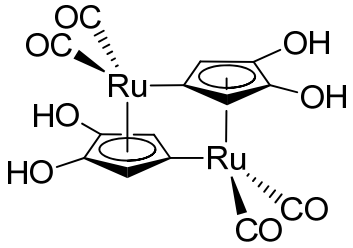
C	-0.595700854	4.450167460	-0.069619500
C	1.737123685	4.557547580	0.088117142
C	1.200867423	5.867523580	0.331534909
O	-1.082724082	6.857915379	0.224445000
H	-0.588684760	7.653501070	0.513388419
H	-1.612937678	4.100821906	-0.227936012
H	2.792836129	4.294986079	0.063237525
O	1.829163967	7.080161389	0.443019236
H	2.725178107	6.963013624	0.813211608
Ru	0.458869833	4.365912220	1.948309213
C	-0.969555812	4.489973095	3.200384289
O	-1.863551406	4.619517726	3.940348862
C	1.715177304	4.557494185	3.359905566
O	2.511267077	4.735931407	4.197284558
C	0.050380059	0.016021999	0.170676696
C	0.688567087	2.224944534	-0.202513193
C	-0.451626595	1.333908396	-0.101034643

C	1.881851646	1.440152883	0.046555235
C	1.480890645	0.079418793	0.240337657
O	-0.585892338	-1.197531664	0.164663727
H	-1.522999839	-1.088104449	0.416479960
H	-1.495626103	1.599547241	-0.254509374
H	2.910624617	1.791349332	0.031282556
O	2.330347011	-0.976247717	0.329146052
H	1.804598205	-1.779215315	0.527442803
Ru	0.575725333	1.467787559	1.913239747
C	-0.852012670	1.237545609	3.144585237
O	-1.749706797	1.036389790	3.866071148
C	1.831693916	1.304302965	3.334420241
O	2.623827771	1.151590327	4.178631705

Photoisomer



Energy: -525.3448023309

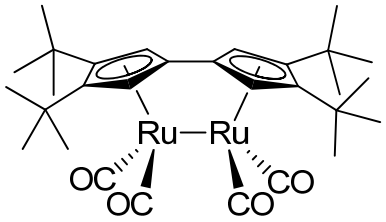
Molecular coordinates

C	-0.219223597	5.822581503	0.133058114
C	0.499045327	3.612546082	-0.253053606
C	-0.659087147	4.470616250	-0.132983742
C	1.649812693	4.440500697	0.035452873
C	1.201646882	5.802658215	0.251346668
O	-1.019859545	6.921939014	0.111341030
H	-0.476519142	7.706399372	0.333861412
H	-1.695548795	4.185648445	-0.302442223
H	2.690973706	4.120115216	0.013655736
O	1.912303573	6.971952480	0.336965914
H	2.835120303	6.785048347	0.595235854
Ru	0.360552553	4.357833210	1.889092645
C	-1.101421739	4.631011291	3.088426496
O	-2.016562879	4.798090570	3.792744747
C	1.636733662	4.585116909	3.288814573
O	2.447638633	4.733280349	4.116220232
C	1.044853059	0.037381807	1.641731884
C	0.322642892	2.245859573	2.029391088
C	1.482428375	1.390174759	1.906770253
C	-0.826849377	1.415427397	1.743558033
C	-0.376281124	0.054174417	1.526141130
O	1.848153698	-1.059955411	1.661034245
H	1.306022149	-1.845795900	1.440450380
H	2.518655138	1.677127523	2.074140896

H	-1.868633058	1.733536115	1.767459025
O	-1.084400979	-1.116823124	1.442006847
H	-2.008065701	-0.932255267	1.185142559
Ru	0.458272279	1.500600216	-0.112880693
C	1.916503067	1.224155058	-1.315994372
O	2.829690847	1.053865843	-2.022076600
C	-0.823029696	1.275356668	-1.508275464
O	-1.637556438	1.128575486	-2.332369617

Entry 3

Parent



Energy: -617.35833390

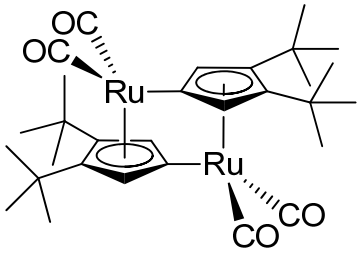
Molecular coordinates

C	0.001101601	5.872167882	0.190572400
C	0.675991982	3.659007197	-0.298038657
C	-0.448267661	4.531550753	-0.108234480
C	1.845315542	4.465078477	-0.094124189
C	1.472860217	5.831129515	0.200950983
H	-1.487452417	4.225135423	-0.184963728
H	2.865149820	4.097868233	-0.157933789
C	-0.191655559	0.037349502	0.152465511
C	0.630799197	2.209945123	-0.301103196
C	-0.547797930	1.404018449	-0.159220482
C	1.743515508	1.336503687	-0.055526670
C	1.278791024	-0.004327366	0.217598758
H	-1.562757130	1.771965984	-0.275255867
H	2.785406086	1.642516870	-0.077704936
Ru	0.685114333	4.387645715	1.849838441
Ru	0.511251314	1.478169173	1.841992081
C	-0.601587941	4.632183086	3.226978404
O	-1.393209536	4.840747057	4.062052626
C	2.053679587	4.395868602	3.166486862
O	2.919412842	4.448121355	3.950509682
C	-0.922442750	1.469385600	3.087374060
O	-1.826978618	1.417357779	3.826332994
C	1.726444966	1.231251646	3.282033750
O	2.475229061	1.021273411	4.155401789
C	-1.040497280	7.008683539	0.216455057
C	2.561039487	6.923889276	0.308752580
C	-1.284235515	-1.055168646	0.204994303
C	2.316887009	-1.141577461	0.296169074

C	1.938168822	-2.313429856	1.215870154
H	2.781623097	-3.022848093	1.259390330
H	1.063429517	-2.873310399	0.860279303
H	1.738452212	-1.962708567	2.241192162
C	3.674273221	-0.608846411	0.811665792
H	4.128884793	0.125182199	0.128384541
H	4.380655846	-1.451466182	0.888167570
H	3.583314366	-0.152503591	1.809039339
C	2.550031075	-1.659315712	-1.145958867
H	2.894408794	-0.844206448	-1.803588463
H	3.327966051	-2.441807624	-1.138412653
H	1.639816978	-2.088055805	-1.589243256
C	-1.030774506	-2.111298382	-0.894957964
H	-1.891316887	-2.799516378	-0.947954662
H	-0.916769379	-1.636732914	-1.883975525
H	-0.135681855	-2.717902347	-0.701511230
C	-1.411764453	-1.737209735	1.583479708
H	-1.765942278	-1.018167807	2.337163652
H	-2.150080475	-2.555418261	1.519170745
H	-0.468155327	-2.158593069	1.946625670
C	-2.668183561	-0.437172421	-0.097128680
H	-2.949282991	0.327089009	0.645500641
H	-3.429375791	-1.232866472	-0.051430490
H	-2.714218808	0.009170880	-1.104255626
C	-0.706091432	8.185561136	1.146652431
H	-1.552141817	8.893143850	1.148598695
H	0.182485272	8.745872510	0.827867025
H	-0.552241073	7.840333544	2.181712320
C	-2.419836628	6.477288140	0.671430531
H	-2.841068113	5.737192307	-0.026441642
H	-3.130106879	7.319403314	0.708164765
H	-2.374991943	6.028881014	1.675470424
C	-1.206461437	7.519768684	-1.237260666
H	-1.518906501	6.701603939	-1.906890223
H	-1.984500090	8.301527815	-1.269423314
H	-0.276602049	7.947642638	-1.639010061
C	2.366857713	7.974316336	-0.808702931
H	3.228511930	8.663062867	-0.818794493
H	2.306806904	7.494275960	-1.799865728
H	1.461939746	8.580934792	-0.667497197
C	2.614790884	7.611917655	1.689044781
H	2.922446482	6.894666421	2.464622191
H	3.360141559	8.425810483	1.662069405
H	1.655049182	8.040422596	1.997054605
C	3.959354638	6.304937182	0.084768655
H	4.199605461	5.543811904	0.844678572

H	4.716795020	7.101124922	0.168459606
H	4.060235482	5.854655515	-0.916621304

Photoisomer



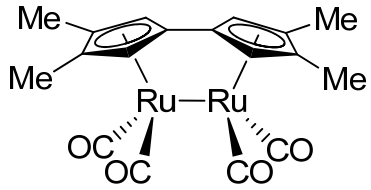
Energy: -617.2888298640

Molecular coordinates:

C	-0.059387504	5.922082487	0.184205560
C	0.613289316	3.685935103	-0.324721453
C	-0.500883891	4.562248404	-0.116421868
C	1.770782153	4.495301439	-0.082565152
C	1.402374362	5.879926584	0.208001593
H	-1.541315513	4.263007434	-0.213758019
H	2.793579332	4.133203262	-0.141454187
Ru	0.604367551	4.439618465	1.851672372
C	-0.736815160	4.662273012	3.189459597
O	-1.564869301	4.783901670	4.004499662
C	1.973228249	4.494119178	3.176653869
O	2.829107123	4.504946695	3.971591198
C	-1.106128773	7.053895500	0.173677751
C	2.494545360	6.969297943	0.311986374
C	-0.781706702	8.265057286	1.062652641
H	-1.627301313	8.972644948	1.027444466
H	0.111137491	8.812735474	0.733976545
H	-0.641188593	7.959787510	2.112354722
C	-2.486351958	6.535364687	0.639844262
H	-2.896682895	5.760586223	-0.025182373
H	-3.201722430	7.374088170	0.633210306
H	-2.447157848	6.134081137	1.664040818
C	-1.265051454	7.514777055	-1.297937503
H	-1.566384138	6.672552691	-1.942053737
H	-2.047294832	8.290272287	-1.362614578
H	-0.333691278	7.934460918	-1.705258133
C	2.323224337	7.991337270	-0.835651695
H	3.184466505	8.680668392	-0.846320771
H	2.283580201	7.485053739	-1.814414833
H	1.414715320	8.599829207	-0.729518282
C	2.525543015	7.694497419	1.673845472
H	2.819643315	6.997957356	2.473749459
H	3.272815355	8.506465076	1.639430421
H	1.561249343	8.132645593	1.953212179
C	3.894801905	6.341614393	0.128795469

H	4.115429700	5.591481048	0.905398939
H	4.653517905	7.136548150	0.214747761
H	4.014858033	5.872667606	-0.861299877
C	1.124995959	0.084851604	1.418412920
C	0.496112201	2.338665952	1.912578167
C	1.592648944	1.434298083	1.730457132
C	-0.675261694	1.558784091	1.643668816
C	-0.334296950	0.165863578	1.364260629
H	2.637651772	1.709548709	1.844054032
H	-1.690529220	1.944705354	1.686359762
Ru	0.539203718	1.583234773	-0.262748905
C	1.966199800	1.407954403	-1.513708946
O	2.858553081	1.320364892	-2.262488544
C	-0.743475967	1.473056241	-1.670235540
O	-1.534176107	1.421483534	-2.528599017
C	2.125724862	-1.092795142	1.371924406
C	-1.471555511	-0.873888477	1.317940165
C	-1.202745263	-2.112424694	0.448345468
H	-2.105944981	-2.745698604	0.437458273
H	-0.378686863	-2.732097111	0.825281599
H	-0.980196377	-1.825309409	-0.592253278
C	-2.776089830	-0.243621332	0.777425724
H	-3.154780505	0.566557536	1.418583514
H	-3.558972277	-1.019088316	0.746075310
H	-2.648078838	0.147356938	-0.243501440
C	-1.747522170	-1.312157662	2.779180473
H	-2.011070929	-0.444131894	3.405360480
H	-2.594489254	-2.018977079	2.802422189
H	-0.877801304	-1.806123700	3.236431728
C	1.808109862	-2.092284662	2.508256429
H	2.605721701	-2.852412513	2.563759495
H	1.760464325	-1.580754844	3.483930538
H	0.857895306	-2.621673545	2.354183100
C	2.168581848	-1.823190320	0.013158906
H	2.562333090	-1.156719797	-0.769364458
H	2.842532539	-2.694569691	0.087052484
H	1.187437332	-2.180485830	-0.317892080
C	3.561992085	-0.584043059	1.630093301
H	3.885858285	0.141976386	0.866856069
H	4.254795403	-1.440148255	1.584318420
H	3.668112524	-0.122981318	2.625450342

Entry 4
Parent



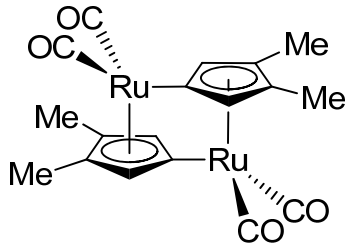
Energy: -452.3428156256

Molecular coordinates

C	-0.112761044	5.779327376	0.226579893
C	0.793144134	3.655805477	-0.172838442
C	-0.427859090	4.430928728	-0.156674373
C	1.858231818	4.545604700	0.210193514
C	1.311325609	5.853573921	0.451722742
C	-1.082636421	4.560306049	3.113663877
C	1.578282972	4.484368316	3.449340026
C	0.129280980	0.008542418	0.181382887
C	0.859138243	2.208195962	-0.162237656
C	-0.270603119	1.320023481	-0.254983987
C	1.964891777	1.428660748	0.348322831
C	1.520794595	0.079170416	0.559208758
C	-1.346061168	1.358028913	2.805469974
C	1.219666432	1.284032804	3.600428020
C	-1.085563056	6.913404490	0.286186059
H	-1.424594468	4.056625604	-0.384870112
H	2.910062500	4.281310388	0.305958040
C	2.111588503	7.080356139	0.752922303
C	-0.718880851	-1.221029656	0.123514399
H	-1.266267820	1.590695454	-0.603508853
H	2.968903750	1.794374210	0.556947474
C	2.393769181	-1.051290778	1.005535999
O	-2.007850664	4.750638870	3.800816618
O	2.330790816	4.614868393	4.331509034
O	-2.402241653	1.219010056	3.285432937
O	1.776560883	1.090708570	4.607624058
Ru	0.410167831	4.363784951	1.953177897
Ru	0.333138916	1.488012217	1.928652807
H	1.858963399	-1.736813366	1.678777280
H	3.275586957	-0.673382629	1.544199202
H	2.751265437	-1.636711254	0.139595122
H	-1.788060820	-0.972578948	0.204612301
H	-0.469486736	-1.915407149	0.938109284
H	-0.568147875	-1.757002594	-0.831728737
H	3.082368865	6.819722967	1.201073207
H	1.585801982	7.745134492	1.453564052
H	2.309638121	7.653783776	-0.171406486
H	-2.101246884	6.548503390	0.500045119
H	-1.112773279	7.458753154	-0.674507221

H	-0.813458752	7.630369946	1.074080151

Photoisomer



Energy: -452.2750369447

Molecular coordinates

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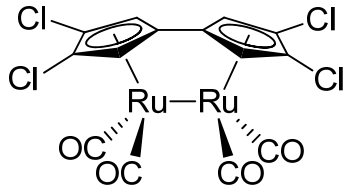
C	0.410755868	3.560665158	-0.285051474
C	-0.655890614	4.503376990	-0.073815276
C	1.630002931	4.308668747	-0.101259473
C	1.321978116	5.704128836	0.157714818
C	-0.853095498	4.712454487	3.160705304
C	1.888063034	4.576253527	3.167313769
C	0.995680663	0.056992182	1.550266098
C	0.404022774	2.298369484	2.047929248
C	1.499535475	1.397314663	1.787778103
C	-0.787829732	1.502573843	1.914952203
C	-0.436592912	0.120436297	1.632426198
C	1.489076618	1.122648605	-1.504643386
C	-1.224270607	1.326825654	-1.302448324
C	-0.902811247	7.089924542	0.282984167
H	-1.720290693	4.276702735	-0.127304569
H	2.638790213	3.905032512	-0.183900043
C	2.328944943	6.809665962	0.242646372
C	1.849248249	-1.162387630	1.382266540
H	2.557130599	1.659099996	1.807325727
H	-1.809048293	1.863499916	2.035856374
C	-1.403340401	-1.022723398	1.588234545
O	-1.712220841	4.915834831	3.924380099
O	2.752933350	4.701083296	3.940986804
O	2.260082134	0.900726718	-2.352089793
O	-2.146014386	1.226012778	-2.011840176
Ru	0.508038916	4.390464618	1.862818273
Ru	0.248094048	1.472774454	-0.098451674
H	-1.128882679	-1.765916080	0.825101335
H	-2.421440559	-0.668172963	1.365405585
H	-1.433727575	-1.538980808	2.564942382
H	1.387273098	-1.894689385	0.703110513
H	2.012274877	-1.656850170	2.356914938
H	2.838651108	-0.901337952	0.974581605
H	-1.916589318	6.891883281	0.664550147
H	-1.002309221	7.561211447	-0.711901396

H	-0.419790096	7.816311672	0.954837966
H	3.293809481	6.437067934	0.620079714
H	1.994451070	7.622946544	0.903728810
H	2.506568397	7.244933324	-0.757389314

Entry 6

Parent

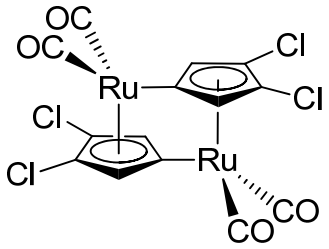


Energy: -520.6483057796

Molecular coordinates

C	-0.343584478	5.674273535	0.096206413
C	0.734481970	3.639569288	-0.236168070
C	-0.557206230	4.294069500	-0.223229635
C	1.730557064	4.625271926	0.099912511
C	1.066397301	5.883534953	0.297288010
C	-1.131583279	4.523634809	3.082149486
C	1.541182374	4.526794734	3.333510017
C	0.410656773	-0.043960871	0.141196219
C	0.927631171	2.201328910	-0.203239490
C	-0.121605183	1.217079585	-0.292925494
C	2.109190651	1.542433099	0.313100055
C	1.785727664	0.160500845	0.513011478
C	-1.213359246	1.315268962	2.765692096
C	1.352876898	1.318521947	3.570486181
Cl	-1.545681339	6.890630835	0.044239469
H	-1.521459399	3.845497887	-0.447314529
H	2.806357682	4.479691640	0.163021974
Cl	1.832132268	7.396361391	0.488864062
Cl	-0.367320680	-1.556980449	-0.000903282
H	-1.133646973	1.365601068	-0.661687130
H	3.082713642	1.991125763	0.493888597
Cl	2.906777335	-1.061755846	0.930581157
O	-2.038135895	4.703900447	3.791135198
O	2.319401572	4.669942678	4.187256776
O	-2.265081810	1.185138709	3.249719266
O	1.917984683	1.150971241	4.574432314
Ru	0.330269106	4.354876985	1.872006358
Ru	0.469213357	1.478236430	1.888980995

Photoisomer



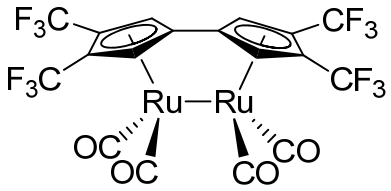
Energy: -520.5843010649

Molecular coordinates

C	-0.050486939	5.780451104	-0.028753959
C	0.429758687	3.492997550	-0.332275007
C	-0.630671765	4.457574850	-0.167517327
C	1.668524705	4.223840569	-0.219337749
C	1.371783775	5.634583043	-0.061560144
C	-0.733342226	4.880427833	3.083617606
C	1.993355538	4.650845252	3.015648429
C	0.852299265	0.072164427	1.780741900
C	0.376998989	2.359423620	2.084380823
C	1.435189325	1.393307002	1.913433007
C	-0.863131147	1.629647454	1.978913435
C	-0.569318864	0.217727442	1.820294837
C	1.497296292	0.931350273	-1.340702522
C	-1.216259982	1.265507646	-1.259043235
Cl	-0.903985087	7.263263095	-0.048666981
H	-1.700064260	4.261050217	-0.216447204
H	2.675776127	3.820866282	-0.303660671
Cl	2.511598246	6.910368058	-0.131497509
Cl	1.704769037	-1.411356162	1.797857448
H	2.506116358	1.582281861	1.947854755
H	-1.865822961	2.040691260	2.077165023
Cl	-1.699972783	-1.065231261	1.904455580
O	-1.552365541	5.150623677	3.865004753
O	2.884665500	4.798837890	3.749504332
O	2.296700755	0.616611912	-2.125634961
O	-2.114117785	1.184285915	-1.995400416
Ru	0.570525148	4.430233657	1.757391822
Ru	0.218571592	1.424445535	-0.005366064

Entry 7

Parent



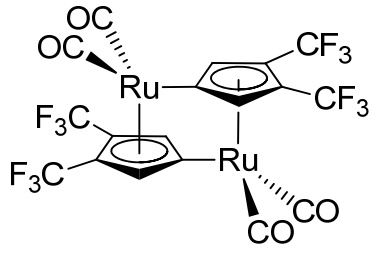
Energy: -1023.1261205428

Molecular coordinates

C	-0.433869527	5.665727148	0.347254523

C	0.718212379	3.717353124	-0.196813972
C	-0.583611057	4.326467234	-0.137118592
C	1.676488148	4.687804248	0.232335699
C	0.979982700	5.891550919	0.577778829
C	-1.149312143	4.295987900	3.252917598
C	1.473672566	4.456998621	3.459981927
C	0.457541080	0.043033523	0.105464128
C	0.944037509	2.290101091	-0.233437405
C	-0.077137437	1.294353597	-0.347730245
C	2.125276217	1.651456224	0.284249622
C	1.832157694	0.269432831	0.503939503
C	-1.226884570	1.172753551	2.681347055
C	1.245814025	1.301559553	3.590182431
C	-1.606446490	6.605585804	0.409877844
H	-1.527705981	3.849131651	-0.379630223
H	2.751941834	4.562137453	0.316235074
C	1.741783867	7.126957793	0.947340696
C	-0.340249528	-1.214214439	-0.049498797
H	-1.095582020	1.424361911	-0.703958830
H	3.079342396	2.120985138	0.502927684
C	2.913782405	-0.687929668	0.923782330
O	-2.010421880	4.363382486	4.030763176
O	2.224546536	4.630211505	4.329221838
O	-2.266663928	0.930439390	3.140706129
O	1.710571674	1.142360378	4.643146782
Ru	0.276632577	4.287953427	1.989998407
Ru	0.464239837	1.465188057	1.859935046
F	2.527566675	-1.562227237	1.893239318
F	4.007098861	-0.001898600	1.406537156
F	3.353453705	-1.416542218	-0.159107656
F	-1.683017909	-0.922394024	-0.167206021
F	-0.210438482	-2.074646760	0.993500492
F	0.019796318	-1.870965813	-1.207423786
F	3.056006593	6.818773978	1.227322676
F	1.237245968	7.763721384	2.039073042
F	1.768528862	8.004293676	-0.113574494
F	-2.791163589	5.901956386	0.323645607
F	-1.591708684	7.471719208	-0.660322444
F	-1.656637195	7.349489565	1.549007852

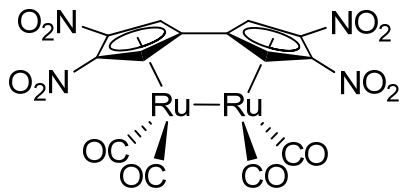
Photoisomer



Energy: -1023.0644205428
Molecular coordinates

C	0.092213009	5.768509172	0.035646520
C	0.477879072	3.478121189	-0.345617760
C	-0.535009683	4.480828134	-0.171807748
C	1.741737852	4.149677680	-0.219667348
C	1.515031509	5.564702102	0.002845889
C	-0.634870208	4.901097165	3.105925002
C	2.044121827	4.504637869	3.089569504
C	0.769093336	0.096011186	1.703704169
C	0.353880754	2.378741389	2.103579026
C	1.379079560	1.391865684	1.905030799
C	-0.899792338	1.687441338	2.001375508
C	-0.656660972	0.276230465	1.766205372
C	1.379399533	0.943304220	-1.399390931
C	-1.284029044	1.389339770	-1.283850670
C	-0.686280344	7.049287806	0.155994457
H	-1.610742962	4.325441670	-0.204125318
H	2.729327284	3.700750841	-0.302468014
C	2.625537809	6.580651879	0.014160545
C	1.576319250	-1.165793803	1.566354911
H	2.452701301	1.561579335	1.920886455
H	-1.892351577	2.120472824	2.106148448
C	-1.756579179	-0.751371496	1.766585638
O	-1.442777206	5.177253925	3.892542333
O	2.898339439	4.539222433	3.875454789
O	2.142949769	0.655726379	-2.225167527
O	-2.167823428	1.375681346	-2.037286534
Ru	0.653092338	4.418538210	1.779005901
Ru	0.151818020	1.442664344	-0.021507108
F	-1.764479458	-1.550195978	0.656022400
F	-2.986702264	-0.133319243	1.825985397
F	-1.670392470	-1.575504185	2.862786230
F	1.265283536	-1.877393524	0.441396962
F	1.399940213	-1.990766327	2.649762533
F	2.919711755	-0.872760842	1.497335112
F	-2.037841981	6.791888554	0.191261141
F	-0.461548531	7.874659913	-0.918534666
F	-0.382166131	7.748316209	1.291429794
F	3.851012821	5.951370361	0.001980414
F	2.606708274	7.401758540	1.107571087
F	2.578369512	7.382533463	-1.100952711

Entry 8
Parent

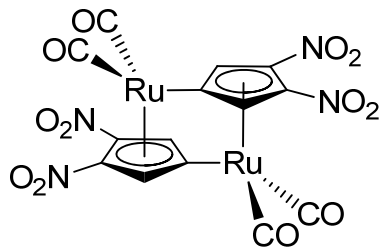


Energy: -727.5187274148

Molecular coordinates

C	-0.175863454	5.796419948	0.344259855
C	0.590039875	3.679391525	-0.223692977
C	-0.595832316	4.487507773	-0.057678474
C	1.738228188	4.499698733	0.073271931
C	1.259168027	5.801152898	0.422929334
H	-1.630108321	4.197320475	-0.228480260
H	2.787434919	4.215956565	0.046269008
C	-0.155710370	0.072637556	0.155166685
C	0.595059373	2.225921716	-0.275465472
C	-0.587806415	1.402691679	-0.146172892
C	1.749459196	1.392229975	-0.057303830
C	1.279408331	0.065628993	0.205215496
H	-1.624703887	1.704062420	-0.277424062
H	2.797438002	1.680564177	-0.081498680
Ru	0.445699975	4.318387507	1.961777465
Ru	0.492662318	1.433098238	1.860245523
C	-0.973105771	4.403233156	3.238785902
O	-1.846813145	4.505155759	3.995528726
C	1.683076626	4.427181207	3.411444448
O	2.446622279	4.555161992	4.277288865
C	-0.877367795	1.191081328	3.170598311
O	-1.717628912	0.995585053	3.946469372
C	1.782698737	1.282219358	3.260276036
O	2.580992829	1.130664722	4.089940711
N	2.149769520	-1.097779985	0.407156960
O	3.346164937	-0.938700445	0.105571644
O	1.629739950	-2.127294555	0.858121497
N	-1.078245083	-1.082847035	0.117144904
O	-0.821395309	-1.938119046	-0.738578371
O	-2.052216504	-1.054971460	0.879511472
N	2.134221584	6.942018161	0.731769246
O	3.308389113	6.840115348	0.333520786
O	1.643753531	7.888896042	1.358082676
N	-1.104011987	6.944720132	0.368509512
O	-0.743202017	7.948958478	-0.256636254
O	-2.185964640	6.774375855	0.948458197

Photoisomer



Energy: -727.4596040857

Molecular coordinates

C	-0.117156945	5.780187234	0.205683920
C	0.503256011	3.569134476	-0.268506817
C	-0.620235620	4.464249006	-0.100759231
C	1.692795255	4.337642020	-0.020228112
C	1.307401924	5.705987201	0.250131254
H	-1.673887828	4.226818369	-0.236736410
H	2.724742959	3.995790239	-0.057984459
Ru	0.460688321	4.366730958	1.907528731
C	-0.906748446	4.709606442	3.209673397
O	-1.746231329	4.913424060	3.981803385
C	1.788357227	4.447739413	3.284918255
O	2.607582220	4.500703351	4.104609943
C	0.920005167	0.075648215	1.597488218
C	0.296595695	2.285515610	2.072957697
C	1.421789638	1.392238867	1.902008950
C	-0.891987489	1.515170665	1.827820623
C	-0.504611358	0.147280390	1.556859234
H	2.475151420	1.632430601	2.035288232
H	-1.924462270	1.855036755	1.868481086
Ru	0.333817915	1.488398054	-0.103115390
C	1.691826886	1.140820343	-1.414081203
O	2.524986425	0.934553143	-2.192430453
C	-1.003613837	1.414613955	-1.471443203
O	-1.830126032	1.367383407	-2.284136137
N	1.772120568	-1.134609981	1.603481247
O	2.558211381	-1.295653103	0.663337777
O	1.656673585	-1.840580960	2.612968009
N	-1.425125451	-0.973999375	1.370529056
O	-0.931858897	-2.063789772	1.038320298
O	-2.629416492	-0.734747302	1.569083537
N	2.230795019	6.824677720	0.442766239
O	3.432875892	6.587185163	0.229070634
O	1.742050823	7.909901382	0.794984179
N	-0.970797612	6.988536983	0.196820224
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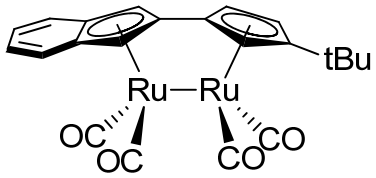
O	-1.790889233	7.122948890	1.112336318

Entry 9

Parent



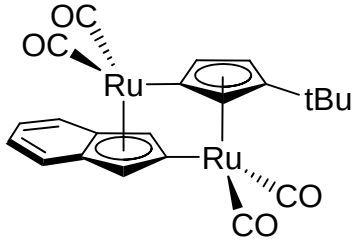
Energy: -555.1863846481

Molecular coordinates

C	-0.002368146	5.900381027	0.191369561
C	0.686613232	3.690306571	-0.283801169
C	-0.443341587	4.556394886	-0.105756162
C	1.851547279	4.501346305	-0.080139341
C	1.469545664	5.866750837	0.209920749
H	-1.480163529	4.244251969	-0.188833845
H	2.873273835	4.138902478	-0.139816542
Ru	0.680460914	4.419689983	1.857292859
C	-0.622273696	4.664809776	3.220872704
O	-1.423606253	4.871403128	4.045835533
C	2.039806087	4.476783787	3.184117342
O	2.897080427	4.562103619	3.973359406
C	-1.050462678	7.030992499	0.205700741
C	2.550421463	6.966616232	0.319691077
C	-0.731247637	8.212349839	1.135577397
H	-1.581256854	8.915072111	1.126252737
H	0.157889792	8.775976141	0.824228197
H	-0.586826065	7.872115691	2.173664157
C	-2.430638414	6.492324917	0.649423202
H	-2.841925139	5.749859175	-0.051816903
H	-3.145629058	7.330487603	0.679329414
H	-2.392796339	6.044899606	1.654178718
C	-1.206594462	7.536396635	-1.251241602
H	-1.507198044	6.714126097	-1.921196722
H	-1.990192164	8.311962104	-1.292457920
H	-0.276812649	7.970319611	-1.646264076
C	2.354369640	8.013434672	-0.800913576
H	3.212452358	8.706486015	-0.808591795
H	2.300875591	7.532126455	-1.791681077
H	1.445988936	8.615761116	-0.664203609
C	2.592693255	7.659974132	1.697758842
H	2.911051273	6.951354993	2.476743075
H	3.326295922	8.484217414	1.668398492
H	1.626564220	8.075843609	2.003280652
C	3.953320534	6.355664516	0.103236622
H	4.194309500	5.595833749	0.864258607
H	4.705720745	7.156051327	0.190970149
H	4.061947077	5.906271364	-0.897702295
C	-0.168981765	0.072094868	0.073566805

C	0.643718053	2.236961926	-0.283191109
C	-0.556471021	1.446913121	-0.142522937
C	1.775588547	1.371806605	-0.041523016
C	1.282616760	0.025725361	0.136971338
H	-1.575952998	1.806504865	-0.266962060
H	2.822754364	1.666048693	-0.073628023
C	-0.244355560	-2.322590184	0.361977839
C	1.177090524	-2.368132510	0.425140203
C	-0.921761367	-1.127954520	0.201176746
C	1.941979895	-1.220419348	0.327933517
H	-0.808780184	-3.255084743	0.450198129
H	-2.013815705	-1.099640932	0.155770786
H	3.033253136	-1.263155661	0.379481166
H	1.670375417	-3.334736201	0.560508478
Ru	0.527581506	1.526787588	1.850295598
C	-0.906741772	1.481925646	3.101400225
O	-1.809141314	1.408432664	3.838377967
C	1.804127875	1.321937473	3.249049253
O	2.599477468	1.136681937	4.083163137

Photoisomer



Energy: -555.1225812337

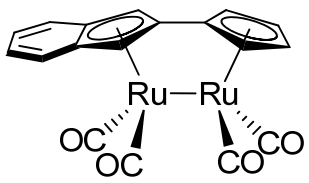
Molecular coordinates

C	0.983154164	5.840506964	0.937319977
C	0.311140629	3.641287173	1.572135089
C	1.426987654	4.500046938	1.311579573
C	-0.849235356	4.432822954	1.290229655
C	-0.478915031	5.797874779	0.921685574
H	2.467082887	4.205001998	1.422209979
H	-1.871296259	4.074382670	1.374934594
Ru	0.311982119	4.259813334	-0.638912680
C	1.654075899	4.389618597	-1.989463605
O	2.482981911	4.454562085	-2.809074667
C	-1.057904813	4.245797402	-1.965286243
O	-1.914606543	4.216138663	-2.757907408
C	2.030910223	6.970067310	0.881698926
C	-1.570595697	6.880629415	0.760189124
C	1.702843023	8.133301229	-0.067840200
H	2.549850555	8.839954975	-0.074370718
H	0.812328829	8.698779942	0.236108681
H	1.556825986	7.774690426	-1.099688765

C	3.407543290	6.425550780	0.434919662
H	3.821500650	5.685927787	1.136717463
H	4.124034468	7.262194803	0.393328319
H	3.361479847	5.971788721	-0.566851928
C	2.198204149	7.507094348	2.326332204
H	2.501456901	6.699483587	3.012489639
H	2.982280490	8.283119293	2.346365874
H	1.269610619	7.949481893	2.715700027
C	-1.396215108	7.963154621	1.850585622
H	-2.255941539	8.653881286	1.823877869
H	-1.357690668	7.510938230	2.855525987
H	-0.485938820	8.562393400	1.711668500
C	-1.602882125	7.529540373	-0.639577413
H	-1.900615175	6.790633023	-1.399143098
H	-2.348508118	8.343507590	-0.648621533
H	-0.638720520	7.949772797	-0.945320676
C	-2.971023667	6.265062258	0.979491664
H	-3.193261977	5.473410989	0.245722573
H	-3.729114127	7.054594517	0.850188821
H	-3.090804141	5.852108284	1.994273777
C	-0.239684360	-0.049765402	-0.015595964
C	0.401489205	2.157220393	-0.572456503
C	-0.724104670	1.292283515	-0.314405648
C	1.586934692	1.392231958	-0.269175807
C	1.208809495	0.012862251	0.012390416
H	-1.771083886	1.562019859	-0.446286117
H	2.610846206	1.751923188	-0.361451132
C	-0.130400827	-2.423787881	0.407938731
C	1.288205472	-2.362462215	0.435280633
C	-0.898374767	-1.288860329	0.201344488
C	1.963015274	-1.165337481	0.256390015
H	-0.623440481	-3.388822048	0.555442480
H	-1.990292487	-1.343764815	0.178544558
H	3.055676611	-1.126045050	0.275885821
H	1.856421235	-3.281725809	0.603315756
Ru	0.383820245	1.560463784	1.643132092
C	-1.029949275	1.452505701	2.928440462
O	-1.909716432	1.397201756	3.691511326
C	1.745564723	1.558021964	2.987613867
O	2.593895422	1.568275231	3.787314285

Entry 10

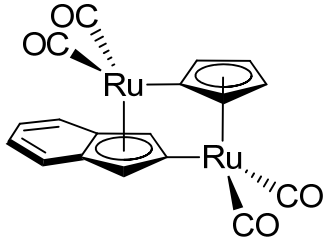
Parent



Energy: -445.1472779172
Molecular coordinates

C	-0.013899067	8.149026778	-0.017268356
C	0.731293306	5.996880640	-0.517467084
C	-0.442223358	6.828126554	-0.375894145
C	1.880729257	6.829058953	-0.245394227
C	1.413988268	8.149666037	0.063081065
H	-0.663701018	9.007271023	0.142609395
H	-1.472403766	6.508304260	-0.515752471
H	2.920347489	6.510065536	-0.269097982
H	2.041072409	9.008493362	0.294516268
C	-0.011159808	2.349050517	-0.218403015
C	0.733759456	4.542197603	-0.543453721
C	-0.442064767	3.711658565	-0.429252087
C	1.889780527	3.714093667	-0.290801061
C	1.439858784	2.350664268	-0.131979994
H	-1.470988653	4.037934545	-0.567017068
H	2.927016366	4.042757899	-0.305617672
C	-0.009312724	-0.048883275	0.047868114
C	1.411841208	-0.047209367	0.133100866
C	-0.724748580	1.123032227	-0.113383453
C	2.138703173	1.126333118	0.057884348
H	-0.542956963	-1.000653169	0.117948587
H	-1.816144632	1.114341867	-0.176880886
H	3.229896224	1.120285009	0.125307826
H	1.935464806	-0.997698677	0.266932154
Ru	0.609767613	6.695848033	1.642252903
Ru	0.608655168	3.811943395	1.582724784
C	-0.801547668	6.871286188	2.903802735
O	-1.682407848	7.046739989	3.648572762
C	1.874609985	6.868435496	3.051043221
O	2.669612462	7.042222772	3.887168626
C	-0.828074050	3.673116956	2.824953963
O	-1.725226308	3.538998662	3.559165758
C	1.884911192	3.671682844	2.989371406
O	2.685461502	3.536653504	3.827669802

Photoisomer



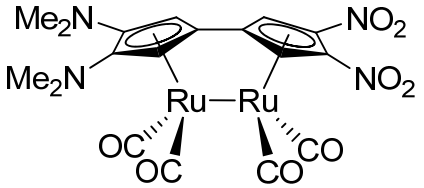
Energy: -445.0857779802
Molecular coordinates

C	0.668367146	7.125959493	-0.897789325

C	0.962616321	4.852047120	-0.359458706
C	-0.010252744	5.863441366	-0.696795767
C	2.240219254	5.522230513	-0.316194843
C	2.056893305	6.915476221	-0.662878388
H	0.201214148	8.063197546	-1.196400260
H	-1.079833722	5.699017197	-0.814615483
H	3.195350157	5.050992276	-0.091427462
H	2.844482143	7.662575275	-0.749047004
Ru	0.929966436	6.466124909	1.281985320
C	-0.474789403	7.406580198	2.164927827
O	-1.350437503	7.978840316	2.680174762
C	2.184665295	7.001307135	2.615034896
O	2.973396582	7.319487923	3.412694186
C	0.785791316	2.375845701	2.852440897
C	0.492959607	4.634721095	2.219507416
C	1.471201969	3.624902554	2.543164570
C	-0.785151992	3.968078176	2.161117784
C	-0.628105164	2.591014412	2.613224659
H	2.539790852	3.796731913	2.665225788
H	-1.738155469	4.447327097	1.941094456
C	-1.081261228	0.339458207	3.354948384
C	0.303985381	0.128519201	3.589072382
C	-1.554994390	1.543790626	2.860607445
C	1.238728800	1.118310738	3.332700943
H	-1.784719520	-0.469708427	3.569416889
H	-2.623125416	1.700437921	2.686387883
H	2.303022689	0.950174741	3.519296839
H	0.635037875	-0.838108009	3.978503848
Ru	0.530034723	3.036906577	0.567130516
C	1.965908214	2.127816067	-0.313408457
O	2.858702032	1.588665777	-0.833893262
C	-0.743195877	2.538125873	-0.772496048
O	-1.535546818	2.253121273	-1.578433685

Entry 11

Parent



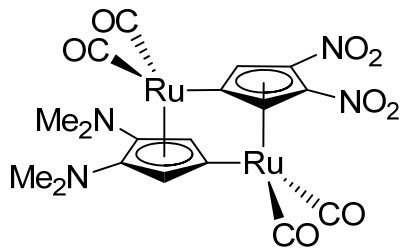
Energy: -659.5203506974

Molecular coordinates

C	-0.210102153	5.860632556	0.428247536
C	0.453797694	3.653779020	-0.011913149
C	-0.681951117	4.520380948	0.186018812
C	1.643211308	4.447572665	0.189207534

C	1.251496648	5.811113021	0.465901937
H	-1.726202965	4.238744356	0.074361414
H	2.665444933	4.087545868	0.111577420
Ru	0.472901016	4.276563868	2.128009645
C	-0.894989120	4.475731126	3.437079610
O	-1.756078330	4.662393948	4.203308423
C	1.807563521	4.487147366	3.469758842
O	2.645113710	4.661605657	4.265061454
C	-0.366972571	0.058390753	0.445277870
C	0.410758901	2.203601036	-0.022771967
C	-0.775647631	1.411081488	0.205301913
C	1.549268115	1.327851449	0.094438680
C	1.070070199	0.007490718	0.374776581
H	-1.811244987	1.740764967	0.172951279
H	2.599648825	1.586782690	-0.010553521
Ru	0.461374285	1.362047276	2.117467954
C	-0.789672482	1.243876739	3.548198654
O	-1.564533145	1.125879405	4.408450035
C	1.853785876	1.275209440	3.412493478
O	2.717268053	1.174913736	4.187392123
N	1.938302023	-1.164706854	0.485069009
O	3.075027535	-1.047681733	-0.016217197
O	1.498696771	-2.169900668	1.063425732
N	-1.334406576	-1.048401155	0.454422697
O	-1.039675349	-2.056809055	-0.204781792
O	-2.399621683	-0.855267406	1.063452003
N	2.113492348	6.882759137	0.624420319
C	3.541870876	6.604485180	0.479525336
C	1.822655564	7.825570294	1.713858922
N	-0.986723776	7.010472351	0.507706936
C	-0.678699712	8.082998276	-0.451287486
C	-2.416552158	6.822506847	0.733816160
H	3.735231154	6.085483869	-0.471266709
H	3.941117466	5.994766136	1.317540895
H	4.081805671	7.562956999	0.464033212
H	0.743141634	8.010919912	1.781937201
H	2.345673735	8.775212443	1.523117498
H	2.161724588	7.410579539	2.685131805
H	0.408119788	8.181628730	-0.578669576
H	-1.080747003	9.036427265	-0.073416123
H	-1.129326946	7.878613542	-1.444468644
H	-2.865240026	7.798418936	0.975421721
H	-2.575267975	6.146556275	1.588060869
H	-2.944273150	6.414074960	-0.155001178

Photoisomer



Energy: -659.4501058514

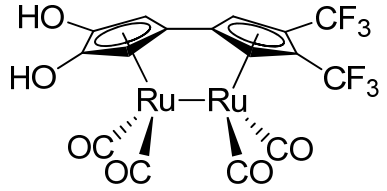
Molecular coordinates

C	-0.239211150	5.897436168	0.431802990
C	0.360238523	3.675036075	-0.110406461
C	-0.742040493	4.561795314	0.133958428
C	1.558569024	4.429989508	0.150268366
C	1.210045508	5.815512656	0.450462210
H	-1.795429898	4.316340310	0.014204006
H	2.573098126	4.050281158	0.055984118
Ru	0.379769565	4.282189703	2.079914808
C	-1.012504853	4.473292644	3.372807787
O	-1.883196201	4.586278295	4.141906077
C	1.730318285	4.426604030	3.427269935
O	2.573043685	4.478377966	4.233709433
C	1.006828208	0.039760631	1.360258311
C	0.325551447	2.175412599	2.081947209
C	1.467568504	1.348474354	1.759771405
C	-0.839495993	1.363003124	1.844176062
C	-0.422565638	0.044639693	1.419661281
H	2.518153564	1.619265414	1.848531213
H	-1.880106905	1.652696449	1.973180985
Ru	0.254254121	1.573439361	-0.157881477
C	1.528039946	1.441647342	-1.579264455
O	2.317428231	1.363377708	-2.427355773
C	-1.167793890	1.619729787	-1.431581695
O	-2.047893336	1.646557844	-2.190527689
N	1.917693691	-1.106038374	1.206889500
O	2.866067201	-0.978436949	0.416667659
O	1.704179230	-2.075176751	1.950240260
N	-1.318027005	-1.081135745	1.168152545
O	-0.858292244	-2.069554862	0.570555535
O	-2.486428223	-0.955747683	1.582994646
N	2.108322471	6.859805770	0.606363840
C	3.527669779	6.531220278	0.484702962
C	1.833867995	7.822351006	1.680282309
N	-0.989443958	7.075857930	0.511186528
C	-0.702565675	8.073269698	-0.531996791
C	-2.415218159	6.920354787	0.782978047
H	3.717429200	5.992895941	-0.455625498
H	3.894999554	5.918839382	1.336023935

H	4.100678828	7.470296473	0.464811644
H	0.764613238	8.070536315	1.705463195
H	2.419618466	8.738191347	1.507690339
H	2.110924454	7.393088234	2.666565778
H	0.383406299	8.173827516	-0.672511600
H	-1.110726639	9.048460327	-0.221661549
H	-1.157174417	7.793599770	-1.505677194
H	-2.842102965	7.911550581	1.002349376
H	-2.559625941	6.276659291	1.664322824
H	-2.977621072	6.488645423	-0.073441655

Entry 12

Parent



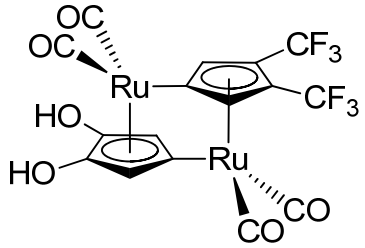
Energy: -774.2835420382

Molecular coordinates

C	-0.481129837	5.728008970	1.642198474
C	0.243560852	3.563780495	2.095831074
C	-0.927689623	4.387176079	1.872896325
C	1.415091007	4.405585352	1.947814862
C	0.954837850	5.737104702	1.670458439
O	-1.290935932	6.808064335	1.553672807
H	-0.747411756	7.599394099	1.353913123
H	-1.967911773	4.076296592	1.929920067
H	2.451994021	4.102959310	2.079906239
O	1.628337882	6.922137919	1.626739984
H	2.575994443	6.777048533	1.439637787
Ru	0.317785194	4.263691599	-0.029036641
C	-0.983591372	4.502623997	-1.402649823
O	-1.798448566	4.708230403	-2.209994231
C	1.713825404	4.488887143	-1.302867287
O	2.592884044	4.694384100	-2.042373567
C	0.997856652	-0.040820680	1.563484852
C	0.253130723	2.113316003	2.071972693
C	1.422468630	1.288377650	1.903879612
C	-0.897743667	1.278607589	1.834486107
C	-0.444719023	-0.047389616	1.521131199
H	2.459548412	1.596630571	2.012072115
H	-1.941074029	1.579818330	1.881558399
Ru	0.325191307	1.365759057	-0.098617782
C	1.690367868	1.277280763	-1.419644911
O	2.536937094	1.174413748	-2.212932059
C	-0.951871146	1.277553711	-1.506189813

O	-1.744253384	1.175144489	-2.353404339
C	1.941767341	-1.204575508	1.497309812
C	-1.367612414	-1.225633826	1.370538457
F	1.558320288	-2.174979436	0.615209805
F	2.057428462	-1.809730765	2.734329514
F	3.206989818	-0.795689280	1.143406377
F	-1.224391878	-1.906539705	0.193599055
F	-2.681377951	-0.821206287	1.445711406
F	-1.170174940	-2.137399433	2.387208869

Photoisomer



Energy: -774.2149920973

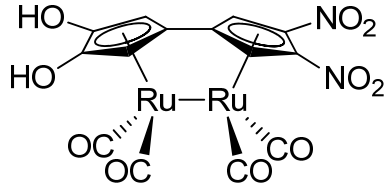
Molecular coordinates

C	-0.259974720	5.844352895	0.222171908
C	0.463924863	3.645495999	-0.182934189
C	-0.698685942	4.494342563	-0.058069873
C	1.613455037	4.464615836	0.126407905
C	1.161010918	5.824795787	0.351106318
H	-1.733362128	4.211378610	-0.240553746
H	2.655118958	4.146659850	0.104700506
Ru	0.308352955	4.361541460	1.969444376
C	-1.157792092	4.649116115	3.164976511
O	-2.071200619	4.827093219	3.865736791
C	1.577954139	4.574829581	3.379855783
O	2.383449269	4.713323027	4.212143727
C	0.963659273	0.069822886	1.544926372
C	0.247762883	2.255816819	2.089149047
C	1.392869264	1.394965879	1.950189691
C	-0.895693862	1.448798088	1.747510408
C	-0.466575989	0.103112453	1.419200211
H	2.430454692	1.666505581	2.135069023
H	-1.935003713	1.770350875	1.749706750
Ru	0.427432250	1.542299621	-0.111602134
C	1.895660095	1.385053044	-1.323002832
O	2.803937401	1.290795864	-2.042582503
C	-0.796114775	1.431449848	-1.575171393
O	-1.557078091	1.364507862	-2.451063706
C	1.884661613	-1.112506260	1.495669087
C	-1.410264396	-1.042569915	1.171680321
O	-1.064750986	6.936030700	0.204834314
H	-0.531843585	7.728300205	0.426768353

O	1.867320900	6.991524382	0.448703376
H	2.792435273	6.811907330	0.704526009
F	1.504570366	-2.072576197	0.597563200
F	1.956193837	-1.723906366	2.730938801
F	3.167371770	-0.730433417	1.173444460
F	-1.226275352	-1.676167415	-0.029680754
F	-2.715223339	-0.606974911	1.197101343
F	-1.287306165	-2.002161896	2.153036542

Entry 13

Parent



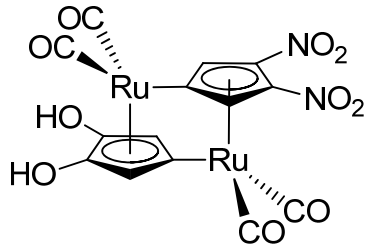
Energy: -626.4800387130

Molecular coordinates

C	-0.361892663	5.768997359	0.203314969
C	0.520326126	3.658793019	-0.219554498
C	-0.710242808	4.413786465	-0.101956091
C	1.625248415	4.553520637	0.066857734
C	1.068039612	5.851939654	0.322827061
H	-1.721039082	4.053032769	-0.275867913
H	2.684741509	4.307211489	0.034576343
C	-0.029805387	0.010747925	0.199169819
C	0.604108427	2.209682779	-0.224241134
C	-0.527217190	1.319689841	-0.106164918
C	1.797458923	1.438683661	0.020556108
C	1.405158085	0.085866527	0.275420912
H	-1.578506983	1.557109162	-0.250698275
H	2.827445357	1.785967543	0.016180380
Ru	0.338387332	4.296702017	1.913462000
Ru	0.511355430	1.400734200	1.921740801
C	-1.117494990	4.429727184	3.140588778
O	-2.026678116	4.570139909	3.854746258
C	1.573927167	4.590502172	3.333337656
O	2.353271420	4.842260228	4.163631771
C	-0.875952391	1.198799512	3.212658251
O	-1.729333163	1.030248230	3.984398003
C	1.762603650	1.392293650	3.357221338
O	2.543443413	1.339391411	4.218745754
N	2.355868031	-1.007130034	0.497823164
O	3.519250623	-0.801141984	0.099563362
O	1.947091075	-2.031520772	1.061763627
N	-0.893711245	-1.178549926	0.135690862
O	-0.447838904	-2.161179211	-0.473866227

O	-2.024429288	-1.073264400	0.637716450
O	-1.232631773	6.801628065	0.231741860
H	-0.756357375	7.619199640	0.490159695
O	1.665067520	7.066629678	0.466387248
H	2.606112936	6.970557077	0.710507863

Photoisomer



Energy: -626.4115839610

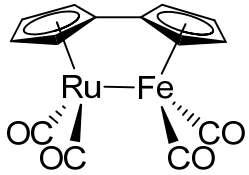
Molecular coordinates

C	-0.246170596	5.834463019	0.236242295
C	0.451280321	3.630491553	-0.179186182
C	-0.701263592	4.491655783	-0.053540979
C	1.611469451	4.430699918	0.140144814
C	1.174724043	5.795515720	0.369204698
H	-1.738910837	4.223351648	-0.241186993
H	2.649072805	4.099982954	0.116428874
Ru	0.295798698	4.328794957	1.974941761
C	-1.182622446	4.611099530	3.158557931
O	-2.102364079	4.784560667	3.850894015
C	1.553217165	4.540662894	3.398894881
O	2.351007781	4.677935111	4.237977511
C	0.988088270	0.065408139	1.522094831
C	0.236609745	2.223104326	2.084014480
C	1.407358548	1.391155493	1.907604133
C	-0.899750160	1.396669668	1.771565155
C	-0.439027434	0.064305698	1.445110070
H	2.443482047	1.673899481	2.084911383
H	-1.948676622	1.684333292	1.790157752
Ru	0.377662354	1.529226164	-0.123415343
C	1.782433485	1.335457707	-1.409662782
O	2.648536401	1.221467150	-2.173921537
C	-0.918184801	1.484741570	-1.528255749
O	-1.721138093	1.453992280	-2.366906495
N	1.907145888	-1.087866948	1.504110943
O	2.858013634	-1.053322215	0.710054784
O	1.685220829	-1.960326870	2.355216978
N	-1.297131389	-1.083698514	1.164605702
O	-0.760284733	-2.109064891	0.710880019
O	-2.508740709	-0.938149816	1.412505277
O	-1.037237099	6.934217627	0.221342096
H	-0.497944351	7.722468311	0.443185097

O	1.892947829	6.951620730	0.478039913
H	2.819728262	6.762234834	0.720805533

Entry 14

Parent

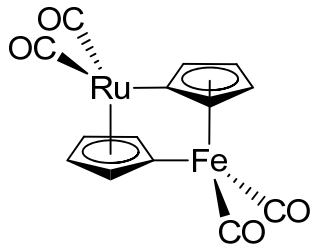


Energy: -600.5427948774

Molecular coordinates

C	-0.077352328	5.802847997	0.244576631
C	0.672018828	3.650120143	-0.251089180
C	-0.502128011	4.484614550	-0.126854949
C	1.818213635	4.480232057	0.045104130
C	1.348195588	5.800147703	0.350240899
H	-0.728044865	6.661505105	0.398590178
H	-1.530621918	4.168582455	-0.286546499
H	2.857796913	4.160209330	0.039036029
H	1.972359858	6.656301958	0.598932391
C	-0.091184959	0.068035982	0.309361144
C	0.668815312	2.197270869	-0.247611045
C	-0.506807752	1.376724786	-0.099368695
C	1.806863500	1.371424917	0.068581398
C	1.330529226	0.064750096	0.412605110
H	-0.750097749	-0.774041381	0.512712671
H	-1.535916578	1.702306756	-0.234741728
H	2.846236538	1.692205309	0.083349925
H	1.949344661	-0.780257410	0.708690147
Ru	0.513692349	4.325465201	1.903914474
Fe	0.523617448	1.505823314	1.728726758
C	-0.921346836	4.476058133	3.143270358
O	-1.815757670	4.639792029	3.874836250
C	1.751081284	4.473022885	3.340822599
O	2.528779872	4.635082611	4.195727362
C	-0.812705876	1.369616934	2.842042297
O	-1.715416631	1.208265033	3.56879923

Photoisomer



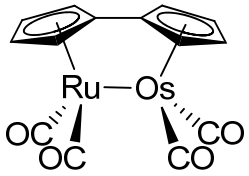
Energy: -600.4851623805

Molecular coordinates

C	-0.248156222	5.420229972	-0.573961832
C	0.179786012	3.113093792	-0.298794314
C	-0.828771098	4.146102228	-0.209492311
C	1.394858076	3.789356969	-0.697946003
C	1.125855585	5.199679388	-0.875863757
H	-0.773877566	6.372530697	-0.626594998
H	-1.870835858	3.990173308	0.065790318
H	2.359101603	3.311269824	-0.863961184
H	1.842208528	5.952735086	-1.201075810
Ru	0.776479551	4.617656538	1.317229564
C	-0.192622811	5.465242604	2.726264227
O	-0.809338826	5.977736976	3.573082961
C	2.439714910	5.050719289	2.147556739
O	3.469413853	5.305567211	2.632235200
C	1.025175836	0.368154920	2.169595353
C	0.649569217	2.689685836	2.129794887
C	1.634453709	1.656125959	1.942956173
C	-0.582015854	2.010191361	2.437001924
C	-0.346690665	0.587270627	2.475295049
H	1.525878847	-0.597309541	2.113034260
H	2.676570661	1.816714191	1.671631260
H	-1.543147918	2.490824112	2.612166516
H	-1.087728322	-0.179853723	2.695303215
Fe	0.081031661	1.329305508	0.552180585
C	0.990014106	0.533688493	-0.710232705
O	1.610448608	-0.000041649	-1.544226948
C	-1.461930787	0.927602720	-0.162662123
O	-2.501078837	0.659102307	-0.624771246

Entry 16

Parent



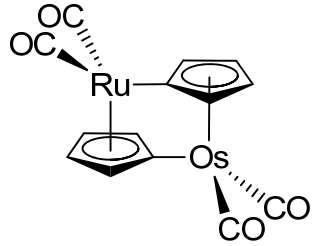
Energy: -413.83380098

Molecular coordinates

C	-0.074477915	5.829821202	0.177253943
C	0.680536440	3.674330204	-0.296712554
C	-0.494822726	4.505946137	-0.179787830
C	1.821533199	4.509765555	-0.002636130
C	1.347147796	5.832209974	0.286085065
H	-0.729088185	6.687154579	0.321480418
H	-1.522749892	4.185803953	-0.336493281
H	2.862486173	4.193377046	-0.001397903
H	1.969266313	6.691771312	0.527863923
C	-0.076672577	0.074607109	0.228451262

C	0.682075411	2.215225010	-0.294631253
C	-0.494812890	1.384030744	-0.182693559
C	1.827927070	1.386649802	0.004232606
C	1.352425746	0.076168622	0.343595973
H	-0.728715928	-0.781605378	0.388840528
H	-1.521730755	1.702402706	-0.347816303
H	2.867211228	1.707716224	0.006100387
H	1.972430030	-0.778549743	0.606312405
Ru	0.513950726	4.353709395	1.870538315
Os	0.509027181	1.537343013	1.868801770
C	-0.899145250	4.494051242	3.130209855
O	-1.774704782	4.629026055	3.888482571
C	1.721031823	4.500193460	3.328487583
O	2.472653384	4.639079900	4.209133248
C	-0.871313204	1.289640878	3.111437889
O	-1.753057337	1.070672224	3.856016640
C	1.674598657	1.295514384	3.315480653
O	2.427104263	1.080129388	4.191297779

Photoisomer



Energy: -413.79514730

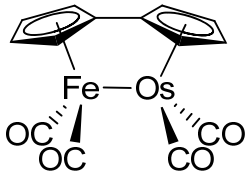
Molecular coordinates

C	-0.367352349	5.337032166	-0.704133971
C	0.384073750	3.118172157	-0.399173380
C	-0.782423434	3.971533734	-0.483621598
C	1.521208490	4.005471439	-0.526493335
C	1.058228944	5.358024739	-0.730640145
H	-1.025407634	6.193029042	-0.846535307
H	-1.815013427	3.630716374	-0.426869307
H	2.564760906	3.695161252	-0.508579827
H	1.685071416	6.233001864	-0.896594611
Ru	0.394413161	4.647741026	1.343979945
C	-0.962800676	5.282712117	2.526885553
O	-1.811608998	5.664767760	3.228128121
C	1.772929790	5.328098543	2.475748376
O	2.633656219	5.738805360	3.145578022
C	1.197954815	0.515091816	2.444370471
C	0.442372976	2.730782774	2.208907145
C	1.611920147	1.889957492	2.269449907
C	-0.697255381	1.854757871	2.318276003
C	-0.234631007	0.493193641	2.474637217

H	1.857482397	-0.342582678	2.567050185
H	2.643599422	2.232425182	2.214017179
H	-1.740310409	2.165587957	2.306607395
H	-0.861855145	-0.384105044	2.624839006
Os	0.428421979	1.208763249	0.437850534
C	1.756707194	0.581809665	-0.738861711
O	2.617502319	0.186520725	-1.432051659
C	-0.929811322	0.543615384	-0.682393916
O	-1.807468143	0.123469394	-1.338841291

Entry 17

Parent

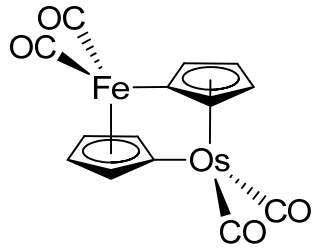


Energy: -617.0977998553

Molecular coordinates

C	-0.015200042	5.819892365	0.334576043
C	0.733011357	3.693495371	-0.250183832
C	-0.435121799	4.526433478	-0.109757107
C	1.873693597	4.498622231	0.103009372
C	1.402384382	5.802197554	0.466728402
H	-0.668301605	6.664485903	0.545460846
H	-1.465089609	4.213575695	-0.267845859
H	2.909999289	4.168502088	0.129394730
H	2.024651668	6.632037430	0.796982444
C	-0.110221031	0.113174159	0.205136315
C	0.711836627	2.234325282	-0.283990842
C	-0.486286697	1.426544919	-0.230839798
C	1.827715317	1.386247611	0.063242805
C	1.313023229	0.085249775	0.389582908
H	-0.786101728	-0.728446817	0.344384937
H	-1.496830177	1.761615190	-0.452663806
H	2.870574150	1.690575564	0.116764016
H	1.903629501	-0.781728173	0.677722538
Fe	0.562829291	4.322842334	1.741293597
Os	0.433903266	1.571666046	1.856301801
C	-0.802962387	4.306674433	2.833597324
O	-1.718757801	4.378286365	3.556550796
C	1.641180497	4.541139425	3.093920766
O	2.365694448	4.745063598	3.988338219
C	-0.960038325	1.245553881	3.074553545
O	-1.845578479	0.973002749	3.796499715
C	1.605291349	1.426637376	3.311439089
O	2.371185711	1.268519163	4.187735036

Photoisomer



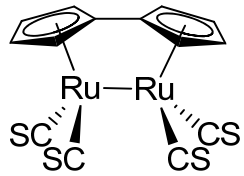
Energy: -617.0628409129

Molecular coordinates

C	-0.000860060	5.164748634	-0.969405441
C	0.421259971	2.929783677	-0.341263429
C	-0.609547478	3.914876360	-0.587378580
C	1.677948795	3.609371767	-0.570406186
C	1.424105904	4.974354676	-0.958905090
H	-0.524438929	6.078541269	-1.247291672
H	-1.681140997	3.740828724	-0.503469714
H	2.664987825	3.160380000	-0.471433542
H	2.173088323	5.718180396	-1.227395142
Os	0.646539769	4.699169402	1.145482529
C	-0.605329212	5.615110646	2.218650025
O	-1.416251947	6.185100594	2.845682650
C	2.078567940	5.257080376	2.239074857
O	3.000697155	5.596185378	2.879654991
C	0.809552091	0.615200165	2.601987594
C	0.396023360	2.877144347	2.125436098
C	1.423752716	1.881872102	2.303131453
C	-0.859340265	2.186869914	2.286394313
C	-0.603393308	0.804028631	2.591678717
H	1.330754647	-0.320582648	2.798713199
H	2.494836781	2.060173253	2.225233094
H	-1.844838577	2.639936545	2.193672486
H	-1.354713053	0.038251919	2.779084795
Fe	0.192371341	1.274442967	0.697506862
C	1.374671218	0.393662565	-0.231740078
O	2.184196311	-0.198112931	-0.833912544
C	-1.165908195	0.733210818	-0.250805961
O	-2.093226129	0.373745455	-0.866441283

Entry 19

Parent



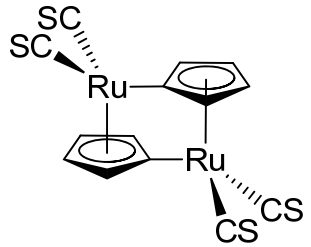
Energy: -350.6388364622

Molecular coordinates

C	-0.078079568	5.808833998	0.179159262

C	0.658659557	3.660137411	-0.316081728
C	-0.509542525	4.500157343	-0.195138003
C	1.812912459	4.485546421	-0.045211054
C	1.353618789	5.799659369	0.271227500
H	-0.722277580	6.670212172	0.344724611
H	-1.541439305	4.183984724	-0.331429531
H	2.849539256	4.155796985	-0.047343254
H	1.982002308	6.652768014	0.519659096
C	-0.108365405	0.062427070	0.154043740
C	0.650424634	2.207024614	-0.325705604
C	-0.527491254	1.379633625	-0.202480842
C	1.796472121	1.364998574	-0.075193493
C	1.324071259	0.053224216	0.232927113
H	-0.761254493	-0.792727678	0.317979425
H	-1.556724199	1.709828572	-0.324866372
H	2.837153244	1.681619874	-0.084620570
H	1.944336049	-0.810125280	0.465980310
Ru	0.521121692	4.367348258	1.882503331
Ru	0.526019487	1.481646760	1.865673404
C	-0.882387107	4.591930392	3.106374116
S	-2.071249544	4.904513036	4.073162471
C	1.740866900	4.591961999	3.290053303
S	2.778907317	4.903820838	4.417380741
C	-0.849317178	1.250030084	3.119401194
S	-2.007831986	0.935357413	4.120954936
C	1.770668291	1.250638723	3.249085031

Photoisomer



Energy: -350.5741720793

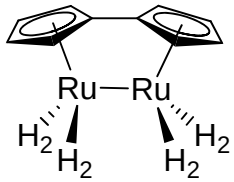
Molecular coordinates

C	-0.111950620	5.782641259	0.162791614
C	0.533842620	3.569919480	-0.274807362
C	-0.590682377	4.465586100	-0.171903058
C	1.708466265	4.353559682	0.014007858
C	1.311759769	5.713299613	0.277940744
H	-0.722752272	6.676161526	0.283305819
H	-1.632660286	4.193536907	-0.330674100
H	2.731245847	3.980853369	0.022579671
H	1.979058276	6.544274695	0.502130926
Ru	0.396097195	4.377348663	1.919710011
C	-1.025330992	4.674983431	3.117674393

S	-2.218727231	4.930882396	4.094106366
C	1.641650385	4.547654188	3.319835192
S	2.699466747	4.700619804	4.459746374
C	0.931315453	0.072962498	1.608363182
C	0.283907962	2.285291719	2.048051082
C	1.409034617	1.390337752	1.943885540
C	-0.890238392	1.500594952	1.759039085
C	-0.492492667	0.141223201	1.493661481
H	1.543303532	-0.819450309	1.485109869
H	2.451180008	1.663160699	2.100436443
H	-1.913245991	1.872435235	1.749847065
H	-1.158764795	-0.690180774	1.268115851
Ru	0.421950542	1.478906222	-0.145691417
C	1.858758683	1.181647478	-1.322607945
S	3.079780181	0.924587011	-2.262696735
C	-0.817202285	1.314796414	-1.553071085
S	-1.872404176	1.175921792	-2.697351866

Entry 20

Parent



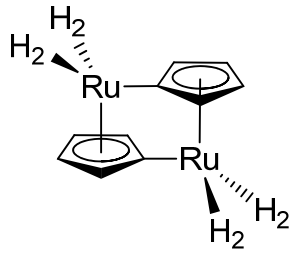
Energy: -232.8050148903

Molecular coordinates

C	-0.010341889	5.929514792	-0.240143752
C	0.736759693	3.757991324	-0.642973858
C	-0.440413935	4.602794144	-0.572332439
C	1.886300512	4.589967441	-0.341709415
C	1.413905694	5.921691953	-0.098933155
H	-0.656594526	6.798925536	-0.134158186
H	-1.465184267	4.291515696	-0.761739762
H	2.924854118	4.267304581	-0.326645693
H	2.036117197	6.784232627	0.132622443
C	-0.052013849	0.159183726	-0.149818027
C	0.726287882	2.306022144	-0.620206961
C	-0.462956810	1.480957104	-0.523331063
C	1.863805786	1.467330395	-0.292942485
C	1.372228426	0.150829559	-0.008706494
H	-0.710650812	-0.697144019	-0.016956528
H	-1.483166612	1.800863588	-0.722784708
H	2.906937070	1.775213529	-0.287744299
H	1.981966561	-0.712927097	0.249949907
Ru	0.533614130	4.516073622	1.447298979
Ru	0.512951467	1.616702929	1.492731262
H	-0.729271131	4.112276103	2.461635024

H	-0.568938449	5.149665388	2.508840006
H	1.567807037	4.098941466	2.689827601
H	1.413872140	5.137400624	2.705795669
H	-0.743621467	2.070574742	2.493794509
H	-0.598564242	1.033438859	2.573856908
H	1.553950441	2.057131788	2.721319868
H	1.384170836	1.021822455	2.770084649

Photoisomer

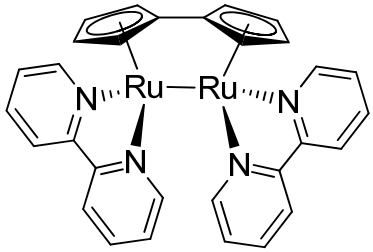


Energy: -232.7397903887

Molecular coordinates

C	-0.091121879	5.789545875	0.108504988
C	0.532020100	3.540471538	-0.252330063
C	-0.585832087	4.455108377	-0.153084039
C	1.713762487	4.334249561	0.011306775
C	1.328780201	5.714912195	0.210048607
H	-0.695091729	6.691922686	0.192787868
H	-1.631900676	4.190690740	-0.297541864
H	2.736394814	3.961045751	0.014777882
H	2.005595593	6.549882199	0.385851133
Ru	0.429678776	4.442993985	1.843159688
C	0.928458225	0.099750463	1.687015571
C	0.305256501	2.348773625	2.047909906
C	1.423122588	1.434206524	1.948454845
C	-0.876464668	1.554917457	1.784519353
C	-0.491454144	0.174272027	1.585695050
H	1.532539758	-0.802557999	1.602856210
H	2.469176414	1.698700812	2.092815805
H	-1.899118472	1.928042248	1.781276221
H	-1.168172663	-0.660839226	1.410190715
Ru	0.407228441	1.446265184	-0.047624100
H	-0.857168807	4.275945255	2.922636351
H	-0.633831784	5.239278713	2.871657080
H	1.525503946	4.150920232	3.093321215
H	1.413403913	5.131919959	3.018160301
H	-0.688789126	1.738701127	-1.297476455
H	-0.577311065	0.757621115	-1.222028131
H	1.693850512	1.613110948	-1.127241904
H	1.470107387	0.649688574	-1.076401317

Entry 21
Parent

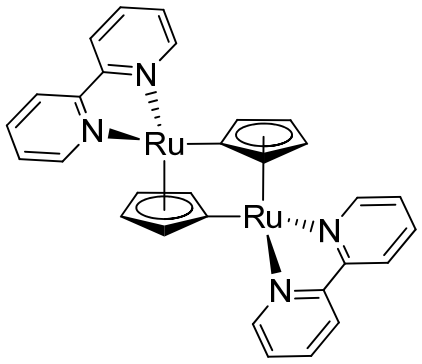


Energy: -549.4451852243
Molecular coordinates

C	0.124624476	5.770340009	-0.841516000
C	0.632251844	3.511944733	-1.094134831
C	-0.451815390	4.473209119	-1.058388992
C	1.877876031	4.233014272	-0.920642020
C	1.555979806	5.622723523	-0.756736841
H	-0.423314431	6.709990106	-0.776705338
H	-1.508012495	4.250938543	-1.198228275
H	2.875662066	3.798778411	-0.938832186
H	2.272044647	6.432139199	-0.617325212
C	-0.492019565	0.058601201	-0.316797185
C	0.476528289	2.075263944	-0.962741112
C	-0.785772735	1.389075424	-0.769870185
C	1.544547019	1.148102523	-0.646049041
C	0.939739512	-0.089547451	-0.240827008
H	-1.224725290	-0.716093536	-0.092513480
H	-1.774042066	1.802824453	-0.961209637
H	2.610958866	1.349292398	-0.728527486
H	1.471384009	-0.994917597	0.050743731
Ru	0.615546830	4.488554530	0.891912280
Ru	0.303121988	1.493286750	1.165878098
C	-0.208196542	5.189665631	3.661752643
C	-2.064013614	5.149317799	2.211815976
C	-1.048825493	5.560221273	4.728104850
C	-2.921632932	5.530939391	3.226986529
H	-2.425395526	4.964084817	1.198424540
C	-2.409684352	5.738239373	4.525417130
H	-0.617374154	5.712893129	5.720182831
H	-3.984511294	5.657920185	3.008140122
H	-3.064442106	6.030681487	5.349348767
C	3.194751657	4.601589288	2.534190258
C	1.225277648	5.039398129	3.749731229
C	3.982952489	4.808493234	3.651145266
H	3.630211288	4.334555545	1.569349406
C	1.988537516	5.239202340	4.915422866
C	3.371089689	5.129591499	4.881453154
H	5.067608851	4.710009481	3.564493166

H	1.480749203	5.487160249	5.850468243
H	3.967026807	5.287616606	5.783116470
C	0.862581438	1.339226665	4.082532710
C	2.843983711	1.118225384	2.828509295
C	1.598305944	1.187772800	5.272901318
C	3.601199418	0.945672791	3.972505548
H	3.298750630	1.109114958	1.836054319
C	2.970467356	0.987115958	5.234003880
H	1.076247127	1.224105556	6.231947192
H	4.678509507	0.788493799	3.880684362
H	3.544227544	0.864526096	6.155344703
C	-2.417197229	1.668956173	2.555860061
C	-0.571582948	1.489552256	4.008115191
C	-3.306405963	1.671061679	3.614611125
H	-2.760041068	1.743288151	1.522029394
C	-1.440334208	1.507951546	5.115443447
C	-2.812964943	1.595785245	4.934437290
H	-4.377649918	1.740779881	3.411392707
H	-1.022614023	1.446945410	6.123141699
H	-3.490604411	1.606187617	5.791053445
N	-0.718131794	4.972667619	2.386377278
N	1.830358166	4.708259715	2.542228508
N	1.489424156	1.313064793	2.841531674
N	-1.060221037	1.579145899	2.709262130

Photoisomer



Energy: -549.3930993372

Molecular coordinates

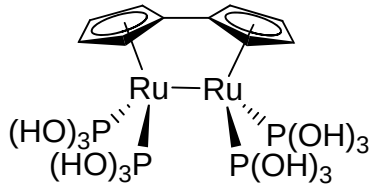
C	0.235722207	5.518165026	0.006640742
C	0.576719328	3.190434243	-0.097357724
C	-0.421446284	4.238247659	-0.128451826
C	1.851981804	3.846983904	0.099831639
C	1.642563742	5.275990981	0.148074106
H	-0.247516898	6.495441469	-0.013984043
H	-1.490269497	4.088048032	-0.279251578
H	2.818471826	3.346274337	0.153074956
H	2.416315109	6.036993947	0.253594647
Ru	0.574729698	4.324057896	1.870293704

C	0.544543459	-0.023225671	2.134675486
C	0.196764695	2.303238675	2.241786851
C	1.198728448	1.258391831	2.266680862
C	-1.077256978	1.643179853	2.052043252
C	-0.863866337	0.214714931	2.002144202
H	1.030733520	-0.999110567	2.151581732
H	2.267861473	1.411712466	2.411789033
H	-2.045504586	2.141069116	2.004389531
H	-1.635932981	-0.548578285	1.900839727
Ru	0.191203040	1.170501358	0.274095305
C	-0.306633789	5.097568339	4.598728094
C	-2.102000810	5.191249002	3.077584002
C	-1.174386943	5.454371803	5.648153430
C	-2.986129622	5.558972948	4.076418515
H	-2.426841741	5.066968112	2.042554814
C	-2.518964264	5.691565279	5.400586436
H	-0.779309593	5.543780066	6.662724810
H	-4.033819623	5.737551007	3.823132334
H	-3.195678765	5.971217406	6.211098765
C	1.111031285	4.853239980	4.742937001
C	3.096445598	4.294053474	3.606695108
C	1.824822296	4.936755113	5.953404119
C	3.838818581	4.380038288	4.771233400
H	3.557236164	4.033987978	2.651539701
C	3.192638104	4.704936241	5.982041026
H	1.291474943	5.185727177	6.873703775
H	4.914070065	4.189842381	4.734402174
H	3.751087919	4.770211218	6.918502973
C	-0.372959747	0.635683506	-2.592286678
C	-2.345622834	1.205380245	-1.438998435
C	-1.098966606	0.548332486	-3.795163780
C	-3.099683621	1.115992823	-2.595711526
H	-2.796204480	1.471142866	-0.480567120
C	-2.466436315	0.783594063	-3.811292733
H	-0.575521502	0.293386492	-4.719508582
H	-4.174008956	1.309297254	-2.549198028
H	-3.034359338	0.715225792	-4.741833903
C	1.045410159	0.388163823	-2.460741386
C	2.855277176	0.296618298	-0.956849772
C	1.901924023	0.024719449	-3.517072235
C	3.728848441	-0.077045332	-1.962811840
H	3.190454575	0.424413154	0.074460701
C	3.248363829	-0.214563139	-3.281664851
H	1.496652101	-0.068208863	-4.527296620
H	4.778630547	-0.256638448	-1.719114618
H	3.916429131	-0.499475525	-4.097506354

N	-0.772401810	4.957994974	3.298166387
N	1.749298102	4.524405694	3.554531221
N	1.524075499	0.531529919	-1.165262563
N	-0.998602965	0.971483453	-1.399208364

Entry 22

Parent



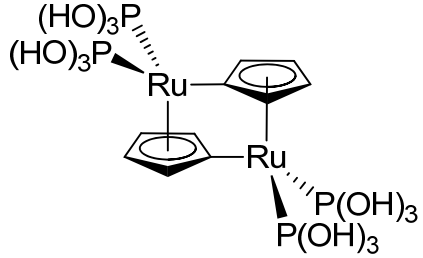
Energy: -675.9324075160

Molecular coordinates

C	-0.430775350	5.882902739	-0.084672883
C	0.535997798	3.802737536	-0.529054350
C	-0.714696157	4.512291990	-0.405560293
C	1.586363481	4.752401002	-0.245314721
C	0.987601325	6.034177828	0.010012146
H	-1.168392604	6.677533362	0.014446408
H	-1.705007365	4.084785400	-0.547107579
H	2.653111163	4.538865140	-0.247330092
H	1.524684434	6.966855520	0.174864230
C	0.165283392	0.126435912	-0.234236678
C	0.687905535	2.362389299	-0.590003896
C	-0.396680145	1.409321952	-0.539129334
C	1.923336440	1.644431407	-0.371736802
C	1.591567454	0.271101580	-0.132167731
H	-0.389143916	-0.804504441	-0.130815881
H	-1.453746396	1.625482631	-0.675005237
H	2.924246044	2.069114545	-0.362170953
H	2.300499877	-0.531863226	0.061126796
Ru	0.315253802	4.553145961	1.621402966
Ru	0.627201854	1.483399191	1.494096736
P	-1.346207646	4.545951219	3.014887274
O	-2.103238968	5.957393874	3.505077498
O	-1.130814416	3.928398386	4.588036518
O	-2.765951538	3.800331825	2.581785832
P	1.805294260	4.782472084	3.222360623
O	2.189034543	6.328858451	3.701413613
O	1.617329274	4.139796196	4.730092172
O	3.353988758	4.262624025	2.937652131
P	-1.012555974	0.710299063	2.775881756
O	-1.078848765	-0.916681917	2.848893700
O	-2.546753954	0.950255729	2.214522421
O	-1.179563595	1.015535770	4.380879139
P	2.176461484	0.977945638	3.012702172

O	2.443765467	-0.621368196	3.162282566
O	2.106792776	1.343662805	4.607625884
O	3.711829205	1.430834227	2.611028274
H	-1.040126148	1.971989529	4.567997491
H	-1.848641239	-1.208791297	3.381678472
H	-2.735662864	1.918685040	2.191087499
H	1.963013811	2.315052533	4.739651131
H	3.736282562	2.417295298	2.559862591
H	3.120517720	-0.796601745	3.850132923
H	0.640020583	4.081818274	4.909156484
H	-1.529748413	6.712797373	3.269701627
H	-1.751837278	4.349569753	5.220835698
H	-3.554132618	4.283866564	2.908093487
H	3.990407371	4.732536527	3.518241583
H	1.808891935	6.941827649	3.041739598

Photoisomer



Energy: -675.8771473303

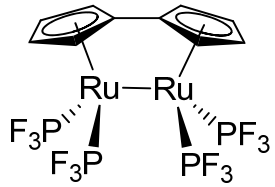
Molecular coordinates

C	-0.005151544	5.515255630	-0.437552173
C	0.672228557	3.242799530	-0.327966488
C	-0.459231447	4.139308773	-0.466719992
C	1.827356198	4.114770859	-0.203307129
C	1.410309351	5.500272339	-0.275162085
H	-0.626414713	6.400130041	-0.572942372
H	-1.496299386	3.823210216	-0.593284081
H	2.855668038	3.791340736	-0.037934438
H	2.067167316	6.368054200	-0.244173886
Ru	0.491488937	4.548936050	1.574608959
C	1.158716985	0.303940154	2.356540265
C	0.449154349	2.561346379	2.283893336
C	1.601435003	1.683804319	2.368813349
C	-0.697487272	1.683818083	2.202549406
C	-0.264133155	0.303894350	2.258518305
H	1.801690279	-0.571612442	2.431898093
H	2.642377505	2.001410820	2.424244294
H	-1.735848115	2.001917909	2.130361867
H	-0.912195617	-0.570993748	2.254865920
Ru	0.587854871	1.253531234	0.385527146
P	-1.134436252	5.254390146	2.873034486

O	-2.636340897	5.453287768	2.206318577
O	-1.067359224	6.780599247	3.575802562
O	-1.430776194	4.453686442	4.257936513
P	1.955724920	5.207755800	3.113057594
O	3.487531983	5.351792553	2.567630701
O	1.823049342	6.667112155	3.831642222
O	2.136429521	4.271985265	4.447953913
P	-0.915306809	0.618175008	-1.120930046
O	-0.870449328	-0.866483271	-1.792464719
O	-1.023004040	1.505059564	-2.509522399
O	-2.462151283	0.584244413	-0.591737855
P	2.211385492	0.523969206	-0.904482016
O	1.950448600	-0.721189839	-2.006003409
O	3.507642079	-0.075076390	-0.108963823
O	2.924170016	1.529463382	-2.013454723
H	-3.050766509	0.140599503	-1.238771855
H	-0.658144028	2.397672488	-2.327601626
H	0.077515473	-1.101120472	-1.958968384
H	4.207885351	-0.397848958	-0.714198091
H	2.606690030	2.444283143	-1.850026243
H	2.203322008	-0.418764144	-2.903352699
H	1.700513064	3.408404273	4.280139237
H	-1.229847119	7.467115352	2.897118460
H	-2.093944981	4.909037700	4.819030459
H	-2.712155304	4.872401564	1.422769439
H	4.083537598	5.726431059	3.250011489
H	0.867561313	6.893686976	3.944663329

Entry 23

Parent



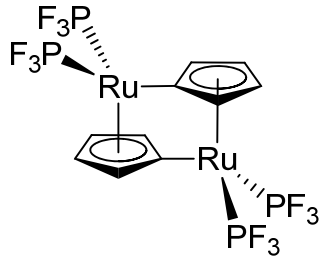
Energy: -862.4428406087

Molecular coordinates

C	-0.117880333	5.814483912	-0.141991546
C	0.700213702	3.674138686	-0.587840936
C	-0.500698436	4.473490242	-0.486237507
C	1.816393601	4.540479556	-0.286203603
C	1.305355973	5.856319825	-0.020072118
H	-0.795140337	6.657288036	-0.016138045
H	-1.517900482	4.125912396	-0.653993370
H	2.865085269	4.251760160	-0.268428465
H	1.902228017	6.737892095	0.206313853
C	0.051643094	0.029252778	-0.240441262

C	0.744588980	2.227868501	-0.608902923
C	-0.405537068	1.355758825	-0.547828527
C	1.908839541	1.420883371	-0.317748044
C	1.473110715	0.069935767	-0.097911334
H	-0.574439908	-0.857386711	-0.159371364
H	-1.440580533	1.647917429	-0.711688133
H	2.938443831	1.770661227	-0.283528264
H	2.118145482	-0.779551271	0.119021039
Ru	0.494214939	4.421360480	1.546801309
Ru	0.558039647	1.402692761	1.499742017
P	-1.180084874	4.773382460	2.894831986
F	-1.740845521	6.284389451	2.927359989
F	-1.118448443	4.573158510	4.479219672
F	-2.614963808	4.094910497	2.635035584
P	1.942596723	4.804420055	3.126856983
F	2.006747671	6.298871054	3.721159635
F	2.009314165	4.067069552	4.544288951
F	3.500656225	4.710884934	2.745325660
P	-1.155751735	0.967972728	2.768017262
F	-1.321977103	-0.546339799	3.287828108
F	-2.616049315	1.076087533	2.105902392
F	-1.490435507	1.655128085	4.172630399
P	1.948022995	0.990091015	3.126096510
F	2.488307911	-0.526094440	3.211946077
F	1.586246645	1.137178683	4.675962195
F	3.407142277	1.664842621	3.167875825

Photoisomer



Energy: -862.3942313969

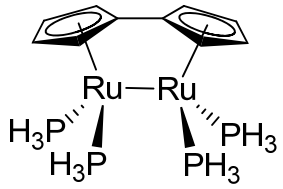
Molecular coordinates

C	-0.244185841	5.559220124	-0.357949293
C	0.528475606	3.322805547	-0.385688673
C	-0.646861717	4.166964161	-0.394285286
C	1.651236718	4.226615129	-0.288234087
C	1.176535661	5.597070734	-0.291911234
H	-0.910266727	6.419763911	-0.402781893
H	-1.676197743	3.817698823	-0.459036105
H	2.700040454	3.936639201	-0.256704027
H	1.800057893	6.489638810	-0.280224646
Ru	0.403090536	4.545456584	1.569194388

C	1.075020444	0.257825115	2.147796284
C	0.358137707	2.512945858	2.142382028
C	1.507622755	1.640750438	2.209068112
C	-0.782844152	1.637051817	1.984347828
C	-0.341040847	0.256435421	2.009330769
H	1.717948196	-0.617237548	2.227938633
H	2.541625085	1.959861309	2.327389795
H	-1.819962548	1.958160709	1.900127500
H	-0.982887817	-0.622036725	1.959696437
Ru	0.547172652	1.290496644	0.192603849
P	-1.233816519	5.127909509	2.895248409
F	-2.683071461	4.466807304	2.667405607
F	-1.742606191	6.648728836	2.938861115
F	-1.153612472	4.902530707	4.477881323
P	1.945223992	5.142732403	2.998753248
F	3.406734669	5.457610170	2.411242529
F	1.800553382	6.471072915	3.885533656
F	2.417806205	4.184603081	4.196101684
P	-0.867373510	0.660889100	-1.349782063
F	-1.354523221	-0.865606509	-1.429386241
F	-0.551357125	0.848561851	-2.907683070
F	-2.339004750	1.312042286	-1.360436912
P	2.293113378	0.740638495	-1.002883959
F	2.322208677	-0.601215994	-1.880396628
F	3.671336522	0.490174587	-0.216644630
F	2.887746074	1.705142558	-2.139007061

Entry 24

Parent



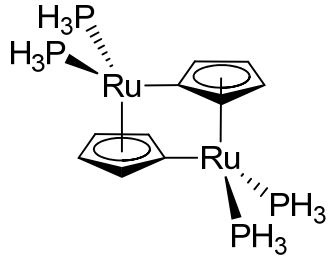
Energy: -290.4928313521

Molecular coordinates

C	0.014989477	5.852260844	-0.155770435
C	0.765878901	3.685146571	-0.615691608
C	-0.406397475	4.528519976	-0.531028780
C	1.907096267	4.507233040	-0.277844314
C	1.437593091	5.838880694	0.000599497
H	-0.631425123	6.722677982	-0.054174656
H	-1.428786676	4.218715008	-0.738032280
H	2.944417811	4.179073200	-0.259822620
H	2.062283316	6.697544704	0.242186132
C	-0.019994722	0.056580096	-0.323388772
C	0.757309856	2.236558596	-0.660908380

C	-0.425332428	1.404025235	-0.625725706
C	1.888060298	1.382378846	-0.369187696
C	1.402341807	0.043023251	-0.166077260
H	-0.677081603	-0.810243609	-0.270356282
H	-1.443774766	1.736662688	-0.816054652
H	2.929259778	1.696288695	-0.330790192
H	2.015762675	-0.835804443	0.026871731
Ru	0.540018910	4.423111936	1.508229976
Ru	0.519613535	1.390518522	1.414880357
P	-1.199201241	4.653289169	2.898874667
H	-1.798502768	5.944296908	3.089740542
H	-1.099209109	4.356284881	4.297971252
H	-2.457091777	3.987085242	2.711343048
P	1.929023643	4.661865472	3.248592957
H	2.471766262	5.954656186	3.558236498
H	1.521641529	4.374268884	4.592888682
H	3.196808181	3.994974327	3.349987877
P	-1.223895392	1.093516783	2.788404709
H	-1.796095704	-0.213449239	2.953487407
H	-2.493236877	1.734392629	2.591624322
H	-1.151953971	1.371738081	4.193069782
P	1.923780596	1.095743208	3.134373607
H	2.444448331	-0.210821228	3.425276177
H	1.548528988	1.380677070	4.488364234
H	3.205960377	1.735440792	3.213740181

Photoisomer



Energy: -290.4579846310

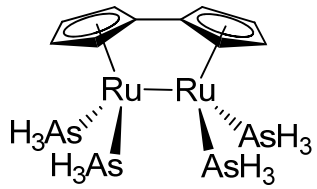
Molecular coordinates

C	-0.046944790	5.489062731	-0.586805729
C	0.648323824	3.227298108	-0.417821921
C	-0.490136839	4.106629983	-0.580762591
C	1.792921047	4.104987521	-0.292809577
C	1.366264349	5.487884490	-0.408459299
H	-0.675315541	6.366337543	-0.737421432
H	-1.523240707	3.785004419	-0.710121187
H	2.825258728	3.780839251	-0.163059805
H	2.013848857	6.364188915	-0.397191015
Ru	0.417756794	4.575011833	1.428033681
C	1.043552869	0.355519023	2.341694669

C	0.337510206	2.613272363	2.179827907
C	1.482142714	1.739304236	2.329721934
C	-0.804829898	1.731312500	2.070278617
C	-0.372179047	0.350047552	2.182592567
H	1.678067223	-0.519053130	2.482789295
H	2.515138194	2.066065541	2.446620739
H	-1.839625384	2.051447803	1.950954475
H	-1.016067043	-0.528833356	2.181783729
Ru	0.551297522	1.264170426	0.334061381
P	-1.351130462	5.238949800	2.643826619
H	-2.413057046	5.983156159	2.038750123
H	-1.199225203	6.102024461	3.778833224
H	-2.207821498	4.297736449	3.307793067
P	1.841927349	5.256286855	3.019545615
H	3.009166206	6.007747463	2.672220224
H	1.426023965	6.121946839	4.084523814
H	2.530432563	4.325797447	3.868904775
P	-0.897377725	0.618389499	-1.251907343
H	-0.504022919	-0.252950134	-2.320772117
H	-1.563064034	1.569509290	-2.096228025
H	-2.081914331	-0.105405769	-0.904935447
P	2.295101363	0.549352963	-0.885467724
H	2.117473506	-0.314629867	-2.016008432
H	3.337168213	-0.220603717	-0.278290433
H	3.178650937	1.460941868	-1.556826992

Entry 25

Parent



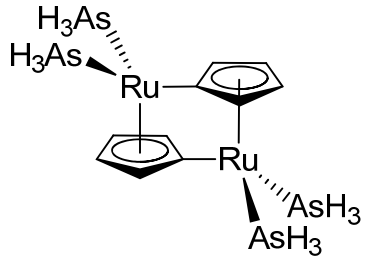
Energy: -381.2910552806

Molecular coordinates

C	-0.014956584	5.876568986	-0.191239749
C	0.740075473	3.704340354	-0.638272021
C	-0.436288239	4.543755489	-0.544963387
C	1.881717072	4.534372203	-0.313987618
C	1.409549103	5.870771560	-0.049114442
H	-0.664668263	6.745135601	-0.092144016
H	-1.458857414	4.229544752	-0.744798193
H	2.921044708	4.211783270	-0.308110376
H	2.033818938	6.734187593	0.177032167
C	-0.019510608	0.062794722	-0.376554447
C	0.738798422	2.257885082	-0.684529043
C	-0.439048805	1.416299016	-0.643066726

C	1.879399941	1.406805241	-0.416503727
C	1.405301001	0.056902848	-0.237332156
H	-0.670685268	-0.809185228	-0.331981483
H	-1.461394550	1.744492410	-0.820208248
H	2.919354239	1.726513780	-0.392062897
H	2.028412800	-0.820368841	-0.068569079
Ru	0.534986370	4.468309706	1.451233714
Ru	0.536147162	1.360883734	1.352038984
As	-1.287173128	4.774550512	2.934094361
H	-2.062229175	6.103533734	2.911823256
H	-1.085372773	4.769979382	4.457730320
H	-2.572655941	3.922488776	2.974268251
As	2.028648074	4.762771654	3.266693859
H	2.799315017	6.087607248	3.401941391
H	1.528471816	4.757029854	4.719925194
H	3.276289553	3.903729960	3.558476912
As	-1.281453974	0.958415577	2.817410429
H	-2.058722013	-0.364971946	2.708036432
H	-2.565542577	1.807268254	2.920663639
H	-1.073406987	0.859035724	4.336962372
As	2.035316501	0.947303141	3.139627472
H	2.810946301	-0.380864776	3.179833285
H	1.538344910	0.849175477	4.590678860
H	3.280632895	1.788266151	3.488856710

Photoisomer



Energy: -381.2615336225

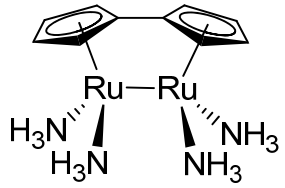
Molecular coordinates

C	-0.069697483	5.500929240	-0.555455217
C	0.623858978	3.230059757	-0.409243102
C	-0.516212534	4.116314340	-0.539523939
C	1.770657876	4.109896739	-0.294011930
C	1.345323689	5.496942472	-0.403569628
H	-0.700852412	6.378612513	-0.692377702
H	-1.552326221	3.797580339	-0.653259220
H	2.805472059	3.785193012	-0.185607609
H	1.995999548	6.371056215	-0.402931796
Ru	0.431121645	4.572006450	1.424944005
C	1.044113508	0.336157814	2.317780931
C	0.348228039	2.606200912	2.172635975

C	1.489523691	1.721052795	2.300763143
C	-0.797950993	1.725464063	2.059862620
C	-0.371245833	0.338794310	2.168955879
H	1.676270299	-0.541026965	2.453371854
H	2.525525916	2.040775655	2.412574561
H	-1.833249617	2.049247177	1.953300680
H	-1.021172487	-0.535866864	2.170057580
Ru	0.538481537	1.264206853	0.338315634
As	-1.420350568	5.294501263	2.726722180
H	-2.531224186	6.162395043	2.123336733
H	-1.238129325	6.157672911	3.986213002
H	-2.386924996	4.300666339	3.396162562
As	1.966308559	5.286923523	3.091323204
H	3.183073315	6.151515533	2.740139126
H	1.522922182	6.149001653	4.284939944
H	2.764501678	4.288176253	3.948716213
As	-1.003640925	0.552690827	-1.322966737
H	-0.567726444	-0.313166372	-2.516595291
H	-1.800803730	1.553096133	-2.179421940
H	-2.222657354	-0.306272653	-0.966014481
As	2.384181647	0.537551006	-0.969493350
H	2.194499963	-0.321341710	-2.230798968
H	3.492951293	-0.337141803	-0.371994718
H	3.353223644	1.528882588	-1.638982813

Entry 26

Parent



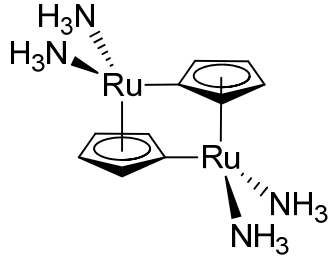
Energy: -317.1497943335

Molecular coordinates

C	-0.543905135	5.655595709	0.075166172
C	0.585281691	3.672125090	-0.444164546
C	-0.734757779	4.253181549	-0.218867181
C	1.546830999	4.745752220	-0.272808694
C	0.850797961	5.983254790	-0.022870070
H	-1.351157441	6.369173529	0.255265326
H	-1.692488390	3.748582780	-0.339763500
H	2.626251896	4.635167008	-0.390809730
H	1.292311218	6.977337398	0.043050335
C	0.544144385	-0.082828049	-0.238011651
C	0.883353160	2.246194711	-0.459906582
C	-0.088650324	1.172438332	-0.561357790
C	2.129059375	1.641934633	0.003200509

C	1.885691518	0.226830228	0.170328965
H	0.103155863	-1.075701544	-0.323080677
H	-1.118326534	1.298180107	-0.900701420
H	3.088271036	2.145284542	0.118072487
H	2.638482532	-0.503116061	0.476041463
Ru	0.473078974	4.409194315	1.591516679
Ru	0.561789447	1.395626975	1.499773178
N	-0.593027146	5.033068623	3.448029097
H	-1.313211002	4.395309112	3.797708404
H	-1.051746501	5.933866130	3.267890415
H	0.062219644	5.183252423	4.229299107
N	2.267385779	4.128338362	2.843737736
H	3.093266723	4.653650128	2.531799321
H	2.204939336	4.205362164	3.869313527
H	2.354057767	3.125093736	2.587243131
N	-1.454956494	1.612828820	2.375254370
H	-2.205804702	1.125796820	1.871465486
H	-1.465793775	2.631366962	2.162197610
H	-1.597786248	1.477360653	3.385256916
N	1.220634170	0.720551280	3.524554069
H	2.120631116	0.233696223	3.462610586
H	0.538526072	0.038832014	3.885014799
H	1.316054810	1.454529287	4.232442154

Photoisomer

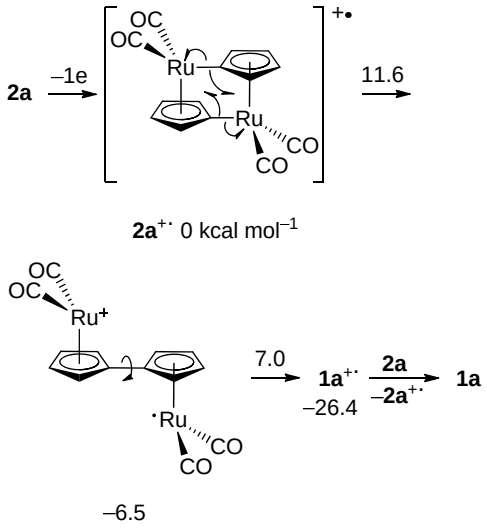


Energy: -317.1537002025

Molecular coordinates

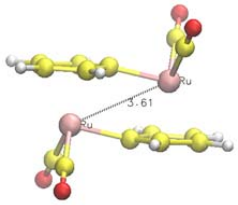
C	-0.075131460	5.518197461	-0.595265651
C	0.621183199	3.235563977	-0.429423700
C	-0.524107500	4.128680441	-0.574673478
C	1.773516838	4.126336923	-0.335034146
C	1.341412730	5.516890180	-0.447936829
H	-0.703489507	6.398954604	-0.740561745
H	-1.566544784	3.814418125	-0.676175615
H	2.813836934	3.809838245	-0.219524701
H	1.988034318	6.396291459	-0.461268691
Ru	0.438085978	4.531757580	1.342099792
C	1.039274971	0.317431389	2.359506981
C	0.344830248	2.600533295	2.192535577
C	1.489245742	1.706644829	2.339253899

C	-0.808091755	1.710667177	2.096629660
C	-0.377016164	0.319910003	2.209959080
H	1.666664259	-0.563804461	2.505968671
H	2.531770026	2.020136675	2.442211043
H	-1.848003044	2.027974301	1.979976916
H	-1.024301106	-0.559033438	2.222005488
Ru	0.529320349	1.304309656	0.421127128
N	-1.243579335	5.100059271	2.675825575
H	-2.006157845	5.519076151	2.136035829
H	-1.030339833	5.751781427	3.442865036
H	-1.594804111	4.231581214	3.098361232
N	1.813823162	5.090388503	2.992559793
H	2.674320328	5.501791878	2.619992439
H	1.453414421	5.746017275	3.698817662
H	2.063801180	4.220347507	3.479103625
N	-0.842486004	0.743220558	-1.232013222
H	-0.478006040	0.090974415	-1.939326010
H	-1.095319102	1.613317485	-1.716938391
H	-1.701851581	0.327118195	-0.862046068
N	2.214095036	0.738072095	-0.909784403
H	2.004399404	0.083529081	-1.675398489
H	2.977205716	0.323127542	-0.367622803
H	2.563068290	1.606646342	-1.333974096



Scheme 11. One-electron-transfer catalysis by $AgNO_3$ in the conversion of **2a** to **1a**. ΔH (below the respective species) and $\Delta H^{\ddagger}$ values (above reaction arrows) are relative to $\mathbf{2a}^{+\cdot}$ (0).

2a^{+}

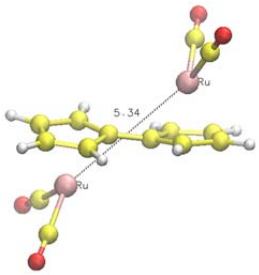


Energy: -397.262963

Molecular coordinates

C	-0.2258644930	5.7441351310	0.1750181840
C	0.3816208590	3.5190521350	-0.2356400470
C	-0.7333229920	4.4129264820	-0.0058321240
C	1.5826965400	4.3148728520	-0.1051736920
C	1.2054374060	5.6840368970	0.1127550740
C	-0.8194552960	4.6156926910	3.2929397600
C	1.9942311430	4.4404045860	3.1487074560
C	0.9817022820	0.1053747470	1.5863055490
C	0.4035593050	2.3401309250	1.9884083310
C	1.5075369870	1.4293128490	1.7754737920
C	-0.8076769550	1.5601726460	1.8417512340
C	-0.4492787000	0.1854672650	1.6282025980
C	1.6614678230	1.2752186560	-1.5047388040
C	-1.1628897540	1.3801506580	-1.4313138090
H	-0.8249246260	6.6430357370	0.3168544980
H	-1.7853952140	4.1340034650	-0.0211713710
H	2.6048397310	3.9524887160	-0.2040627460
H	1.8856889050	6.5304399710	0.2009110070
H	1.5663627930	-0.8037124260	1.4499659550
H	2.5660110360	1.6847736050	1.8021628080
H	-1.8244786710	1.9377392940	1.9315523380
H	-1.1408832320	-0.6518979650	1.5316990180
O	-1.6378125860	4.7249451000	4.1018743240
O	2.9026601890	4.4285738550	3.8635682740
O	2.5130511310	1.1982266560	-2.2824516430
O	-2.0520929130	1.3521241850	-2.1689721400
Ru	0.5131177100	4.4128468300	1.8997744280
Ru	0.2884716950	1.4462887550	-0.1481772020

Intermediate meta-stable state between $2a^+$ and $1a^+$



Energy: -397.28377

Molecular coordinates

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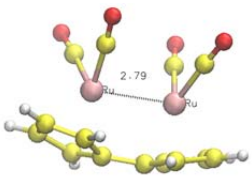
C	1.7240710057	4.8496978257	0.1666376607
C	1.2884000627	6.1679307949	0.5142521074
C	-0.5179077225	5.0321751880	3.6431476813
C	2.2911832983	5.1008498746	3.3844790496
C	1.2097237042	0.3967032980	-0.6180347120
C	0.5674112749	2.5557910366	-0.0252092032
C	1.6525328727	1.7564082177	-0.5555583233
C	-0.5534811281	1.6693602414	0.2105488022
C	-0.1479773158	0.3412315444	-0.1398873085
C	0.7880626325	1.1490264179	-3.6639264881
C	-1.8402810695	1.1155468246	-2.6786611841
H	-0.7699943942	7.0024790574	0.9075375808
H	-1.6344314442	4.4759426100	0.4506824335
H	2.7515344033	4.5477545995	-0.0275661034
H	1.9247599333	7.0450733011	0.6208843842
H	1.8013372444	-0.4540972942	-0.9522505432
H	2.6390718885	2.1203960269	-0.8366407562
H	-1.5147809662	1.9515848769	0.6359194052
H	-0.7514711073	-0.5593425713	-0.0391914551
O	-1.3430602655	5.1973836545	4.4374495891
O	3.2235018027	5.3064307512	4.0376839831
O	1.3550916494	0.8318622273	-4.6212160034
O	-2.8993666215	0.7809743066	-3.0032521214
Ru	0.7718352729	4.7932788673	2.2188139515
Ru	-0.0929741747	1.5848236244	-1.9952318072

1a^{+}



Energy: -397.347106

Molecular coordinates

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C	1.9826542380	4.4525704550	0.0608764610
C	1.5380634270	5.7733310440	0.3834268420
C	-0.8858960980	4.3148434830	3.0685914820
C	1.7140654380	4.8308261600	3.4156217480
C	-0.1415139410	0.0874140630	0.0679559390
C	0.7599517500	2.2030472750	-0.2746757470

C	-0.4442222200	1.4094701640	-0.3872865830
C	1.8008170950	1.3368697010	0.2388486350
C	1.2348378120	0.0387011670	0.4582223990
C	-1.3828253360	1.0141740500	2.8381658550
C	1.1710326690	1.5343167390	3.4429208060
H	-0.5152299780	6.6957867180	0.4230762930
H	-1.3719138900	4.2371788270	-0.3321611780
H	3.0171304920	4.1149190990	0.0448070620
H	2.1807964190	6.6066605430	0.6634925450
H	-0.8410061190	-0.7468941250	0.0997708490
H	-1.4066593850	1.7476916090	-0.7668349560
H	2.8324463480	1.6243492100	0.4364325520
H	1.7650123400	-0.8362547790	0.8300595700
O	-1.8128703410	4.3909691340	3.7588122730
O	2.3652866850	5.2114591640	4.2924536490
O	-2.3034580050	0.6266810290	3.4212737260
O	1.7910423660	1.4584255530	4.4181435200
Ru	0.6382049000	4.2993438370	1.8998169240
Ru	0.1614552260	1.5550947730	1.8087184750

Method B: BP86/Lanl2dz&631+g(d,p)

All calculations are performed with the Gaussian09 software package[8] using the BP86,[9] the 6–31+G(d,p) basis set for C, O, and H, and the LANL2DZ[10] basis set for Fe. This combination has been employed previously and with satisfactory results for other organometallic species.[11]

Entry 1

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[8] Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, **2010**.

[9] A. D. Becke, *Phys. Rev. A*, **1988**, *38*, 3098.

[10] a) P. J. Hay, W. R. Wadt, *J. Chem. Phys.*, **1985**, *82*, 299; b) T. H. Dunning, P. J. Hay, in *Methods of Electronic Structure Theory*, *Vol. 2*, (Ed.: H. F. Schaefer), Plenum, New York, **1977**.

[11] a) M. R. Harpham, S. C. Nguyen, Z. Hou, J. C. Grossman, C. B. Harris, M. W. Mara, A. B. Stickrath, Y. Kanai, A. M. Kolpak, D. Lee, D. Liu, J. P. Lomont, K. Moth-Poulsen, N. Vinokurov, L. X. Chen, K. P. C. Vollhardt, *Angew. Chem.* **2012**, *124*, 7812; *Angew. Chem., Int. Ed.* **2012**, *51*, 7692; b) K. R. Sawyer, J. F. Cahoon, J. E. Shanoski, E. A. Glascoe, M. F. Kling, J. P. Schlegel, M. C. Zoerb, M. Hapke, J. F. Hartwig, C. E. Webster, C. B. Harris, *J. Am. Chem. Soc.* **2010**, *132*, 1848; c) J. F. Cahoon, K. R. Sawyer, J. P. Schlegel, C. B. Harris, *Science* **2008**, *319*, 1820.

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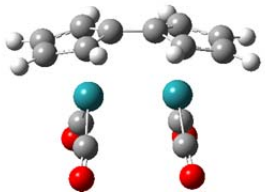

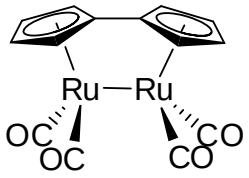

Energy (a.u., sum of electronic and thermal enthalpies, corrected at 298 K, 1 atm):
-1027.156471

Molecular coordinates

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C	-0.72727200	-2.06066400	-0.00001200
C	-1.56350200	-1.85331200	1.16517000
C	-1.56347200	-1.85330100	-1.16521400
C	-2.89225300	-1.54362000	-0.71673400
H	-3.75386300	-1.35196600	1.35628500
H	-1.24276600	-1.92537200	2.20392800
H	-1.24270900	-1.92535100	-2.20396400
H	-3.75382900	-1.35195400	-1.35638100
C	2.89227600	-1.54359000	0.71673000
C	0.72730100	-2.06065900	0.00000700
C	1.56349900	-1.85328600	1.16520900
C	1.56353000	-1.85329900	-1.16517500
C	2.89229500	-1.54359600	-0.71666300
H	3.75384900	-1.35191300	1.35637700
H	1.24273600	-1.92533800	2.20396000
H	1.24279400	-1.92536400	-2.20393300
H	3.75388500	-1.35192700	-1.35628900
Ru	-1.44086700	0.14201900	-0.00001000
Ru	1.44086700	0.14203100	0.00000600
C	-1.61392300	1.45733600	1.32385400
O	-1.79199400	2.24646500	2.17385100
C	-1.61386300	1.45736500	-1.32385400
O	-1.79189100	2.24651900	-2.17383700
C	1.61384300	1.45737000	1.32385800
O	1.79185800	2.24652000	2.17384900
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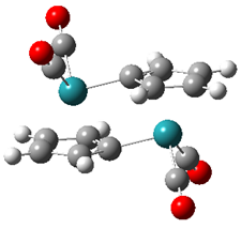
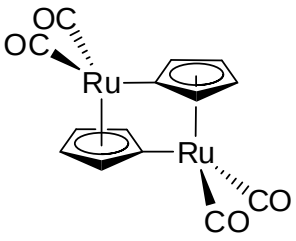
Photoisomer





Energy (a.u.): -1027.124493

Molecular coordinates

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C	-0.48262000	-1.70220600	1.15477600
C	-0.48262100	-1.70224700	-1.15472800
C	-1.68606300	-2.38438600	-0.71316700
C	-2.78046500	0.65004200	1.35110200
C	-2.78047200	0.65000400	-1.35112000
C	1.68606300	2.38437500	-0.71322000
C	-0.29287100	1.30730500	-0.00001800
C	0.48262400	1.70222000	-1.15476900
C	0.48262000	1.70222700	1.15473500
C	1.68605500	2.38438500	0.71318700
C	2.78047000	-0.65004200	-1.35111000
C	2.78046600	-0.65000200	1.35111900
H	-2.44676500	-2.82601700	1.35831600
H	-0.19342900	-1.55066300	2.19509900
H	-0.19344400	-1.55073000	-2.19505900
H	-2.44675800	-2.82607400	-1.35823100
H	2.44675600	2.82605500	-1.35829100
H	0.19344800	1.55068100	-2.19509700
H	0.19342900	1.55070800	2.19506100
H	2.44676100	2.82605200	1.35825300
O	-3.40678100	1.13940500	2.21243800
O	-3.40679500	1.13934200	-2.21246500
O	3.40678900	-1.13940600	-2.21244100
O	3.40678100	-1.13933000	2.21247500
Ru	-1.75705200	-0.17541200	0.00000000
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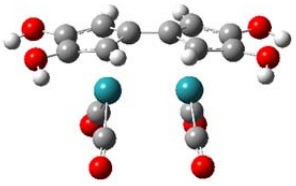

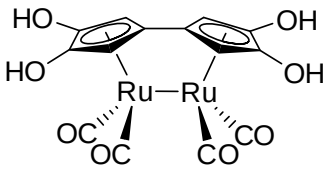

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Molecular coordinates

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C	1.55814800	-1.66465700	1.13497000
C	2.90670200	-1.44673700	0.69946800
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H	1.24646800	-1.77704900	2.17190800
C	-2.91104500	-1.37130300	-0.73491300
C	-0.72499700	-1.80918500	-0.04652900

C	-1.56907300	-1.58651600	-1.20879000
C	-1.55815900	-1.66466800	1.13495900
C	-2.90670900	-1.44674100	0.69944900
H	-1.26224400	-1.64087300	-2.25296400
H	-1.24648800	-1.77707200	2.17189800
Ru	1.44394600	0.35613300	0.00766100
Ru	-1.44394600	0.35613300	0.00767300
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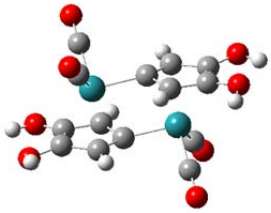
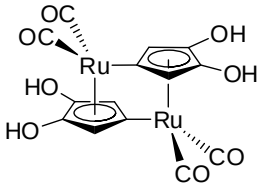
O	1.80873500	2.48817000	-2.13632400
C	1.64403500	1.63669700	1.36687300
O	1.82760200	2.40496300	2.23480300
C	-1.62542000	1.69195900	-1.29039300
O	-1.80874600	2.48821200	-2.13626900
C	-1.64402500	1.63667300	1.36690900
O	-1.82758200	2.40492200	2.23485700
O	-3.99415000	-1.43315600	1.50853900
H	-4.77216700	-1.17255700	0.97327000
O	-4.09955500	-1.31534500	-1.41347700
H	-3.96192300	-0.93767000	-2.30269900
O	3.99413600	-1.43314300	1.50856600
H	4.77215700	-1.17255100	0.97330000
O	4.09956500	-1.31536300	-1.41344900
H	3.96194200	-0.93768600	-2.30267200

Photoisomer





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Molecular coordinates

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C	-1.18470900	-1.31518800	-1.19113900
C	-2.55904200	-1.50952600	-0.77040000
C	-2.19815100	1.72588500	1.40158400
C	-2.25837800	1.77942000	-1.31305800
C	2.55900100	1.50940000	-0.77079000
C	0.33265600	1.29821800	-0.01888300
C	1.18464400	1.31499100	-1.19142200
C	1.21348700	1.36286900	1.12831600
C	2.58248100	1.51483100	0.65683900
C	2.25830100	-1.77962800	-1.31290100
C	2.19823100	-1.72566200	1.40173900
H	-0.90431400	-1.38953600	2.17452400

H	-0.85710500	-1.29826600	-2.23010300
H	0.85698300	1.29789500	-2.23036400
H	0.90443400	1.38989600	2.17424400
O	-2.54464200	2.40121700	2.29850700
O	-2.63914600	2.49657000	-2.15866200
O	2.63901800	-2.49691000	-2.15841500
O	2.54477100	-2.40085200	2.29875100
Ru	-1.63787000	0.58400700	0.01241100
Ru	1.63787100	-0.58400600	0.01241500
O	-3.59932200	-1.76609900	-1.60406400
H	-4.41837200	-1.81951000	-1.06958100
O	-3.72938800	-1.84400100	1.33318300
H	-3.65379100	-1.57824000	2.26883700
O	3.59923600	1.76583600	-1.60455100
H	4.41831400	1.81933400	-1.07012200
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Entry 3
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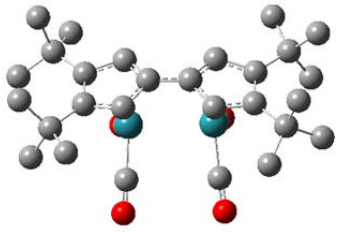

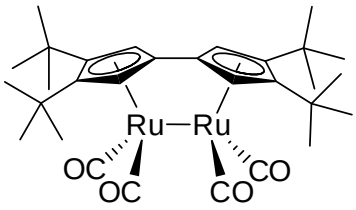

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Molecular coordinates

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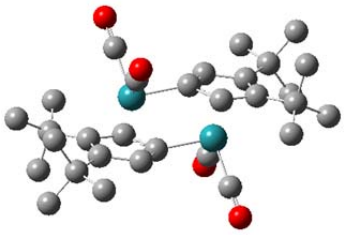
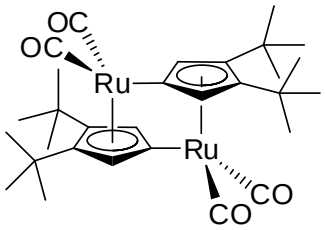
C	1.49679300	-1.56274500	1.20455800
C	2.88897100	-1.31274100	0.89093000
H	1.33139700	-1.25822600	-2.12538500
C	-2.88317900	-0.90748000	-0.87675300
C	-0.74050000	-1.52501400	-0.06879300
C	-1.51558800	-1.21827500	-1.24025800
C	-1.63007500	-1.36272300	1.05036300
C	-2.95493400	-1.00126400	0.59342000
H	-1.34682600	-1.50782300	2.09060700
Ru	1.52518900	0.53434000	0.27497700
Ru	-1.36983000	0.68132900	0.03728800
C	1.86722800	2.01335100	-0.82458600
O	2.14597300	2.92006700	-1.51899700
C	1.56693700	1.66029300	1.77085000
O	1.64258000	2.32722600	2.73587700

C	-1.30413900	2.04844500	-1.24091700
O	-1.31537900	2.87648400	-2.07519200
C	-1.59145000	1.97188400	1.37840200
O	-1.79644900	2.76541100	2.22122200
C	-4.11526500	-0.99157100	1.61734900
C	-4.69289200	-2.43729200	1.68617000
H	-5.49127500	-2.48311700	2.44844300
H	-5.12037900	-2.76327100	0.72531100
H	-3.90842400	-3.16013700	1.97058800
C	-5.25088300	0.01183300	1.31783500
H	-5.98111100	-0.01244100	2.14570300
H	-4.85957700	1.04045200	1.24180400
H	-5.80153500	-0.22461400	0.39628400
C	-3.58994200	-0.64188400	3.03848900
H	-2.89240700	-1.39954400	3.43273000
H	-3.09172300	0.34071500	3.06028100
H	-4.44415200	-0.60421400	3.73611400
C	4.12978200	-1.07099200	-1.58841300
C	4.57949700	-2.52777600	-1.91076700
H	3.73770200	-3.11864100	-2.31202400
H	5.37833600	-2.51058100	-2.67375200
H	4.96727400	-3.05164500	-1.02335700
C	3.64927900	-0.43520100	-2.92354900
H	4.50971200	-0.35079200	-3.60933000
H	2.89258200	-1.04955500	-3.43931600
H	3.23777700	0.57551400	-2.77081600
C	5.34623400	-0.23859100	-1.12646600
H	5.04559300	0.79071900	-0.86757900
H	5.86708900	-0.68072300	-0.26529300
H	6.07783700	-0.18056300	-1.95142000
H	1.10140800	-1.71925700	2.20547600
C	3.96453200	-1.37968400	2.00671900
C	3.30379800	-1.73899100	3.36627900
H	2.57059100	-0.97797400	3.68372500
H	2.80844200	-2.72553800	3.34187600
H	4.08689700	-1.78042400	4.14259300
C	4.98042800	-2.51518900	1.70222800
H	4.46378500	-3.47554400	1.52822000
H	5.60687100	-2.29900300	0.82438000
H	5.65691600	-2.64596900	2.56542000
C	4.70668900	-0.03566200	2.22963500
H	4.01097900	0.72929500	2.60918900
H	5.50439900	-0.17687900	2.98136800
H	5.16635800	0.35942100	1.31567500
H	-1.12883400	-1.23420000	-2.25657400
C	-3.95324200	-0.68851900	-1.97820100

C	-5.06729800	-1.76542700	-1.86284700
H	-4.63839900	-2.78303300	-1.85891400
H	-5.67856500	-1.64752400	-0.95610500
H	-5.74652500	-1.68748700	-2.73027300
C	-4.57255200	0.73394800	-1.96215300
H	-3.81169100	1.48771900	-2.21969500
H	-5.38010200	0.79155800	-2.71445900
H	-4.99427000	1.00909000	-0.98786500
C	-3.31821600	-0.86769100	-3.38477000
H	-2.51832600	-0.13162500	-3.57414000
H	-2.91241700	-1.88385200	-3.53308100
H	-4.09677900	-0.70655100	-4.14995900

Photoisomer





(H atoms are omitted)

Energy (a.u.): -1655.656452

Molecular coordinates

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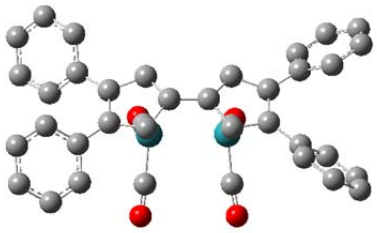
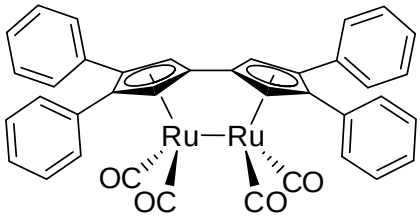
C	-0.16958000	1.29085500	-0.02728100
C	0.65183700	1.54371500	1.12252000
C	0.62142200	1.70894400	-1.14852300
C	1.88965100	2.30112300	-0.71441700
C	2.66536200	-1.04417300	1.13179200
C	2.68631900	-0.85312100	-1.54551300
C	-1.93250100	-2.20940500	-1.00060000
C	0.14685400	-1.30512300	-0.22790600
C	-0.67456100	-1.55797800	-1.37770900
C	-0.64415000	-1.72321400	0.89333300
C	-1.91237900	-2.31539200	0.45922400
C	-2.68809900	1.02992700	-1.38695400
C	-2.70903700	0.83884100	1.29034300
H	0.35698200	1.32097400	2.14601200
H	0.29770800	1.64371400	-2.18589700
H	-0.37970400	-1.33523900	-2.40120100
H	-0.32043900	-1.65798400	1.93070900
O	3.19808200	-1.70081600	1.94687100
O	3.24353600	-1.39388700	-2.42656500
O	-3.22082500	1.68658700	-2.20201500
O	-3.26624800	1.37959700	2.17140500
Ru	1.76616200	0.00842000	-0.14479900
Ru	-1.78888900	-0.02268500	-0.11038600

C	2.74894000	3.05388700	-1.75814200
C	2.59214600	2.41765800	-3.16802900
H	1.56186100	2.48264800	-3.55394200
H	3.23445100	2.96361800	-3.88047800
H	2.90326500	1.36036900	-3.17482500
C	2.19668800	4.50878800	-1.84555800
H	2.30052900	5.04998700	-0.89201800
H	2.74725800	5.07152700	-2.62076200
H	1.12746500	4.50768400	-2.11936500
C	4.26596100	3.09096300	-1.46998500
H	4.51685600	3.64739600	-0.55572800
H	4.67883600	2.07100600	-1.38744300
H	4.77965100	3.59624200	-2.30686200
C	2.86843000	2.73531600	1.83919300
C	2.97085600	4.28241200	1.73069600
H	3.48209800	4.61022600	0.81343400
H	1.96989400	4.74783400	1.75052000
H	3.54511300	4.67618500	2.58819900
C	4.28159100	2.09631500	1.79998600
H	4.92781600	2.58423700	2.55223500
H	4.22491300	1.02362500	2.04612500
H	4.77020000	2.18793900	0.82234100
C	2.29778700	2.43414500	3.25248800
H	1.32361800	2.92405400	3.42281000
H	2.18688900	1.35097200	3.43129700
H	3.00092300	2.82093400	4.01008800
C	-2.89115900	-2.74956800	-2.09438800
C	-2.77166500	-3.06816700	1.50294100
C	-4.30431300	-2.11055200	-2.05518000
H	-4.95054400	-2.59846700	-2.80742900
H	-4.79292400	-2.20217200	-1.07753500
H	-4.24762400	-1.03786300	-2.30131900
C	-2.99360300	-4.29666300	-1.98589700
H	-3.50484800	-4.62447600	-1.06863600
H	-3.56786700	-4.69042600	-2.84340100
H	-1.99264700	-4.76209800	-2.00572500
C	-2.32051200	-2.44840000	-3.50768200
H	-2.20960300	-1.36522700	-3.68648800
H	-1.34634700	-2.93831800	-3.67800300
H	-3.02365000	-2.83518000	-4.26528400
C	-4.28868900	-3.10523300	1.21478900
H	-4.53958900	-3.66164200	0.30051800
H	-4.80237700	-3.61052900	2.05165600
H	-4.70155900	-2.08527200	1.13227100
C	-2.21941800	-4.52307100	1.59033500
H	-2.76998500	-5.08581900	2.36553500

H	-2.32326300	-5.06425600	0.63678800
H	-1.15019300	-4.52197200	1.86413800
C	-2.61486700	-2.43195900	2.91283700
H	-1.58458100	-2.49695500	3.29874700
H	-2.92598600	-1.37466900	2.91964800
H	-3.25717100	-2.97792700	3.62528000

Entry 5
Parent





(H atom are omitted)
Energy (a.u.): -1950.573469
Molecular coordinates

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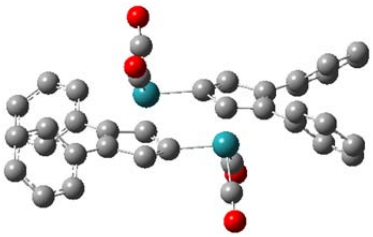
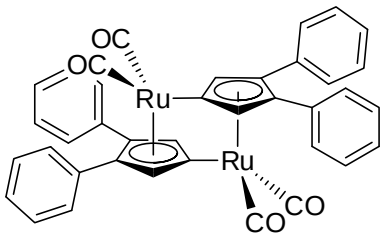
C	-5.24370800	1.76477400	-3.34281300
C	-0.57348500	0.08413300	-3.47124700
C	-4.53323400	3.99339900	-2.66413700
C	2.59764200	0.16771700	-3.04970500
C	-4.24374800	1.19490100	-2.53848300
C	-3.53145700	3.42604200	-1.85611200
C	-0.68936200	-2.00585600	-1.83853200
C	-3.37319000	2.01926100	-1.78206300
C	2.47317600	-1.87863600	-1.36368400
C	-2.30358700	1.45262600	-0.92588000
C	-0.97153300	2.01043700	-0.81342900
C	2.13480800	2.13644900	-0.39560500
C	3.49100300	1.69725100	-0.13421300
C	-2.38494900	0.32086300	-0.00696600
C	-3.48917300	-1.86864600	0.58927500
C	-3.58135300	-0.47165400	0.36757300
C	-4.60864000	-2.60143700	1.01801200
C	4.46382300	-0.57589900	2.74093500
C	-4.82476800	0.17169100	0.59278400
C	-0.22397200	1.26180300	0.17955700
C	-5.84021500	-1.95288200	1.23506600
C	-5.94264600	-0.56500400	1.02195600
C	1.21279600	1.32070000	0.37383500
C	5.50055800	-1.31631300	3.33702600
C	-1.09366000	0.19390100	0.63865000
C	3.41217300	0.55291800	0.76924600
C	4.52462400	-0.22183700	1.36962900

C	2.01200500	0.32329600	1.06061700
C	6.61418700	-1.71330500	2.57365900
C	5.65051500	-0.62844600	0.61024500
C	6.68434400	-1.36616000	1.20907200
H	-6.16987100	3.60560700	-4.04166700
H	-5.90080900	1.11508800	-3.92899500
H	-4.64197000	5.08155800	-2.70920900
H	-4.11398300	0.10935700	-2.50798700
H	-2.87569400	4.07247200	-1.26337400
H	-0.60555100	2.86383000	-1.38116700
H	1.87219900	3.00398100	-0.99742200
H	3.60709100	-0.25305900	3.34177800
H	-2.54278400	-2.38302900	0.39641100
H	5.43779300	-1.58074300	4.39725300
H	-4.52097800	-3.68122300	1.17297400
H	-4.90814000	1.25142000	0.44195000
H	-6.71260400	-2.52509200	1.56544400
H	-6.89392500	-0.05158500	1.19333600
H	-0.86075800	-0.53145600	1.41546300
H	7.41928200	-2.29310700	3.03540900
H	5.69543600	-0.38206800	-0.45439100
H	7.54158400	-1.68180300	0.60658000
O	-0.59854700	0.27457600	-4.64966700
O	2.91051700	0.33791300	-4.19091300
O	-0.79031200	-3.19203500	-1.94806400
O	2.70321800	-3.04986000	-1.39332400
Ru	-0.63903900	-0.15301300	-1.61879600
Ru	2.20341400	-0.03380800	-1.23648900
C	4.70109500	2.42481700	-0.58821100
C	4.79493600	2.92848100	-1.90983600
C	5.75310100	2.70228400	0.32117900
C	5.91036300	3.68231800	-2.31179200
H	4.00246200	2.70218800	-2.62968700
C	6.86753600	3.45714700	-0.08475200
H	5.68819500	2.33472900	1.34888100
C	6.95176900	3.94878200	-1.40130800
H	5.97029100	4.05315000	-3.33966700
H	7.66913700	3.66384100	0.63122100
H	7.82197300	4.53284100	-1.71635400
H	1.63328000	-0.46867500	1.70398500

Photoisomer





Energy (a.u.): -1950.537623

Molecular coordinates

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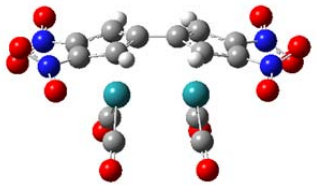
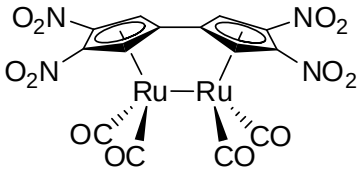
C	0.63889800	1.57644200	1.17976600
C	0.66358300	1.73860800	-1.12678300
C	1.90869200	2.34553900	-0.63842200
C	2.69187600	-0.99334200	1.22329600
C	2.71236100	-0.83767300	-1.47574200
C	-1.87202100	-2.24049100	-0.97384000
C	0.18230300	-1.31865500	-0.17504000
C	-0.61881700	-1.57638700	-1.35518700
C	-0.63751800	-1.71643200	0.95278200
C	-1.88739900	-2.31731000	0.47493400
C	-2.66620300	1.02442200	-1.40268500
C	-2.69192700	0.82898700	1.29385300
H	0.36284200	1.72583700	-2.17296600
H	-0.29833700	-1.42732000	-2.38482300
H	-0.35695200	-1.63771000	2.00202200
O	3.25576200	-1.60983100	2.07424500
O	3.29094200	-1.35576700	-2.38265200
O	-3.23025300	1.65569500	-2.24467900
O	-3.27077400	1.33065800	2.20786400
Ru	1.78136500	0.00661700	-0.08160600
Ru	-1.75803100	0.00583300	-0.11388500
C	2.88963900	2.73507300	1.78859900
C	4.28644100	2.60589500	1.58108400
C	2.43417600	3.36288400	2.97549600
C	5.19705400	3.09364500	2.53211200
H	4.64963200	2.10504300	0.67890200
C	3.34926300	3.84889800	3.92681000
H	1.35857700	3.48291100	3.14106900
C	4.73320500	3.71666100	3.70877200
H	6.27166100	2.97773400	2.36031500
H	2.97929000	4.33182100	4.83666000
H	5.44564200	4.09084800	4.45039900
C	-2.80223100	-2.86602800	-1.94492900
C	-3.29722500	-4.17624100	-1.72093100
C	-3.14226300	-2.21211400	-3.15610700
C	-4.11496100	-4.80501600	-2.67613100

H	-3.02690000	-4.70396800	-0.80250000
C	-3.95901000	-2.84365400	-4.10876100
H	-2.78108300	-1.19529300	-3.33826200
C	-4.45083000	-4.14238900	-3.87200400
H	-4.48469200	-5.81761400	-2.48670600
H	-4.21755200	-2.31805900	-5.03326600
H	-5.08917000	-4.63291100	-4.61329200
C	-2.89865500	-2.94017800	1.36333400
C	-2.46581200	-3.71881400	2.46637500
C	-4.29128600	-2.78031200	1.14914700
C	-3.39883000	-4.32145400	3.32948100
H	-1.39356300	-3.86297000	2.63450000
C	-5.21980500	-3.38463600	2.01178000
H	-4.63726800	-2.16487200	0.31355100
C	-4.77838100	-4.15721600	3.10545600
H	-3.04621200	-4.92003600	4.17522400
H	-6.29093400	-3.24360400	1.83707000
H	-5.50477100	-4.62237000	3.77894000
H	0.33886800	1.36143500	2.20426500
C	2.85702200	3.09113400	-1.50122200
C	3.22948900	2.59588900	-2.77634700
C	3.33856100	4.36414800	-1.10199500
C	4.06458200	3.34501800	-3.62192800
H	2.87918000	1.60870300	-3.09309400
C	4.17465800	5.11085700	-1.95042000
H	3.04359800	4.77073700	-0.13099400
C	4.54257500	4.60516300	-3.21173900
H	4.34829200	2.94085600	-4.59863800
H	4.53378500	6.09259500	-1.62614300
H	5.19527000	5.18711000	-3.86971600

Entry 8

Parent





Energy (a.u.): -1845.197250

Molecular coordinates

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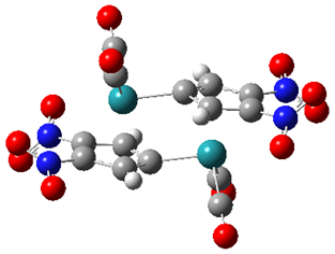
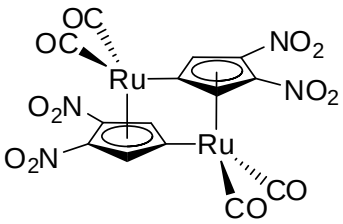
C	-1.55680000	-1.46157500	-1.18364300
C	-1.54782900	0.82947600	-1.66396000
C	-2.87347200	0.45861200	-1.26575700
H	-1.26745200	-2.50127000	-1.03896600
H	-1.25611900	1.83101100	-1.97686600

C	2.87677100	-0.95112900	-0.97185300
C	0.72860600	-0.36208200	-1.62030600
C	1.55681100	-1.46157100	-1.18365900
C	1.54782400	0.82948600	-1.66395300
C	2.87346900	0.45862800	-1.26575000
H	1.26747000	-2.50126900	-1.03899600
H	1.25610800	1.83102200	-1.97685000
Ru	-1.43399400	0.11625200	0.54064900
Ru	1.43399200	0.11623600	0.54064400
C	-1.58407100	-0.89051400	2.12172500
O	-1.74037800	-1.53878300	3.07991400
C	-1.59670800	1.67792500	1.57762200
O	-1.75410300	2.65496600	2.19484100
C	1.58404300	-0.89057400	2.12169500
O	1.74033000	-1.53887600	3.07986500
C	1.59672800	1.67788300	1.57765500
O	1.75414200	2.65490500	2.19489800
N	4.02188800	1.36739600	-1.42384100
N	4.02025300	-1.78265600	-0.57069000
O	5.04691200	0.88184600	-1.92102800
O	4.96896500	-1.22503100	-0.00385000
O	3.92112600	-2.99514100	-0.83630900
O	3.83771000	2.55456500	-1.11030700
N	-4.02023900	-1.78266700	-0.57066600
N	-4.02189900	1.36736900	-1.42386600
O	-3.92108200	-2.99516700	-0.83620800
O	-4.96897800	-1.22502500	-0.00388700
O	-5.04689300	0.88181600	-1.92111200
O	-3.83775200	2.55453200	-1.11029200

Photoisomer





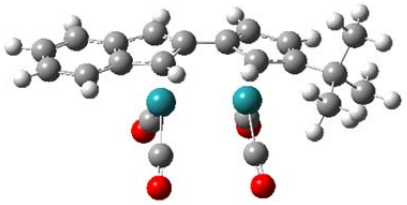
Energy (a.u.): -1845.169196

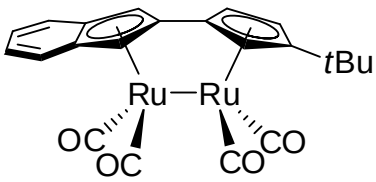
Molecular coordinates

C	-2.78692400	0.96377500	-0.54644900
C	-0.58813500	1.18745400	0.23543300
C	-1.42645400	1.26624500	-0.93418800
C	-1.43042400	0.77218800	1.33331200
C	-2.79045500	0.65440600	0.85114200
C	-1.69510900	-1.95301000	-1.79596100
C	-1.74837300	-2.51444000	0.81664000
C	2.78692000	-0.96377700	0.54645000

C	0.58813100	-1.18745800	-0.23543500
C	1.42645000	-1.26624700	0.93419000
C	1.43042200	-0.77219300	-1.33331200
C	2.79045300	-0.65441000	-0.85114000
C	1.69510600	1.95301200	1.79595200
C	1.74836700	2.51443200	-0.81664800
H	-1.13210800	1.54443800	-1.94560500
H	-1.14262900	0.63426500	2.37542400
H	1.13210200	-1.54444100	1.94560600
H	1.14262600	-0.63427300	-2.37542300
O	-1.83701900	-2.55010900	-2.78704000
O	-1.91880300	-3.46568300	1.46617000
O	1.83703100	2.55014000	2.78701600
O	1.91880500	3.46568800	-1.46615700
Ru	-1.46873100	-0.94858100	-0.20977300
Ru	1.46872700	0.94857700	0.20977000
N	3.93929000	-1.01792600	1.45277100
N	3.93811200	-0.49112800	-1.75909200
O	3.79078200	-1.71522300	2.47355100
O	4.95149900	-0.37361400	1.14032900
O	4.88901700	-1.26670700	-1.59280600
O	3.82119100	0.35820100	-2.65822700
N	-3.93929700	1.01793000	-1.45276600
N	-3.93811400	0.49112100	1.75909600
O	-4.95149700	0.37359600	-1.14034200
O	-3.79077900	1.71520600	-2.47356200
O	-4.88899700	1.26673600	1.59284400
O	-3.82118200	-0.35819200	2.65824500

Entry 9
Parent



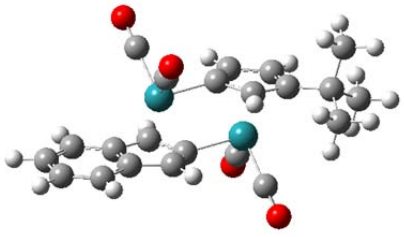


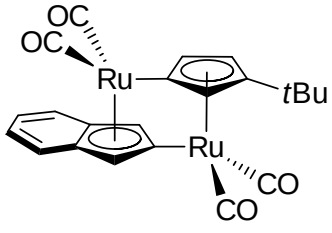
Energy (a.u.): -1337.891123
Molecular coordinates

C	2.88222400	-1.47030400	-0.84366300
C	0.67145900	-1.96305600	-0.19076900
C	1.52397500	-1.61950700	-1.30987900
C	1.51202400	-2.00122000	0.98539600
C	2.85514100	-1.69457700	0.58031400
H	1.19057600	-1.50537100	-2.34044100
H	1.18591400	-2.22019000	2.00178700

H	3.71834000	-1.66513900	1.24538400
C	-2.96331200	-1.32488900	-0.83523800
C	-0.78433300	-1.89872100	-0.18593600
C	-1.60113000	-1.47781600	-1.30357900
C	-1.60759400	-1.86118300	1.00399400
C	-2.96730600	-1.56457800	0.60316000
H	-1.27404700	-1.39946200	-2.34024400
H	-1.28571600	-2.12266600	2.01187100
Ru	1.49454300	0.15060600	0.17511100
Ru	-1.38143900	0.27370300	0.17350300
C	1.73840000	1.68183200	-0.88051300
O	1.95207000	2.61527500	-1.56010800
C	1.75086900	1.18017900	1.72107500
O	1.98471100	1.77574500	2.70474200
C	-1.45607700	1.78375100	-0.94121000
O	-1.56481700	2.70152000	-1.66448400
C	-1.46195400	1.35244900	1.70932400
O	-1.57081000	1.99741300	2.68361900
C	-4.18979100	-1.48794600	1.33258900
H	-4.19915500	-1.66260300	2.41323100
C	-4.18201400	-1.01650500	-1.50756400
H	-4.18534400	-0.83270300	-2.58674500
C	-5.36253600	-1.20876000	0.64040800
H	-6.31156200	-1.15958900	1.18414900
C	-5.35878600	-0.97505900	-0.76875000
H	-6.30497200	-0.75256300	-1.27268300
C	4.13094200	-1.29129700	-1.70343200
C	5.18572500	-0.42444400	-0.97601000
H	6.08671800	-0.32379700	-1.60592400
H	4.79242300	0.58424400	-0.76618400
H	5.50140300	-0.87521900	-0.01929500
C	4.71971800	-2.71030400	-1.95589500
H	3.99127800	-3.35969700	-2.47204200
H	5.62229600	-2.63727500	-2.58836100
H	5.00385400	-3.20052300	-1.00854900
C	3.78805600	-0.64018500	-3.06299700
H	3.33905300	0.35816700	-2.93101100
H	4.70784800	-0.52254300	-3.66164100
H	3.09154000	-1.26149000	-3.65276400

Photoisomer



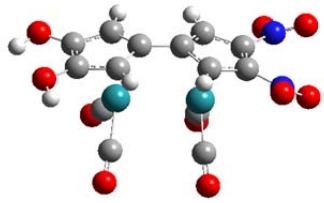


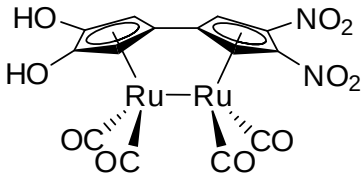
Energy (a.u.): -1337.860889
Molecular coordinates

C	1.75757100	2.30010400	0.83059800
C	-0.26412900	1.32805200	0.03956000
C	0.53420800	1.60271700	1.21230400
C	0.50720100	1.79383000	-1.08853500
C	1.73232400	2.39792400	-0.59950500
C	2.71238900	-0.90389700	1.12694100
C	2.66233400	-0.60616300	-1.55079100
C	-1.80592100	-2.30848600	-0.99202100
C	0.16739400	-1.26348400	-0.19964600
C	-0.63801000	-1.51325100	-1.37311400
C	-0.60053500	-1.72178300	0.93541800
C	-1.78247200	-2.43917800	0.45584100
C	-2.77005500	0.96884600	-1.32857800
C	-2.72220600	0.72022600	1.40842800
H	0.24036200	1.36575700	2.23470700
H	0.20655900	1.73636600	-2.13504300
H	2.49074200	2.87208400	-1.22380600
H	-0.34770200	-1.28350600	-2.39910400
H	-0.27662800	-1.67827900	1.97606800
O	3.31451200	-1.54787600	1.90111300
O	3.23884900	-1.03411400	-2.47777400
O	-3.35257300	1.58803200	-2.13499100
O	-3.27363600	1.18184500	2.33378300
Ru	1.71805200	0.13061700	-0.09579200
Ru	-1.80212200	-0.04518500	-0.05706400
C	2.75789600	2.96886100	1.77116000
C	4.17708000	2.98314000	1.15670000
H	4.20593600	3.52743900	0.19698000
H	4.87810800	3.48950300	1.84309400
H	4.54328000	1.95733400	0.98121900
C	2.27458700	4.43456500	1.97820600
H	1.26049400	4.46328800	2.41312300
H	2.95775400	4.96455000	2.66569500
H	2.25201900	4.98599200	1.02237600
C	2.80667400	2.25975400	3.14422700
H	3.12870300	1.20978400	3.04529100
H	3.52632800	2.77493600	3.80401200
H	1.82668800	2.27663600	3.65158100
C	-2.84273900	-2.92708300	-1.74467200
C	-2.79698400	-3.18465100	1.11850800
C	-3.80505500	-3.67447200	-1.06822600
C	-3.78237200	-3.80213300	0.35043100
H	-2.86449600	-2.83455000	-2.83547600
H	-2.78390000	-3.28855700	2.20843300

H	-4.59723900	-4.17388400	-1.63567100
H	-4.55782500	-4.39676100	0.84444600

Entry 13
Parent

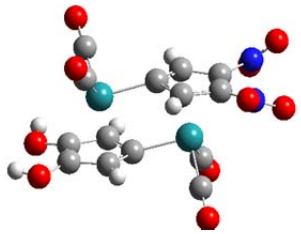


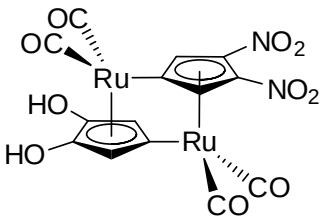


Energy (a.u.): -1586.621956
Molecular coordinates

C	-3.21231300	-1.65390700	0.65496400
C	-1.00298700	-1.83824400	-0.05562600
C	-1.85556400	-1.76844300	1.11858400
C	-1.84490200	-1.70820900	-1.23064800
C	-3.20633300	-1.63808500	-0.78465800
H	-1.53914800	-1.86155200	2.15719900
H	-1.52939000	-1.73958300	-2.27211800
C	2.54029700	-0.99708800	0.69619700
C	0.44065500	-1.66947700	-0.04559000
C	1.24708100	-1.43158500	1.12899400
C	1.24431500	-1.34674200	-1.20391600
C	2.54077200	-0.94212600	-0.74347700
H	0.96227400	-1.56102800	2.17159900
H	0.96589200	-1.43089700	-2.25320400
Ru	-1.89561700	0.24369000	0.00784700
Ru	0.96363000	0.60759300	0.01664200
C	-2.27049600	1.47183000	1.37691200
O	-2.57703600	2.18137800	2.25901400
C	-2.27749400	1.55346400	-1.28878900
O	-2.57833200	2.32337900	-2.11791800
C	0.91364100	1.90660700	1.36836200
O	0.93692300	2.69891900	2.22913700
C	0.93152500	1.99779100	-1.24371400
O	0.96151300	2.85020600	-2.04304100
O	-4.28792400	-1.67227200	-1.59335500
H	-5.09381500	-1.54381600	-1.05097000
O	-4.39584800	-1.73467400	1.32535300
H	-4.27247300	-1.52899700	2.27171700
N	3.67842800	-0.79294200	-1.66035200
N	3.64732100	-0.71365200	1.61425400
O	4.76622300	-1.25525600	-1.28575600
O	4.55360800	0.03536700	1.22474000
O	3.57054800	-1.25720300	2.73498500
O	3.43840700	-0.27723400	-2.76623900

Photoisomer





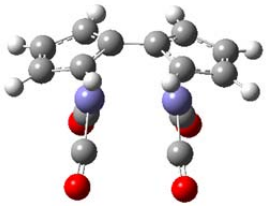
Energy (a.u.): -1586.589062

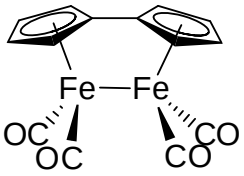
Molecular coordinates

C	3.17862100	1.21022000	0.68983600
C	0.94122100	1.30706600	-0.02670200
C	1.79439600	1.24161800	1.14012100
C	1.79944300	1.20039700	-1.18623500
C	3.18015200	1.20441500	-0.73892000
C	2.39148100	-1.96015900	1.40082900
C	2.42038600	-2.00424700	-1.31553000
C	-2.30556900	-0.97483300	-0.70369500
C	-0.07373500	-1.18113200	0.01193600
C	-0.93409800	-1.10782100	-1.14433500
C	-0.92874000	-1.03844400	1.16854800
C	-2.30424400	-0.92608100	0.72815600
C	-1.40940700	2.18690500	-1.40170700
C	-1.44656200	2.25911800	1.26702100
H	1.47319000	1.31657200	2.17976700
H	1.49292900	1.23166500	-2.23118000
H	-0.63955700	-1.17082200	-2.19134700
H	-0.63287700	-1.07520300	2.21665600
O	2.66091600	-2.67937100	2.28624400
O	2.70106800	-2.75665300	-2.16653000
O	-1.59626200	2.94742700	-2.26742700
O	-1.65080400	3.06657300	2.08411600
Ru	1.96690500	-0.74324900	0.02088600
Ru	-1.10495800	0.92771700	-0.02829600
O	4.25350200	1.32010000	-1.55742500
H	5.06896200	1.27667800	-1.01638700
O	4.34424300	1.37757000	1.38417400
H	4.21240000	1.16889800	2.32837300
N	-3.46503500	-0.93556700	-1.59870900
N	-3.43936000	-1.01066400	1.65542000
O	-3.29801100	-1.44807000	-2.72254300
O	-4.50557200	-0.40215600	-1.18392000
O	-4.37059100	-1.76333100	1.33345000
O	-3.33724400	-0.37995000	2.72326900

Entry 15

Parent



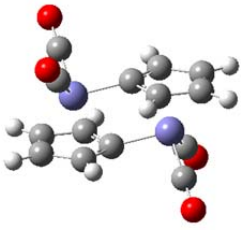


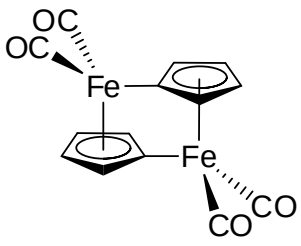
Energy (a.u.): -1086.246095

Molecular coordinates

C	-2.86047000	-1.26648000	0.71425700
C	-0.72786300	-1.89780000	-0.00000300
C	-1.55039300	-1.65319900	1.16401500
C	-1.55038600	-1.65319400	-1.16402500
C	-2.86046500	-1.26647700	-0.71427300
H	-3.70109300	-0.99955100	1.35470100
H	-1.22870200	-1.71914400	2.20255400
H	-1.22868900	-1.71913500	-2.20256200
H	-3.70108400	-0.99954500	-1.35472100
C	2.86047000	-1.26647200	0.71427000
C	0.72786900	-1.89779900	0.00000100
C	1.55039100	-1.65319100	1.16402200
C	1.55039700	-1.65319600	-1.16401700
C	2.86047300	-1.26647500	-0.71426000
H	3.70108800	-0.99953800	1.35471700
H	1.22869500	-1.71913300	2.20256000
H	1.22870600	-1.71914300	-2.20255600
H	3.70109500	-0.99954400	-1.35470400
Fe	-1.37056600	0.10331900	0.00000000
Fe	1.37056700	0.10332100	-0.00000200
C	-1.50380600	1.30587600	1.25269400
O	-1.67997900	2.09393500	2.10384300
C	-1.50381100	1.30589300	-1.25267700
O	-1.67998700	2.09396600	-2.10381400
C	1.50380700	1.30589200	1.25267900
O	1.67997900	2.09396200	2.10381900
C	1.50380200	1.30588500	-1.25269000
O	1.67997100	2.09395000	-2.10383500

Photoisomer





Energy (a.u.): -1086.221596

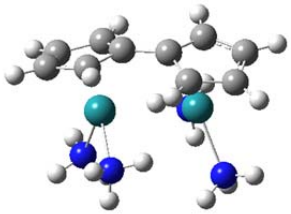
Molecular coordinates

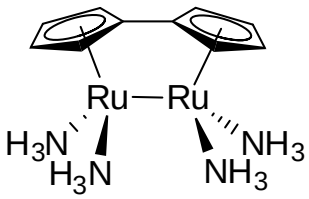
C	1.80682500	2.15812700	0.71280100

C	-0.21885900	1.17010400	-0.00005800
C	0.57110200	1.54462200	1.15261800
C	0.57109400	1.54451000	-1.15277700
C	1.80681800	2.15805900	-0.71303000
C	2.58424800	-0.61574700	1.27188200
C	2.58423700	-0.61590200	-1.27182600
C	-1.80681900	-2.15812900	-0.71280600
C	0.21885900	-1.17009900	0.00005700
C	-0.57109600	-1.54462500	-1.15262000
C	-0.57109900	-1.54449900	1.15277500
C	-1.80682100	-2.15805300	0.71302400
C	-2.58425100	0.61576700	-1.27188100
C	-2.58423400	0.61587700	1.27183300
H	2.60022700	2.53907100	1.35699000
H	0.28990500	1.38091700	2.19320100
H	0.28988500	1.38070900	-2.19334200
H	2.60021900	2.53892900	-1.35726300
H	-2.60022000	-2.53907100	-1.35699800
H	-0.28989400	-1.38092800	-2.19320300
H	-0.28989500	-1.38069100	2.19334000
H	-2.60022200	-2.53892600	1.35725600
O	3.19425000	-1.11923500	2.13648600
O	3.19423000	-1.11950900	-2.13636500
O	-3.19426100	1.11927000	-2.13647000
O	-3.19422400	1.11945400	2.13639300
Fe	1.66569800	0.14919100	-0.00001400
Fe	-1.66569800	-0.14918800	0.00000300

Entry 26

Parent





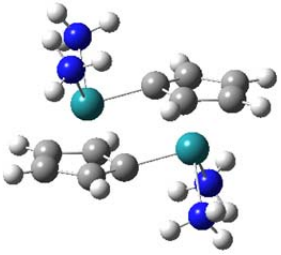
Energy (a.u.): -799.785630

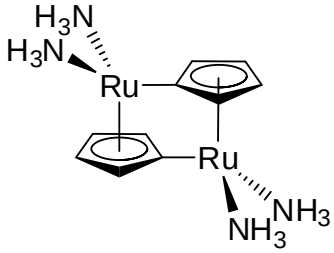
Molecular coordinates

C	-2.70274800	-1.44429400	1.29553600
C	-0.72993100	-2.00450500	0.15413300
C	-1.27915800	-1.66167000	1.46749500
C	-1.84277300	-1.95868400	-0.78298900
C	-3.07503800	-1.71101100	-0.06845100
H	-3.39640100	-1.20679200	2.10732700
H	-0.74394500	-1.67700100	2.41795500
H	-1.76084800	-2.17853000	-1.85051700
H	-4.08406700	-1.71630800	-0.48306800

C	3.03229700	-1.70572000	0.04559100
C	0.68931700	-2.00628200	-0.19089200
C	1.79845100	-1.97517700	0.75250200
C	1.24292400	-1.64305700	-1.49715900
C	2.66480200	-1.42155700	-1.31587400
H	4.04039800	-1.71450700	0.46260400
H	1.71406000	-2.21786000	1.81482700
H	0.71055300	-1.64226800	-2.44943300
H	3.36151300	-1.16612500	-2.11923600
Ru	-1.52464800	0.02404800	0.09009000
Ru	1.47185400	0.01195200	-0.08241900
N	1.27343600	1.06153200	1.84556900
H	0.26527800	0.80859500	1.92041700
H	1.81321800	0.65297200	2.61855600
H	1.36829000	2.08597100	1.88773000
N	2.04893900	1.99338000	-0.94258900
H	2.89039500	2.32446700	-0.45146300
H	2.29434700	1.91114000	-1.93433600
H	1.33156000	2.72224100	-0.86061200
N	-1.31654300	1.08698000	-1.82393700
H	-0.30249300	0.85757500	-1.89371700
H	-1.84017600	0.66652200	-2.60206400
H	-1.43183000	2.11084000	-1.87388100
N	-2.20454500	1.95992900	0.96230900
H	-3.12810200	1.80809900	1.38564400
H	-1.60804800	2.37128300	1.68634700
H	-2.32335300	2.68537100	0.23899800

Photoisomer





Energy (a.u.): -799.791276

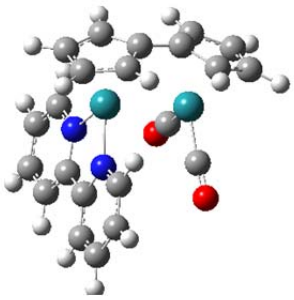
Molecular coordinates

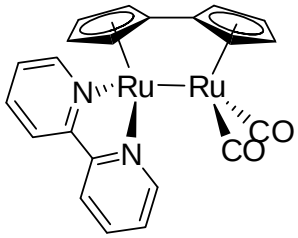
C	-1.62375900	-2.46956100	0.75298300
C	0.34118100	-1.30589200	0.01189100
C	-0.43038800	-1.73204300	1.18080200
C	-0.44923900	-1.75776600	-1.13458600
C	-1.63540500	-2.48522900	-0.67111600
C	1.62375900	2.46956200	-0.75297900
C	-0.34118200	1.30589300	-0.01188700
C	0.43038800	1.73204400	-1.18079800
C	0.44923900	1.75776700	1.13459000
C	1.63540500	2.48523000	0.67112000

H	-2.36187100	-2.94091400	1.40714000
H	-0.14783100	-1.56456200	2.22527800
H	-0.18381600	-1.61326500	-2.18696400
H	-2.38416000	-2.97051800	-1.30259300
H	2.36187100	2.94091500	-1.40713600
H	0.14783100	1.56456300	-2.22527400
H	0.18381600	1.61326600	2.18696800
H	2.38415900	2.97051900	1.30259700
Ru	-1.63942800	-0.32310200	0.01713000
Ru	1.63942800	0.32310300	-0.01712600
N	-2.84319100	0.73166500	-1.51817400
H	-2.29399100	1.54832400	-1.81835100
H	-2.98796000	0.13201400	-2.33662700
N	-2.81730900	0.76628000	1.54841100
H	-3.75262300	1.09689500	1.27374200
H	-2.94394800	0.18652600	2.38401500
N	2.84319100	-0.73166400	1.51817800
H	2.98796000	-0.13201300	2.33663100
H	2.29399000	-1.54832300	1.81835500
N	2.81730900	-0.76627900	-1.54840700
H	2.94394800	-0.18652500	-2.38401100
H	3.75262300	-1.09689400	-1.27373800
H	-3.77185900	1.07255300	-1.23367600
H	-2.26537100	1.59180100	1.81776900
H	3.77185900	-1.07255200	1.23368000
H	2.26537100	-1.59180000	-1.81776500

Entry 28

Parent





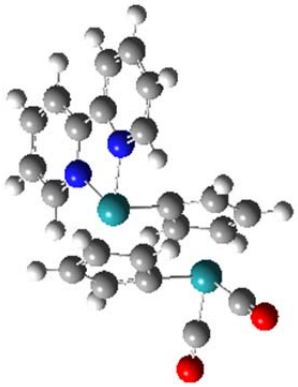
Energy (a.u.): -1295.707468

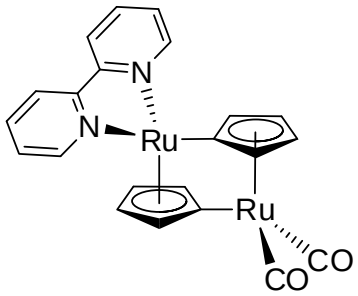
Molecular coordinates

C	-0.09738400	-0.72180900	3.26643100
C	-1.88190700	-0.00000700	1.95041300
C	-1.20263600	-1.17650200	2.46390700
C	-1.20263500	1.17648300	2.46391800
C	-0.09738400	0.72178100	3.26643800
H	0.60688400	-1.35894900	3.80353500
H	-1.49511400	-2.21206100	2.29219000
H	-1.49511200	2.21204400	2.29221100

H	0.60688500	1.35891600	3.80354800
C	-3.83505400	-0.71499500	-1.14562900
C	-2.82463200	-0.00000100	0.84179200
C	-3.20227800	-1.16192600	0.06462100
C	-3.20227300	1.16193000	0.06462900
C	-3.83505100	0.71500900	-1.14562400
H	-4.24467200	-1.35568900	-1.92670200
H	-3.04657200	-2.20053600	0.35517100
H	-3.04656300	2.20053700	0.35518500
H	-4.24466600	1.35571000	-1.92669400
C	-0.61412400	-1.31610200	-2.01664100
O	-0.05983100	-2.16858400	-2.61316800
C	-0.61412100	1.31610800	-2.01663700
O	-0.05982600	2.16859200	-2.61316100
C	2.66869800	-0.72619300	-0.30752200
C	1.51778300	-2.64400200	0.43723200
C	3.66321300	-1.53985900	-0.89102000
C	2.66869600	0.72619900	-0.30751800
C	2.48272500	-3.48669300	-0.10279800
H	0.63764200	-3.03524700	0.95212700
C	3.58346400	-2.92850600	-0.79149500
H	4.49751700	-1.07241500	-1.42162900
C	3.66320900	1.53987100	-0.89101000
H	2.36508000	-4.56928400	-0.00035100
H	4.34932800	-3.56633400	-1.24186200
C	1.51777700	2.64400100	0.43724900
C	3.58345800	2.92851700	-0.79147700
H	4.49751400	1.07243200	-1.42162200
C	2.48271700	3.48669700	-0.10277600
H	0.63763500	3.03524100	0.95214700
H	4.34932000	3.56635000	-1.24184000
H	2.36507000	4.56928700	-0.00032100
N	1.58190500	1.27880000	0.35610000
N	1.58190700	-1.27880000	0.35609200
Ru	-1.57907200	0.00000300	-1.11453200
Ru	0.21854500	-0.00000400	1.17638000

Photoisomer





Energy (a.u.): -1295.677734

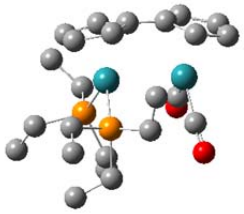
Molecular coordinates

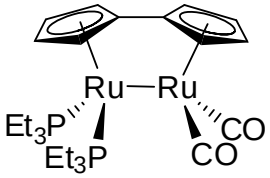
C	0.00308600	0.71725600	2.90021700
C	1.56468500	0.00000000	1.29534300
C	0.95181300	1.16277500	1.89808000
C	0.95181300	-1.16277500	1.89808100
C	0.00308600	-0.71725500	2.90021800
C	1.78602500	-0.71354700	-2.62668200
C	0.24570600	0.00000000	-0.96860100
C	0.86290400	-1.15235600	-1.59570900
C	0.86290400	1.15235500	-1.59571000
C	1.78602500	0.71354600	-2.62668200
C	3.76236000	-1.34968900	-0.04955300
C	3.76235900	1.34968900	-0.04955300
H	-0.59375400	1.36079600	3.54932300
H	1.20735000	2.19988200	1.67761500
H	1.20735000	-2.19988200	1.67761500
H	-0.59375400	-1.36079500	3.54932400
H	2.37079100	-1.35724200	-3.28575300
H	0.64424700	-2.19407700	-1.35674200
H	0.64424700	2.19407700	-1.35674300
H	2.37079100	1.35724000	-3.28575400
O	4.50249400	-2.21363400	0.24112100
O	4.50249100	2.21363600	0.24112100
C	-3.25521500	0.72603600	-0.40474100
C	-2.06641900	2.64655500	0.27926100
C	-4.26943000	1.54080700	-0.95349800
C	-3.25521500	-0.72603600	-0.40474100
C	-3.04716300	3.48936400	-0.23265500
H	-1.17148400	3.03684800	0.76977700
C	-4.17838900	2.92987900	-0.87144800
H	-5.12841400	1.07359900	-1.44366600
C	-4.26943000	-1.54080800	-0.95349800
H	-2.92545500	4.57222500	-0.13659500
H	-4.96078200	3.56752100	-1.29278900
C	-2.06641900	-2.64655500	0.27926200

C	-4.17838900	-2.92988000	-0.87144800
H	-5.12841400	-1.07359900	-1.44366600
C	-3.04716300	-3.48936400	-0.23265400
H	-1.17148500	-3.03684800	0.76977800
H	-4.96078100	-3.56752200	-1.29278900
H	-2.92545500	-4.57222500	-0.13659400
N	-2.13955300	1.28033900	0.21101300
N	-2.13955300	-1.28033900	0.21101400
Ru	-0.69362400	0.00000000	0.86687800
Ru	2.54752500	0.00000000	-0.54538200

Entry 29

Parent





(H atoms are omitted)

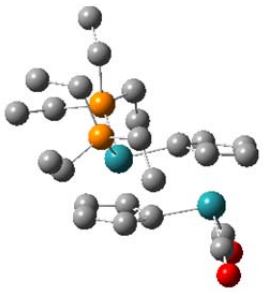
Energy (a.u.): -1958.166022

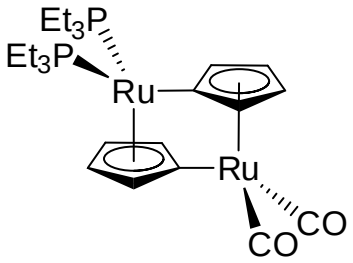
Molecular coordinates

C	-4.21719000	0.97649400	-0.30276400
C	-2.70616400	0.47391400	1.41666100
C	-3.17154800	1.51373500	0.52011900
C	-3.45637500	-0.71643700	1.09070700
C	-4.39170900	-0.39850400	0.04468500
H	-4.77572700	1.52087700	-1.06434700
H	-2.80668500	2.53928700	0.49128400
H	-3.35255100	-1.68755100	1.57434200
H	-5.11262700	-1.08597600	-0.39802100
C	0.63607500	1.16361900	2.92985900
C	-1.48338000	0.50834700	2.20168500
C	-0.61361500	1.64518600	2.39730600
C	-0.76797300	-0.67337300	2.64695600
C	0.54014100	-0.26073800	3.08478700
H	1.48086000	1.77820000	3.24100600
H	-0.87294600	2.68623700	2.21779000
H	-1.16694300	-1.68626900	2.65789900
H	1.30533500	-0.90138200	3.52416700
C	-1.43446600	0.58851900	-2.29753500
O	-1.00930700	1.04057300	-3.30482900
C	-1.86841300	-1.84820200	-1.49254700
O	-1.78613300	-2.93793100	-1.94482800
P	1.39113500	-1.70065800	0.08608100
P	1.48429800	1.79842900	-0.42054600
C	2.80442000	2.68921200	0.59696800

H	3.54098300	1.91237400	0.87154200
H	2.31127400	2.97245900	1.54258800
C	0.53989800	3.28950600	-1.10821600
H	1.28072000	3.89973800	-1.65736900
H	-0.15742200	2.89375200	-1.86426200
C	2.44143400	1.43488200	-2.01662000
H	1.80750900	0.74829400	-2.60178000
H	2.48012200	2.37695400	-2.59340100
C	0.63322000	-3.33968300	0.64586100
H	0.98299500	-4.13136000	-0.03891600
H	-0.45160400	-3.24042400	0.47634500
C	3.15033800	-1.88743700	0.74101000
H	3.03996800	-1.93168000	1.83988800
H	3.64696000	-0.92182400	0.54376000
C	1.59275800	-1.96197000	-1.77898900
H	0.77146000	-1.38456500	-2.23286900
H	2.52561500	-1.43639700	-2.04661900
C	0.91441500	-3.77722500	2.09428600
H	0.61021000	-3.02099600	2.83450500
H	0.35656300	-4.70345200	2.32133500
H	1.98308400	-3.99467500	2.26074700
C	4.01777100	-3.05333200	0.23529700
H	4.99354500	-3.06279900	0.75419200
H	3.54184400	-4.03367400	0.41006200
H	4.22258700	-2.97017100	-0.84555100
C	1.61027900	-3.38349700	-2.37044000
H	1.80448500	-3.32468000	-3.45683600
H	2.39549700	-4.02096700	-1.93082100
H	0.63913400	-3.88750300	-2.24291100
C	3.50414600	3.91795200	-0.01292900
H	2.80733300	4.76218100	-0.14812000
H	4.31391100	4.26679300	0.65331400
H	3.95785100	3.70328000	-0.99541000
C	3.86851300	0.87785700	-1.87802000
H	3.90970500	-0.04304500	-1.27560600
H	4.28149000	0.63768100	-2.87415400
H	4.55196900	1.60480600	-1.40812600
C	-0.20748500	4.17717500	-0.10538400
H	-0.63502800	5.05721300	-0.61831800
H	-1.03894300	3.63368000	0.36744400
H	0.45160500	4.55125100	0.69826300
Ru	-2.19314400	-0.16661400	-0.77762200
Ru	0.32944700	0.20981100	0.87604800

Photoisomer





Energy (a.u.): -1958.136393

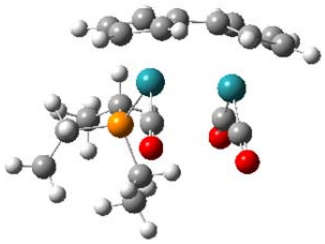
Molecular coordinates

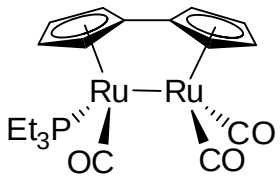
C	2.68016100	0.25695000	-2.52502600
C	0.75358500	-0.23989000	-1.18260700
C	1.51837000	0.80477700	-1.84667800
C	1.56197000	-1.43674200	-1.41185900
C	2.70509700	-1.14088700	-2.25488400
C	3.91450700	1.48360700	0.28670700
C	4.10289100	-1.18392600	0.68514000
C	-0.25722800	-0.60446400	2.65135000
C	1.58500700	0.08313400	1.34410800
C	0.88661400	-1.06254500	1.88060500
C	0.83449100	1.24319900	1.75144200
C	-0.28883800	0.81520800	2.57710800
H	3.39278300	0.81441000	-3.13491000
H	1.26014700	1.85892800	-1.87772500
H	1.33806700	-2.43166400	-1.03451700
H	3.44471200	-1.85859300	-2.61369800
H	-0.93549400	-1.23286200	3.22999600
H	1.21860200	-2.09627300	1.80104500
H	1.10874900	2.27852400	1.54941200
H	-0.99366500	1.46624600	3.09368600
O	4.50920500	2.44996300	0.59190000
O	4.82180900	-1.92571000	1.24453500
Ru	2.93664900	-0.03587700	-0.24345700
Ru	-0.55363500	-0.02612500	0.44260700
P	-1.88180000	-1.85808000	-0.16708200
P	-1.82071000	1.81280300	-0.35125200
C	-2.31315700	2.97660800	1.05444600
H	-1.37950800	3.20486500	1.59684400
H	-2.92266000	2.36930500	1.74735800
C	-3.04258300	4.28602000	0.70196200
H	-3.26918600	4.85215400	1.62338700
H	-2.43368900	4.94303700	0.05856600
H	-4.00037800	4.11090600	0.18410100
C	-0.99470600	3.06035000	-1.51421800
H	-0.65282100	2.48582000	-2.39345700
H	-1.78053000	3.74600600	-1.88076200
C	0.15648300	3.88231800	-0.90895700

H	0.91946400	3.24503900	-0.43372700
H	0.65785500	4.48386600	-1.68801500
H	-0.20799300	4.58415900	-0.13968300
C	-3.47045400	1.72481900	-1.27755800
H	-3.64678900	2.71625100	-1.73340800
C	-4.69159800	1.32950100	-0.43047000
H	-4.97971700	2.13600900	0.26460300
H	-5.56607300	1.12389200	-1.07336600
H	-4.50171500	0.43365000	0.18123600
C	-3.12152600	-1.69085500	-1.57832600
H	-3.80086100	-0.88233900	-1.27286800
C	-1.07569800	-3.47266400	-0.74104400
H	-1.90687600	-4.14177100	-1.02570700
H	-0.53143000	-3.23834700	-1.67336100
C	-0.16712700	-4.22192400	0.24702000
H	0.20760700	-5.15376300	-0.21283300
H	0.70880900	-3.62731000	0.54981600
H	-0.70674500	-4.50742000	1.16606500
C	-2.91751900	-2.60125900	1.22348600
H	-3.39741300	-3.52486600	0.84722300
H	-2.18213800	-2.92068400	1.98355600
C	-3.95849800	-1.67815700	1.87123100
H	-3.50327200	-0.71731700	2.16882100
H	-4.79510500	-1.46203000	1.18461800
H	-4.39083700	-2.14804200	2.77261200
C	-3.95447000	-2.90819700	-2.02149600
H	-4.48816500	-3.37833900	-1.17695300
H	-4.72011800	-2.59164100	-2.75264200
H	-3.34399800	-3.68460300	-2.51084800
H	-2.53330600	-1.29470000	-2.42659900
H	-3.32400300	1.02281600	-2.11584000

Entry 30

Parent





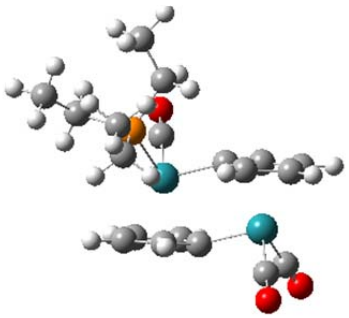
Energy (a.u.): -1492.672259

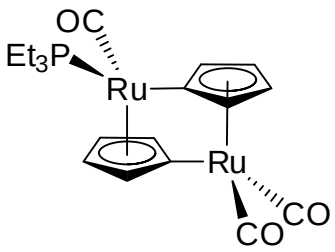
Molecular coordinates

C	-0.62706300	2.96120700	-1.07568700
C	1.50357900	2.03442200	-0.83602500
C	0.34230200	2.10902500	-1.70333300
C	1.23638400	2.86355700	0.31785100
C	-0.07984300	3.42019000	0.17152800

H	-1.59320100	3.24810000	-1.49163700
H	0.23415600	1.61092600	-2.66614400
H	1.90816100	3.02650100	1.15977500
H	-0.56375400	4.10426200	0.86890300
C	3.59323000	-0.99087100	-1.46840700
C	2.55479000	1.03404300	-0.92676000
C	2.63625800	-0.01678800	-1.91798800
C	3.45141300	0.66554200	0.14998700
C	4.09530600	-0.57042200	-0.19605500
H	3.88859800	-1.89125700	-2.00738200
H	2.08449200	-0.05383400	-2.85690200
H	3.61358800	1.23248600	1.06627100
H	4.83806400	-1.09513000	0.40483600
Ru	-0.27367800	1.12527900	0.30797100
Ru	1.78023200	-0.94720300	0.02431700
C	-0.61243200	0.87766800	2.11162500
O	-0.83585100	0.82588600	3.27259500
C	0.71194300	-2.33824700	-0.58889700
O	0.10652100	-3.25258400	-1.02978400
C	1.52389600	-1.51513000	1.78860800
O	1.42756000	-1.90411700	2.89390500
P	-2.16342400	-0.14515100	-0.15057300
C	-2.26631800	-0.72593500	-1.93449700
H	-1.75021600	0.06578500	-2.50575800
H	-1.61453800	-1.61467600	-1.99468500
C	-3.70297400	0.90697800	0.11911600
H	-3.43753600	1.54867800	0.97747000
H	-3.75571700	1.58437400	-0.75434200
C	-2.41737000	-1.64708700	0.94246600
H	-2.79804700	-1.24681700	1.90065300
H	-1.39908100	-2.00877100	1.15644900
C	-3.28983100	-2.81247600	0.44514200
H	-2.88336400	-3.25267700	-0.48035000
H	-3.30264500	-3.61337300	1.20563500
H	-4.33468800	-2.51549300	0.26002400
C	-5.06610000	0.23708900	0.37427000
H	-5.04212800	-0.39742500	1.27591600
H	-5.83661400	1.01083900	0.54249900
H	-5.40022800	-0.38539400	-0.47065600
C	-3.63896300	-1.01124700	-2.57125800
H	-4.28589800	-0.11768900	-2.57144000
H	-3.50285000	-1.31601700	-3.62449000
H	-4.17867100	-1.82407300	-2.06055400

Photoisomer





Energy (a.u.): -1492.644716

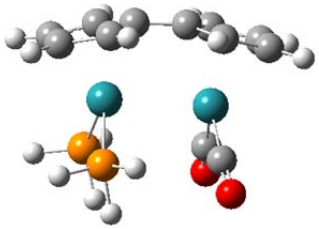
Molecular coordinates

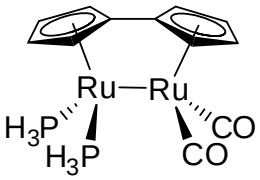
C	-1.84837700	2.35961500	1.27139500
C	-0.38893300	0.49509200	1.04492300
C	-0.71791900	1.81530800	0.53819500
C	-1.39192300	0.22155200	2.05489000
C	-2.26541700	1.37103500	2.21109000
C	-3.26820700	1.28071600	-1.47760200
C	-4.03880600	-0.61928800	0.27936200
C	-0.02655300	-2.78458500	-1.25287300
C	-1.44762100	-0.92279100	-0.98919400
C	-1.16992300	-2.26103300	-0.52804500
C	-0.43709700	-0.61377800	-1.97526500
C	0.42615800	-1.76789500	-2.14764000
C	1.30485300	-1.78396100	1.57447000
H	-2.29200200	3.34671000	1.13257400
H	-0.18239000	2.34634700	-0.25019500
H	-1.45862900	-0.69799900	2.63765500
H	-3.08717800	1.46420300	2.92265200
H	0.39422600	-3.78537200	-1.14585800
H	-1.73920900	-2.80551100	0.22562500
H	-0.36704100	0.31711100	-2.53868300
H	1.24358200	-1.85861700	-2.86466800
O	-3.69973300	1.79213300	-2.44198900
O	-4.96483800	-1.32183400	0.43868700
O	1.68416300	-2.32033200	2.55878900
Ru	-2.54159600	0.50452500	0.07505400
Ru	0.65764200	-0.98092200	0.02924300
P	2.61559100	0.25992200	-0.11589700
C	4.12707200	-0.84227800	-0.28024400
H	4.29661900	-1.25286800	0.73283200
H	3.76596900	-1.69455700	-0.88300400
C	2.91880300	1.34502900	1.38275300
H	2.24069900	2.20996900	1.26293800
H	2.49903400	0.76228400	2.22120100
C	2.65515800	1.39381400	-1.61347200
H	1.60905900	1.72094900	-1.74344500
H	2.86814800	0.73472400	-2.47601200

C	5.43419200	-0.29230800	-0.87976900
H	6.19494400	-1.09257000	-0.91175400
H	5.29042700	0.05941200	-1.91553000
H	5.85417300	0.53966000	-0.29278800
C	3.58590400	2.62034300	-1.61794000
H	3.34655500	3.31316900	-0.79383500
H	4.64884200	2.34529600	-1.53268700
H	3.46168200	3.18046100	-2.56190300
C	4.34518700	1.80612100	1.73168500
H	4.32357200	2.40898000	2.65706500
H	5.01389100	0.94948500	1.91978400
H	4.79909200	2.42737900	0.94322000

Entry 31

Parent





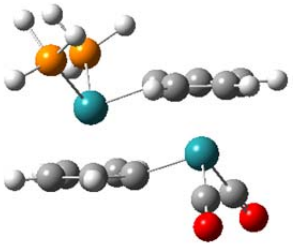
Energy (a.u.): -1486.743919

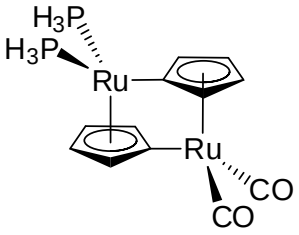
Molecular coordinates

C	-2.97643400	-1.55432200	0.71558400
C	-0.80760400	-2.07004100	-0.00000900
C	-1.64412700	-1.85380300	1.16196800
C	-1.64413500	-1.85379000	-1.16197900
C	-2.97643900	-1.55431400	-0.71558200
H	-3.83777600	-1.36487500	1.35620000
H	-1.32227000	-1.92300100	2.20073100
H	-1.32228400	-1.92297500	-2.20074500
H	-3.83778500	-1.36485900	-1.35619000
C	2.82299300	-1.61768100	0.71751000
C	0.64597800	-2.10355600	-0.00001400
C	1.48484700	-1.91571800	1.16915900
C	1.48484000	-1.91570500	-1.16919100
C	2.82298800	-1.61767400	-0.71754700
H	3.69145500	-1.45586600	1.35694200
H	1.16422200	-2.00447800	2.20679100
H	1.16420800	-2.00445500	-2.20682200
H	3.69144600	-1.45585100	-1.35698200
C	-1.66868300	1.47320000	1.31367200
O	-1.81578700	2.27880500	2.16283700
C	-1.66869400	1.47321700	-1.31364100
O	-1.81580500	2.27883200	-2.16279400
P	1.65363600	1.59060200	-1.61778300
H	2.95033900	1.82227800	-2.19082800

H	0.96408100	1.50043000	-2.86959700
H	1.34955900	2.96886800	-1.37291600
P	1.65364900	1.59058500	1.61778700
H	0.96410500	1.50039900	2.86960700
H	2.95035700	1.82225700	2.19082300
H	1.34956800	2.96885400	1.37293800
Ru	-1.53488100	0.15794700	0.00000700
Ru	1.40467700	0.01013200	-0.00000500

Photoisomer





Energy (a.u.): -1486.716563

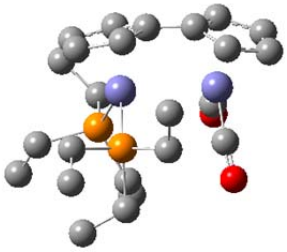
Molecular coordinates

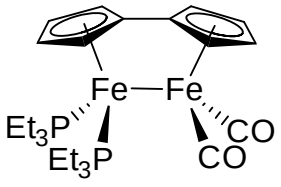
C	1.77786700	-2.37765100	-0.71331600
C	-0.22268200	-1.30173700	-0.00006400
C	0.57096000	-1.69692200	-1.15011600
C	0.57094400	-1.69703100	1.14996000
C	1.77785700	-2.37771800	0.71311300
C	2.87091300	0.65158600	-1.35152000
C	2.87089200	0.65145700	1.35162200
C	-1.59594700	2.38976400	0.71268400
C	0.38700800	1.31594000	0.00006300
C	-0.38568700	1.70980100	1.15704800
C	-0.38567200	1.70990800	-1.15689400
C	-1.59593800	2.38982900	-0.71248300
H	2.54208900	-2.81418000	-1.35823200
H	0.29351900	-1.53866500	-2.19351600
H	0.29348900	-1.53887200	2.19337200
H	2.54207000	-2.81430900	1.35799900
H	-2.35167300	2.83936000	1.35840100
H	-0.08564200	1.57160400	2.19627400
H	-0.08561500	1.57180700	-2.19612900
H	-2.35165600	2.83948400	-1.35816700
O	3.49620000	1.14227500	-2.21510800
O	3.49616600	1.14206300	2.21526700
Ru	1.85256700	-0.17437400	0.00000300
Ru	-1.63605000	0.21780100	0.00000000
P	-2.88066300	-0.74156600	1.64441900
H	-2.38181700	-1.85206500	2.40930300
H	-3.29304400	0.04164000	2.77018500
H	-4.16802400	-1.32010000	1.37887500

P	-2.88064500	-0.74141000	-1.64452300
H	-3.29301400	0.04190300	-2.77022000
H	-2.38179200	-1.85183700	-2.40950700
H	-4.16801100	-1.31996800	-1.37904800

Entry 32

Parent





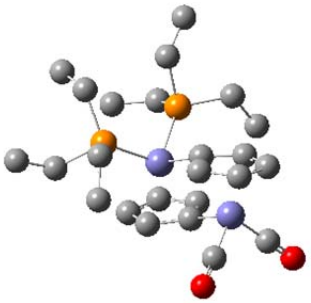
Energy (a.u.): -2017.241220

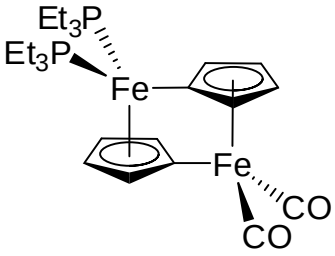
Molecular coordinates

C	-4.14806600	0.74052600	-0.52364700
C	-2.71425400	0.28127500	1.27417900
C	-3.15034900	1.30327600	0.34609300
C	-3.44365300	-0.91757800	0.93766500
C	-4.32841900	-0.62695200	-0.16328700
H	-4.65338100	1.26187600	-1.33668100
H	-2.77238200	2.32225800	0.29889300
H	-3.34198900	-1.88463700	1.42929000
H	-5.00188000	-1.33620100	-0.64435900
C	0.60117100	0.99158900	2.82230500
C	-1.50676100	0.32213800	2.08221900
C	-0.66548600	1.46685300	2.32391500
C	-0.75614300	-0.85834400	2.45135700
C	0.54198800	-0.43239100	2.90024200
H	1.44611200	1.60605100	3.13231500
H	-0.94943900	2.50760600	2.18947600
H	-1.11404700	-1.88339300	2.37473900
H	1.34189400	-1.07539800	3.26767300
Fe	-2.27017100	-0.30814400	-0.71020000
Fe	0.19548100	0.17243600	0.90042500
C	-1.55834200	0.42232600	-2.09921800
O	-1.14205600	0.88545600	-3.10768300
C	-1.90407900	-1.88404400	-1.30701700
O	-1.76713400	-2.97738300	-1.73983600
P	1.33150100	-1.57597500	0.08589100
P	1.10854800	1.88507700	-0.28982900
C	2.39075600	2.86737300	0.69350200
H	3.18967800	2.14675200	0.94659600
H	1.91048300	3.12459000	1.65313400
C	0.00636600	3.32092300	-0.88082300
H	0.64122400	3.92423600	-1.55509000
H	-0.77702800	2.87676400	-1.51546600

C	2.03387300	1.66388000	-1.93245700
H	1.43480800	0.95816300	-2.53017400
H	1.98200100	2.62931700	-2.46757200
C	0.76607700	-3.30703200	0.60513900
H	1.19729900	-4.02095600	-0.11694000
H	-0.32383000	-3.33396200	0.44289400
C	3.12776700	-1.62434800	0.67281700
H	3.07080400	-1.72307800	1.77202200
H	3.53317100	-0.61273200	0.49929500
C	1.49102500	-1.77227400	-1.79292700
H	0.61440000	-1.25057300	-2.20694800
H	2.37056100	-1.16961600	-2.07520000
C	1.11043200	-3.78872600	2.02652900
H	0.65414400	-3.17182900	2.81577300
H	0.73915900	-4.82006600	2.16585000
H	2.19875000	-3.81217000	2.20701700
C	4.07400800	-2.68805900	0.08950500
H	5.06866200	-2.62471400	0.56712500
H	3.69672500	-3.71288100	0.24850300
H	4.22230600	-2.55208500	-0.99521100
C	1.59842800	-3.16977100	-2.43030100
H	1.74318000	-3.06069100	-3.52052000
H	2.44995100	-3.75444700	-2.04368100
H	0.67679400	-3.75480900	-2.28309500
C	2.98485100	4.14059300	0.06212000
H	2.22363100	4.92621900	-0.07669600
H	3.76999600	4.55948600	0.71728300
H	3.44577600	3.95213700	-0.92172100
C	3.50379700	1.21449700	-1.86609800
H	3.63841200	0.27470100	-1.30951200
H	3.89472000	1.05026000	-2.88626400
H	4.14876900	1.97007200	-1.38743200
C	-0.61917000	4.25769800	0.16576800
H	-1.06698000	5.13300700	-0.33829000
H	-1.42353000	3.77576300	0.74174000
H	0.12088500	4.64171100	0.88913300

Photoisomer





Energy (a.u.): -2017.214985

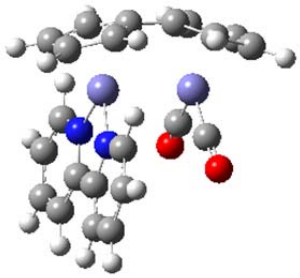
Molecular coordinates

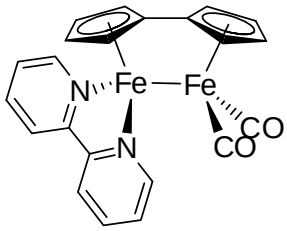
C	-2.84201000	0.38624200	2.35154700
C	-0.90926100	-0.19385700	1.04860500
C	-1.64793100	0.88092000	1.69772300
C	-1.75309300	-1.36088200	1.30313500
C	-2.90586200	-1.01411300	2.10565200
C	-3.79975100	1.46847800	-0.21588200
C	-4.03330200	-1.02907800	-0.58110100
C	0.17279600	-0.66423700	-2.51599900
C	-1.63639400	0.10467100	-1.21491300
C	-0.98351300	-1.06663000	-1.74804000
C	-0.85076200	1.23039600	-1.65035400
C	0.25408100	0.75104900	-2.46308500
H	-3.56375100	0.98086100	2.91361700
H	-1.37346000	1.93058800	1.69265100
H	-1.57300000	-2.36390100	0.92311200
H	-3.68903800	-1.69632100	2.44020100
H	0.84310400	-1.32303300	-3.06954800
H	-1.33332700	-2.08847600	-1.62768500
H	-1.07546400	2.27715600	-1.45072100
H	0.99345000	1.36142500	-2.98015900
O	-4.37599600	2.44529600	-0.52414200
O	-4.76944700	-1.75590600	-1.13776300
Fe	-2.93751400	0.03282600	0.25652300
Fe	0.35714500	-0.04717100	-0.46953100
P	1.56427500	-1.85992600	0.10133100
P	1.61704400	1.73136300	0.27516200
C	2.33724500	2.80119700	-1.11118300
H	1.49164600	3.05592700	-1.77238300
H	2.98840800	2.13050300	-1.70054400
C	3.09014400	4.09134600	-0.73669200
H	3.51195500	4.55812900	-1.64500800
H	2.42648700	4.83714600	-0.26839800
H	3.92869700	3.91202600	-0.04320800
C	0.80704100	3.11554400	1.30117900
H	0.42897000	2.64581100	2.22657000
H	1.63054400	3.78063200	1.61815400
C	-0.28129600	3.97059800	0.63049300
H	-1.17128900	3.38857300	0.34577600
H	-0.61515300	4.76797800	1.31849900
H	0.09329800	4.46445600	-0.28280900
C	3.14841900	1.59789500	1.39161000
H	3.30554600	2.58621000	1.86038000
C	4.45445900	1.15398200	0.71234000
H	4.85125500	1.93707400	0.04487800
H	5.23381500	0.93973900	1.46545900

H	4.32072500	0.25036100	0.09841100
C	2.63881300	-1.76176300	1.65183000
H	3.39675400	-0.99639200	1.43433400
C	0.74534500	-3.52490000	0.52463600
H	1.59156300	-4.19806100	0.74913700
H	0.20835000	-3.38330400	1.47979400
C	-0.16006000	-4.22716200	-0.50179900
H	-0.33689300	-5.27219900	-0.19023100
H	-1.14749900	-3.74994200	-0.59853300
H	0.29178700	-4.26177100	-1.50802800
C	2.74463900	-2.56450700	-1.19752700
H	3.27637700	-3.42835600	-0.75562700
H	2.08185900	-2.98329900	-1.97663500
C	3.74137200	-1.59254200	-1.84343300
H	3.24214100	-0.65750200	-2.15165000
H	4.55928400	-1.32883300	-1.15210000
H	4.20755400	-2.04601300	-2.73641000
C	3.34238300	-3.01969100	2.19508100
H	3.94383500	-3.53092200	1.42256500
H	4.03527200	-2.73670700	3.00801900
H	2.63508900	-3.75345000	2.61445500
H	1.97663600	-1.33003000	2.42485900
H	2.87683600	0.91246200	2.21190800

Entry 33

Parent





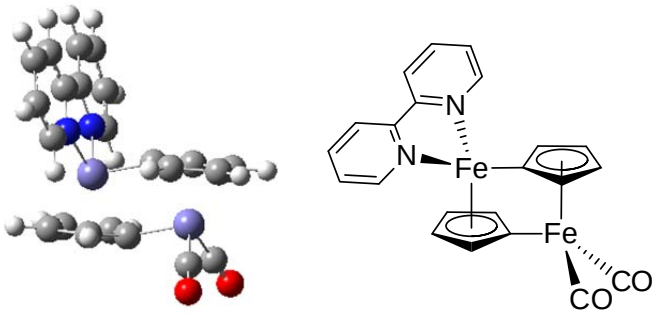
Energy (a.u.): -1354.808169

Molecular coordinates

C	-0.00652200	0.71817700	3.09113600
C	1.83375700	-0.00002600	1.86260800
C	1.13400200	1.17111400	2.34659600
C	1.13398900	-1.17116600	2.34658100
C	-0.00652900	-0.71822600	3.09112800
H	-0.76312900	1.35409800	3.55351500
H	1.42053700	2.20644400	2.16246600
H	1.42051300	-2.20649700	2.16243900
H	-0.76314300	-1.35414400	3.55349900
C	3.69983400	0.71349900	-1.27078300
C	2.78651000	-0.00002200	0.76363700

C	3.13446000	1.16127700	-0.02502400
C	3.13444400	-1.16130800	-0.02505000
C	3.69982400	-0.71350900	-1.27080000
H	4.04518300	1.35512000	-2.08146800
H	2.97278300	2.19966900	0.26194900
H	2.97275300	-2.19970400	0.26189900
H	4.04516400	-1.35511600	-2.08149900
Fe	-0.11802600	-0.00001200	1.12691300
Fe	1.67983200	0.00000600	-1.01994900
C	0.78601100	1.24258800	-1.82866400
O	0.23464300	2.09518600	-2.42797600
C	0.78599300	-1.24253800	-1.82870000
O	0.23461400	-2.09511000	-2.42804000
C	-2.42470500	0.72601200	-0.29461000
C	-1.27281400	2.61750000	0.49245500
C	-3.41027500	1.54805600	-0.87595600
C	-2.42471100	-0.72599800	-0.29462100
C	-2.23225300	3.47413800	-0.03941500
H	-0.39745700	3.00514200	1.01681000
C	-3.32726500	2.93584200	-0.75006200
H	-4.24031200	1.09008800	-1.42170200
C	-3.41028800	-1.54802600	-0.87597700
H	-2.11054500	4.55405100	0.08490500
H	-4.08534300	3.58549600	-1.19664500
C	-1.27283600	-2.61750600	0.49241800
C	-3.32728900	-2.93581400	-0.75010200
H	-4.24032100	-1.09004300	-1.42171700
C	-2.23228200	-3.47412900	-0.03946300
H	-0.39748200	-3.00516200	1.01676900
H	-4.08537300	-3.58545500	-1.19669400
H	-2.11058300	-4.55404400	0.08484200
N	-1.33790500	-1.25512800	0.38597000
N	-1.33789500	1.25512400	0.38598700

Photoisomer



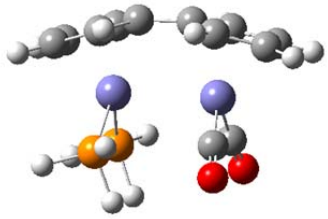
Energy (a.u.): -1354.784817

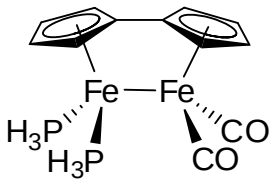
Molecular coordinates

C	0.02229400	-0.71623000	2.75789100

C	-1.57556900	0.00000000	1.18866500
C	-0.95477200	-1.15793900	1.79302100
C	-0.95477300	1.15794100	1.79302000
C	0.02229400	0.71623300	2.75789000
C	-2.01740700	0.71321600	-2.46701200
C	-0.42093000	-0.00000100	-0.86299200
C	-1.05050000	1.15006300	-1.48103200
C	-1.05050100	-1.15006700	-1.48102900
C	-2.01740700	-0.71322200	-2.46701000
C	-3.64842400	1.26980300	-0.07995500
C	-3.64842700	-1.26980000	-0.07995200
H	0.66702100	-1.35664600	3.36315400
H	-1.19420700	-2.19531600	1.55434800
H	-1.19420800	2.19531700	1.55434600
H	0.66702000	1.35664900	3.36315300
H	-2.64483600	1.35641100	-3.08586900
H	-0.84624400	2.19213600	-1.23164500
H	-0.84624500	-2.19213900	-1.23164000
H	-2.64483700	-1.35641800	-3.08586600
O	-4.38526400	2.13656600	0.20976800
O	-4.38527100	-2.13656000	0.20976800
Fe	0.52594400	0.00000000	0.83917000
Fe	-2.54158200	0.00000000	-0.52331800
C	2.94826000	-0.72583300	-0.35178300
C	1.75333600	-2.61896300	0.37359400
C	3.95501100	-1.55000700	-0.89480400
C	2.94826000	0.72583200	-0.35178300
C	2.73004500	-3.47675800	-0.12565800
H	0.86238700	-3.00382200	0.87420000
C	3.85763600	-2.93819700	-0.78556700
H	4.81192900	-1.09329500	-1.39873900
C	3.95501100	1.55000600	-0.89480500
H	2.60320600	-4.55678800	-0.00646400
H	4.63289100	-3.58868800	-1.20041700
C	1.75333600	2.61896300	0.37359100
C	3.85763600	2.93819600	-0.78556900
H	4.81192900	1.09329400	-1.39873900
C	2.73004500	3.47675800	-0.12566100
H	0.86238700	3.00382300	0.87419700
H	4.63289200	3.58868700	-1.20041900
H	2.60320600	4.55678800	-0.00646700
N	1.82999000	-1.25596700	0.27686200
N	1.82999000	1.25596700	0.27686100

Entry 34
Parent



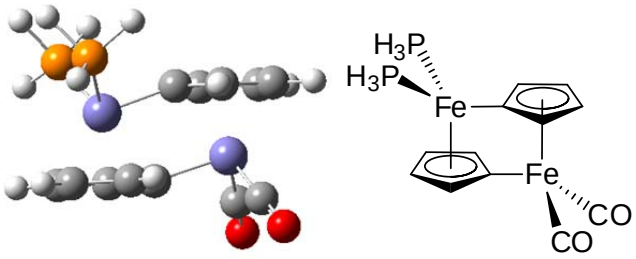


Energy (a.u.): -1545.827065

Molecular coordinates

C	-2.96626900	-1.26612500	0.71367000
C	-0.82776500	-1.89603700	0.00000100
C	-1.65196900	-1.64531700	1.16110700
C	-1.65198600	-1.64532400	-1.16109300
C	-2.96627900	-1.26612900	-0.71364000
H	-3.80706300	-1.00311800	1.35546100
H	-1.32987600	-1.71225300	2.19957100
H	-1.32990800	-1.71226700	-2.19956200
H	-3.80708300	-1.00312500	-1.35541900
C	2.77819400	-1.39656500	0.71458000
C	0.62492400	-1.95971100	-0.00001100
C	1.45322300	-1.74414400	1.16705200
C	1.45320100	-1.74412400	-1.16708600
C	2.77818000	-1.39655200	-0.71463300
H	3.63398100	-1.17178800	1.35293800
H	1.12913100	-1.81749300	2.20509000
H	1.12908800	-1.81745500	-2.20511900
H	3.63395400	-1.17176400	-1.35300400
Fe	-1.48743800	0.11846400	0.00000100
Fe	1.33655600	-0.02962900	-0.00000100
C	-1.58087200	1.32027400	1.24063600
O	-1.72693400	2.12736300	2.09012300
C	-1.58087200	1.32025800	-1.24065100
O	-1.72693100	2.12733400	-2.09015000
P	1.56857400	1.44437300	-1.56347300
H	2.89146300	1.76765300	-2.02721700
H	1.00985700	1.25842200	-2.87000300
H	1.13568900	2.79817900	-1.40043000
P	1.56858100	1.44433500	1.56350700
H	1.00985500	1.25835800	2.87003000
H	2.89147100	1.76758900	2.02726600
H	1.13571100	2.79814900	1.40049500

Photoisomer



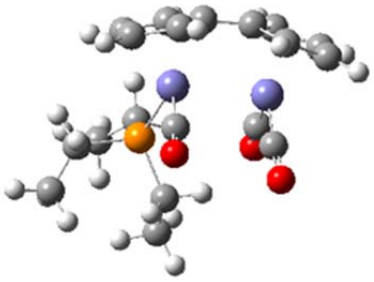
Energy (a.u.): -1545.804813

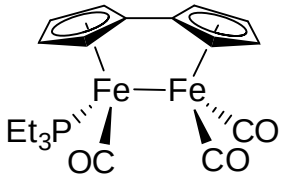
Molecular coordinates

C	-1.91697800	-2.15469200	0.71255000
C	0.12986000	-1.16633300	-0.00020800
C	-0.67753300	-1.54349900	1.14755500
C	-0.67754100	-1.54310700	-1.14809300
C	-1.91698300	-2.15444800	-0.71328700
C	-2.68979500	0.61933900	1.27072700
C	-2.68980200	0.61977100	-1.27051100
C	1.68472900	2.17651400	-0.71217100
C	-0.33231400	1.17595400	0.00019400
C	0.45041000	1.55484900	-1.15520800
C	0.45042900	1.55449200	1.15569900
C	1.68474100	2.17629500	0.71283400
H	-2.71247500	-2.53178800	1.35691400
H	-0.40974500	-1.37182200	2.19135700
H	-0.40975900	-1.37107700	-2.19183900
H	-2.71248500	-2.53132500	-1.35777400
H	2.47044000	2.57751200	-1.35474400
H	0.15740500	1.40365700	-2.19505400
H	0.15743900	1.40298400	2.19550300
H	2.47046100	2.57709800	1.35551800
O	-3.29591100	1.12767300	2.13762400
O	-3.29592300	1.12839600	-2.13723300
Fe	-1.77985500	-0.15100900	-0.00002500
Fe	1.53403300	0.19326000	0.00002800
P	2.68860400	-0.70447200	-1.58446800
H	2.21386900	-1.87320000	-2.27432900
H	2.99589700	0.05066500	-2.76358600
H	4.02151600	-1.20210400	-1.37833300
P	2.68853700	-0.70498200	1.58428400
H	2.99587900	0.04981700	2.76360600
H	2.21371600	-1.87386200	2.27383000
H	4.02141400	-1.20265400	1.37802100

Entry 35

Parent





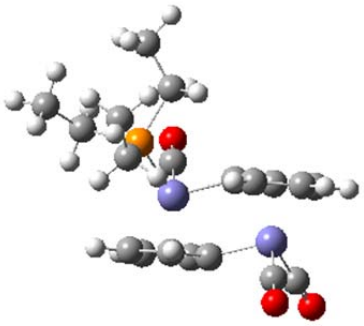
Energy (a.u.): -1551.757288

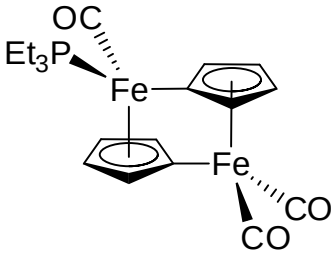
Molecular coordinates

C	-0.63195400	2.71888500	-1.08167400
C	1.53763000	1.92008900	-0.79016600
C	0.39222000	1.91107600	-1.67902200
C	1.20542900	2.75369800	0.33833600
C	-0.13864400	3.23487700	0.15908700
H	-1.61628500	2.91860500	-1.50680200
H	0.31919000	1.37133900	-2.62226000
H	1.84356300	2.95161800	1.19881500
H	-0.68191200	3.88345500	0.84649000
C	3.62155200	-1.12760300	-1.25439500
C	2.60867800	0.93557000	-0.81676000
C	2.73866700	-0.12345400	-1.78979600
C	3.41272100	0.56015800	0.32625700
C	4.03331700	-0.70707000	0.04565200
H	3.90572900	-2.05632400	-1.74906200
H	2.24135800	-0.16689600	-2.75806800
H	3.50428900	1.12045900	1.25579300
H	4.68426600	-1.26101600	0.72209400
Fe	-0.09791000	1.10289800	0.22762200
Fe	1.88635100	-0.86997300	-0.00732400
C	-0.27411400	0.90379000	1.93170800
O	-0.41008000	0.87903100	3.10644200
C	0.85266600	-2.06166600	-0.70501400
O	0.22156500	-2.92354700	-1.21178300
C	1.59721600	-1.45239000	1.60293000
O	1.46904300	-1.90777700	2.68041200
P	-1.95021300	-0.07085400	-0.09934900
C	-2.25355400	-0.62215300	-1.87045800
H	-1.78583300	0.16665600	-2.48580400
H	-1.63061400	-1.52227900	-2.01159100
C	-3.43281000	1.01100400	0.33504900
H	-3.06689700	1.64826400	1.15913300
H	-3.57398600	1.68855600	-0.52803000
C	-2.14405800	-1.58233200	0.99385100
H	-2.42686900	-1.18531600	1.98647700
H	-1.12347300	-1.97703800	1.11561800

C	-3.08804400	-2.71928900	0.56655200
H	-2.77934300	-3.15765800	-0.39690800
H	-3.05201200	-3.52857300	1.31737500
H	-4.13748800	-2.39472400	0.48034900
C	-4.77210600	0.36593300	0.73704100
H	-4.66202600	-0.27466500	1.62793200
H	-5.50420300	1.15317700	0.99198500
H	-5.20932600	-0.24475000	-0.06859000
C	-3.69111100	-0.86977100	-2.36377900
H	-4.31677600	0.03520300	-2.28215100
H	-3.67247700	-1.15784000	-3.43031500
H	-4.19157500	-1.68127600	-1.81292600

Photoisomer





Energy (a.u.): -1551.737475

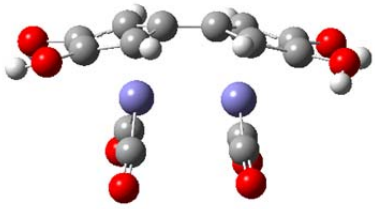
Molecular coordinates

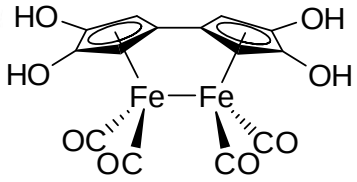
C	-2.07874600	2.16126400	1.31726400
C	-0.58785400	0.33996400	0.96358400
C	-0.91521800	1.70329700	0.58452600
C	-1.61035300	-0.02684300	1.92465600
C	-2.50993400	1.08600400	2.14837800
C	-3.19300300	1.36079900	-1.26692900
C	-3.95751600	-0.56424400	0.20355500
C	-0.04880600	-2.58232200	-1.36016600
C	-1.49540600	-0.76070800	-0.97431200
C	-1.22039500	-2.13540600	-0.63439100
C	-0.46607800	-0.36668200	-1.91038600
C	0.41785800	-1.48705100	-2.14774300
C	0.96113200	-1.88200400	1.27464700
H	-2.54767700	3.14305300	1.23708100
H	-0.38377900	2.30129900	-0.15705900
H	-1.70046900	-1.00506900	2.39841100
H	-3.37114800	1.09551000	2.81793900
H	0.39642200	-3.57679200	-1.30749300
H	-1.78681900	-2.74046600	0.07397700
H	-0.37523800	0.61715600	-2.37092700
H	1.27100900	-1.50317000	-2.82837400
O	-3.60068400	1.96351300	-2.18776700

O	-4.88929000	-1.27224000	0.28554600
O	1.28599800	-2.53857100	2.20403000
Fe	-2.56916900	0.48434500	0.10302000
Fe	0.43818700	-0.95532200	-0.08017500
P	2.33597000	0.16711900	-0.07610700
C	3.80366700	-0.97549100	-0.34501700
H	3.93232200	-1.50823300	0.61574500
H	3.42102800	-1.73589000	-1.04896900
C	2.64930200	1.04327400	1.55231500
H	2.03066700	1.95897300	1.51881200
H	2.16732600	0.39457400	2.30407900
C	2.48055500	1.48790500	-1.40692700
H	1.46136100	1.90077800	-1.50317500
H	2.66779800	0.94068700	-2.35004300
C	5.14888800	-0.42509500	-0.85188100
H	5.87297300	-1.25223500	-0.96111400
H	5.04810000	0.04961700	-1.84267400
H	5.59187900	0.31270500	-0.16446000
C	3.48514600	2.64255500	-1.23816900
H	3.27186300	3.23525900	-0.33281600
H	4.52731800	2.29248400	-1.17691800
H	3.41487200	3.32867900	-2.10113600
C	4.08862700	1.36662000	1.99114400
H	4.60395700	2.04996500	1.29759000
H	4.07433300	1.85063600	2.98398100
H	4.69850700	0.45244500	2.08580200

Entry 36

Parent





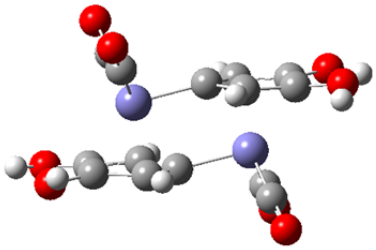
Energy (a.u.): -1387.130853

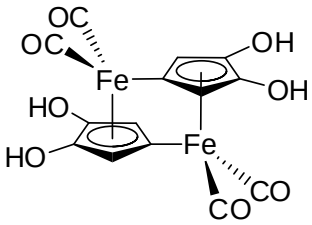
Molecular coordinates

C	2.88009400	-1.12957600	-0.68590500
C	0.72594800	-1.68699900	0.00769800
C	1.56378800	-1.47850800	-1.15630000
C	1.53564000	-1.43500800	1.18491000
C	2.87055900	-1.14870800	0.74538300
H	1.26180500	-1.57053500	-2.19903200
H	1.21767900	-1.48627000	2.22449100
C	-2.87055900	-1.14870800	-0.74538300
C	-0.72594800	-1.68699800	-0.00769900
C	-1.53564000	-1.43500800	-1.18491000

C	-1.56378700	-1.47850800	1.15630000
C	-2.88009400	-1.12957600	0.68590400
H	-1.21767800	-1.48626900	-2.22449200
H	-1.26180500	-1.57053500	2.19903100
Fe	1.36802000	0.28406600	-0.03708300
Fe	-1.36802000	0.28406600	0.03708200
C	1.43153500	1.41702500	-1.35351400
O	1.56434500	2.14903500	-2.26463600
C	1.58600800	1.53797100	1.15593800
O	1.81350500	2.36298700	1.95895900
C	-1.58600800	1.53797200	-1.15593700
O	-1.81350500	2.36298900	-1.95895700
C	-1.43153500	1.41702500	1.35351400
O	-1.56434600	2.14903300	2.26463700
O	-4.06300100	-0.98226100	1.36333700
H	-3.90019800	-0.58791200	2.24140300
O	-3.93738700	-0.96939300	-1.56040800
H	-4.69622200	-0.68114000	-1.01119300
O	3.93738700	-0.96939300	1.56040700
H	4.69622200	-0.68113900	1.01119300
O	4.06300200	-0.98226100	-1.36333800
H	3.90019800	-0.58791000	-2.24140200

Photoisomer





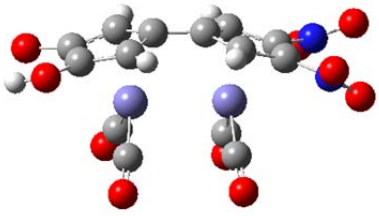
Energy (a.u.): -1387.105417

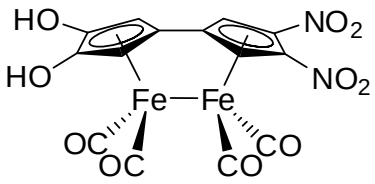
Molecular coordinates

C	-2.58294500	-1.24093300	0.67052600
C	-0.32759100	-1.13907400	-0.01406600
C	-1.21061200	-1.16975200	1.13420600
C	-1.18841300	-1.13479300	-1.18106100
C	-2.56493500	-1.25072300	-0.75717100
C	-2.05033800	1.61792800	1.31033900
C	-2.10194300	1.65819900	-1.24466600
C	2.56498100	1.25070400	-0.75704400
C	0.32759200	1.13907400	-0.01407500
C	1.18848600	1.13476300	-1.18101600
C	1.21054200	1.16978000	1.13425200
C	2.58290300	1.24094900	0.67065400
C	2.10201800	-1.65823100	-1.24449500
C	2.05025800	-1.61789600	1.31050600
H	-0.90214700	-1.17000900	2.18066200

H	-0.86767500	-1.10442700	-2.22178800
H	0.86781300	1.10437100	-2.22176200
H	0.90201200	1.17006400	2.18068800
O	-2.38488200	2.29979400	2.20724800
O	-2.46409000	2.37820500	-2.09552200
O	2.46421800	-2.37825700	-2.09531200
O	2.38475000	-2.29973500	2.20745500
Fe	-1.55491100	0.57055900	0.01007300
Fe	1.55491000	-0.57055900	0.01018400
O	3.62840300	1.41185900	-1.58316500
H	4.44519200	1.40073200	-1.04228500
O	3.75228700	1.45987000	1.35035000
H	3.66055600	1.17170900	2.27817100
O	-3.62830600	-1.41190100	-1.58335400
H	-4.44512800	-1.40075900	-1.04252400
O	-3.75237000	-1.45983600	1.35015500
H	-3.66069700	-1.17165100	2.27797500

Entry 37
Parent



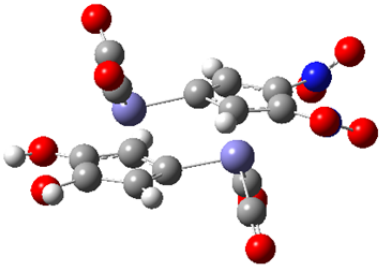


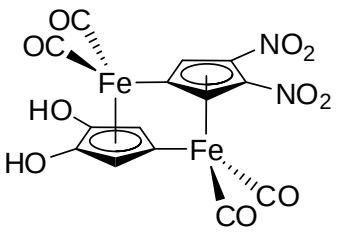
Energy (a.u.): -1645.714863
Molecular coordinates

C	3.31749300	0.59398800	-1.33305900
C	1.14346100	-0.14493500	-1.70525000
C	1.97914100	1.03618000	-1.62500300
C	1.96932000	-1.29974300	-1.41678900
C	3.31545800	-0.83666200	-1.23751300
H	1.66630800	2.06794300	-1.78252100
H	1.65741500	-2.34200500	-1.38419800
C	-2.38272100	0.64942900	-0.88231500
C	-0.30528700	-0.12998700	-1.58440300
C	-1.09572100	1.06031900	-1.37017400
C	-1.11306100	-1.27077200	-1.22719100
C	-2.39184000	-0.78515700	-0.79560300
H	-0.80680500	2.09683500	-1.53421600
H	-0.82540900	-2.32027600	-1.23649200
Fe	1.86807800	0.03881900	0.22020300
Fe	-0.87734500	0.01660300	0.44597300
C	2.08520100	1.42430100	1.25606900
O	2.32500400	2.37048200	1.90647700
C	2.19142700	-1.08639400	1.52073800

O	2.49322500	-1.84264300	2.36130600
C	-0.90049500	1.30693700	1.63032400
O	-0.97886300	2.15880300	2.42558200
C	-0.81314200	-1.16929300	1.73098800
O	-0.84200000	-1.96789900	2.58424100
O	4.38971600	-1.63448900	-1.05892500
H	5.17339300	-1.07456900	-0.87714300
O	4.49720600	1.27619700	-1.29085700
H	4.34454700	2.22168800	-1.10035300
N	-3.50466300	1.59033500	-0.75552200
N	-3.48625000	-1.65436400	-0.35208400
O	-4.34796900	-1.17246700	0.39600100
O	-3.44426500	-2.82887900	-0.76929700
O	-4.61159700	1.19735400	-1.15100800
O	-3.23389600	2.72708700	-0.33068700

Photoisomer





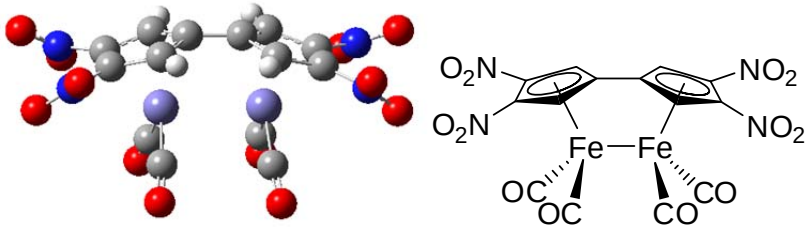
Energy (a.u.): -1645.689709

Molecular coordinates

C	3.19192600	-0.26165300	-1.18470200
C	0.94170900	-0.83116700	-0.80639500
C	1.82330900	0.02594300	-1.56956400
C	1.78052300	-1.58556100	0.10067700
C	3.16481800	-1.27227600	-0.17516800
C	2.38787000	2.17337400	0.32940600
C	2.40080700	0.40108100	2.17153900
C	-2.17537900	0.04067000	1.05097500
C	0.04874600	0.75569800	0.74061700
C	-0.80763600	-0.15233800	1.47385300
C	-0.81784700	1.50439600	-0.13930800
C	-2.18142500	1.07254600	0.05888700
C	-1.34645100	-2.29075200	-0.58231900
C	-1.27826400	-0.46585400	-2.31823600
H	1.52441800	0.73686100	-2.34089600
H	1.45193100	-2.32351000	0.83158900
H	-0.50459900	-0.87602600	2.23015900
H	-0.52390500	2.26288000	-0.86367000
O	2.67853200	3.30187600	0.20197400
O	2.68868700	0.32939000	3.30320600
O	-1.55385200	-3.43710300	-0.58971400

O	-1.45162000	-0.39131900	-3.47005000
Fe	1.96778400	0.48476700	0.47624400
Fe	-0.99788900	-0.56789700	-0.59150000
O	4.22694200	-1.89663600	0.38414800
H	5.04884000	-1.46783300	0.06676000
O	4.37897200	0.14334300	-1.72488500
H	4.26055700	0.96638200	-2.23627300
N	-3.34683600	1.61484100	-0.64620900
N	-3.31994300	-0.57627800	1.74081300
O	-4.21788000	0.19416200	2.10970500
O	-3.25244200	-1.79531800	1.96844700
O	-4.37350200	0.91996700	-0.69103900
O	-3.19924900	2.74514400	-1.14864300

Entry 38
Parent

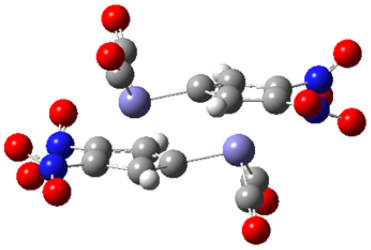


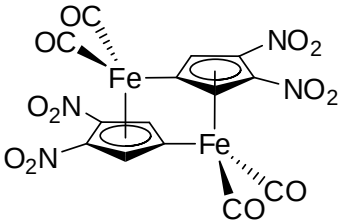
Energy (a.u.): -1904.289282
Molecular coordinates

C	-2.83466000	-0.68164400	-0.95980500
C	-0.72889600	0.07114800	-1.58235900
C	-1.52848100	-1.11345500	-1.36685900
C	-1.54762000	1.22661800	-1.31184300
C	-2.84488800	0.75319200	-0.92683700
H	-1.23092500	-2.15460600	-1.48069300
H	-1.25978000	2.27563600	-1.35196900
C	2.84204300	-0.66837400	-0.97851800
C	0.72755600	0.07699000	-1.58257800
C	1.53910800	-1.10241700	-1.39768100
C	1.53492700	1.23521000	-1.28316200
C	2.83608700	0.76575300	-0.91130900
H	1.25364800	-2.14365200	-1.53833500
H	1.23567900	2.28169400	-1.29736500
Fe	-1.38185800	0.00073200	0.41984800
Fe	1.38261400	-0.03859400	0.41706600
C	-1.52070300	-1.25247900	1.64433400
O	-1.67833700	-2.07207800	2.45698100
C	-1.46538900	1.23949600	1.65961100
O	-1.59995600	2.06915300	2.46841100
C	1.47676900	-1.35737600	1.57469900
O	1.60608200	-2.22747400	2.33844200
C	1.51333700	1.13102800	1.71846100

O	1.67950100	1.90942000	2.57110200
N	3.98838300	-1.58772600	-0.88415000
N	3.94941000	1.65065500	-0.53357200
O	4.81297200	1.19912800	0.22880100
O	3.91018100	2.79550100	-1.02010600
O	5.06563700	-1.17742500	-1.33662400
O	3.75679500	-2.71717800	-0.42310300
N	-3.96868100	1.63064200	-0.57111700
N	-3.97209800	-1.61139800	-0.84170500
O	-5.03026300	-1.25405800	-1.37618000
O	-3.74869300	-2.69732700	-0.28414300
O	-4.85612200	1.16403000	0.15515000
O	-3.91686300	2.78430900	-1.03554400

Photoisomer





Energy (a.u.): -1904.26717

Molecular coordinates

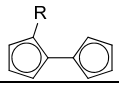
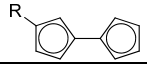
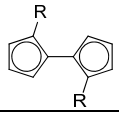
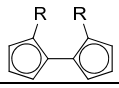
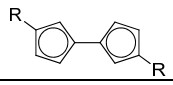
C	2.71171800	0.70243100	-0.71764500
C	0.50270700	0.01024700	-1.09240800
C	1.36295800	1.15998000	-0.95364600
C	1.33560500	-1.15803600	-0.91350700
C	2.69505800	-0.72728300	-0.68531800
C	1.70071000	1.31349700	2.00262200
C	1.73223200	-1.20714900	2.07444600
C	-2.69505500	-0.72729500	0.68530300
C	-0.50270600	0.01023200	1.09240700
C	-1.33560300	-1.15805000	0.91348300
C	-1.36295800	1.15996600	0.95366800
C	-2.71171800	0.70241800	0.71765800
C	-1.73224300	-1.20708800	-2.07448200
C	-1.70069600	1.31355600	-2.00258400
H	1.07859700	2.21056400	-0.99956800
H	1.02745000	-2.20263800	-0.95116900
H	-1.02744400	-2.20265200	0.95112500
H	-1.07859800	2.21055000	0.99961400
O	1.86715100	2.17589200	2.76764200
O	1.90152400	-2.01044600	2.89870800
O	-1.90154400	-2.01035900	-2.89876600
O	-1.86712900	2.17597600	-2.76757700
Fe	1.44020400	0.01846700	0.84393900

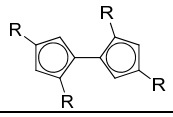
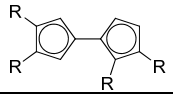
Fe	-1.44020300	0.01849000	-0.84393900
N	-3.87954000	1.57757100	0.55139200
N	-3.83690800	-1.66065700	0.66917900
O	-4.76684300	-1.39548200	1.44210200
O	-3.73200100	-2.66514600	-0.05164100
O	-4.87073900	1.10916600	-0.02717400
O	-3.76308700	2.72726000	1.01198900
N	3.87953500	1.57758700	-0.55135900
N	3.83690900	-1.66064600	-0.66921500
O	4.76686800	-1.39543200	-1.44209600
O	3.73198200	-2.66517200	0.05155100
O	4.87072700	1.10918700	0.02722200
O	3.76308300	2.72727800	-1.01195400

b. Table 2

Method B: BP86/Lanl2dz&631+g(d,p)

Table 2. DFT estimates of $\Delta H_{storage}$ by the $FvRu_2(CO)_4$ frame bearing substituents at the α-positions in comparison with their β-isomers.[a]

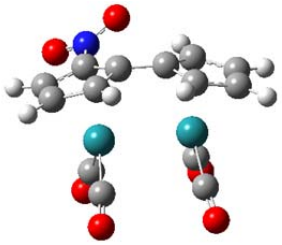
Entry	Fv substitution pattern	$\Delta H_{storage}$ (kcal mol^{-1})	$\Delta H_{isomerization\alpha\rightarrow\beta}$ (kcal mol^{-1}) Parent	Photoisomer
				
1	R=NO_2	18.6	2.5	1.5
2	R=CO_2CH_3	20.4	1.5	1.9
3 (cf. **16→18**)	R=$C_5H_4Re(CO)_3$	20.5	3.3	3.5
4 (cf. **12→14**)	R=2-cyclopentenone-3-yl	21.7	2.8	4.6
5	R=NMe_2	23.8	6.5	10.0
				
6	R=NO_2	19.6		
7	R=CO_2CH_3	20.0		
8 (cf. **17→19**)	R=$C_5H_4Re(CO)_3$	20.3		
9 (cf. **13→15**)	R=2-cyclopentenone-3-yl	19.9		
10	R=NMe_2	20.3		
				
11	R=NO_2	16.8	5.6	3.3
12 (cf. **10→11**)	R=CO_2CH_3	19.6	4.3	4.1
13	R=NMe_2	26.4	12.7	18.7
				
14	R=NO_2	8.6	12.8	2.3
15	R=CO_2CH_3	11.8	11.6	3.6
16	R=NMe_2	18.0	20.9	18.5
				
17	R=NO_2	19.1		
18	R=CO_2CH_3	19.8		
19	R=NMe_2	20.4		

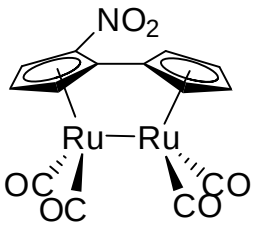
				
20 (cf. **4** and Table 1, entry 3)	R=*t*Bu	24.6	–5.9 (14.1)[b]	–2.3 (17.7)[b]
				
21 (cf. **9**)	R=C_6H_5	23.8	1.6	2.9

[a] Method: BP86/Lanl2dz&631+g(d,p). [b] Corrected for the estimated strain in 2,2',3,3'-tetra-*tert*-butylfulvalene, ~20 kcal mol^{-1}.

Entry 1

Parent





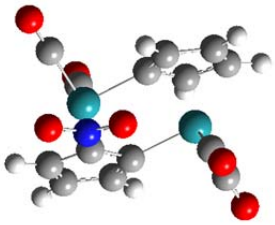
Energy (a.u., sum of electronic and thermal enthalpies, corrected at 298 K, 1 atm): -1231.672543

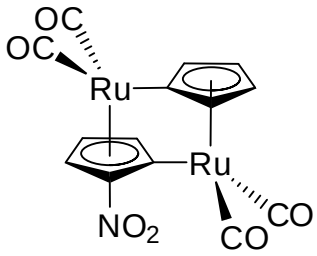
Molecular coordinates

C	2.91710000	-1.50290000	-0.75760000
C	0.69730000	-2.03450000	-0.09460000
C	1.59350000	-1.82410000	-1.23350000
C	1.53280000	-1.83660000	1.07200000
C	2.87490000	-1.53230000	0.66460000
H	3.78110000	-1.34560000	-1.40090000
H	1.19030000	-1.90060000	2.10410000
H	3.71930000	-1.35640000	1.33110000
C	-2.97120000	-1.43180000	-0.52880000
C	-0.76120000	-2.00260000	-0.02500000
C	-1.70720000	-1.79510000	-1.10250000
C	-1.47670000	-1.75320000	1.21860000
C	-2.83020000	-1.40920000	0.89760000
H	-3.88560000	-1.22830000	-1.08610000
H	-1.49090000	-1.91830000	-2.16050000
H	-3.61720000	-1.18140000	1.61690000
Ru	1.45100000	0.18170000	-0.07590000
Ru	-1.41100000	0.21500000	0.01430000
C	1.62160000	1.56210000	-1.33850000
O	1.78320000	2.40470000	-2.13410000
C	1.63040000	1.45190000	1.28040000
O	1.80760000	2.21410000	2.15290000
C	-1.61480000	1.48030000	-1.35940000
O	-1.81300000	2.23680000	-2.23160000
C	-1.55540000	1.58170000	1.29170000
O	-1.72440000	2.40170000	2.11280000

N	1.36030000	-2.06650000	-2.64950000
O	0.33410000	-2.69740000	-2.98070000
O	2.23460000	-1.66960000	-3.44360000
H	-1.06720000	-1.82550000	2.22510000

Photoisomer





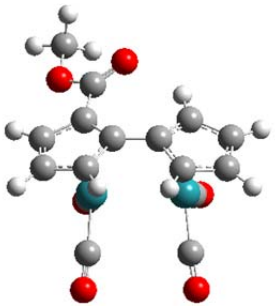
Energy (a.u.): -1231.642901

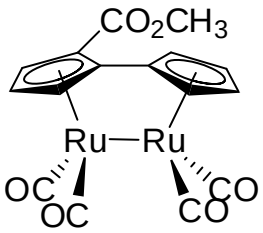
Molecular coordinates

C	1.72100000	2.38020000	0.82110000
C	-0.31170000	1.33760000	0.08660000
C	0.52280000	1.66520000	1.23510000
C	0.44830000	1.82820000	-1.03960000
C	1.66430000	2.48480000	-0.59090000
C	2.87460000	-0.72190000	1.17280000
C	2.70500000	-0.50670000	-1.49170000
C	-1.64400000	-2.35130000	-0.87840000
C	0.31030000	-1.28510000	-0.10390000
C	-0.43420000	-1.65710000	-1.28230000
C	-0.47790000	-1.71500000	1.03200000
C	-1.66640000	-2.38590000	0.54950000
C	-2.65660000	0.69040000	-1.52020000
C	-2.96510000	0.55300000	1.14300000
H	2.47480000	2.77880000	1.49820000
H	0.13230000	1.74710000	-2.08030000
H	2.40190000	2.97540000	-1.22740000
H	-2.38850000	-2.78480000	-1.54720000
H	-0.12980000	-1.47560000	-2.31340000
H	-2.43860000	-2.84160000	1.17080000
O	3.55750000	-1.28740000	1.93350000
O	3.28400000	-0.92560000	-2.41870000
O	-3.20750000	1.18660000	-2.42790000
O	-3.76100000	0.95830000	1.89470000
Ru	1.75940000	0.21070000	-0.03580000
Ru	-1.74290000	-0.16540000	-0.11400000
N	0.23640000	1.47110000	2.65790000
O	1.09530000	1.89240000	3.46090000
O	-0.82960000	0.92060000	2.99130000
H	-0.22100000	-1.57550000	2.08190000

Entry 2

Parent



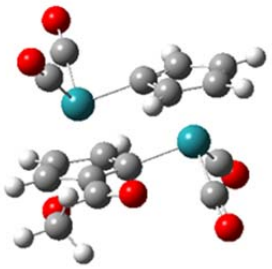


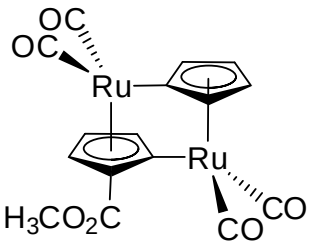
Energy (a.u.): -1254.998038

Molecular coordinates

C	2.73080000	-1.85700000	-0.98830000
C	0.68280000	-2.03620000	0.15390000
C	1.32280000	-2.07410000	-1.14490000
C	1.75020000	-1.78080000	1.12840000
C	2.99570000	-1.66040000	0.39670000
H	3.46900000	-1.84470000	-1.79030000
H	0.81280000	-2.23610000	-2.09370000
H	3.96860000	-1.49980000	0.85790000
C	-2.91060000	-1.21930000	-0.36260000
C	-0.76240000	-1.88070000	0.29610000
C	-1.65520000	-1.71740000	-0.84290000
C	-1.49880000	-1.46270000	1.47060000
C	-2.81310000	-1.05960000	1.05870000
H	-3.78820000	-1.00770000	-0.97390000
H	-1.42350000	-1.94260000	-1.88290000
H	-3.60640000	-0.70950000	1.71930000
Ru	1.58220000	0.06350000	-0.27950000
Ru	-1.25440000	0.36520000	0.06350000
C	1.64660000	1.14420000	-1.80250000
O	1.74780000	1.77910000	-2.78360000
C	2.06430000	1.54540000	0.76320000
O	2.42430000	2.44320000	1.42560000
C	-1.49280000	1.57280000	-1.35110000
O	-1.72410000	2.30030000	-2.24240000
C	-1.13360000	1.79740000	1.26950000
O	-1.12580000	2.66730000	2.05620000
C	1.68900000	-1.77970000	2.61170000
O	0.72530000	-2.10100000	3.30610000
O	2.89190000	-1.41090000	3.14250000
C	2.94130000	-1.39520000	4.59220000
H	3.96780000	-1.09330000	4.83920000
H	2.21450000	-0.67010000	4.99120000
H	2.71670000	-2.39550000	4.99530000
H	-1.10540000	-1.48230000	2.48490000

Photoisomer





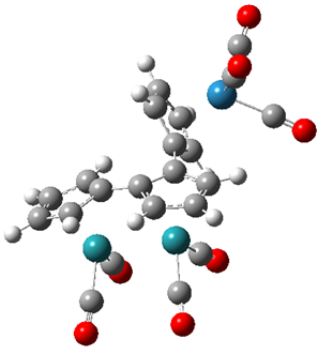
Energy (a.u.): -1254.965507

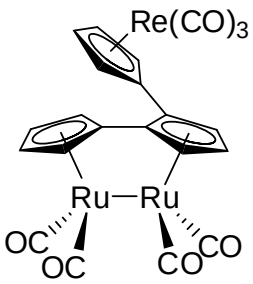
Molecular coordinates

C	-1.67720000	-2.29270000	0.95960000
C	0.29000000	-1.30580000	0.11170000
C	-0.45740000	-1.58940000	1.31390000
C	-0.50960000	-1.79560000	-0.98980000
C	-1.70560000	-2.41890000	-0.46250000
C	-2.66040000	0.80640000	1.38820000
C	-2.91770000	0.52670000	-1.26580000
C	1.73840000	2.28280000	-1.00250000
C	-0.27780000	1.29910000	-0.21270000
C	0.53220000	1.55880000	-1.40050000
C	0.48440000	1.83090000	0.89220000
C	1.70220000	2.45170000	0.40520000
C	2.83590000	-0.83940000	-1.23990000
C	2.73260000	-0.49560000	1.42270000
H	-2.42600000	-2.66980000	1.65730000
H	-0.26430000	-1.70980000	-2.04790000
H	-2.48690000	-2.90130000	-1.05130000
H	2.50560000	2.64200000	-1.68720000
H	0.17260000	1.80090000	1.93670000
H	2.45290000	2.95950000	1.01260000
O	-3.21340000	1.37400000	2.25320000
O	-3.68500000	0.92370000	-2.05290000
O	3.49000000	-1.44470000	-1.99930000
O	3.32600000	-0.87600000	2.35850000
Ru	-1.74690000	-0.15520000	0.05500000
Ru	1.76590000	0.16000000	-0.05040000
C	0.19700000	1.24860000	-2.81620000
O	-0.75290000	0.58100000	-3.21670000
O	1.10530000	1.82960000	-3.66180000
C	0.86990000	1.58070000	-5.07060000
H	-0.12410000	1.95260000	-5.36530000
H	1.66470000	2.12800000	-5.59510000
H	0.93110000	0.50190000	-5.28610000
H	-0.14600000	-1.34630000	2.33030000

Entry 3

Parent





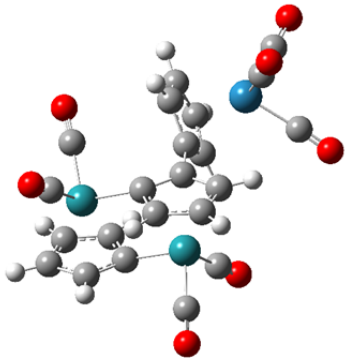
Energy (a.u.): -1638.728486

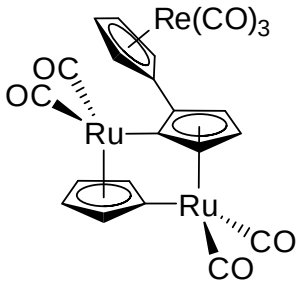
Molecular coordinates

C	2.53260000	-2.02590000	-0.76840000
C	0.34290000	-2.15440000	0.05320000
C	1.15340000	-2.10260000	-1.15020000
C	1.25950000	-2.11460000	1.18970000
C	2.59950000	-2.02150000	0.65940000
H	3.38530000	-1.99370000	-1.44670000
H	0.77570000	-2.11420000	-2.17190000
H	3.50680000	-2.02150000	1.26350000
C	-3.12030000	-1.01540000	-0.71640000
C	-1.08860000	-1.87730000	0.06770000
C	-1.87300000	-1.59930000	-1.12030000
C	-1.87690000	-1.43180000	1.20320000
C	-3.12290000	-0.91300000	0.71250000
H	-3.92920000	-0.71450000	-1.38230000
H	-1.57500000	-1.80810000	-2.14720000
H	-1.58150000	-1.48130000	2.24900000
H	-3.93380000	-0.51870000	1.32510000
Ru	1.44410000	-0.11360000	-0.02730000
Ru	-1.38330000	0.41600000	-0.08760000
C	1.84710000	1.11560000	-1.38080000
O	2.16110000	1.83940000	-2.24830000
C	1.85060000	1.18920000	1.25610000
O	2.16180000	1.95890000	2.08670000
C	-1.31770000	1.65080000	-1.49810000
O	-1.35510000	2.39880000	-2.40090000
C	-1.31350000	1.82470000	1.14560000
O	-1.34260000	2.68690000	1.94080000
C	0.89950000	-2.29070000	2.61470000
C	1.20350000	-1.42020000	3.72850000
C	0.08070000	-3.36940000	3.14720000
C	0.55960000	-1.92280000	4.90850000
H	1.79320000	-0.50540000	3.66600000
C	-0.13660000	-3.13650000	4.54320000
H	-0.31980000	-4.19980000	2.56480000
H	0.57920000	-1.46020000	5.89470000

H	-0.72720000	-3.76400000	5.21070000
C	3.93980000	-2.82070000	4.34970000
Re	2.15150000	-3.50690000	4.22680000
O	5.01130000	-2.34080000	4.40570000
C	2.41430000	-4.48120000	5.85780000
C	2.78490000	-5.00680000	3.21250000
O	2.51240000	-5.05600000	6.87790000
O	3.11940000	-5.91450000	2.54460000

Photoisomer





Energy (a.u.): -1638.695764

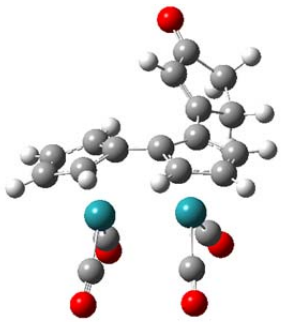
Molecular coordinates

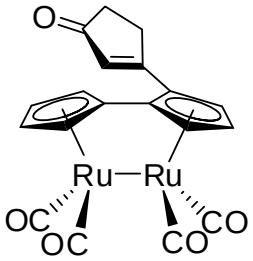
C	-1.72160000	-2.39520000	0.76730000
C	0.28060000	-1.38130000	0.02950000
C	-0.49360000	-1.74710000	1.19180000
C	-0.51510000	-1.76470000	-1.11870000
C	-1.73160000	-2.40670000	-0.65990000
C	-2.64120000	0.68660000	1.43030000
C	-2.92340000	0.54930000	-1.22870000
C	1.81390000	2.24530000	-0.74910000
C	-0.22930000	1.26000000	-0.07510000
C	0.58940000	1.61320000	-1.23080000
C	0.53690000	1.64740000	1.08870000
C	1.77740000	2.27200000	0.67200000
C	2.83840000	-0.87200000	-1.24820000
C	2.73140000	-0.74070000	1.43300000
H	-2.48830000	-2.81180000	1.42170000
H	-0.19340000	-1.59210000	2.22860000
H	-0.23210000	-1.63100000	-2.16270000
H	-2.51210000	-2.82930000	-1.29440000
H	2.58940000	2.66430000	-1.39130000
H	0.21520000	1.52140000	2.12290000
H	2.53710000	2.69970000	1.32750000
O	-3.19180000	1.20620000	2.32410000
O	-3.70820000	0.95540000	-1.99990000
O	3.48490000	-1.43850000	-2.04550000
O	3.30770000	-1.20840000	2.33900000

Ru	-1.73740000	-0.19610000	0.03040000
Ru	1.78590000	0.05570000	0.01070000
C	0.17820000	1.53530000	-2.65450000
C	0.75040000	0.74360000	-3.72170000
C	-0.97080000	2.21620000	-3.22440000
C	-0.04600000	0.90020000	-4.90570000
H	1.63180000	0.10850000	-3.62850000
C	-1.11560000	1.82100000	-4.59180000
H	-1.62470000	2.90030000	-2.68430000
H	0.11990000	0.40230000	-5.86060000
H	-1.90280000	2.14910000	-5.27030000
C	0.95520000	4.69740000	-3.55180000
Re	0.91170000	2.97650000	-4.39900000
O	0.93680000	5.72810000	-2.98600000
C	2.82780000	2.95980000	-4.49420000
C	0.83040000	3.81190000	-6.12360000
O	4.00140000	2.88830000	-4.52940000
O	0.73060000	4.27830000	-7.19780000

Entry 4

Parent





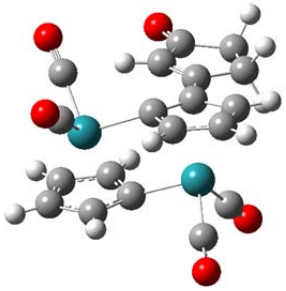
Energy (a.u.): -1295.244091

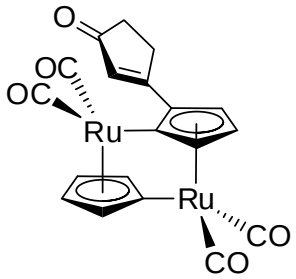
Molecular coordinates

C	2.77930000	-1.52040000	-0.59350000
C	0.60220000	-1.99260000	0.14200000
C	1.44990000	-1.83450000	-1.02480000
C	1.44880000	-1.77950000	1.31820000
C	2.77770000	-1.45330000	0.83240000
H	3.64220000	-1.36050000	-1.24010000
H	1.12520000	-1.92130000	-2.06100000
H	3.64930000	-1.27410000	1.46130000
C	-2.93790000	-1.44070000	-0.88690000
C	-0.85510000	-1.94090000	0.06300000
C	-1.58900000	-1.82920000	-1.18450000
C	-1.78230000	-1.59110000	1.12430000
C	-3.05660000	-1.29490000	0.53360000
H	-3.73560000	-1.29660000	-1.61570000
H	-1.19360000	-2.02270000	-2.18090000
H	-1.55520000	-1.56220000	2.18740000

H	-3.96030000	-1.01880000	1.07700000
Ru	1.35920000	0.20800000	0.05030000
Ru	-1.50150000	0.26910000	-0.20900000
C	1.62060000	1.44300000	-1.32930000
O	1.85610000	2.18340000	-2.20760000
C	1.48240000	1.60650000	1.29280000
O	1.62270000	2.45520000	2.09130000
C	-1.55740000	1.45700000	-1.66070000
O	-1.66790000	2.16100000	-2.59260000
C	-1.74060000	1.70380000	0.97370000
O	-1.95920000	2.57160000	1.73190000
C	1.15600000	-2.00050000	2.73640000
C	1.88340000	-1.23320000	3.83830000
C	0.31250000	-2.94190000	3.25580000
C	1.32320000	-1.80920000	5.15760000
H	2.97710000	-1.37510000	3.75360000
H	1.70530000	-0.14830000	3.73190000
H	-0.29360000	-3.65510000	2.69190000
H	0.78380000	-1.05540000	5.75670000
H	2.09790000	-2.24170000	5.81320000
C	0.33830000	-2.91700000	4.73360000
O	-0.30350000	-3.64460000	5.49490000

Photoisomer





Energy (a.u.): -1295.209469

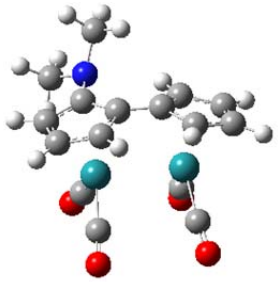
Molecular coordinates

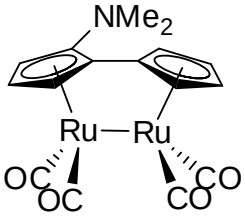
C	-1.64350000	-2.49000000	0.75300000
C	0.25410000	-1.32180000	-0.02510000
C	-0.42960000	-1.79760000	1.14970000
C	-0.58000000	-1.69090000	-1.15490000
C	-1.72800000	-2.42540000	-0.67170000
C	-2.55810000	0.51480000	1.70020000
C	-3.22680000	0.49590000	-0.85750000
C	1.56620000	2.38050000	-0.83220000
C	-0.40960000	1.28580000	-0.11080000
C	0.36720000	1.67220000	-1.29850000
C	0.35130000	1.74760000	1.02630000
C	1.54580000	2.43740000	0.58420000
C	2.77730000	-0.66090000	-1.32080000

C	2.66770000	-0.53020000	1.36200000
H	-2.34670000	-2.98890000	1.42080000
H	-0.08730000	-1.67460000	2.17800000
H	-0.36240000	-1.48140000	-2.20230000
H	-2.51840000	-2.85490000	-1.28920000
H	2.32650000	2.82430000	-1.47500000
H	0.05800000	1.61900000	2.06850000
H	2.28770000	2.91880000	1.22260000
O	-2.99900000	0.95320000	2.69340000
O	-4.14370000	0.92640000	-1.44580000
O	3.45720000	-1.18030000	-2.12080000
O	3.27600000	-0.95810000	2.26700000
Ru	-1.81730000	-0.25460000	0.14920000
Ru	1.67410000	0.20330000	-0.05780000
C	0.09290000	1.52900000	-2.73280000
C	1.14250000	1.97900000	-3.75530000
C	-1.03000000	1.06770000	-3.36170000
C	0.52720000	1.66210000	-5.13450000
H	1.34840000	3.05930000	-3.63610000
H	2.10290000	1.45740000	-3.58920000
H	-1.94360000	0.71120000	-2.89120000
H	1.10070000	0.90450000	-5.69620000
H	0.43860000	2.54540000	-5.78930000
C	-0.87670000	1.10640000	-4.82900000
O	-1.70810000	0.75010000	-5.66850000

Entry 5

Parent





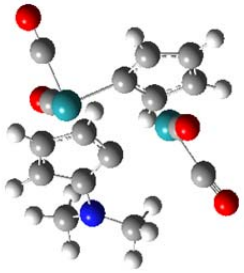
Energy (a.u.): -1161.049312

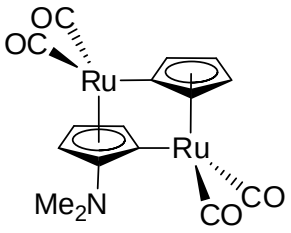
Molecular coordinates

C	2.87240000	-1.37440000	-0.81890000
C	0.72080000	-1.87250000	-0.03660000
C	1.54910000	-1.77720000	-1.23630000
C	1.58170000	-1.60050000	1.10340000
C	2.89120000	-1.28740000	0.61290000
H	3.72810000	-1.21530000	-1.47400000
H	1.27980000	-1.62260000	2.14950000
H	3.76390000	-1.04950000	1.22140000
C	-2.92430000	-1.26620000	-0.57040000
C	-0.73240000	-1.84040000	0.01830000

C	-1.62620000	-1.58130000	-1.09750000
C	-1.50740000	-1.65540000	1.22940000
C	-2.85290000	-1.31360000	0.86060000
H	-3.81350000	-1.03900000	-1.15870000
H	-1.33640000	-1.60030000	-2.14670000
H	-3.67800000	-1.13600000	1.55040000
Ru	1.43570000	0.34050000	-0.10700000
Ru	-1.42730000	0.37640000	0.11970000
C	1.49810000	1.60290000	-1.49280000
O	1.61650000	2.36400000	-2.38030000
C	1.73190000	1.70400000	1.13910000
O	1.98880000	2.52310000	1.94030000
C	-1.68820000	1.73810000	-1.13950000
O	-1.92620000	2.56030000	-1.94290000
C	-1.48220000	1.64300000	1.49950000
O	-1.58400000	2.39940000	2.39150000
N	1.11410000	-2.07550000	-2.54030000
C	0.66720000	-3.46590000	-2.74010000
H	-0.01270000	-3.76980000	-1.93020000
H	0.12090000	-3.53550000	-3.69610000
H	1.52060000	-4.17840000	-2.77030000
C	1.98180000	-1.60170000	-3.62130000
H	2.18940000	-0.52820000	-3.48930000
H	2.94760000	-2.15260000	-3.67690000
H	1.45760000	-1.73680000	-4.58160000
H	-1.13920000	-1.77050000	2.24840000

Photoisomer





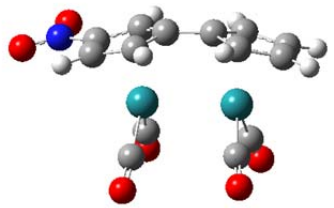
Energy (a.u.): -1161.011323

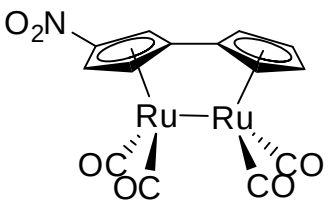
Molecular coordinates

C	1.43720000	2.84730000	0.43430000
C	-0.46400000	1.48230000	0.05140000
C	0.29880000	2.18810000	1.08490000
C	0.17600000	1.82460000	-1.21010000
C	1.32050000	2.66940000	-0.97290000
C	2.84680000	-0.05310000	1.28770000
C	2.88500000	-0.06840000	-1.42580000
C	-1.29070000	-2.43700000	-0.74850000
C	0.51740000	-1.07490000	-0.06810000
C	-0.20200000	-1.59340000	-1.20510000

C	-0.17350000	-1.58190000	1.10400000
C	-1.26530000	-2.43280000	0.68100000
C	-2.72430000	0.42710000	-1.43310000
C	-3.06930000	0.13880000	1.17990000
H	2.18710000	3.46460000	0.92700000
H	-0.17970000	1.52020000	-2.19400000
H	1.97560000	3.10440000	-1.72890000
H	-1.98610000	-2.99210000	-1.37940000
H	0.04360000	-1.39820000	-2.24960000
H	-1.94660000	-2.97840000	1.33590000
O	3.57700000	-0.45970000	2.11370000
O	3.58890000	-0.47060000	-2.27450000
O	-3.35740000	0.82990000	-2.33330000
O	-3.97010000	0.30930000	1.91420000
Ru	1.73140000	0.60430000	-0.09380000
Ru	-1.68920000	-0.27650000	-0.02480000
N	0.03080000	2.36010000	2.43340000
C	1.15950000	2.51040000	3.35100000
H	1.71530000	1.55680000	3.48310000
H	1.86690000	3.27310000	2.99260000
H	0.78210000	2.84010000	4.33160000
C	-1.18560000	1.82010000	3.02770000
H	-2.04140000	2.04560000	2.37900000
H	-1.14580000	0.72500000	3.20020000
H	-1.34800000	2.31970000	3.99710000
H	0.11320000	-1.39240000	2.13840000

Entry 6
Parent



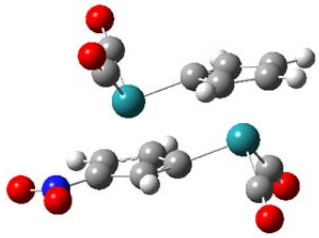


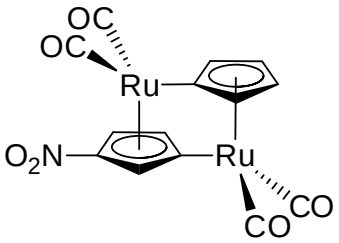
Energy (a.u.): -1231.676479
Molecular coordinates

C	2.89170000	-1.54030000	-0.68190000
C	0.73030000	-2.00450000	-0.00300000
C	1.57290000	-1.84500000	-1.16230000
C	1.55330000	-1.77010000	1.17370000
C	2.88820000	-1.48760000	0.75000000
H	1.29860000	-1.95550000	-2.20950000
H	1.21440000	-1.80930000	2.20840000
H	3.75880000	-1.29190000	1.37420000
C	-2.87980000	-1.43810000	-0.71440000
C	-0.72560000	-1.99790000	-0.00810000

C	-1.55510000	-1.74910000	-1.17140000
C	-1.56060000	-1.82170000	1.16080000
C	-2.88480000	-1.48180000	0.71910000
H	-3.73730000	-1.21460000	-1.34940000
H	-1.23150000	-1.79340000	-2.21080000
H	-1.24540000	-1.93530000	2.19760000
Ru	1.46000000	0.20010000	-0.05870000
Ru	-1.41370000	0.20490000	0.05780000
C	1.48040000	1.45520000	-1.45460000
O	1.55330000	2.21050000	-2.34520000
C	1.69740000	1.59700000	1.16810000
O	1.90200000	2.44180000	1.95370000
C	-1.68230000	1.58370000	-1.18780000
O	-1.93050000	2.41110000	-1.97970000
C	-1.53000000	1.45040000	1.45700000
O	-1.66840000	2.18790000	2.35710000
N	4.07740000	-1.41810000	-1.52030000
O	5.16570000	-1.21430000	-0.94780000
O	3.91660000	-1.54460000	-2.75060000
H	-3.74710000	-1.30480000	1.36190000

Photoisomer





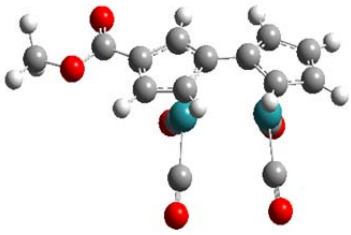
Energy (a.u.): -1231.645239

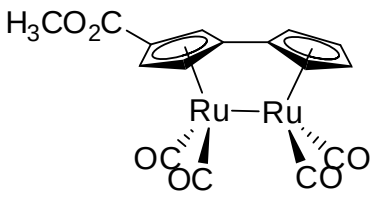
Molecular coordinates

C	1.72120000	2.34080000	0.75620000
C	-0.25470000	1.32610000	0.02360000
C	0.50660000	1.67780000	1.19520000
C	0.54640000	1.72570000	-1.12020000
C	1.75570000	2.37120000	-0.66930000
C	2.66540000	-0.81930000	1.39070000
C	2.85040000	-0.68420000	-1.28730000
C	-1.71120000	-2.28310000	-0.90890000
C	0.27170000	-1.29740000	-0.09800000
C	-0.48680000	-1.60170000	-1.28970000
C	-0.52900000	-1.74400000	1.01900000
C	-1.73720000	-2.37140000	0.51430000
C	-2.74960000	0.80160000	-1.36800000
C	-2.76510000	0.64620000	1.33050000
H	0.22210000	1.53940000	2.23710000
H	0.26310000	1.59940000	-2.16550000
H	2.54030000	2.82390000	-1.27520000

H	-2.46840000	-2.66820000	-1.59310000
H	-0.17350000	-1.39740000	-2.31380000
H	-0.25610000	-1.66240000	2.07140000
O	3.20920000	-1.39500000	2.24950000
O	3.50380000	-1.17300000	-2.12530000
O	-3.36250000	1.34970000	-2.20160000
O	-3.38840000	1.09500000	2.21360000
Ru	1.77350000	0.13490000	0.02730000
Ru	-1.74610000	-0.11980000	-0.06180000
N	2.70570000	2.96720000	1.63100000
O	2.50610000	2.88410000	2.85920000
O	3.66210000	3.55790000	1.09120000
H	-2.51760000	-2.83620000	1.11810000

Entry 7
Parent



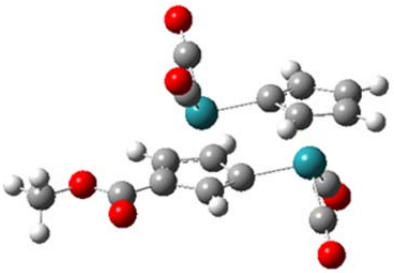


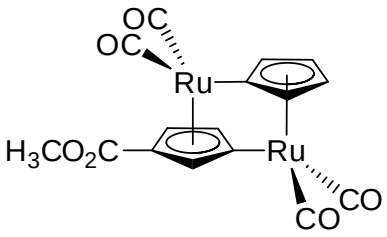
Energy (a.u.): -1255.000359
Molecular coordinates

C	2.90550000	-1.50460000	-0.64500000
C	0.73960000	-2.03640000	0.05630000
C	1.58480000	-1.80790000	-1.10340000
C	1.56130000	-1.85340000	1.22720000
C	2.89900000	-1.53850000	0.79420000
H	3.77690000	-1.29930000	-1.26560000
H	1.27010000	-1.86200000	-2.14520000
H	1.25650000	-1.94920000	2.26850000
C	-2.86790000	-1.54350000	-0.72980000
C	-0.71540000	-2.04000000	0.03450000
C	-1.53270000	-1.86920000	-1.14820000
C	-1.56780000	-1.79730000	1.18210000
C	-2.88810000	-1.49940000	0.70330000
H	-3.72030000	-1.37340000	-1.38750000
H	-1.19780000	-1.97750000	-2.17940000
H	-1.26070000	-1.83670000	2.22670000
H	-3.75840000	-1.28440000	1.32350000
Ru	1.45220000	0.17020000	0.09790000
Ru	-1.42490000	0.15980000	-0.04360000
C	1.69950000	1.53520000	-1.16150000
O	1.91890000	2.35810000	-1.96810000
C	1.48450000	1.44920000	1.47080000

O	1.56910000	2.22130000	2.34780000
C	-1.53010000	1.41220000	-1.43500000
O	-1.66150000	2.15700000	-2.33150000
C	-1.69340000	1.53190000	1.20680000
O	-1.93960000	2.35700000	2.00290000
C	4.04570000	-1.36010000	1.72150000
O	3.97090000	-1.47390000	2.94200000
O	5.19680000	-1.07810000	1.04700000
C	6.36040000	-0.87430000	1.88950000
H	7.18350000	-0.65970000	1.19510000
H	6.19230000	-0.02680000	2.57280000
H	6.56960000	-1.78070000	2.47970000

Photoisomer





Energy (a.u.): -1254.968515

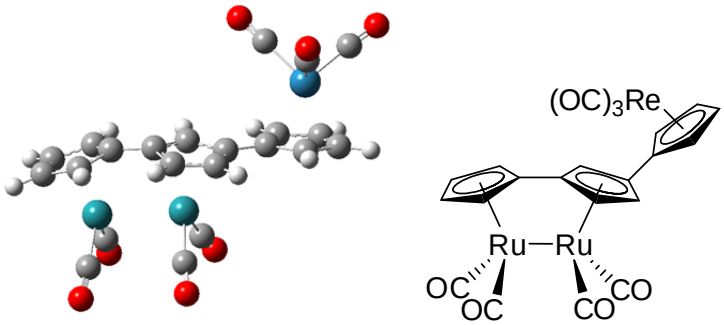
Molecular coordinates

C	1.73880000	2.24690000	0.91460000
C	-0.26270000	1.33680000	0.05520000
C	0.50210000	1.56860000	1.25960000
C	0.54880000	1.82500000	-1.03710000
C	1.76740000	2.40560000	-0.50260000
C	2.71260000	-0.88050000	1.22050000
C	2.74580000	-0.58760000	-1.46450000
C	-1.79090000	-2.21550000	-1.02830000
C	0.21720000	-1.28090000	-0.20950000
C	-0.55130000	-1.54530000	-1.39880000
C	-0.59300000	-1.73630000	0.90320000
C	-1.81270000	-2.32560000	0.40010000
C	-2.68560000	0.96820000	-1.44310000
C	-2.84320000	0.68220000	1.23290000
H	2.50260000	2.58320000	1.61690000
H	0.18520000	1.31680000	2.27200000
H	0.27560000	1.79950000	-2.09230000
H	2.55690000	2.88530000	-1.08240000
H	-0.25650000	-1.33760000	-2.42720000
H	-0.31230000	-1.68110000	1.95560000
H	-2.60420000	-2.78940000	0.98900000
O	3.30800000	-1.48580000	2.02810000
O	3.36390000	-1.00620000	-2.36700000
O	-3.23520000	1.59260000	-2.26580000

O	-3.48610000	1.12190000	2.10780000
Ru	1.73860000	0.12870000	-0.03970000
Ru	-1.78970000	-0.06350000	-0.14190000
C	-2.78080000	-2.73350000	-2.00700000
O	-2.66560000	-2.63700000	-3.22590000
O	-3.82480000	-3.35640000	-1.38530000
C	-4.83420000	-3.88810000	-2.28130000
H	-5.58730000	-4.34590000	-1.62620000
H	-5.27700000	-3.07800000	-2.88240000
H	-4.39140000	-4.63860000	-2.95540000

Entry 8

Parent



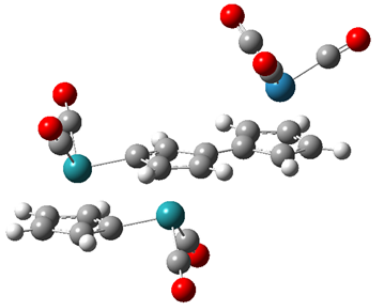
Energy (a.u.): -1638.733693

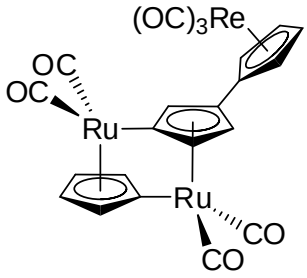
Molecular coordinates

C	3.00410000	-1.07010000	-0.93120000
C	0.91460000	-1.89790000	-0.30030000
C	1.70540000	-1.43150000	-1.41900000
C	1.74620000	-1.79430000	0.87930000
C	3.05260000	-1.32080000	0.48690000
H	3.82960000	-0.70820000	-1.54400000
H	1.37770000	-1.36820000	-2.45590000
H	1.45050000	-2.07990000	1.88800000
C	-2.74870000	-1.64790000	-0.92380000
C	-0.53200000	-2.04630000	-0.29780000
C	-1.40330000	-1.74480000	-1.41590000
C	-1.36510000	-2.11350000	0.88550000
C	-2.72520000	-1.87340000	0.49170000
H	-3.63560000	-1.44730000	-1.52480000
H	-1.09400000	-1.62070000	-2.45320000
H	-1.02270000	-2.31920000	1.89910000
H	-3.59140000	-1.87570000	1.15340000
Ru	1.40740000	0.33330000	0.03960000
Ru	-1.46310000	0.04210000	0.05180000
C	1.42420000	1.84790000	-1.06460000
O	1.50550000	2.77320000	-1.78140000
C	1.44840000	1.44020000	1.55260000
O	1.54530000	2.10060000	2.51790000

C	-1.79430000	1.52650000	-1.04460000
O	-2.06720000	2.41810000	-1.75640000
C	-1.75400000	1.10290000	1.56980000
O	-2.00300000	1.72030000	2.53590000
C	4.21860000	-1.15090000	1.35990000
C	5.55120000	-0.74370000	0.95900000
C	4.25290000	-1.29000000	2.80340000
C	6.36430000	-0.58960000	2.12710000
H	5.87620000	-0.55250000	-0.06400000
C	5.55530000	-0.93080000	3.27590000
H	3.41240000	-1.57920000	3.43440000
H	7.40440000	-0.26530000	2.14440000
H	5.87330000	-0.90820000	4.31780000
Re	5.76750000	-2.85380000	1.94810000
C	6.26070000	-3.72790000	0.31240000
C	7.29620000	-3.60650000	2.82850000
C	4.70830000	-4.37170000	2.45240000
O	6.54710000	-4.20070000	-0.72500000
O	8.24500000	-4.00600000	3.39520000
O	4.00330000	-5.25410000	2.77910000

Photoisomer





Energy (a.u.): -1638.701296

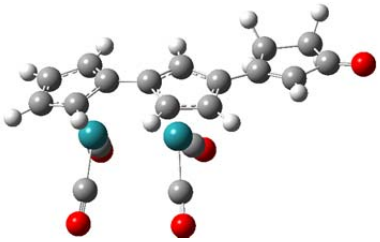
Molecular coordinates

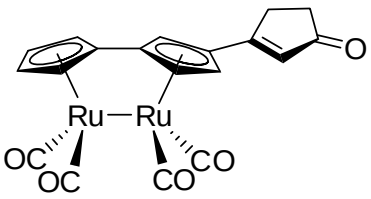
C	-2.00580000	-2.18130000	0.51930000
C	0.06360000	-1.37660000	-0.28690000
C	-0.62270000	-1.91050000	0.86850000
C	-0.93240000	-1.26790000	-1.32910000
C	-2.19730000	-1.78450000	-0.83720000
C	-2.21760000	0.71740000	2.06260000
C	-2.56470000	1.46720000	-0.51080000
C	2.22960000	2.04280000	-0.32560000
C	0.15920000	1.18890000	0.46540000
C	0.84600000	1.73930000	-0.67880000
C	1.15560000	1.06720000	1.50470000
C	2.41660000	1.59390000	1.02290000
C	2.41560000	-0.88760000	-1.90970000
C	2.79960000	-1.65370000	0.65340000
H	-2.75900000	-2.61920000	1.17570000

H	-0.16790000	-2.11840000	1.83740000
H	-0.75710000	-0.89700000	-2.33930000
H	-3.12340000	-1.86420000	-1.40810000
H	0.38290000	1.96190000	-1.64040000
H	0.98450000	0.68170000	2.51000000
H	3.33170000	1.68410000	1.60970000
O	-2.58390000	1.06720000	3.11880000
O	-3.15240000	2.29280000	-1.09850000
O	2.76160000	-1.23110000	-2.97560000
O	3.39850000	-2.48470000	1.22240000
Ru	-1.61560000	0.10470000	0.38320000
Ru	1.83870000	-0.28550000	-0.21800000
C	3.21640000	2.71520000	-1.17800000
C	4.62380000	2.92830000	-0.88560000
C	2.99270000	3.24370000	-2.50650000
C	5.24750000	3.52440000	-2.02670000
H	5.13290000	2.64000000	0.03410000
C	4.23570000	3.72060000	-3.04000000
H	2.03770000	3.25190000	-3.03230000
H	6.30340000	3.77960000	-2.11510000
H	4.38810000	4.14300000	-4.03250000
Re	3.68070000	5.04900000	-1.18460000
C	3.67420000	5.49950000	0.68020000
C	4.69920000	6.62390000	-1.58040000
C	2.05090000	6.03210000	-1.43880000
O	3.68790000	5.70410000	1.83780000
O	5.36340000	7.55100000	-1.86530000
O	1.02990000	6.58040000	-1.63210000

Entry 9

Parent





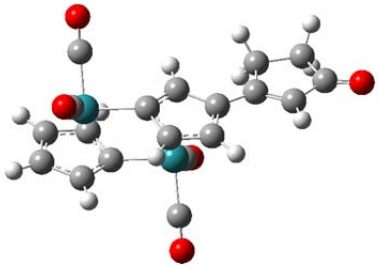
Energy (a.u.): -1295.248598

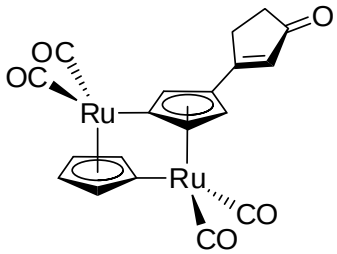
Molecular coordinates

C	-2.86740000	-1.59110000	0.71320000
C	-0.68770000	-2.05360000	0.00770000
C	-1.53300000	-1.86140000	1.16950000
C	-1.52500000	-1.88130000	-1.16180000
C	-2.86330000	-1.60410000	-0.72050000
H	-3.73620000	-1.41670000	1.34810000
H	-1.21440000	-1.91640000	2.21000000
H	-1.20010000	-1.95710000	-2.19900000

H	-3.72820000	-1.44400000	-1.36430000
C	2.94130000	-1.47670000	0.73160000
C	0.76620000	-2.00980000	0.00960000
C	1.60030000	-1.80270000	1.17040000
C	1.59160000	-1.76120000	-1.15660000
C	2.90910000	-1.42840000	-0.71140000
H	1.28520000	-1.91550000	2.20720000
H	1.26620000	-1.81410000	-2.19500000
H	3.75770000	-1.19840000	-1.35590000
Ru	-1.46150000	0.12500000	-0.01290000
Ru	1.42130000	0.21000000	0.04820000
C	-1.73170000	1.45270000	1.28370000
O	-1.97620000	2.24490000	2.11340000
C	-1.63990000	1.41350000	-1.36410000
O	-1.81710000	2.18120000	-2.23260000
C	1.46140000	1.49930000	1.40840000
O	1.55240000	2.27410000	2.28440000
C	1.59790000	1.56830000	-1.23190000
O	1.77290000	2.38620000	-2.05370000
C	4.10480000	-1.28570000	1.59400000
C	3.97370000	-1.17250000	3.10960000
C	5.41000000	-1.22160000	1.19420000
C	5.42120000	-0.97920000	3.61550000
H	3.31170000	-0.32950000	3.37930000
H	3.50520000	-2.08510000	3.52450000
H	5.78840000	-1.29600000	0.17190000
H	5.74330000	-1.75380000	4.33180000
H	5.57390000	-0.00400000	4.10890000
C	6.30700000	-1.04660000	2.35430000
O	7.53780000	-0.97020000	2.33280000

Photoisomer





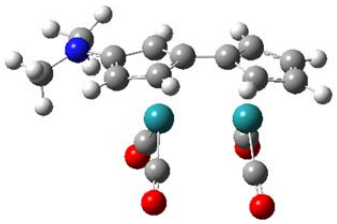
Energy (a.u.): -1295.216841

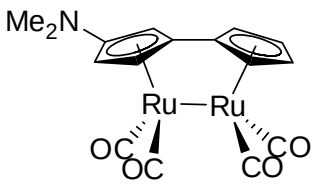
Molecular coordinates

C	-0.25410000	5.82530000	0.35760000
C	0.34870000	3.64260000	-0.31070000
C	-0.76010000	4.50270000	0.03690000
C	1.54350000	4.43760000	-0.13810000
C	1.16750000	5.78550000	0.24960000
C	-0.69720000	4.49930000	3.33660000

C	1.99410000	4.39270000	3.11810000
C	1.02420000	0.00350000	1.31800000
C	0.45270000	2.22380000	1.94880000
C	1.54270000	1.33810000	1.62540000
C	-0.75680000	1.45320000	1.75280000
C	-0.40840000	0.10210000	1.37820000
C	1.57490000	1.42520000	-1.67220000
C	-1.11890000	1.44520000	-1.53530000
H	-0.85670000	6.69490000	0.62310000
H	-1.81310000	4.22040000	0.01910000
H	2.56450000	4.09670000	-0.31140000
H	1.85090000	6.61900000	0.41650000
H	2.60070000	1.59780000	1.67260000
H	-1.77350000	1.82010000	1.89740000
H	-1.11250000	-0.71120000	1.19640000
O	-1.48680000	4.63030000	4.19180000
O	2.92050000	4.45420000	3.83270000
O	2.39150000	1.33890000	-2.50780000
O	-2.01920000	1.36790000	-2.27980000
Ru	0.53740000	4.30250000	1.92400000
Ru	0.29680000	1.56040000	-0.29330000
C	1.82460000	-1.19320000	1.06740000
C	3.33600000	-1.12170000	0.87200000
C	1.37180000	-2.48240000	1.02260000
C	3.77330000	-2.58640000	0.64570000
H	3.58790000	-0.46490000	0.01910000
H	3.81640000	-0.67450000	1.76250000
H	0.34160000	-2.82110000	1.15610000
H	4.51280000	-2.94160000	1.38320000
H	4.21270000	-2.75290000	-0.35290000
C	2.48240000	-3.42190000	0.77230000
O	2.40730000	-4.64980000	0.67970000

Entry 10
Parent



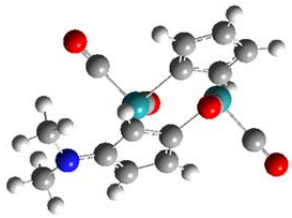


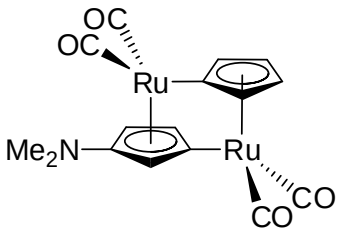
Energy (a.u.): -1161.059604
Molecular coordinates

C	2.91740000	-1.63230000	-0.77400000
C	0.72710000	-2.04210000	-0.00700000
C	1.54270000	-1.82050000	-1.18800000
C	1.58530000	-1.86370000	1.13950000

C	2.91130000	-1.56150000	0.67140000
H	1.18570000	-1.88070000	-2.21410000
H	1.28990000	-1.94840000	2.18470000
H	3.77910000	-1.40950000	1.31100000
C	-2.90630000	-1.56940000	-0.69850000
C	-0.72620000	-2.04160000	0.00810000
C	-1.57730000	-1.87560000	-1.15120000
C	-1.55340000	-1.80770000	1.17670000
C	-2.89060000	-1.53080000	0.73380000
H	-3.77720000	-1.41040000	-1.33430000
H	-1.26770000	-1.97500000	-2.19120000
H	-1.22050000	-1.84440000	2.21350000
Ru	1.41970000	0.13980000	0.05000000
Ru	-1.46670000	0.15530000	-0.04680000
C	1.67280000	1.52750000	-1.18960000
O	1.88110000	2.37480000	-1.97840000
C	1.53520000	1.36200000	1.46250000
O	1.68010000	2.08890000	2.37390000
C	-1.57820000	1.40900000	-1.43280000
O	-1.71010000	2.15690000	-2.32870000
C	-1.67790000	1.53140000	1.20590000
O	-1.88110000	2.36560000	2.00720000
N	4.01850000	-1.54540000	-1.59650000
C	5.23470000	-0.95070000	-1.03710000
H	6.05900000	-1.08410000	-1.75430000
H	5.10730000	0.13230000	-0.82770000
H	5.51420000	-1.46300000	-0.10310000
C	3.78390000	-1.27600000	-3.01680000
H	3.06450000	-2.00200000	-3.42710000
H	3.39690000	-0.24970000	-3.18870000
H	4.73190000	-1.39620000	-3.56350000
H	-3.74700000	-1.32910000	1.37740000

Photoisomer





Energy (a.u.): -1161.02721

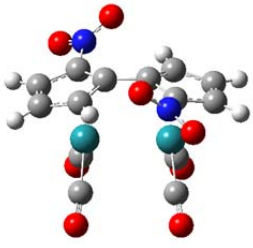
Molecular coordinates

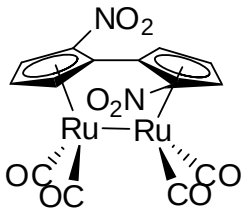
C	1.70110000	2.37900000	0.77240000
C	-0.15420000	1.22150000	-0.16080000
C	0.49180000	1.61440000	1.07330000
C	0.74690000	1.59680000	-1.21920000
C	1.90300000	2.27380000	-0.64930000

C	2.78150000	-0.77640000	1.44740000
C	2.89640000	-0.81010000	-1.26320000
C	-1.61740000	-2.45080000	-0.88380000
C	0.32630000	-1.40230000	-0.03350000
C	-0.35340000	-1.82890000	-1.23700000
C	-0.56840000	-1.72150000	1.05820000
C	-1.74990000	-2.38410000	0.53510000
C	-2.49970000	0.60230000	-1.75890000
C	-2.79750000	0.70430000	0.92540000
H	0.06690000	1.47140000	2.06580000
H	0.57940000	1.44560000	-2.28580000
H	2.71380000	2.71990000	-1.22410000
H	-2.33110000	-2.89690000	-1.57770000
H	0.03560000	-1.73330000	-2.25120000
H	-0.37030000	-1.53340000	2.11390000
O	3.34090000	-1.30400000	2.33630000
O	3.55870000	-1.31060000	-2.09300000
O	-3.00400000	1.08440000	-2.70120000
O	-3.49170000	1.25040000	1.69720000
Ru	1.83290000	0.04340000	0.03280000
Ru	-1.66800000	-0.20940000	-0.27460000
N	2.47590000	3.07750000	1.67200000
C	3.81490000	3.47770000	1.23760000
H	3.75580000	4.02930000	0.28600000
H	4.25050000	4.15000000	1.99280000
H	4.48560000	2.60220000	1.10210000
C	2.35420000	2.73500000	3.09000000
H	2.77900000	1.73300000	3.31340000
H	2.88890000	3.48990000	3.68700000
H	1.29720000	2.74920000	3.39640000
H	-2.58430000	-2.76930000	1.12290000

Entry 11

Parent





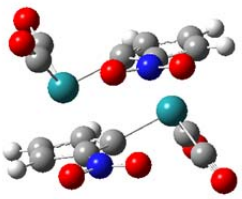
Energy (a.u.): -1436.185637

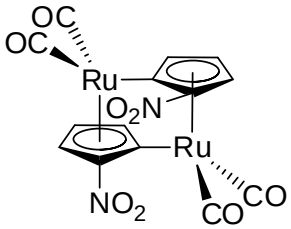
Molecular coordinates

C	2.89350000	-1.47260000	-0.80290000
C	0.71730000	-2.04520000	-0.03370000
C	1.56150000	-1.83620000	-1.21760000
C	1.59890000	-1.81040000	1.09250000
C	2.91170000	-1.47980000	0.62040000

H	3.72600000	-1.31130000	-1.48580000
H	1.30300000	-1.89120000	2.13550000
H	3.77860000	-1.27670000	1.24900000
C	-2.92860000	-1.41410000	-0.62390000
C	-0.74710000	-2.02940000	0.02830000
C	-1.62300000	-1.77050000	-1.09710000
C	-1.58710000	-1.80750000	1.21280000
C	-2.91090000	-1.41380000	0.79930000
H	-3.79070000	-1.18970000	-1.25200000
H	-1.32820000	-1.85260000	-2.14030000
H	-3.74000000	-1.23770000	1.48280000
Ru	1.43050000	0.18340000	-0.08530000
Ru	-1.41250000	0.21380000	0.08970000
C	1.60630000	1.55160000	-1.36480000
O	1.78130000	2.37920000	-2.17220000
C	1.63290000	1.46480000	1.26270000
O	1.82620000	2.23610000	2.12140000
C	-1.58720000	1.50540000	-1.25250000
O	-1.76400000	2.28450000	-2.10760000
C	-1.55910000	1.57980000	1.37530000
O	-1.71670000	2.40730000	2.18620000
N	1.30410000	-2.14290000	-2.62030000
O	0.35030000	-2.90290000	-2.89260000
O	2.09550000	-1.67070000	-3.45710000
N	-1.33680000	-2.12530000	2.61430000
O	-2.11900000	-1.64080000	3.45280000
O	-0.39870000	-2.90550000	2.88390000

Photoisomer





Energy (a.u.): -1436.158809

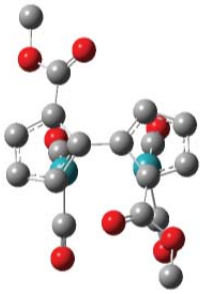
Molecular coordinates

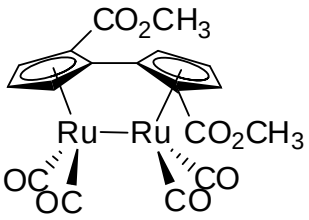
C	1.73060000	2.36390000	0.81580000
C	-0.30390000	1.33000000	0.10190000
C	0.52260000	1.68280000	1.24590000
C	0.45430000	1.78940000	-1.03710000
C	1.67890000	2.43710000	-0.60060000
C	2.96480000	-0.69750000	1.16050000
C	2.68150000	-0.51570000	-1.48330000
C	-1.65070000	-2.33790000	-0.92660000
C	0.31770000	-1.32770000	-0.05740000
C	-0.41930000	-1.64230000	-1.25780000

C	-0.52880000	-1.81800000	1.01920000
C	-1.72790000	-2.43990000	0.48690000
C	-2.63950000	0.70210000	-1.45720000
C	-2.97240000	0.55760000	1.18310000
H	2.48750000	2.77000000	1.48510000
H	0.13920000	1.68930000	-2.07640000
H	2.42280000	2.90580000	-1.24620000
H	-2.38230000	-2.72270000	-1.63830000
H	-0.08570000	-1.41520000	-2.27100000
H	-2.49630000	-2.92460000	1.08740000
O	3.75830000	-1.19910000	1.84920000
O	3.24570000	-0.91400000	-2.42830000
O	-3.18630000	1.21410000	-2.35660000
O	-3.77880000	0.97230000	1.91340000
Ru	1.75470000	0.18320000	-0.01130000
Ru	-1.73960000	-0.17380000	-0.06530000
N	0.19320000	1.57360000	2.66690000
O	1.03360000	2.02270000	3.46940000
O	-0.90280000	1.07810000	2.98830000
N	-0.22410000	-1.88600000	2.44810000
O	0.86630000	-1.43630000	2.84670000
O	-1.07820000	-2.42870000	3.17470000

Entry 12

Parent





(H atoms are omitted)

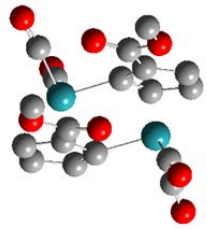
Energy (a.u.): -1482.837452

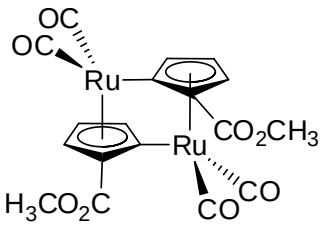
Molecular coordinates

C	2.84850000	-1.52410000	-0.87760000
C	0.73060000	-2.06880000	0.00920000
C	1.49920000	-1.90730000	-1.24280000
C	1.65850000	-1.79910000	1.08610000
C	2.94260000	-1.47690000	0.54130000
H	3.65390000	-1.36290000	-1.59200000
H	1.39700000	-1.85740000	2.14090000
H	3.83770000	-1.24250000	1.11760000
C	-2.95070000	-1.60420000	-0.43450000
C	-0.72830000	-2.07190000	0.17190000
C	-1.66080000	-1.97790000	-0.93040000

C	-1.50040000	-1.74700000	1.38960000
C	-2.85630000	-1.44500000	0.97620000
H	-3.84980000	-1.47160000	-1.03650000
H	-1.39850000	-2.18340000	-1.96640000
H	-3.66510000	-1.19760000	1.66170000
Ru	1.40710000	0.14490000	-0.16490000
Ru	-1.44500000	0.13010000	0.02750000
C	1.53420000	1.45920000	-1.49830000
O	1.67990000	2.25540000	-2.34650000
C	1.61310000	1.47010000	1.13920000
O	1.80980000	2.26730000	1.97620000
C	-1.67340000	1.24960000	-1.45360000
O	-1.88330000	1.91440000	-2.39640000
C	-1.59730000	1.62040000	1.15780000
O	-1.75810000	2.52760000	1.88270000
C	-1.14400000	-1.85310000	2.82880000
O	-0.15150000	-2.40280000	3.30730000
O	-2.11990000	-1.29880000	3.60670000
C	-1.88880000	-1.38970000	5.03580000
H	-1.80520000	-2.44340000	5.34580000
H	-0.96490000	-0.85560000	5.30830000
H	-2.76400000	-0.91250000	5.49640000
C	1.14700000	-2.22200000	-2.65210000
O	0.16430000	-2.84980000	-3.04760000
O	2.11480000	-1.76660000	-3.50120000
C	1.88550000	-2.05790000	-4.90360000
H	0.95380000	-1.58030000	-5.24550000
H	2.75360000	-1.63600000	-5.42730000
H	1.81780000	-3.14540000	-5.06480000

Photoisomer





(H atoms are omitted)

Energy (a.u.): -1482.80627

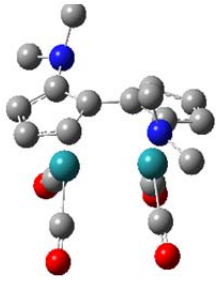
Molecular coordinates

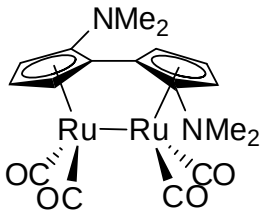
C	-1.40950000	-2.61540000	0.58330000
C	0.46220000	-1.28880000	-0.02060000
C	-0.29630000	-1.82640000	1.10240000
C	-0.22580000	-1.73980000	-1.20590000
C	-1.35570000	-2.57090000	-0.83480000
C	-3.00570000	0.22610000	1.17970000
C	-2.73570000	0.29150000	-1.47020000

C	1.34730000	2.57490000	-0.75840000
C	-0.47010000	1.26890000	0.01810000
C	0.21710000	1.75540000	-1.15360000
C	0.28900000	1.77250000	1.15620000
C	1.40190000	2.57670000	0.66040000
C	2.72710000	-0.26710000	-1.48030000
C	2.99830000	-0.28080000	1.17040000
H	-2.12300000	-3.16450000	1.19640000
H	0.07390000	-1.51400000	-2.22980000
H	-2.03710000	-3.07440000	-1.52200000
H	2.02830000	3.09890000	-1.43060000
H	-0.08320000	1.56040000	-2.18360000
H	2.11580000	3.10710000	1.28930000
O	-3.85720000	0.56820000	1.90060000
O	-3.35560000	0.69350000	-2.38060000
O	3.34640000	-0.64160000	-2.40270000
O	3.84990000	-0.64420000	1.88080000
Ru	-1.71670000	-0.40450000	-0.06040000
Ru	1.70880000	0.38630000	-0.04970000
C	0.03960000	-1.73490000	2.54610000
O	1.03890000	-1.20380000	3.02460000
O	-0.90400000	-2.37230000	3.30100000
C	-0.68790000	-2.30950000	4.73180000
H	-1.49100000	-2.91670000	5.17090000
H	0.30150000	-2.71830000	4.99170000
H	-0.75930000	-1.26510000	5.07470000
C	-0.04600000	1.63790000	2.59670000
O	-1.04760000	1.09720000	3.05930000
O	0.90110000	2.24710000	3.37020000
C	0.68610000	2.14020000	4.79840000
H	-0.30090000	2.54580000	5.07240000
H	0.75220000	1.08500000	5.10780000
H	1.49290000	2.72890000	5.25570000

Entry 13

Parent





(H atoms are omitted)

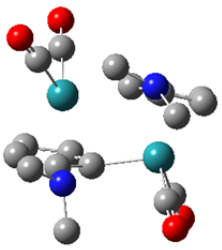
Energy (a.u.): -1294.941926

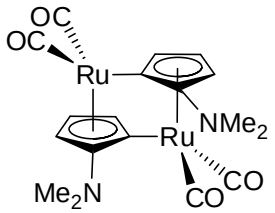
Molecular coordinates

C	2.86720000	-1.35950000	-0.81440000

C	0.71460000	-1.84760000	-0.02180000
C	1.54530000	-1.77620000	-1.22250000
C	1.57590000	-1.54080000	1.11340000
C	2.88320000	-1.23460000	0.61500000
H	3.72380000	-1.21980000	-1.47270000
H	1.24700000	-1.51890000	2.15100000
H	3.75420000	-0.97540000	1.21730000
C	-2.89560000	-1.16960000	-0.61640000
C	-0.74060000	-1.83210000	0.01700000
C	-1.59530000	-1.50190000	-1.11660000
C	-1.56930000	-1.74800000	1.21830000
C	-2.88200000	-1.30100000	0.81240000
H	-3.76090000	-0.88900000	-1.21730000
H	-1.26670000	-1.48300000	-2.15430000
H	-3.73520000	-1.14570000	1.47150000
Ru	1.43400000	0.37060000	-0.14490000
Ru	-1.41190000	0.40070000	0.14990000
C	1.45530000	1.58710000	-1.57220000
O	1.54540000	2.31610000	-2.49000000
C	1.76640000	1.77090000	1.04890000
O	2.04880000	2.61610000	1.81450000
C	-1.71370000	1.81300000	-1.03770000
O	-1.97740000	2.66760000	-1.79960000
C	-1.40670000	1.61130000	1.58240000
O	-1.48070000	2.33820000	2.50330000
N	1.11870000	-2.10420000	-2.52330000
N	-1.14980000	-2.09150000	2.51750000
C	-2.02600000	-1.64660000	3.60330000
H	-2.22430000	-0.56770000	3.50400000
H	-2.99690000	-2.19100000	3.63030000
H	-1.51390000	-1.81660000	4.56470000
C	-0.71050000	-3.48830000	2.67810000
H	-0.00760000	-3.76240000	1.87730000
H	-0.18990000	-3.59330000	3.64520000
H	-1.56470000	-4.20080000	2.65960000
C	0.64830000	-3.49010000	-2.69100000
H	-0.06030000	-3.75250000	-1.89130000
H	0.12510000	-3.57840000	-3.65840000
H	1.48630000	-4.22160000	-2.67660000
C	2.00430000	-1.67330000	-3.60710000
H	2.22650000	-0.59960000	-3.50230000
H	2.96290000	-2.23900000	-3.63720000
H	1.48840000	-1.82700000	-4.56920000

Photoisomer





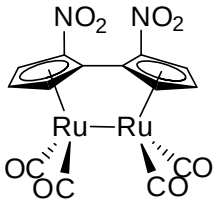
(H atoms are omitted)
Energy (a.u.): -1294.899781
Molecular coordinates

C	1.39910000	2.86780000	0.39890000
C	-0.49300000	1.48310000	0.05440000
C	0.22990000	2.27020000	1.05910000
C	0.18960000	1.73950000	-1.20700000
C	1.33070000	2.59080000	-0.99650000
C	2.80130000	0.20490000	1.53170000
C	2.93020000	-0.15890000	-1.15970000
C	-1.33530000	-2.36130000	-0.82030000
C	0.46790000	-1.10670000	0.07450000
C	-0.19110000	-1.53390000	-1.13970000
C	-0.28450000	-1.71810000	1.16980000
C	-1.40060000	-2.46660000	0.60150000
C	-2.75250000	0.43050000	-1.44260000
C	-3.11630000	0.19840000	1.16930000
H	2.14810000	3.49900000	0.87380000
H	-0.13990000	1.37090000	-2.17760000
H	2.01530000	2.96490000	-1.75870000
H	-2.00880000	-2.84130000	-1.53190000
H	0.13170000	-1.27760000	-2.14890000
H	-2.13740000	-3.04220000	1.16240000
O	3.56020000	0.05930000	2.41920000
O	3.68930000	-0.61050000	-1.93320000
O	-3.37520000	0.82820000	-2.35310000
O	-4.03420000	0.39920000	1.87760000
Ru	1.69750000	0.59930000	0.05100000
Ru	-1.73460000	-0.26060000	-0.01680000
N	-0.06740000	2.53950000	2.38080000
N	0.08200000	-1.69790000	2.53440000
C	0.99960000	3.09490000	3.21620000
H	1.84620000	2.38770000	3.34620000
H	1.38510000	4.03390000	2.78750000
H	0.58420000	3.33120000	4.20710000
C	-1.06200000	1.73420000	3.08820000
H	-2.02170000	1.78150000	2.56110000
H	-0.74200000	0.67710000	3.18490000
H	-1.20710000	2.16280000	4.09210000
C	-0.97530000	-2.08490000	3.47110000

H	-1.88130000	-1.48360000	3.29130000
H	-1.24600000	-3.16400000	3.40470000
H	-0.62610000	-1.89170000	4.49950000
C	1.33300000	-2.43100000	2.81220000
H	1.72420000	-2.13040000	3.79850000
H	1.16950000	-3.53240000	2.81300000
H	2.08510000	-2.19240000	2.04960000

Entry 14

Parent



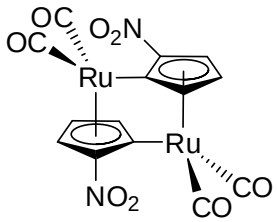
Energy (a.u.): -1436.174148

Molecular coordinates

C	2.85960000	-1.71900000	-0.62780000
C	0.68070000	-2.02600000	0.22470000
C	1.50570000	-2.04950000	-0.96320000
C	1.60000000	-1.64580000	1.31030000
C	2.92420000	-1.47720000	0.77250000
H	3.69790000	-1.67930000	-1.32300000
H	3.80290000	-1.23060000	1.36620000
C	-2.80140000	-1.28620000	-0.83820000
C	-0.77500000	-2.00630000	0.12150000
C	-1.43980000	-1.61960000	-1.12200000
C	-1.80020000	-1.92270000	1.13640000
C	-3.02780000	-1.44700000	0.56310000
H	-3.54360000	-0.96250000	-1.56820000
H	-0.96500000	-1.55850000	-2.10000000
H	-3.96280000	-1.33460000	1.10970000
Ru	1.46370000	0.12850000	-0.13260000
Ru	-1.38200000	0.23500000	0.22610000
C	1.53520000	1.16870000	-1.69000000
O	1.62890000	1.76620000	-2.69340000
C	1.76000000	1.68090000	0.88170000
O	1.99460000	2.63470000	1.51660000
C	-1.58560000	1.70140000	-0.90240000
O	-1.76990000	2.59850000	-1.63380000
C	-1.39970000	1.41550000	1.69770000
O	-1.46680000	2.12780000	2.62050000
N	-1.77180000	-2.52690000	2.46790000
O	-2.63970000	-2.16260000	3.27700000
O	-0.93050000	-3.42570000	2.65590000

H	1.15170000	-2.31620000	-1.95840000
N	1.37560000	-1.43290000	2.74310000
O	2.35180000	-1.65190000	3.48400000
O	0.27050000	-1.01180000	3.12570000

Photoisomer



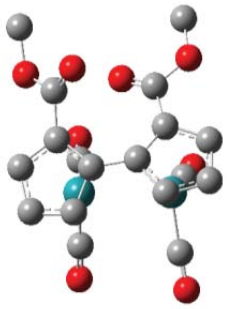
Energy (a.u.): -1436.160446

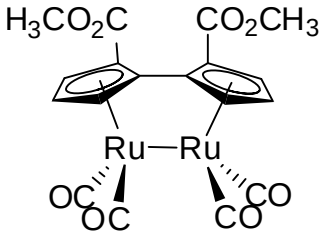
Molecular coordinates

C	1.73550000	2.30590000	0.76910000
C	-0.24740000	1.30280000	-0.06850000
C	0.50290000	1.63120000	1.12250000
C	0.60040000	1.75740000	-1.15930000
C	1.80670000	2.38730000	-0.64610000
C	2.91240000	-0.72210000	1.19010000
C	2.81640000	-0.66370000	-1.45690000
C	-1.65550000	-2.35090000	-0.91930000
C	0.32730000	-1.34770000	-0.08170000
C	-0.42300000	-1.67620000	-1.27260000
C	-0.52050000	-1.80240000	1.00910000
C	-1.72670000	-2.43230000	0.49590000
C	-2.83240000	0.67720000	-1.34030000
C	-2.73650000	0.61870000	1.30670000
H	2.47870000	2.68770000	1.47050000
H	0.18510000	1.41150000	2.14190000
H	2.57380000	2.85900000	-1.25780000
H	-2.39880000	-2.73270000	-1.62070000
H	-0.10520000	-1.45640000	-2.29210000
H	-2.49390000	-2.90390000	1.10760000
O	3.65750000	-1.20400000	1.94650000
O	3.43310000	-1.12880000	-2.33360000
O	-3.57760000	1.15910000	-2.09660000
O	-3.35310000	1.08380000	2.18340000
Ru	1.79940000	0.12580000	-0.07840000
Ru	-1.71950000	-0.17080000	-0.07170000
N	0.33400000	1.73340000	-2.59840000
O	1.15760000	2.32370000	-3.32580000
O	-0.68060000	1.14330000	-3.01840000
N	-0.25400000	-1.77840000	2.44820000
O	-1.07760000	-2.36870000	3.17570000
O	0.76060000	-1.18830000	2.86830000

Entry 15

Parent



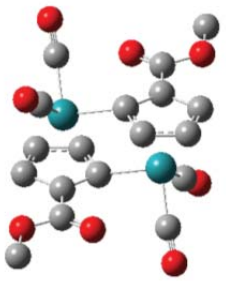


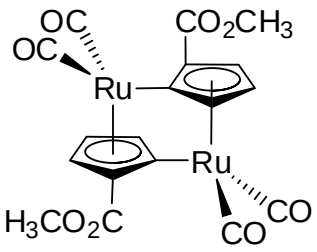
(H atoms are omitted)
Energy (a.u.): -1482.825767
Molecular coordinates

C	2.75570000	-1.97130000	-0.91430000
C	0.65030000	-2.09540000	0.13160000
C	1.35770000	-2.20330000	-1.12440000
C	1.67070000	-1.76630000	1.14520000
C	2.95000000	-1.70650000	0.46980000
H	3.53220000	-2.00480000	-1.67840000
H	0.89840000	-2.45350000	-2.08000000
H	3.89690000	-1.49910000	0.96530000
C	-2.84940000	-1.13640000	-0.64860000
C	-0.80660000	-1.97170000	0.15530000
C	-1.54610000	-1.56900000	-1.04150000
C	-1.71250000	-1.80320000	1.27170000
C	-2.94960000	-1.25130000	0.77310000
H	-3.63030000	-0.77250000	-1.31700000
H	-1.15820000	-1.56350000	-2.05880000
H	-3.82660000	-1.04520000	1.38510000
Ru	1.55110000	-0.01660000	-0.34150000
Ru	-1.24480000	0.29420000	0.25480000
C	1.54200000	0.98310000	-1.92600000
O	1.58170000	1.55290000	-2.95090000
C	2.05350000	1.52030000	0.60500000
O	2.41820000	2.46000000	1.20400000
C	-1.44430000	1.76970000	-0.86650000
O	-1.63320000	2.67800000	-1.58560000
C	-1.04620000	1.46120000	1.71820000
O	-0.97870000	2.16880000	2.64820000
C	-1.57310000	-2.40640000	2.62740000
O	-0.93690000	-3.43120000	2.85450000
O	-2.35720000	-1.76920000	3.53530000
C	-2.33110000	-2.33970000	4.86760000
H	-2.66480000	-3.38960000	4.84480000
H	-1.30990000	-2.28730000	5.27580000
H	-3.01960000	-1.72110000	5.45870000
C	1.54770000	-1.44340000	2.59360000

O	0.55070000	-1.04120000	3.18530000
O	2.75620000	-1.61270000	3.21050000
C	2.77930000	-1.24620000	4.61390000
H	3.81570000	-1.41510000	4.93590000
H	2.49490000	-0.18960000	4.74000000
H	2.08480000	-1.88270000	5.18450000

Photoisomer





(H atoms are omitted)

Energy (a.u.): -1482.806996

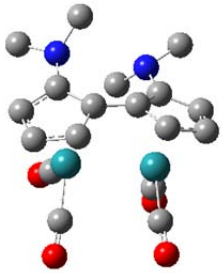
Molecular coordinates

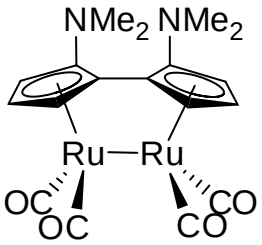
C	-1.74770000	-2.27400000	0.97510000
C	0.27270000	-1.30080000	0.19800000
C	-0.53630000	-1.56510000	1.38250000
C	-0.48720000	-1.81600000	-0.91630000
C	-1.70890000	-2.42610000	-0.43630000
C	-2.74720000	0.86360000	1.29580000
C	-2.86700000	0.51340000	-1.33560000
C	1.74770000	2.27400000	-0.97510000
C	-0.27270000	1.30080000	-0.19800000
C	0.53630000	1.56510000	-1.38250000
C	0.48720000	1.81600000	0.91630000
C	1.70890000	2.42610000	0.43630000
C	2.74720000	-0.86360000	-1.29580000
C	2.86700000	-0.51340000	1.33560000
H	-2.51770000	-2.63660000	1.65470000
H	-0.19390000	-1.74960000	-1.96370000
H	-2.46550000	-2.91450000	-1.05210000
H	2.51770000	2.63660000	-1.65470000
H	0.19390000	1.74960000	1.96370000
H	2.46550000	2.91450000	1.05210000
O	-3.34480000	1.46410000	2.10560000
O	-3.60980000	0.89260000	-2.15350000
O	3.34480000	-1.46410000	-2.10560000
O	3.60980000	-0.89260000	2.15350000
Ru	-1.76100000	-0.13960000	0.04810000
Ru	1.76100000	0.13960000	-0.04810000
C	0.20990000	1.25000000	-2.79810000
O	-0.71880000	0.55220000	-3.20000000

O	1.09880000	1.85890000	-3.64310000
C	0.87550000	1.59950000	-5.05200000
H	-0.13020000	1.93610000	-5.34980000
H	1.65200000	2.17340000	-5.57550000
H	0.97520000	0.52310000	-5.26520000
C	-0.20990000	-1.25000000	2.79810000
O	0.71880000	-0.55220000	3.20000000
O	-1.09880000	-1.85890000	3.64310000
C	-0.87550000	-1.59950000	5.05200000
H	-1.65200000	-2.17340000	5.57550000
H	0.13010000	-1.93610000	5.34980000
H	-0.97520000	-0.52310000	5.26520000

Entry 16

Parent





(H atoms are omitted)

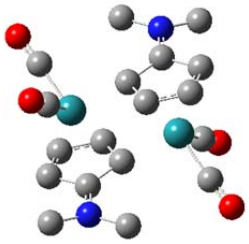
Energy (a.u.): -1294.928787

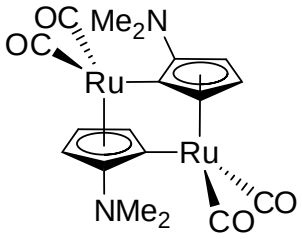
Molecular coordinates

C	2.69810000	-1.95000000	-0.71640000
C	0.55620000	-2.03930000	0.26620000
C	1.30180000	-2.11990000	-0.97790000
C	1.55400000	-1.79570000	1.33120000
C	2.85000000	-1.73430000	0.68590000
H	3.50010000	-1.99740000	-1.45290000
H	3.79630000	-1.57650000	1.20240000
C	-2.86680000	-0.97630000	-0.68970000
C	-0.89460000	-1.85830000	0.23070000
C	-1.57530000	-1.48920000	-1.01570000
C	-1.86920000	-1.68270000	1.30450000
C	-3.03000000	-1.03630000	0.73310000
H	-3.61630000	-0.62190000	-1.39760000
H	-1.16440000	-1.57840000	-2.01900000
H	-3.93110000	-0.75460000	1.27610000
Ru	1.57930000	0.01780000	-0.19030000
Ru	-1.26390000	0.43800000	0.12510000
C	1.70480000	1.00890000	-1.77440000
O	1.85070000	1.56720000	-2.79770000
C	2.09520000	1.53330000	0.78670000
O	2.48440000	2.46830000	1.38350000
C	-1.36330000	1.80290000	-1.14540000

O	-1.49500000	2.63710000	-1.96190000
C	-1.15340000	1.73770000	1.48030000
O	-1.16550000	2.54250000	2.33770000
N	-1.73110000	-2.09850000	2.62060000
H	0.86610000	-2.31720000	-1.95600000
N	1.38250000	-1.78900000	2.73750000
C	-2.75350000	-1.65560000	3.56570000
H	-2.89350000	-0.56510000	3.48670000
H	-3.73450000	-2.15620000	3.40750000
H	-2.41420000	-1.88510000	4.58900000
C	-1.25480000	-3.46880000	2.85190000
H	-0.46330000	-3.72340000	2.13540000
H	-0.82790000	-3.54020000	3.86550000
H	-2.08290000	-4.20530000	2.75700000
C	0.81890000	-0.57390000	3.34460000
H	-0.04990000	-0.23080000	2.77030000
H	0.49560000	-0.79970000	4.37550000
H	1.56650000	0.24880000	3.37610000
C	2.55120000	-2.25880000	3.49170000
H	2.92910000	-3.19950000	3.06000000
H	3.38290000	-1.51860000	3.52730000
H	2.23850000	-2.45470000	4.53190000

Photoisomer





(H atoms are omitted)

Energy (a.u.): -1294.900109

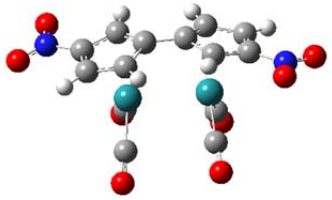
Molecular coordinates

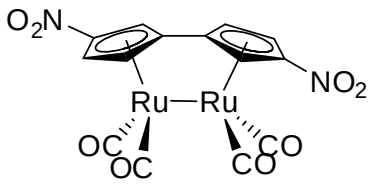
C	1.52270000	2.27390000	0.45300000
C	-0.31570000	1.05460000	-0.42780000
C	0.33130000	1.54570000	0.78710000
C	0.47760000	1.58910000	-1.53500000
C	1.66630000	2.23610000	-0.96840000
C	3.21850000	-0.24010000	1.10850000
C	2.77210000	-0.85310000	-1.44420000
C	-1.32280000	-2.77730000	-0.67880000
C	0.51570000	-1.55800000	0.20210000
C	-0.13130000	-2.04920000	-1.01290000
C	-0.27760000	-2.09260000	1.30920000
C	-1.46630000	-2.73960000	0.74260000
C	-3.01850000	-0.26340000	-1.33430000
C	-2.57210000	0.34970000	1.21840000

H	2.20060000	2.77240000	1.14760000
H	-0.05710000	1.40990000	1.79560000
H	2.46000000	2.72760000	-1.52890000
H	-2.00060000	-3.27590000	-1.37330000
H	0.25710000	-1.91330000	-2.02140000
H	-2.26010000	-3.23100000	1.30310000
O	4.12510000	-0.37700000	1.84620000
O	3.40220000	-1.41980000	-2.25830000
O	-3.92510000	-0.12660000	-2.07200000
O	-3.20220000	0.91630000	2.03250000
Ru	1.82630000	0.09770000	-0.10730000
Ru	-1.62630000	-0.60120000	-0.11850000
N	0.22640000	1.58600000	-2.89040000
N	-0.02640000	-2.08940000	2.66460000
C	1.35580000	1.71470000	-3.81110000
H	1.94480000	2.62100000	-3.59520000
H	2.03400000	0.83690000	-3.76450000
H	0.96950000	1.80710000	-4.83720000
C	-0.99200000	0.99740000	-3.43600000
H	-0.96220000	-0.10970000	-3.48470000
H	-1.85030000	1.29730000	-2.82270000
H	-1.14120000	1.39030000	-4.45490000
C	1.19200000	-1.50080000	3.21020000
H	2.05030000	-1.80080000	2.59690000
H	1.16220000	-0.39370000	3.25880000
H	1.34120000	-1.89370000	4.22920000
C	-1.15590000	-2.21810000	3.58530000
H	-1.83400000	-1.34020000	3.53870000
H	-1.74480000	-3.12440000	3.36940000
H	-0.76950000	-2.31050000	4.61150000

Entry 17

Parent





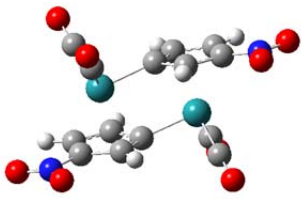
Energy (a.u.): -1436.194557

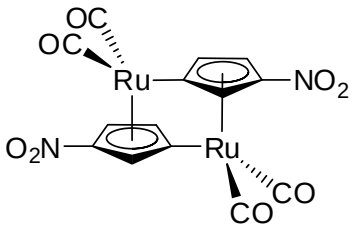
Molecular coordinates

C	2.89100000	-1.53280000	-0.64840000
C	0.72780000	-2.00180000	0.01380000
C	1.58300000	-1.86830000	-1.13790000
C	1.53110000	-1.73010000	1.19760000
C	2.86700000	-1.44330000	0.78220000
H	1.32580000	-2.01470000	-2.18530000
H	1.17750000	-1.74570000	2.22800000

H	3.72660000	-1.21830000	1.41220000
C	-2.86810000	-1.44120000	-0.78210000
C	-0.72930000	-2.00120000	-0.01370000
C	-1.53240000	-1.72890000	-1.19750000
C	-1.58440000	-1.86720000	1.13800000
C	-2.89210000	-1.53070000	0.64860000
H	-3.72750000	-1.21560000	-1.41200000
H	-1.17880000	-1.74470000	-2.22790000
H	-1.32730000	-2.01380000	2.18540000
Ru	1.43000000	0.20140000	-0.09270000
Ru	-1.42990000	0.20240000	0.09290000
C	1.42060000	1.38750000	-1.55060000
O	1.46990000	2.09180000	-2.48200000
C	1.72920000	1.65390000	1.05960000
O	1.97990000	2.53200000	1.79100000
C	-1.72810000	1.65520000	-1.05940000
O	-1.97810000	2.53350000	-1.79080000
C	-1.41960000	1.38850000	1.55080000
O	-1.46840000	2.09280000	2.48230000
N	4.08750000	-1.41940000	-1.47550000
O	5.16280000	-1.18130000	-0.89390000
O	3.94310000	-1.58520000	-2.70240000
N	-4.08860000	-1.41650000	1.47560000
O	-5.16370000	-1.17750000	0.89400000
O	-3.94430000	-1.58240000	2.70250000

Photoisomer





Energy (a.u.): -1436.164036

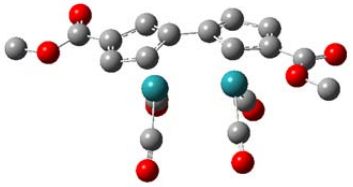
Molecular coordinates

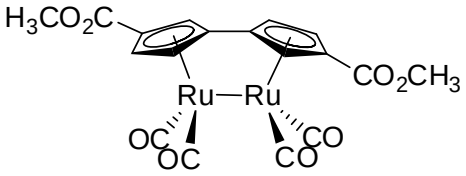
C	1.70780000	2.34570000	0.73590000
C	-0.25720000	1.31450000	0.01070000
C	0.49340000	1.68770000	1.18170000
C	0.54500000	1.69480000	-1.13770000
C	1.74990000	2.35090000	-0.68940000
C	2.64070000	-0.80300000	1.44030000
C	2.87390000	-0.70640000	-1.23730000
C	-1.69640000	-2.27450000	-0.97950000
C	0.27370000	-1.30960000	-0.09590000
C	-0.47340000	-1.58300000	-1.31010000
C	-0.52980000	-1.78570000	1.00030000
C	-1.72070000	-2.39820000	0.44070000

C	-2.80030000	0.82250000	-1.30030000
C	-2.69190000	0.67550000	1.38330000
H	0.20460000	1.56560000	2.22460000
H	0.26530000	1.55440000	-2.18210000
H	2.53620000	2.79540000	-1.29910000
H	-2.45260000	-2.66050000	-1.66280000
H	-0.14560000	-1.34950000	-2.32330000
H	-0.29030000	-1.75920000	2.06220000
O	3.17330000	-1.35970000	2.31670000
O	3.54710000	-1.20140000	-2.05440000
O	-3.43570000	1.39070000	-2.09960000
O	-3.26560000	1.15140000	2.28110000
Ru	1.76530000	0.12560000	0.04550000
Ru	-1.75080000	-0.12460000	-0.04780000
N	2.68750000	2.99010000	1.60550000
O	2.47660000	2.93360000	2.83240000
O	3.64870000	3.56460000	1.05850000
N	-2.73820000	-3.11680000	1.20210000
O	-2.58400000	-3.17300000	2.43740000
O	-3.67220000	-3.63670000	0.56130000

Entry 18

Parent





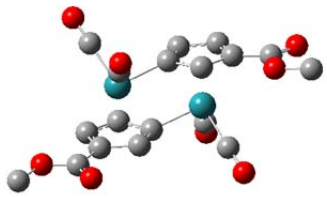
Energy (a.u.): -1482.844285

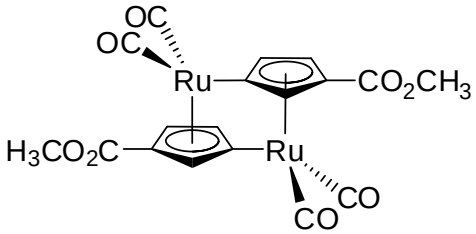
Molecular coordinates

C	2.89490000	-1.50270000	-0.81050000
C	0.78940000	-1.93980000	0.10180000
C	1.53770000	-1.87490000	-1.12980000
C	1.69600000	-1.58050000	1.17950000
C	2.98120000	-1.31690000	0.61310000
H	1.44100000	-1.52330000	2.23710000
H	3.88950000	-1.03750000	1.14680000
C	-2.87170000	-1.48800000	-0.39340000
C	-0.66250000	-1.95330000	0.20890000
C	-1.57750000	-1.80780000	-0.91120000
C	-1.41530000	-1.70640000	1.41310000
C	-2.78050000	-1.43250000	1.04260000
H	-3.78040000	-1.32820000	-0.97260000
H	-1.32280000	-1.92240000	-1.96450000
Ru	1.45560000	0.25170000	-0.22410000
Ru	-1.39780000	0.24110000	0.15640000
C	1.35830000	1.34690000	-1.74350000

O	1.35850000	1.99350000	-2.72070000
C	1.80890000	1.76340000	0.83020000
O	2.10000000	2.68010000	1.49980000
C	-1.79210000	1.53570000	-1.14120000
O	-2.10930000	2.31200000	-1.96070000
C	-1.33030000	1.58810000	1.46240000
O	-1.34680000	2.40050000	2.30560000
H	-1.04910000	-1.73660000	2.43850000
C	-3.87130000	-1.20470000	2.02540000
O	-3.71960000	-1.23950000	3.24350000
O	-5.06390000	-0.97510000	1.40640000
C	-6.17660000	-0.72550000	2.30430000
H	-7.04240000	-0.56100000	1.64920000
H	-6.33990000	-1.59380000	2.96210000
H	-5.97580000	0.16490000	2.92080000
H	1.16540000	-2.08900000	-2.13030000
C	4.05610000	-1.38660000	-1.73070000
O	5.20300000	-1.13640000	-1.37210000
O	3.68890000	-1.61610000	-3.02430000
C	4.76780000	-1.51230000	-3.98990000
H	4.30330000	-1.72060000	-4.96280000
H	5.20010000	-0.49950000	-3.97010000
H	5.55540000	-2.24850000	-3.76380000

Photoisomer





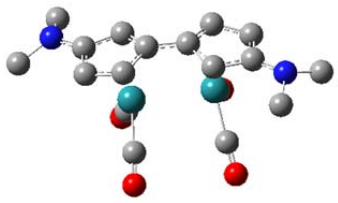
Energy (a.u.): -1482.812748

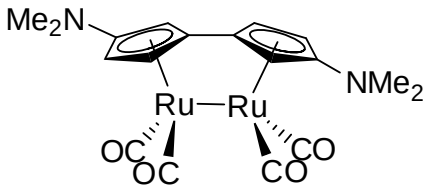
Molecular coordinates

C	-1.50880000	-2.55890000	0.58450000
C	0.37980000	-1.29300000	-0.04720000
C	-0.36430000	-1.80270000	1.07520000
C	-0.35460000	-1.68600000	-1.23360000
C	-1.49980000	-2.47730000	-0.84590000
C	-2.76760000	0.42380000	1.39790000
C	-2.88970000	0.46920000	-1.29390000
C	1.48010000	2.47500000	-0.74280000
C	-0.40400000	1.25950000	-0.00800000
C	0.34280000	1.69530000	-1.17130000
C	0.32710000	1.72840000	1.14140000
C	1.47580000	2.50530000	0.68780000
C	2.87950000	-0.45570000	-1.27690000
C	2.72900000	-0.49850000	1.41440000

H	-0.06840000	-1.45960000	-2.26120000
H	-2.22240000	-2.94750000	-1.51310000
H	2.21290000	2.97620000	-1.37620000
H	0.06840000	1.50480000	-2.20910000
O	-3.38660000	0.86860000	2.28490000
O	-3.58030000	0.94050000	-2.11380000
O	3.57870000	-0.89810000	-2.10510000
O	3.34080000	-0.96400000	2.29620000
Ru	-1.75510000	-0.32020000	-0.01030000
Ru	1.72880000	0.28700000	0.02120000
H	-0.11050000	-1.70020000	2.13010000
C	-2.44040000	-3.31670000	1.45900000
O	-2.34910000	-3.37320000	2.68230000
O	-3.39660000	-3.96560000	0.73250000
C	-4.34550000	-4.72790000	1.52250000
H	-5.03150000	-5.17730000	0.79220000
H	-3.82370000	-5.50590000	2.10220000
H	-4.88800000	-4.06360000	2.21380000
H	0.05440000	1.58050000	2.18570000
C	2.44950000	3.27590000	1.50470000
O	3.35190000	3.96870000	1.04250000
O	2.19620000	3.13770000	2.83790000
C	3.09910000	3.86760000	3.70840000
H	2.75590000	3.64680000	4.72780000
H	4.13470000	3.52340000	3.55930000
H	3.04180000	4.94770000	3.49940000

Entry 19
Parent



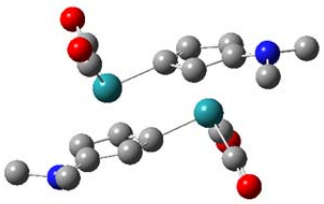


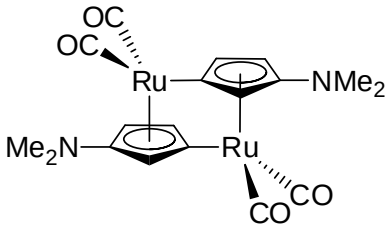
(H atoms are omitted)
Energy (a.u.): -1294.962163
Molecular coordinates

C	2.91530000	-1.63100000	-0.78510000
C	0.72540000	-2.03420000	-0.01220000
C	1.53710000	-1.79750000	-1.19420000
C	1.59330000	-1.88450000	1.13050000
C	2.92080000	-1.59060000	0.66070000
H	1.17300000	-1.83190000	-2.21900000
H	1.30420000	-1.98670000	2.17600000
H	3.79460000	-1.46340000	1.29750000
C	-2.92180000	-1.58960000	-0.66000000

C	-0.72660000	-2.03380000	0.01330000
C	-1.59440000	-1.88450000	-1.12960000
C	-1.53820000	-1.79600000	1.19510000
C	-2.91630000	-1.62910000	0.78590000
H	-3.79550000	-1.46250000	-1.29680000
H	-1.30530000	-1.98760000	-2.17500000
H	-1.17410000	-1.82980000	2.22000000
Ru	1.44310000	0.14180000	0.07970000
Ru	-1.44320000	0.14240000	-0.08010000
C	1.71280000	1.56490000	-1.11360000
O	1.93140000	2.44000000	-1.86970000
C	1.51550000	1.32570000	1.52500000
O	1.62460000	2.02760000	2.46190000
C	-1.51500000	1.32540000	-1.52630000
O	-1.62380000	2.02670000	-2.46370000
C	-1.71220000	1.56650000	1.11220000
O	-1.93040000	2.44220000	1.86770000
N	4.01320000	-1.53690000	-1.61440000
N	-4.01410000	-1.53380000	1.61510000
C	-5.23230000	-0.94720000	1.05180000
H	-6.05230000	-1.06370000	1.77690000
H	-5.10330000	0.13100000	0.81870000
H	-5.51920000	-1.47780000	0.13030000
C	-3.76810000	-1.22690000	3.02580000
H	-3.04340000	-1.94050000	3.44850000
H	-3.38160000	-0.19570000	3.16800000
H	-4.71110000	-1.33490000	3.58360000
C	5.23170000	-0.95050000	-1.05150000
H	6.05160000	-1.06790000	-1.77660000
H	5.10330000	0.12790000	-0.81920000
H	5.51830000	-1.48050000	-0.12960000
C	3.76740000	-1.23090000	-3.02530000
H	3.04220000	-1.94430000	-3.44750000
H	3.38130000	-0.19950000	-3.16830000
H	4.71030000	-1.33970000	-3.58310000

Photoisomer





(H atoms are omitted)

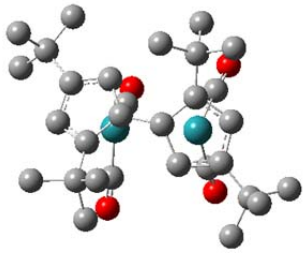
Energy (a.u.): -1294.929627

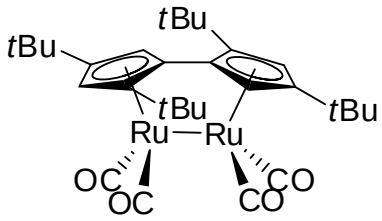
Molecular coordinates

C	1.70420000	2.39300000	0.78390000

C	-0.15930000	1.25170000	-0.15900000
C	0.49220000	1.63020000	1.07780000
C	0.74090000	1.64180000	-1.21370000
C	1.90140000	2.30740000	-0.63980000
C	2.78250000	-0.77020000	1.40840000
C	2.85400000	-0.78760000	-1.30430000
C	-1.64490000	-2.46380000	-0.81150000
C	0.30160000	-1.36840000	-0.03440000
C	-0.39600000	-1.82930000	-1.20740000
C	-0.56440000	-1.67230000	1.08590000
C	-1.70780000	-2.45910000	0.62700000
C	-2.44250000	0.57760000	-1.83080000
C	-2.86480000	0.73060000	0.84520000
H	0.06790000	1.47770000	2.06930000
H	0.57130000	1.50240000	-2.28170000
H	2.71290000	2.75800000	-1.21020000
H	-2.34280000	-2.95390000	-1.48950000
H	-0.03590000	-1.75650000	-2.23400000
H	-0.32490000	-1.45530000	2.12610000
O	3.34910000	-1.31070000	2.28610000
O	3.49650000	-1.29200000	-2.14770000
O	-2.91830000	1.02420000	-2.80690000
O	-3.57880000	1.32150000	1.56950000
Ru	1.82060000	0.06790000	0.01450000
Ru	-1.67030000	-0.18750000	-0.29550000
N	2.48670000	3.07540000	1.69080000
N	-2.64420000	-3.08820000	1.41920000
C	-3.88960000	-3.51290000	0.77880000
H	-4.50900000	-2.64630000	0.46190000
H	-3.66960000	-4.13250000	-0.10480000
H	-4.46640000	-4.12630000	1.48820000
C	-2.77730000	-2.63870000	2.80560000
H	-1.79380000	-2.63180000	3.29980000
H	-3.21940000	-1.62150000	2.87260000
H	-3.42380000	-3.34480000	3.34970000
C	3.82770000	3.46950000	1.25770000
H	3.77070000	4.03450000	0.31390000
H	4.27200000	4.12730000	2.02060000
H	4.49000000	2.58970000	1.10750000
C	2.36970000	2.70970000	3.10310000
H	2.78970000	1.70150000	3.30760000
H	2.91140000	3.45150000	3.71050000
H	1.31400000	2.72440000	3.41430000

Entry 20
Parent



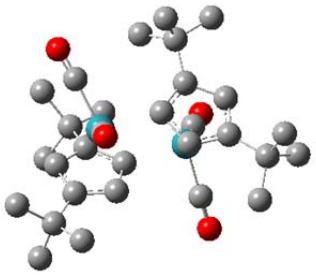


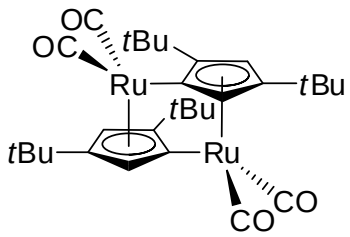
(H atoms are omitted)
Energy (a.u.): -1655.699258
Molecular coordinates

C	2.92000000	-1.13720000	-0.55190000
C	0.70760000	-1.79290000	0.00130000
C	1.58800000	-1.29520000	-1.05740000
C	1.53640000	-1.95980000	1.19470000
C	2.86160000	-1.50220000	0.83560000
H	1.26520000	-1.05600000	-2.06620000
H	3.72140000	-1.52360000	1.50350000
C	-2.87350000	-1.10570000	-0.85440000
C	-0.75780000	-1.71980000	-0.10160000
C	-1.59060000	-1.60740000	-1.29840000
C	-1.59810000	-1.33670000	1.03460000
C	-2.90860000	-0.98070000	0.57570000
H	-3.72770000	-0.93770000	-1.50860000
H	-1.26040000	-1.30170000	2.06590000
Ru	1.45390000	0.33540000	0.50840000
Ru	-1.31450000	0.52050000	-0.22910000
C	1.83280000	1.94600000	-0.35560000
O	2.11670000	2.94790000	-0.90130000
C	1.37430000	1.27330000	2.13510000
O	1.38280000	1.82830000	3.17110000
C	-1.14350000	1.71330000	-1.67150000
O	-1.09750000	2.43660000	-2.59680000
C	-1.55960000	1.98570000	0.90090000
O	-1.76020000	2.90000000	1.61230000
C	-1.37730000	-2.15640000	-2.73170000
C	-2.74150000	-2.67940000	-3.27040000
H	-3.46520000	-1.86390000	-3.43660000
H	-2.58250000	-3.17580000	-4.24350000
H	-3.19510000	-3.41410000	-2.58270000
C	-0.41980000	-3.37750000	-2.71650000
H	-0.79880000	-4.16290000	-2.03940000
H	-0.35900000	-3.80680000	-3.73210000
H	0.60240000	-3.12600000	-2.39930000
C	-0.88260000	-1.08290000	-3.73570000
H	0.08480000	-0.63940000	-3.45280000
H	-0.76720000	-1.53250000	-4.73820000
H	-1.60820000	-0.25660000	-3.81410000

C	-4.14730000	-0.70670000	1.42660000
C	-4.94660000	-2.04040000	1.50640000
H	-5.84930000	-1.90340000	2.12820000
H	-5.26810000	-2.37520000	0.50490000
H	-4.33890000	-2.84420000	1.95750000
C	-5.03970000	0.38030000	0.78280000
H	-5.94400000	0.53540000	1.39720000
H	-4.50220000	1.33960000	0.70480000
H	-5.37260000	0.09270000	-0.22940000
C	-3.76180000	-0.27010000	2.85830000
H	-3.18010000	-1.04920000	3.38160000
H	-3.17200000	0.66130000	2.85390000
H	-4.67530000	-0.08970000	3.45130000
C	1.26500000	-2.72890000	2.51260000
C	0.20690000	-3.84240000	2.29180000
H	0.52370000	-4.52840000	1.48660000
H	0.10030000	-4.43420000	3.21800000
H	-0.78700000	-3.45290000	2.02880000
C	0.85570000	-1.80910000	3.69230000
H	0.70130000	-2.41520000	4.60300000
H	1.64540000	-1.06990000	3.90470000
H	-0.07240000	-1.24760000	3.50200000
C	2.57530000	-3.45240000	2.94250000
H	2.97050000	-4.09150000	2.13400000
H	3.36430000	-2.74310000	3.24410000
H	2.36630000	-4.09580000	3.81490000
C	4.18530000	-0.82910000	-1.35040000
C	4.86750000	-2.19320000	-1.66300000
H	4.19690000	-2.85170000	-2.24230000
H	5.78450000	-2.03030000	-2.25690000
H	5.14940000	-2.72190000	-0.73580000
C	3.85200000	-0.12130000	-2.68350000
H	4.78300000	0.07960000	-3.24140000
H	3.21110000	-0.74630000	-3.33000000
H	3.34370000	0.84240000	-2.51550000
C	5.16190000	0.05020000	-0.53440000
H	4.70800000	1.02450000	-0.28950000
H	5.45950000	-0.43460000	0.41150000
H	6.08180000	0.23000000	-1.11810000

Photoisomer





(H atoms are omitted)
Energy (a.u.): -1655.660102
Molecular coordinates

C	-0.15270000	5.67980000	0.21270000
C	0.83860000	3.57000000	-0.34600000
C	-0.39730000	4.27440000	-0.03180000
C	1.89510000	4.57460000	-0.28100000
C	1.26280000	5.83750000	0.10360000
C	-0.34410000	4.57760000	3.24650000
C	2.26090000	4.90130000	3.03370000
C	0.95070000	-0.05160000	1.63350000
C	0.81660000	2.24900000	2.09430000
C	1.74360000	1.12740000	1.98540000
C	-0.50640000	1.69550000	1.83750000
C	-0.43990000	0.27150000	1.58750000
C	1.92110000	0.76890000	-1.34060000
C	-0.63550000	1.39380000	-1.43800000
H	-1.38200000	3.80830000	-0.02190000
H	1.79450000	6.78450000	0.20460000
H	1.36230000	-1.05440000	1.51170000
H	-1.42860000	2.27460000	1.86900000
O	-1.12720000	4.69790000	4.11330000
O	3.07060000	5.34170000	3.76170000
O	2.64060000	0.23840000	-2.10250000
O	-1.46560000	1.36680000	-2.26830000
Ru	0.89320000	4.38020000	1.84800000
Ru	0.67750000	1.44330000	-0.09670000
C	-1.60340000	-0.71470000	1.50390000
C	-1.29580000	-1.86850000	0.52100000
H	-0.38400000	-2.42070000	0.80690000
H	-2.13160000	-2.59020000	0.51550000
H	-1.15780000	-1.49000000	-0.50560000
C	-2.91470000	-0.01530000	1.07780000
H	-3.20680000	0.77610000	1.78960000
H	-2.82910000	0.43260000	0.07400000
H	-3.73680000	-0.75150000	1.04970000
C	-1.79310000	-1.30100000	2.93440000
H	-2.64090000	-2.00910000	2.94310000
H	-0.89030000	-1.84140000	3.26750000

H	-2.00430000	-0.50370000	3.66790000
C	3.19220000	0.92240000	2.46450000
C	3.33470000	4.60970000	-0.82540000
C	-1.18720000	6.79560000	0.34800000
C	-1.37140000	7.40720000	-1.07250000
H	-2.12890000	8.21070000	-1.04260000
H	-0.42710000	7.83870000	-1.44710000
H	-1.70880000	6.64410000	-1.79510000
C	-2.55080000	6.25290000	0.83390000
H	-2.47270000	5.79270000	1.83270000
H	-3.27860000	7.08050000	0.89960000
H	-2.96610000	5.50500000	0.13640000
C	-0.70190000	7.90040000	1.31540000
H	-0.55970000	7.50250000	2.33410000
H	0.25300000	8.34520000	0.98630000
H	-1.44730000	8.71390000	1.36110000
C	4.29040000	5.36940000	0.12900000
H	5.28600000	5.46150000	-0.34020000
H	3.93850000	6.38990000	0.35590000
H	4.41440000	4.83660000	1.08550000
C	3.26430000	5.39200000	-2.17360000
H	2.92800000	6.43290000	-2.02630000
H	4.26420000	5.42040000	-2.64300000
H	2.56870000	4.90350000	-2.87770000
C	3.92870000	3.22390000	-1.12880000
H	3.90310000	2.56350000	-0.24950000
H	3.38860000	2.72810000	-1.94800000
H	4.98170000	3.33650000	-1.44270000
C	4.00920000	0.06060000	1.46890000
H	5.00620000	-0.15140000	1.89430000
H	3.52920000	-0.90950000	1.25650000
H	4.15440000	0.58060000	0.50830000
C	3.09220000	0.14820000	3.81550000
H	4.10210000	0.00330000	4.23950000
H	2.48970000	0.71090000	4.54930000
H	2.63210000	-0.84650000	3.68500000
C	3.95620000	2.22850000	2.73930000
H	3.96960000	2.89030000	1.86090000
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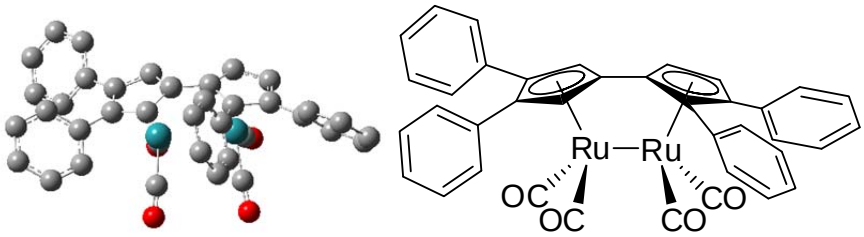
H	5.00150000	1.99310000	3.00760000

Entry 21
Parent



(H atoms are omitted)
Energy (a.u.): -1950.570929
Molecular coordinates

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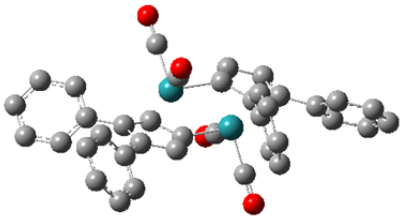
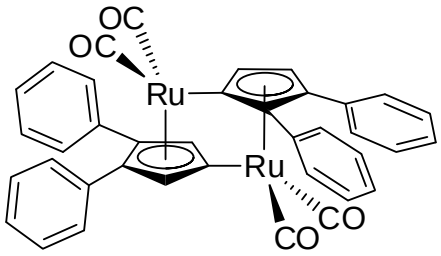
C	-5.14880000	1.90260000	-3.40630000
C	-0.54720000	0.13860000	-3.36260000
C	-4.45960000	4.09970000	-2.61290000
C	2.59470000	0.30730000	-2.84150000
C	-4.19650000	1.29620000	-2.57140000
C	-3.50550000	3.49560000	-1.77440000
C	-0.70150000	-1.97270000	-1.75680000
C	-3.36100000	2.08590000	-1.74200000
C	2.46450000	-1.83250000	-1.29080000
C	-2.34090000	1.47990000	-0.85250000
C	-1.01270000	2.01950000	-0.65710000
C	2.01730000	2.13940000	-0.19420000
C	3.36280000	1.69190000	0.03080000
C	-2.47490000	0.31940000	0.02240000
C	-3.62170000	-1.87340000	0.51620000
C	-3.69470000	-0.47220000	0.31460000
C	-4.76700000	-2.60740000	0.86730000
C	5.65430000	-0.37460000	0.68580000
C	-4.94590000	0.17370000	0.48200000
C	-0.31530000	1.23180000	0.34700000
C	-6.00620000	-1.95640000	1.02590000
C	-6.08980000	-0.56430000	0.83350000
C	1.11860000	1.30400000	0.58910000
C	6.83320000	-0.91370000	1.22640000
C	-1.21780000	0.15770000	0.72630000
C	3.34090000	0.58010000	0.95560000
C	4.55550000	-0.05540000	1.52270000
C	1.94310000	0.32030000	1.29980000
C	6.93580000	-1.14540000	2.61260000
C	1.73220000	-2.01880000	2.27750000
C	1.46550000	-0.62950000	2.34080000
C	4.66930000	-0.29030000	2.91540000
C	5.85100000	-0.83140000	3.45270000
C	1.29910000	-2.87740000	3.30360000
C	0.75830000	-0.12290000	3.46250000
C	0.59300000	-2.36500000	4.40960000

C	0.32400000	-0.98450000	4.48600000
H	-6.02420000	3.77480000	-4.08710000
H	-5.77870000	1.27950000	-4.04860000
H	-4.55840000	5.18970000	-2.62510000
H	-4.07620000	0.20910000	-2.57200000
H	-2.87720000	4.11510000	-1.12570000
H	-0.61760000	2.88910000	-1.17850000
H	1.72370000	2.97390000	-0.82690000
H	5.56350000	-0.22250000	-0.39490000
H	4.26580000	2.14780000	-0.37130000
H	-2.66770000	-2.38910000	0.37140000
H	7.66810000	-1.16340000	0.56430000
H	-4.69270000	-3.69020000	1.00810000
H	-5.01600000	1.25650000	0.34780000
H	-6.89850000	-2.52970000	1.29560000
H	-7.04680000	-0.04850000	0.96060000
H	-1.02680000	-0.59620000	1.48440000
H	2.26750000	-2.42420000	1.41520000
H	7.85250000	-1.57070000	3.03280000
H	3.83590000	-0.03790000	3.57630000
H	1.50820000	-3.94910000	3.23370000
H	0.55510000	0.95120000	3.52540000
H	5.92330000	-1.00520000	4.53090000
H	0.25360000	-3.03620000	5.20450000
H	-0.22200000	-0.57690000	5.34250000
O	-0.54210000	0.33910000	-4.53960000
O	2.94190000	0.55540000	-3.95740000
O	-0.79250000	-3.15850000	-1.87920000
O	2.72360000	-2.99430000	-1.40160000
Ru	-0.66500000	-0.12280000	-1.51480000
Ru	2.15850000	-0.00310000	-1.05600000

Photoisomer





(H atoms are omitted)

Energy (a.u.): -1950.532959

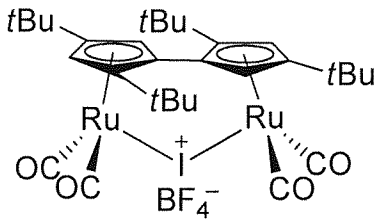
Molecular coordinates

C	1.65310000	2.36110000	0.93310000
C	-0.41630000	1.45120000	0.14590000
C	0.41500000	1.65490000	1.34060000
C	0.35320000	1.95410000	-0.97820000
C	1.60050000	2.52150000	-0.49510000

C	2.65990000	-0.86780000	0.99160000
C	2.45260000	-0.41460000	-1.65020000
C	-1.94750000	-2.19260000	-1.02870000
C	0.05950000	-1.18460000	-0.22110000
C	-0.72590000	-1.46800000	-1.40130000
C	-0.73630000	-1.63920000	0.90690000
C	-1.95240000	-2.29260000	0.42060000
C	-2.77770000	1.06200000	-1.46420000
C	-3.14170000	0.68830000	1.16400000
H	0.02370000	1.95900000	-2.01550000
H	2.34170000	3.04620000	-1.09660000
H	-0.41830000	-1.28390000	-2.42940000
H	-0.46400000	-1.54450000	1.95690000
O	3.34040000	-1.55290000	1.69380000
O	2.99050000	-0.77860000	-2.65110000
O	-3.28640000	1.69240000	-2.34230000
O	-3.95640000	1.04660000	1.95790000
Ru	1.58970000	0.21580000	-0.10870000
Ru	-1.94480000	0.03910000	-0.13170000
C	2.71360000	2.92710000	1.80380000
C	4.07630000	2.85190000	1.41840000
C	2.38270000	3.61930000	2.99530000
C	5.07760000	3.45110000	2.19980000
H	4.34530000	2.29790000	0.51260000
C	3.38850000	4.21700000	3.77600000
H	1.33690000	3.69710000	3.30260000
C	4.73750000	4.13580000	3.38360000
H	6.12470000	3.37490000	1.89060000
H	3.11420000	4.74920000	4.69230000
H	5.51820000	4.59800000	3.99570000
C	0.00280000	1.42420000	2.75320000
C	0.74720000	0.61090000	3.64240000
C	-1.14070000	2.09740000	3.25210000
C	0.35270000	0.46440000	4.98420000
H	1.63770000	0.09200000	3.27730000
C	-1.53670000	1.94780000	4.59390000
H	-1.71230000	2.74560000	2.58190000
C	-0.79230000	1.12970000	5.46440000
H	0.93980000	-0.17230000	5.65340000
H	-2.42860000	2.46880000	4.95480000
H	-1.10150000	1.01070000	6.50750000
C	-2.84500000	-2.85420000	-2.00690000
C	-3.26240000	-4.19450000	-1.80390000
C	-3.22850000	-2.20050000	-3.20520000
C	-4.04710000	-4.85320000	-2.76660000
H	-2.95770000	-4.72130000	-0.89570000

C	-4.01150000	-2.86210000	-4.16580000
H	-2.92810000	-1.16130000	-3.37100000
C	-4.42630000	-4.19100000	-3.94970000
H	-4.35690000	-5.88860000	-2.59320000
H	-4.30410000	-2.33680000	-5.08020000
H	-5.03870000	-4.70500000	-4.69700000
C	-2.93180000	-2.97830000	1.29870000
C	-2.46010000	-3.74040000	2.39710000
C	-4.33010000	-2.89760000	1.07780000
C	-3.36090000	-4.40430000	3.24920000
H	-1.38230000	-3.82200000	2.57040000
C	-5.22650000	-3.56210000	1.93020000
H	-4.70770000	-2.29720000	0.24500000
C	-4.74650000	-4.31800000	3.01910000
H	-2.97840000	-4.98920000	4.09160000
H	-6.30300000	-3.48140000	1.75090000
H	-5.44810000	-4.83080000	3.68420000

X-Ray Structural determination of 7



7

TABLE I

Crystal and Data Collection Parameters

Compound: [(t-Bu_4-fulvalene) $Ru_2I(CO)_4]^+ BF_4^- \cdot CH_2Cl_2$

A) Crystal Parameters at 25°C [a,b]

a = 17.5793(27) Å	Space Group: $P2_1/n$
b = 10.0733(12) Å	Formula Weight = 965.4 amu
c = 22.1112(30) Å	Z = 4
β = 96.533(12) °	d_c = 1.65 g cm^{-3}
V = 3890.1(17) $Å^3$	d_o = _____
μ (calc.)= 17.3 cm^{-1}	

Size of crystal : 0.11×0.16×0.29 mm

B) Data Measurement Parameters [8]

Radiation : Mo Kα (λ = 0.71073 Å)

Monochromator: Highly-oriented graphite (2θ = 12.2°)

Detector: Crystal scintillation counter, with PHA.

Reflections measured: ± h, + k, + ℓ

2θ Range: 3 ° -> 45° Scan Type : θ-2θ

Scan width: Δθ = 0.5 + .347 tan(θ)

Scan speed: 0.6 -> 6.7 (θ, °/min)

Background : Measured over 0.25(Δθ) added to each end of the scan.

Aperture -> crystal = 173 mm Vertical aperture = 3.0 mm

Horizontal aperture = 2.0 + 1.0 tan(θ) mm (variable).

No. of reflections collected: 5241

No. of unique reflections: 5069

Intensity standards: ($\bar{9}28$), ($\bar{2}64$), (2,1,10); measured every 2 hours of x-ray exposure time. Over the data collection period no decrease in intensity was observed.

Orientation: 3 reflections were checked after every 250 measurements. Crystal orientation was redetermined if any of the reflections were offset from their predicted positions by more than 0.1 °. Reorientation was performed once during data collection.

[a] Unit cell parameters and their esd's were derived by a least-squares fit to the setting angles of the unresolved Mo Kα components of 24 reflections with 2θ near 26°.

[b] In this and all subsequent tables the esd's of all parameters are given in parentheses, right-justified to the least significant digit(s) given.

EXPERIMENTAL

Orange blade-like crystals of the compound were obtained by slow crystalization from dichloromethane/hexanes. Fragments cleaved from some of these crystals were mounted on glass fibers using polycyanoacrylate cement, then coated with epoxy to preserve them from possible reaction. Precession photographs indicated monoclinic Laue symmetry and yielded preliminary cell dimensions. Systematic absences were consistent only with space group $P2_1/n$.

The crystal used for data collection was then transferred to our Enraf-Nonius CAD-4 diffractometer [8] and centered in the beam. Automatic peak search and indexing procedures yielded the same reduced primitive cell as the photographs. The final cell parameters and specific data collection parameters are given in Table I.

STRUCTURE DETERMINATION

The 5241 raw intensity data were converted to structure factor amplitudes and their esds by correction for scan speed, background and Lorentz and polarization effects [2-4]. No correction for crystal decompositon was necessary. Inspection of the azimuthal scan data [11] showed a variation Imin/Imax =Ø.81 for the average curve. An empirical correction for absorption, based on the azimuthal scan data, was applied to the intensities. Removal of systematically absent data left 5Ø69 unique data.

The structure was solved by Patterson methods and refined via standard least-squares and Fourier techniques. Following the discovery and inclusion of the dichloromethane solvate, numerous models were used to attempt to account for the disorder of the BF4 anion. The model used in the final refinements has three orienta-

tions of a tetrahedral BF4 with occupancies of Ø.4, Ø.3 and Ø.3. All B-F distances were constrained to be equal, all F-B-F angles within each fractional molecule were constrained to be 1Ø9.5 degrees, and the thermal parameters of the fluorines in each partial molecule were constrained to be the same. In a difference Fourier map calculated following refinement of all non-hydrogen atoms (except those in the BF4) with anisotropic thermal parameters, peaks corresponding to the expected positions of most of the hydrogen atoms were found. The hydrogens of the fulvalene ligand were included in the structure factor calculations in their expected positions based on idealized bonding geometry but were not refined in least squares. The hydrogens of the dichloromethane were not included. All hydrogens were assigned isotropic thermal parameters 1-2 A**2 larger than the equivalent Biso of the atom to which they were bonded. A secondary extinction parameter [1Ø] was refined in the final cycles of least-squares.

The final residuals [5] for 4Ø5 variables refined against the 3653 data for which F**2 > 3 sigma(F**2) were R = 3.97 %, wR = 5.42 % and GOF = 2.1Ø6. The R value for all 5Ø69 data was 7.37 %.

The quantity minimized by the least squares program was $\sum$ w(|Fo|-|Fc|)**2, where w is the weight of a given observation. The p-factor [5], used to reduce the weight of intense reflections, was set to Ø.ØØ35 in the final stages of refinement. The analytical forms of the scattering factor tables for the neutral atoms were used [6] and all non-hydrogen scattering factors were corrected for both the real and imaginary components of anomalous dispersion [7].

Inspection of the residuals ordered in ranges of sin(theta)/lambda, |Fo|, and parity and value of the individual indexes showed no unusual features or trends. The largest peak in the final difference Fourier map had an electron density of Ø.82

e-/A3. The largest ten peaks in the map were all near the BF4 or the CH2C12 solvate.

The positional and thermal parameters of the non-hydrogen atoms are given in Table II. The positions of the hydrogen atoms, and a listing of the values of Fo and Fc are available as supplementary material.

Notes on the Figures

All Figures are ORTEP [9] stereopair drawings. In each Figure the stereopair is set up for cross-eyed viewing, with the left- and right-eye views interchanged -- I(R) (L)I. Before submitting the Figures for photographic reduction, the two images should be restored to their correct positions for viewing with a stereopticon -- I(L) (R)I. The correct distance between the centers of the drawings after reduction is 2 1/4 inches or 55 mm.

In Figures 1-3 the ellipsoids are scaled to represent the 50% probability surface. In Figure 4 they are scaled to represent the 20% probability surface. Hydrogen atoms, where represented, are given as arbitrary small spheres for clarity.

Figure 1 - Labeling diagram for the cationic complex. Hydrogen atoms are labeled according to the carbon to which they are bound.

Figure 2 -The same view as Figure 1, but with hydrogen atoms removed and the methyl groups of the t-butyl side chains reduced in size for clarity.

Figure 3 -"End" view of the molecule, showing the twist ot the fulvalene ligand and the coordination of the ruthenium atoms.

Figure 4 - Packing diagram, showing the contents of somewhat more than one unit cell. Note the ball-like BF4 anion.

An overall view of the crystal structure is given in Fig. 4, and views of the cationic complex are given in Fig 1-3. No detailed view of the BF4 anion is given or needed. The structure consists of well separated molecules of the cation with the anion and the dichloromethane filling the intertices. There are no abnormally short inter-molecular contacts. Distances and angles in the structure are given in the Tables. Angles are not given for the BF4 anion because they were constrained to be 1Ø9.5. The disorder in the anion is undoubtedly more complex than the model, most likely corresponding to some hindered rotor, but the refined model seems to fit reasonably well.

The complex consists of the two Ru atoms bridged on one side by an iodine atom and on the other by the subsituted fulvalene. The Ru-Ru distance of 4.Ø9 A is much too long for bonding. The line drawn in the Figures is given to lead the eye, not to imply electron density. The Ru-Ru distance is actually longer than the distance between the centroids of the rings of the ligand, which is 3.93 A. Each Ru atom is thus coordinated in a "three-leg piano stool" manner, with the two CO and the I as the legs. The molecule as a whole is twisted away from the usual "bench" shape, but maintains good C2 symmetry along an axis passing through the I and the midpoint of the C5-C6 bond. The angle between the two five-carbon planes of the ligand is 59.2 deg, and the torsion angle between the centroids of the rings along the Ru-Ru vector is 56.5 deg. Nothing in the structure inherently determines the reason for the extreme twist, though the structure as determined does not have much steric stress.

The five-carbon rings are not totally planar, but are distorted in such a way that the subsituted carbons are displaced away from the Ru. This is seen both in the Planes output, and in the Ru-C distances. This effect is strongly significant, but whether to blame it on electronics or sterics I leave to you. All other variations in chemically equivalent bond distances are not statistically significant.

Footnotes for CHEXRAY WRITEUPS

1) R. B. Roof, Jr., "A Theoretical Extension of the Reduced-Cell Concept in Crystallography", Publication LA-4038, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, 1969.

2) Calculations were performed on DEC Microvax II using locally modified Nonius-SDP[3] software operating under Micro-VMS operating system.

3) Structure Determination Package User's Guide, 1985, B.A. Frenz and Associates, Inc., College Station, Texas 77840.

4) The data reduction formulae are:

$$F_o^2 = \frac{\omega}{Lp}(C-2B) \qquad \sigma_o(F_o^2) = \frac{\omega}{Lp}(C + 4B)^{1/2}$$

$$F_o = \sqrt{F_o^2} \qquad \sigma_o(F) = \sqrt{F_o^2 + \sigma_o(F_o^2)} - F_o$$

where C is the total count in the scan, B the sum of the two background counts, ω is the scan speed used in deg/min, and

$$\frac{1}{Lp} = \frac{\sin 2\theta\,(1 + \cos^2 2\theta_m)}{1 + \cos^2 2\theta_m - \sin^2 2\theta}$$

is the correction for Lorentz and polarization effects for a reflection with scattering angle 2θ and radiation monochromatized with a 50% perfect single-crystal monochrometer with scattering angle $2\theta_m$.

5) $$R = \frac{\Sigma||F_o| - |F_c||}{\Sigma|F_o|} \qquad wR = \left\{\frac{\Sigma w(|F_o| - |F_c|)^2}{\Sigma wF_o^2}\right\}^{1/2}$$

$$GOF = \left\{\frac{\Sigma w(|F_o| - |F_c|)^2}{(n_o - n_v)}\right\}^{1/2}$$

where n_o is the number of observations, n_v the number of variable parameters, and the weights w were given by

$$w = \frac{1}{\sigma^2(F_o)} \quad , \quad \sigma(F_o^2) = \sqrt{\sigma_o^2(F_o^2) + (pF^2)^2}$$

where $\sigma^2(F_o)$ is calculated as above from $\sigma(F_o^2)$ and where p is the factor used to lower the weight of intense reflections.

6) D. T. Cromer, J. T. Waber, "International Tables for X-ray Crystallography," Vol. IV, The Kynoch Press, Birmingham, England, 1974, Table 2.2B.

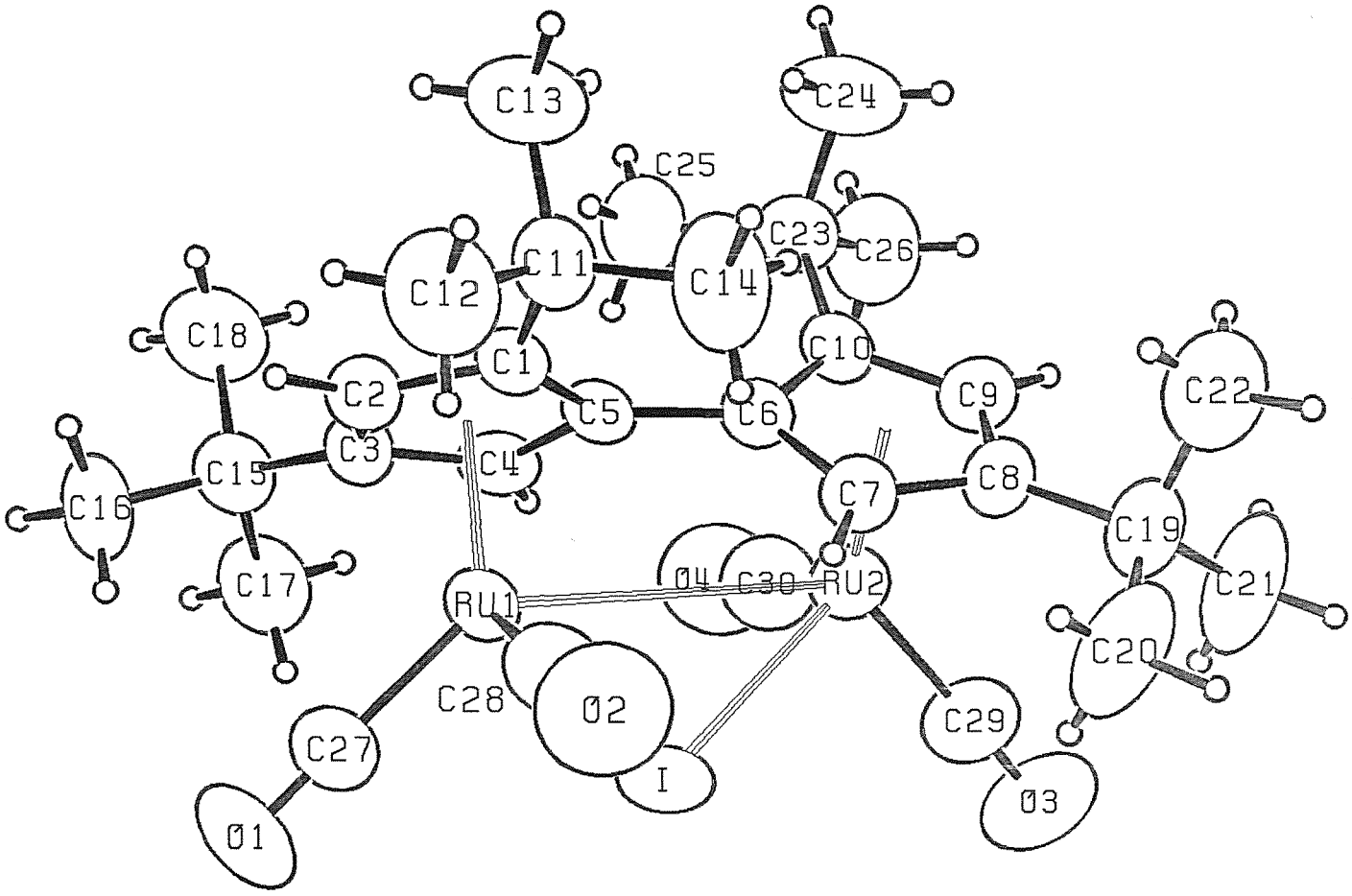
7) D. T. Cromer, ibid., Table 2.3.1.

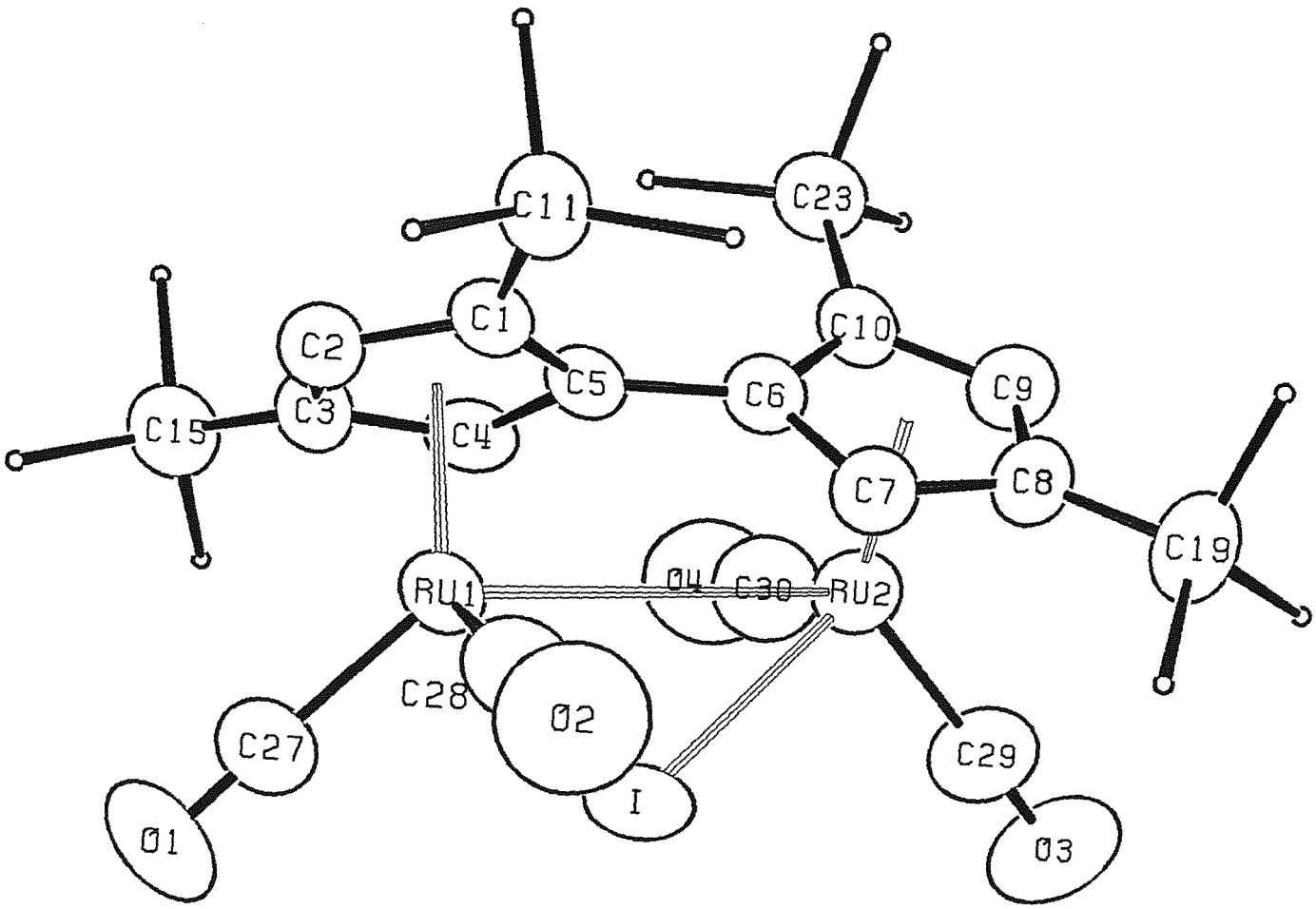
8) Instrumentation at the University of California Chemistry Department X-ray Crystallographic Facility (CHEXRAY) consists of two Enraf-Nonius CAD-4 diffractometers, one controlled by a DEC PDP 8/a with an RK05 disk and the other by a DEC PDP 8/e with an RL01 disk. Both use Enraf-Nonius software as described in the CAD4 Operation Manual, Enraf-Nonius, Delft, Nov. 1977, updated Jan. 1980.

9) C. K. Johnson, Report ORNL-3794, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1965.

10) Zachariesen, W. H., Acta Crystallogr., 16, 1139 (1963).

11) Reflections used for azimuthal scans were located near x = 90° and the intensities were measured at 10° increments of rotation of the crystal about the diffraction vector.


C13
C24
C25
C23
C26
C11
C12
C14
C18
C10
C1
C2
C9
C22
C5
C6
C3
C4
C15
C7
C8
C16
C19
C17
RU1
04
C30
RU2
C21
C20
C28
02
C27
C29
I
03
01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C1
C10
C2
C5
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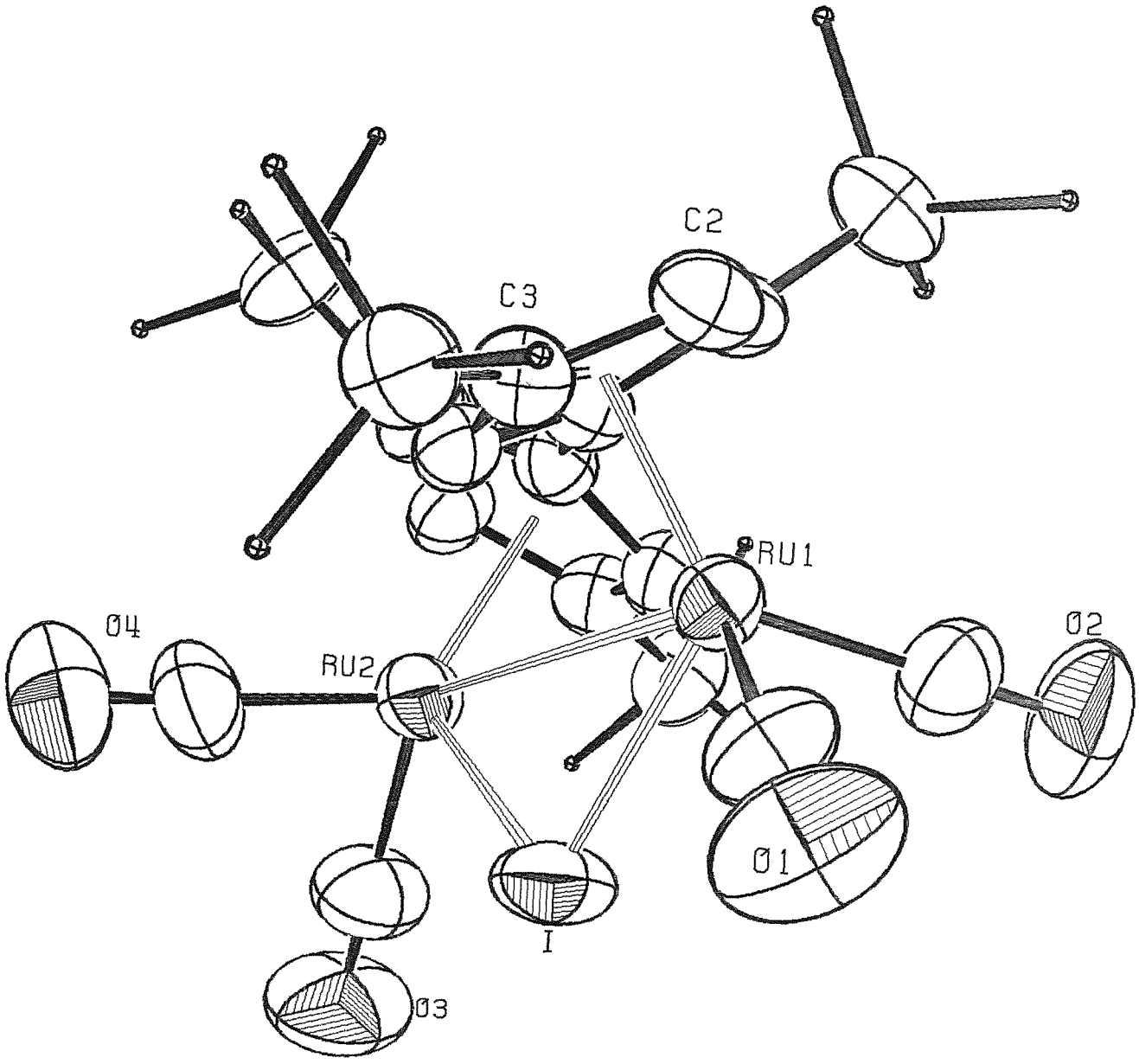
C9
C15
C3
C4
C7
C8
C19
RU1
O4
C30
RU2
C28
O2
C27
I
C29
O1
O3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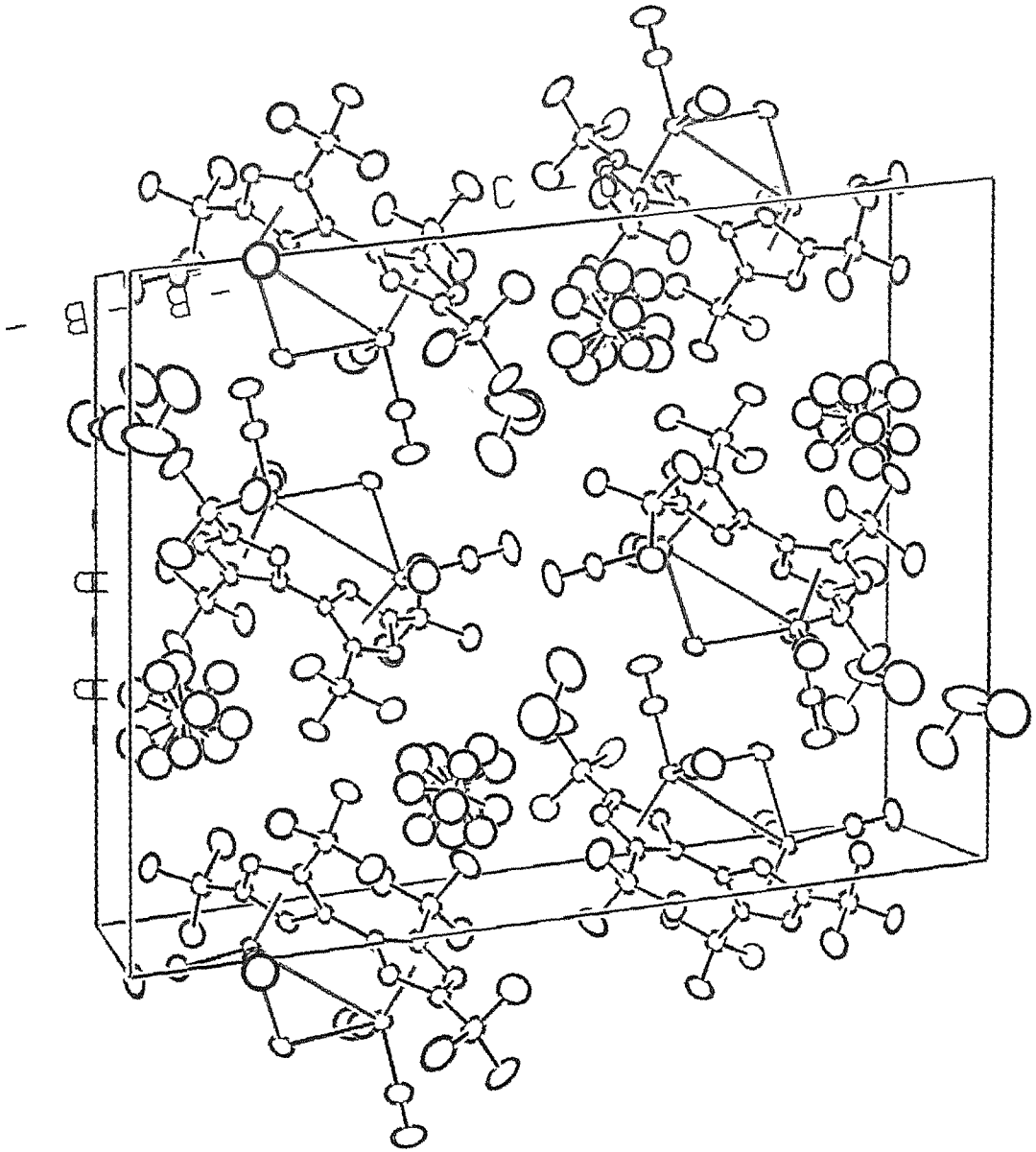
C3
RU1
O4
RU2
O2
O1
I
O3


C
B
B
a
a

Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
I	RU1	2.707(1)
I	RU2	2.717(1)
RU1	RU2	4.092(1)
RU1	C1	2.255(5)
RU1	C2	2.200(5)
RU1	C3	2.278(5)
RU1	C4	2.204(5)
RU1	C5	2.205(5)
RU1	CNT1	1.870
RU2	C6	2.214(5)
RU2	C7	2.201(5)
RU2	C8	2.274(5)
RU2	C9	2.201(6)
RU2	C10	2.268(5)
RU2	CNT2	1.874
RU1	C27	1.894(7)
RU1	C28	1.905(7)
RU2	C29	1.903(7)
RU2	C30	1.870(8)
C27	O1	1.136(7)
C28	O2	1.127(7)
C29	O3	1.132(8)
C30	O4	1.138(8)
C1	C2	1.426(7)
C1	C5	1.421(7)
C2	C3	1.430(7)
C3	C4	1.391(7)
C4	C5	1.463(7)
C5	C6	1.492(7)
C6	C7	1.435(7)
C6	C10	1.434(7)
C7	C8	1.407(7)
C8	C9	1.430(7)
C9	C10	1.417(7)
C11	C1	1.525(7)
C11	C12	1.555(9)
C11	C13	1.511(10)
C11	C14	1.520(9)
C15	C3	1.511(7)
C15	C16	1.528(8)
C15	C17	1.520(9)
C15	C18	1.554(9)
C19	C8	1.533(8)
C19	C20	1.501(10)
C19	C21	1.506(9)
C19	C22	1.537(10)
C23	C10	1.524(8)
C23	C24	1.529(10)
C23	C25	1.537(9)
C23	C26	1.538(9)

Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
C31	CL1	1.633(14)
C31	CL2	1.629(15)
B	F1	1.394(7)
B	F2	1.372(6)
B	F3	1.358(6)
B	F4	1.372(7)
B	F1'	1.369(7)
B	F2'	1.365(7)
B	F3'	1.385(7)
B	F4'	1.379(7)
B	F1"	1.345(7)
B	F2"	1.374(7)
B	F3"	1.401(7)
B	F4"	1.378(7)

Intramolecular Angles

ATOM 1	ATOM 2	ATOM 3	ANGLE
RU1	I	RU2	97.92(2)
CNT1	RU1	I	117.1
CNT1	RU1	C27	128.Ø
CNT1	RU1	C28	128.3
CNT1	RU1	RU2	8Ø.8
I	RU1	C27	92.72(2Ø)
I	RU1	C28	91.49(21)
C27	RU1	C28	88.9(3)
CNT2	RU2	I	117.2
CNT2	RU2	C29	129.6
CNT2	RU2	C3Ø	127.4
CNT2	RU2	RU1	81.6
I	RU2	C29	91.32(21)
I	RU2	C3Ø	92.42(21)
C29	RU2	C3Ø	88.4(3)
RU1	C27	O1	179.3(6)
RU1	C28	O2	178.4(6)
RU2	C29	O3	178.2(7)
RU2	C3Ø	O4	176.8(7)

CNT1 and CNT2 are the centroids of the
five-carbon rings of the fulvalene ligand.

Intramolecular Angles

ATOM 1	ATOM 2	ATOM 3	ANGLE
C2	C1	C5	1Ø6.2(4)
C2	C1	C11	122.4(5)
C5	C1	C11	13Ø.6(5)
C1	C2	C3	111.3(5)
C2	C3	C4	1Ø5.2(4)
C2	C3	C15	129.3(5)
C4	C3	C15	125.3(5)
C3	C4	C5	11Ø.4(4)
C1	C5	C4	1Ø6.7(4)
C1	C5	C6	13Ø.3(5)
C4	C5	C6	123.Ø(4)
C5	C6	C7	123.3(4)
C5	C6	C1Ø	13Ø.Ø(5)
C7	C6	C1Ø	1Ø6.7(4)
C6	C7	C8	11Ø.4(5)
C7	C8	C9	1Ø5.4(5)
C7	C8	C19	126.8(5)
C9	C8	C19	127.5(5)
C8	C9	C1Ø	11Ø.4(5)
C6	C1Ø	C9	1Ø6.7(5)
C6	C1Ø	C23	13Ø.4(5)
C9	C1Ø	C23	122.Ø(5)
C1	C11	C12	11Ø.5(5)
C1	C11	C13	1Ø6.7(5)
C1	C11	C14	113.7(5)
C12	C11	C13	1Ø6.5(6)
C12	C11	C14	1Ø9.3(6)
C13	C11	C14	1Ø9.8(6)
C3	C15	C16	112.Ø(5)
C3	C15	C17	111.9(5)
C3	C15	C18	1Ø5.Ø(5)
C16	C15	C17	1Ø9.4(5)
C16	C15	C18	1Ø9.5(6)
C17	C15	C18	1Ø9.Ø(6)
C8	C19	C2Ø	11Ø.5(5)
C8	C19	C21	113.Ø(5)
C8	C19	C22	1Ø4.7(5)
C2Ø	C19	C21	1Ø8.7(6)
C2Ø	C19	C22	11Ø.5(7)
C21	C19	C22	1Ø9.5(7)
C1Ø	C23	C24	1Ø5.2(5)
C1Ø	C23	C25	113.6(5)
C1Ø	C23	C26	111.4(5)
C24	C23	C25	1Ø8.4(6)
C24	C23	C26	1Ø8.6(6)
C25	C23	C26	1Ø9.5(6)
CL1	C31	CL2	119.9(8)

Table of Torsional Angles in Degrees

Atom 1	Atom 2	Atom 3	Atom 4	Angle	Atom 1	Atom 2	Atom 3	Atom 4	Angle
CNT1	RU1	RU2	CNT2	56.5	C5	C1	C11	C13	9Ø.4
C27	RU1	RU2	C29	-32.5	C2	C3	C15	C18	89.3
C28	RU1	RU2	C3Ø	162.4	C7	C8	C19	C22	-98.2
C1	C5	C6	C7	61.8	C6	C1Ø	C23	C24	91.Ø
C4	C5	C6	C1Ø	59.4					

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	$B(A^2)$
RU1	-Ø.ØØ544(3)	Ø.16Ø11(6)	Ø.14489(3)	3.59(1)
RU2	Ø.13597(4)	Ø.23135(7)	Ø.3Ø16Ø(3)	4.12(1)
I	Ø.14627(3)	Ø.17895(7)	Ø.18225(3)	5.64(1)
CL1	Ø.3286(3)	Ø.4156(5)	Ø.4499(2)	16.5(2)
CL2	Ø.2756(4)	Ø.6484(5)	Ø.5Ø26(3)	18.3(2)
O1	Ø.Ø196(5)	Ø.1716(8)	Ø.Ø117(3)	9.Ø(2)
O2	Ø.ØØ5Ø(5)	-Ø.14ØØ(6)	Ø.1397(4)	8.8(2)
O3	Ø.3Ø73(4)	Ø.1944(9)	Ø.3323(4)	9.7(2)
O4	Ø.1627(5)	Ø.5232(7)	Ø.2847(4)	9.1(2)
C1	-Ø.1Ø23(4)	Ø.1629(7)	Ø.2Ø36(3)	3.5(2)
C2	-Ø.1221(4)	Ø.2361(8)	Ø.1489(3)	4.Ø(2)
C3	-Ø.Ø747(4)	Ø.35Ø9(7)	Ø.1465(3)	3.7(2)
C4	-Ø.Ø21Ø(4)	Ø.3419(7)	Ø.1976(3)	3.6(2)
C5	-Ø.Ø364(4)	Ø.2258(7)	Ø.234Ø(3)	3.4(2)
C6	Ø.Ø116(4)	Ø.1894(7)	Ø.2917(3)	3.4(2)
C7	Ø.Ø533(4)	Ø.Ø67Ø(7)	Ø.2999(3)	3.8(2)
C8	Ø.Ø95Ø(4)	Ø.Ø626(8)	Ø.3581(3)	4.2(2)
C9	Ø.Ø829(4)	Ø.1888(8)	Ø.385Ø(3)	4.2(2)
C1Ø	Ø.Ø281(4)	Ø.2633(7)	Ø.3471(3)	3.9(2)
C11	-Ø.1541(5)	Ø.Ø556(9)	Ø.2252(4)	5.Ø(2)
C12	-Ø.1934(6)	-Ø.Ø24(1)	Ø.17Ø1(5)	7.6(3)
C13	-Ø.2173(5)	Ø.126(1)	Ø.2533(5)	8.2(3)
C14	-Ø.1129(6)	-Ø.Ø4Ø(1)	Ø.2711(5)	8.4(3)
C15	-Ø.Ø83Ø(5)	Ø.4668(8)	Ø.1Ø28(4)	4.9(2)
C16	-Ø.1226(6)	Ø.427(1)	Ø.Ø4Ø4(4)	6.4(2)
C17	-Ø.ØØ63(6)	Ø.53Ø4(9)	Ø.Ø954(4)	6.7(2)
C18	-Ø.1337(6)	Ø.569(1)	Ø.1326(5)	8.2(3)
C19	Ø.1376(5)	-Ø.Ø574(9)	Ø.3881(4)	5.4(2)
C2Ø	Ø.1544(7)	-Ø.157(1)	Ø.34Ø9(6)	9.7(3)
C21	Ø.2116(6)	-Ø.Ø2Ø(1)	Ø.4254(5)	9.1(3)
C22	Ø.Ø822(7)	-Ø.116(1)	Ø.43Ø1(6)	1Ø.1(3)
C23	-Ø.Ø118(5)	Ø.3842(9)	Ø.37Ø5(4)	5.2(2)
C24	-Ø.Ø723(6)	Ø.328(1)	Ø.4Ø79(5)	8.6(3)
C25	-Ø.Ø522(6)	Ø.471(1)	Ø.3195(4)	8.3(3)
C26	Ø.Ø442(7)	Ø.4697(9)	Ø.4125(4)	7.8(3)
C27	Ø.Ø1Ø1(5)	Ø.1681(9)	Ø.Ø616(4)	5.5(2)
C28	Ø.ØØØ6(5)	-Ø.Ø284(9)	Ø.14Ø8(4)	5.6(2)
C29	Ø.2432(5)	Ø.2Ø6(1)	Ø.3213(4)	6.5(2)
C3Ø	Ø.1548(5)	Ø.4123(9)	Ø.2916(4)	6.1(2)
C31	Ø.26ØØ(9)	Ø.498(2)	Ø.477(1)	18.4(7)

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	$B(Å^2)$
B	Ø.65221(7)	Ø.274Ø(1)	Ø.Ø724Ø(6)	8.9(4)*
F1 (a)	Ø.6386(2)	Ø.41ØØ(9)	Ø.Ø757(2)	11.2(2)*
F2	Ø.5882(3)	Ø.2123(4)	Ø.Ø442(2)	11.2
F3	Ø.669Ø(2)	Ø.2243(4)	Ø.1294(3)	11.2
F4	Ø.7127(4)	Ø.2524(4)	Ø.Ø395(2)	11.2
F1'	Ø.7Ø31(3)	Ø.3274(4)	Ø.1173(2)	13.4(4)*
F2'	Ø.585Ø(4)	Ø.3432(5)	Ø.Ø684(2)	13.4
F3'	Ø.6388(2)	Ø.1424(8)	Ø.Ø858(2)	13.4
F4'	Ø.6823(3)	Ø.2812(4)	Ø.Ø175(3)	13.4
F1"	Ø.6125(3)	Ø.2981(4)	Ø.Ø178(3)	1Ø.7(3)*
F2"	Ø.6981(3)	Ø.381Ø(6)	Ø.Ø895(2)	1Ø.7
F3"	Ø.6Ø1Ø(3)	Ø.2533(4)	Ø.1157(3)	1Ø.7
F4"	Ø.6969(3)	Ø.1625(6)	Ø.Ø688(2)	1Ø.7

* -- Atoms refined with isotropic thermal parameters.

Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as:

$$(4/3) * [a^2*B(1,1) + b^2*B(2,2) + c^2*B(3,3) + ab(\cos\gamma)*B(1,2) + ac(\cos\beta)*B(1,3) + bc(\cos\alpha)*B(2,3)]$$

(a) Fn have 4Ø% occupancy, Fn' and Fn" have 3Ø% occupancy.

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	$B(A^2)$
H2	-Ø.163Ø	Ø.2119	Ø.1175	5.Ø**
H4	Ø.Ø216	Ø.4Ø35	Ø.2Ø75	5.Ø**
H7	Ø.Ø526	-Ø.ØØ25	Ø.2692	5.Ø**
H9	Ø.1Ø85	Ø.2196	Ø.4235	5.Ø**
H12A	-Ø.226Ø	-Ø.Ø925	Ø.182Ø	1Ø.Ø**
H12B	-Ø.2232	Ø.Ø331	Ø.1417	1Ø.Ø**
H12C	-Ø.1552	-Ø.Ø659	Ø.1477	1Ø.Ø**
H13A	-Ø.2518	Ø.Ø667	Ø.2684	1Ø.Ø**
H13B	-Ø.1949	Ø.1812	Ø.287Ø	1Ø.Ø**
H13C	-Ø.2445	Ø.1847	Ø.2243	1Ø.Ø**
H14A	-Ø.1454	-Ø.1Ø74	Ø.2835	1Ø.Ø**
H14B	-Ø.Ø713	-Ø.Ø853	Ø.2528	1Ø.Ø**
H14C	-Ø.Ø891	Ø.ØØ54	Ø.3Ø61	1Ø.Ø**
H16A	-Ø.13Ø2	Ø.499Ø	Ø.Ø124	8.Ø**
H16B	-Ø.Ø966	Ø.3572	Ø.Ø217	8.Ø**
H16C	-Ø.1749	Ø.3913	Ø.Ø439	8.Ø**
H17A	-Ø.Ø1Ø3	Ø.6Ø38	Ø.Ø683	8.Ø**
H17B	Ø.Ø193	Ø.5614	Ø.1343	8.Ø**
H17C	Ø.Ø286	Ø.4666	Ø.Ø8Ø3	8.Ø**
H18A	-Ø.1426	Ø.6466	Ø.1Ø83	1Ø.Ø**
H18B	-Ø.1827	Ø.53Ø6	Ø.1382	1Ø.Ø**
H18C	-Ø.11ØØ	Ø.5954	Ø.1721	1Ø.Ø**
H2ØA	Ø.1813	-Ø.2331	Ø.3581	12.Ø**
H2ØB	Ø.1Ø78	-Ø.1888	Ø.3177	12.Ø**
H2ØC	Ø.1852	-Ø.1188	Ø.3116	12.Ø**
H21A	Ø.2381	-Ø.Ø94Ø	Ø.4438	1Ø.Ø**
H21B	Ø.246Ø	Ø.Ø243	Ø.4ØØØ	1Ø.Ø**
H21C	Ø.2Ø34	Ø.Ø431	Ø.4571	1Ø.Ø**
H22A	Ø.1Ø28	-Ø.1916	Ø.4514	12.Ø**
H22B	Ø.Ø692	-Ø.Ø511	Ø.4593	12.Ø**
H22C	Ø.Ø345	-Ø.1418	Ø.4Ø65	12.Ø**
H24A	-Ø.1Ø24	Ø.3953	Ø.4237	1Ø.Ø**
H24B	-Ø.1Ø87	Ø.2717	Ø.3816	1Ø.Ø**
H24C	-Ø.Ø5Ø8	Ø.2726	Ø.44Ø1	1Ø.Ø**
H25A	-Ø.Ø763	Ø.5464	Ø.336Ø	11.Ø**
H25B	-Ø.Ø163	Ø.5Ø4Ø	Ø.2935	11.Ø**
H25C	-Ø.Ø9Ø6	Ø.4218	Ø.295Ø	11.Ø**
H26A	Ø.Ø188	Ø.5465	Ø.426Ø	1Ø.Ø**
H26B	Ø.Ø659	Ø.42Ø7	Ø.4464	1Ø.Ø**
H26C	Ø.Ø852	Ø.5ØØ9	Ø.39Ø2	1Ø.Ø**
CNT1	-Ø.Ø713	Ø.2635	Ø.1861	#
CNT2	Ø.Ø542	Ø.1542	Ø.3363	#

** -- Atoms included but not refined.
# -- Centroids of the delocalized fulvalene rings.

Table of Root-Mean-Square Amplitudes of Thermal Vibration in Angstroms.

Atom	Min.	Int'med.	Max.	Atom	Min.	Int'med.	Max.
RU1	Ø.191	Ø.217	Ø.23Ø	C12	Ø.212	Ø.31Ø	Ø.386
RU2	Ø.198	Ø.224	Ø.259	C13	Ø.213	Ø.336	Ø.392
I	Ø.195	Ø.246	Ø.341	C14	Ø.182	Ø.284	Ø.454
CL1	Ø.355	Ø.425	Ø.566	C15	Ø.215	Ø.257	Ø.27Ø
CL2	Ø.338	Ø.5Ø9	Ø.566	C16	Ø.192	Ø.314	Ø.329
O1	Ø.2Ø4	Ø.338	Ø.433	C17	Ø.2Ø4	Ø.316	Ø.334
O2	Ø.216	Ø.372	Ø.387	C18	Ø.229	Ø.282	Ø.424
O3	Ø.221	Ø.364	Ø.431	C19	Ø.215	Ø.249	Ø.31Ø
O4	Ø.247	Ø.361	Ø.393	C2Ø	Ø.189	Ø.324	Ø.476
C1	Ø.181	Ø.214	Ø.236	C21	Ø.217	Ø.326	Ø.437
C2	Ø.2Ø7	Ø.213	Ø.257	C22	Ø.231	Ø.335	Ø.466
C3	Ø.196	Ø.218	Ø.23Ø	C23	Ø.187	Ø.258	Ø.312
C4	Ø.187	Ø.2ØØ	Ø.251	C24	Ø.2Ø8	Ø.359	Ø.392
C5	Ø.174	Ø.2Ø5	Ø.238	C25	Ø.2Ø6	Ø.258	Ø.455
C6	Ø.199	Ø.2Ø5	Ø.221	C26	Ø.2Ø3	Ø.3Ø3	Ø.4Ø4
C7	Ø.2Ø3	Ø.223	Ø.228	C27	Ø.219	Ø.256	Ø.312
C8	Ø.2Ø3	Ø.232	Ø.254	C28	Ø.229	Ø.27Ø	Ø.295
C9	Ø.198	Ø.23Ø	Ø.26Ø	C29	Ø.229	Ø.278	Ø.344
C1Ø	Ø.187	Ø.219	Ø.259	C3Ø	Ø.215	Ø.299	Ø.311
C11	Ø.21Ø	Ø.227	Ø.3Ø5	C31	Ø.317	Ø.411	Ø.656

Table of General Temperature Factor Expressions - B's

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
RU1	3.89(3)	3.88(3)	3.Ø5(2)	-Ø.19(2)	Ø.56(2)	-Ø.35(2)	3.59(1)
RU2	3.52(3)	4.64(3)	4.14(3)	-Ø.36(3)	Ø.14(2)	-Ø.89(3)	4.12(1)
I	3.64(2)	8.67(4)	4.82(2)	-Ø.33(2)	1.39(2)	-1.43(3)	5.64(1)
CL1	22.4(4)	11.5(3)	16.9(3)	-2.3(3)	7.6(3)	Ø.8(3)	16.5(2)
CL2	24.1(5)	1Ø.5(3)	2Ø.4(4)	3.5(3)	3.3(4)	3.1(3)	18.3(2)
O1	12.1(5)	11.5(5)	3.8(3)	2.8(4)	2.5(3)	1.2(3)	9.Ø(2)
O2	11.8(5)	4.Ø(3)	1Ø.7(5)	Ø.Ø(3)	1.5(4)	-1.4(3)	8.8(2)
O3	4.Ø(3)	13.7(6)	11.Ø(5)	1.Ø(4)	-Ø.4(3)	-1.5(4)	9.7(2)
O4	9.9(4)	6.1(3)	11.4(5)	-2.6(3)	2.Ø(4)	-Ø.7(4)	9.1(2)
C1	3.3(3)	4.3(3)	3.1(3)	-Ø.1(3)	Ø.9(2)	Ø.2(3)	3.5(2)
C2	3.4(3)	5.2(4)	3.6(3)	-Ø.2(3)	Ø.3(3)	Ø.1(3)	4.Ø(2)
C3	3.8(3)	4.Ø(3)	3.2(3)	Ø.1(3)	Ø.4(3)	Ø.4(3)	3.7(2)
C4	3.9(3)	3.1(3)	4.1(3)	-Ø.1(3)	1.5(3)	-Ø.3(3)	3.6(2)
C5	3.3(3)	4.4(3)	2.6(3)	-Ø.1(3)	Ø.6(2)	-Ø.4(3)	3.4(2)
C6	3.3(3)	3.7(3)	3.3(3)	-Ø.3(3)	Ø.5(3)	-Ø.1(3)	3.4(2)
C7	4.Ø(3)	3.6(3)	3.7(3)	Ø.Ø(3)	Ø.3(3)	-Ø.4(3)	3.8(2)
C8	3.8(3)	4.6(4)	4.2(3)	Ø.5(3)	Ø.2(3)	Ø.7(3)	4.2(2)
C9	4.3(4)	4.4(4)	3.9(3)	Ø.5(3)	Ø.4(3)	-Ø.9(3)	4.2(2)
C1Ø	4.8(4)	4.1(3)	3.Ø(3)	Ø.7(3)	Ø.9(3)	-Ø.1(3)	3.9(2)
C11	4.1(4)	6.Ø(4)	4.7(4)	-1.1(3)	Ø.1(3)	1.3(3)	5.Ø(2)
C12	6.8(5)	8.1(5)	7.8(6)	-3.8(4)	-Ø.2(5)	Ø.5(5)	7.6(3)

Table of General Temperature Factor Expressions - B's (Continued)

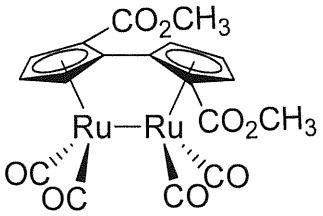
Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
C13	5.5(4)	11.6(7)	8.Ø(5)	-1.5(5)	2.8(4)	1.1(5)	8.2(3)
C14	7.Ø(5)	8.7(5)	9.3(6)	-3.8(4)	-Ø.8(5)	5.1(4)	8.4(3)
C15	5.4(4)	4.7(4)	4.6(4)	Ø.Ø(3)	1.Ø(3)	Ø.9(3)	4.9(2)
C16	7.3(5)	7.3(5)	4.3(4)	Ø.6(4)	-Ø.5(4)	2.2(4)	6.4(2)
C17	7.5(5)	6.Ø(5)	6.7(5)	-1.1(4)	1.6(4)	2.4(4)	6.7(2)
C18	11.1(6)	6.2(5)	7.8(5)	3.8(5)	3.5(5)	1.7(4)	8.2(3)
C19	5.9(4)	5.1(4)	4.9(4)	1.4(4)	-Ø.7(4)	-Ø.1(4)	5.4(2)
C2Ø	11.7(7)	6.6(5)	9.9(7)	5.8(4)	-2.2(6)	-1.5(5)	9.7(3)
C21	8.2(6)	7.8(6)	1Ø.Ø(7)	1.5(5)	-4.2(5)	Ø.8(5)	9.1(3)
C22	9.8(7)	8.3(6)	12.4(7)	2.6(6)	2.9(6)	5.7(5)	1Ø.1(3)
C23	6.3(4)	5.4(4)	4.1(3)	1.8(4)	1.3(3)	-Ø.9(3)	5.2(2)
C24	9.3(6)	9.3(7)	8.Ø(5)	2.Ø(5)	4.6(4)	-1.4(5)	8.6(3)
C25	1Ø.9(6)	9.1(5)	4.9(4)	6.1(4)	Ø.7(4)	-Ø.9(4)	8.3(3)
C26	1Ø.8(7)	6.Ø(5)	6.3(5)	2.2(5)	-Ø.4(5)	-2.7(4)	7.8(3)
C27	6.5(4)	6.Ø(4)	4.2(4)	1.4(4)	1.1(3)	-Ø.4(4)	5.5(2)
C28	6.6(5)	5.1(4)	5.1(4)	-Ø.1(4)	1.3(4)	-Ø.9(4)	5.6(2)
C29	4.2(4)	8.8(6)	6.5(5)	-Ø.Ø(4)	Ø.1(4)	-1.3(5)	6.5(2)
C3Ø	6.Ø(4)	5.3(4)	7.Ø(5)	-1.9(4)	Ø.5(4)	-Ø.8(4)	6.1(2)
C31	11.4(9)	14(1)	32(2)	-3.2(9)	9(1)	-4(1)	18.4(7)

The form of the anisotropic thermal parameter is:

$$\exp[-Ø.25(h^2 a^{*2} B(1,1) + k^2 b^{*2} B(2,2) + l^2 c^{*2} B(3,3)' + 2hka^*b^*B(1,2) + 2hla^*c^*B(1,3) + 2klb^*c^*B(2,3))]$$

, where a*,b*, and c* are reciprocal lattice constants.

X-Ray Structural determination of 10



10

TABLE I -- Crystal and Data Parameters
Compound : Blumel's carboxylated fulvalene

Empirical formula: $Ru_2\ O_8\ C_{18}\ H_{12}$

A)Crystal Parameters at T = -105°C [a,b]

a = 17.5537(20) Å	Space Group: $P2_1/c$
b = 13.8112(20) Å	Formula weight = 558.4 amu
c = 15.4889(20) Å	Z = 8
α = 90.0°	d(calc) = 2.01 g cm^{-3}
β = 101.307(11) °	d(obs) = _____
γ = 90.0°	μ(calc) = 16.5 cm^{-1}
V = 3682.2(15) $Å^3$	

Size: 0.17x0.20x0.25 mm

B) Data Measurement Parameters [8]
Radiation : MoKα (λ = 0.71073 Å)
Monochromator : Highly-oriented graphite (2θ = 1.0)
Detector : Crystal scintillation counter, with PHA.
Reflections measured : +/- H, - K, +L [c]
2θ range: 3 -> 45 deg Scan Type: θ-2θ
Scan width: $\Delta\theta$ = 0.60 + 0.35 tanθ
Scan speed: 5.50 (θ, deg/min)
Background: Measured over 0.25*($\Delta\theta$) added to each end of the scan.
Vert. aperture = 3.0 mm Horiz. aperture = 2.0 + 1.0 tanθ mm
No. of reflections collected: 5239
No. of unique reflections: 4796

Intensity standards: $(\overline{4}39)$, $(\overline{3}92)$, $(10,\overline{4},4)$; measured every 1 hours of x-ray exposure time. Over the data collection period no decrease in intensity was observed.

Orientation: Three reflections were checked after every 250 measurements. Crystal orientation was redetermined if any of the reflections were offset by more than 0.12 degree from their predicted positions. Reorientation was performed once during data collection.

[a] Unit cell parameters and their esd's were derived by a least-squares fit to the setting angles of the unresolved MoKα components of 24 reflections with 2θ between 26° and 30°.
[b] In this and all subsequent tables the esd's of all parameters are given in parentheses, right-justified to the least significant digit(s) of the reported value.
[c] Data were actually collected with a space group setting corresponding to $P2_1/a$. They are given as if they were collected in the current setting.

EXPERIMENTAL

Pale yellow crystals of the compound were obtained by slow crystallization from (EtOAc/hexanes). A fragment cleaved from one of these crystals were mounted on a glass fiber using polycyanoacrylate cement. Preliminary Laue photographs indicated crystal quality.

The crystal used for data collection was then transferred to our Enraf-Nonius CAD-4 diffractometer [8] and centered in the beam. It was cooled to -105°C by a nitrogen flow low-temperature apparatus which had been previously calibrated by a thermocouple placed at the sample position. Automatic peak search and indexing procedures yielded a monoclinic reduced primitive cell. Inspection of the Niggli values [1] revealed no conventional cell of higher symmetry. The final cell parameters and specific data collection parameters for this data set are given in Table I.

STRUCTURE DETERMINATION

The 5239 raw intensity data were converted to structure factor amplitudes and their esds by correction for scan speed, background and Lorentz and polarization effects [2-4]. No correction for crystal decomposition was necessary. Inspection of the azimuthal scan data [11] showed a variation Imin/Imax = 0.94 for the average curve. An empirical correction based on the observed variation was applied to the data. Inspection of the systematic absences indicated uniquely space group $P2_1/a$. The data were transformed to convert the space group to the standard setting of $P2_1/c$. Removal of systematically absent and redundant data left 4796 unique data in the final data set.

The structure was solved via SHELXS and refined via standard least-squares and Fourier techniques. In a difference fourier map calculated following the refinement of all non-hydrogen atoms with anisotropic thermal parameters, peaks were found corresponding to the positions of all of the hydrogen atoms. Hydrogen atoms were assigned idealized locations and values of Biso approximately 1.15 times the Beqv of the atoms to which they were attached. They were included in structure factor calculations, but not refined.

The final residuals [5] for 506 variables refined against the 4039 data for which $F^2 > 3\ \sigma(F^2)$ were R = 2.17%, wR = 2.66% and GOF = 1.190. The R value for all 4796 data was 3.04%. In the final cycles of refinement a secondary extinction parameter [10] was included (maximum correction -- 11% on F).

The quantity minimized by the least squares program was $\Sigma w(|Fo|-|Fc|)^2$, where w is the weight of a given observation. The p-factor [5], used to reduce the weight of intense reflections, was set to 0.03 throughout the refinement. The analytical forms of the scattering factor tables for the neutral atoms were used [6] and all scattering factors were corrected for both the real and imaginary components of anomalous dispersion [7].

Inspection of the residuals ordered in ranges of $\sin\theta/\lambda$, |Fo|, and parity and value of the individual indexes showed no unusual features or trends. The largest peak in the final difference Fourier map had an electron density of 0.46 e^-/A^3, and the lowest excursion -.14 e^-/A^3.

The positional and thermal parameters of the non-hydrogen atoms are given in the Tables. Anisotropic thermal parameters and the positions and thermal parameters of the hydrogen atoms, as well as a listing of the values of Fo and Fc are available as supplementary material.

Notes on the Figures

All Figures are ORTEP [9] stereopair drawings.
In each Figure the stereopair is set up for cross-eyed viewing, with the left- and right-eye views interchanged --¦(R) (L)¦. Before submitting the Figures for photographic reproduction, the two images should be restored to their correct positions for viewing with a stereopticon -- ¦(L) (R)¦. The correct distance between the centers of the drawings after reduction is 2 1/4 inches or 55 mm.

In all Figures the ellipsoids are scaled to represent the 50% probability surface. Hydrogen atoms, where represented, are given as arbitrary small spheres for clarity.

Figure 1 - Labeling diagram for Molecule 1
Hydrogen atoms are numbered according to the atom to which they are attached.

Figure 2 - Labeling diagram for Molecule 2
Hydrogen atoms are numbered according to the atom to which they are attached. View direction is the same, relative to the molecule as it is for Figure 1.

Figure 3 - Labeling diagram showing the contents of the asymmetric unit of the crystal structure.

Notes on the Structure

The structure consists of isolated molecules of the compound packed in the unit cell. There are numerous close contacts between the oxygen atoms of the carbonyls and the atoms of other molecules, but none that are so close as to be unusual. There are two crystallographically distinct molecules in the asymmetric unit of the structure, as shown in Figure 3. Figures 1 and 2 show that while these molecules are crystallographically non-equivalent, they are chemically very similar. The usual tables of crystallographic coordinates, distances, angles and planes are given in the folders.

Overall each of the molecules shows the usual bent fulvalene coordination of the bonded Ru atoms. Bond distances and angles in the fulvalene appear unremarkable. The caboxylates are *trans* to each other on the two rings, and twisted with respect to the ring planes. There is only a small amount of twist of the rings with respect to each other (compare the angles around the C9-C10 and C29-C30 bonds in the Torsion Angle Tables). The coordination twist around the Ru-Ru bond is small also, and not correllated to the twist on the C-C bonds. The angles between the fulvalene rings are 29.1 and 30.8 degrees, the angles of the CO2Me planes to the rings are 17.6, and 29.9 degrees for molecule 1, and 25.1 and 25.5 degrees for molecule 2.

Footnotes for CHEXRAY WRITEUPS

1) R. B. Roof, Jr., "A Theoretical Extension of the Reduced-Cell Concept in Crystallography", Publication LA-4038, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, 1969.

2) Calculations were performed on DEC Microvax II using locally modified Nonius-SDP[3] software operating under Micro-VMS operating system.

3) Structure Determination Package User's Guide, 1985, B.A. Frenz and Associates, Inc., College Station, Texas 77840.

4) The data reduction formulae are:

$$F_o^2 = \frac{\omega}{Lp}(C-2B) \qquad \sigma_o(F_o^2) = \frac{\omega}{Lp}(C + 4B)^{1/2}$$

$$F_o = \sqrt{F_o^2} \qquad \sigma_o(F) = \sqrt{F_o^2 + \sigma_o(F_o^2)} - F_o$$

where C is the total count in the scan, B the sum of the two background counts, ω is the scan speed used in deg/min, and

$$\frac{1}{Lp} = \frac{\sin 2\theta\ (1 + \cos^2 2\theta_m)}{1 + \cos^2 2\theta_m - \sin^2 2\theta}$$

is the correction for Lorentz and polarization effects for a reflection with scattering angle 2θ and radiation monochromatized with a 50% perfect single-crystal monochrometer with scattering angle $2\theta_m$.

5) $R = \frac{\Sigma||F_o| - |F_c||}{\Sigma|F_o|}$ $\qquad wR = \left\{\frac{\Sigma w(|F_o| - |F_c|)^2}{\Sigma wF_o^2}\right\}^{1/2}$

$$GOF = \left\{\frac{\Sigma w(|F_o| - |F_c|)^2}{(n_o - n_v)}\right\}^{1/2}$$

where n_o is the number of observations, n_v the number of variable parameters, and the weights w were given by

$$w = \frac{1}{\sigma^2(F_o)} \quad , \quad \sigma(F_o^2) = \sqrt{\sigma_o^2(F_o^2) + (pF^2)^2}$$

where $\sigma^2(F_o)$ is calculated as above from $\sigma(F_o^2)$ and where p is the factor used to lower the weight of intense reflections.

6) D. T. Cromer, J. T. Waber, "International Tables for X-ray Crystallography," Vol. IV, The Kynoch Press, Birmingham, England, 1974, Table 2.2B.

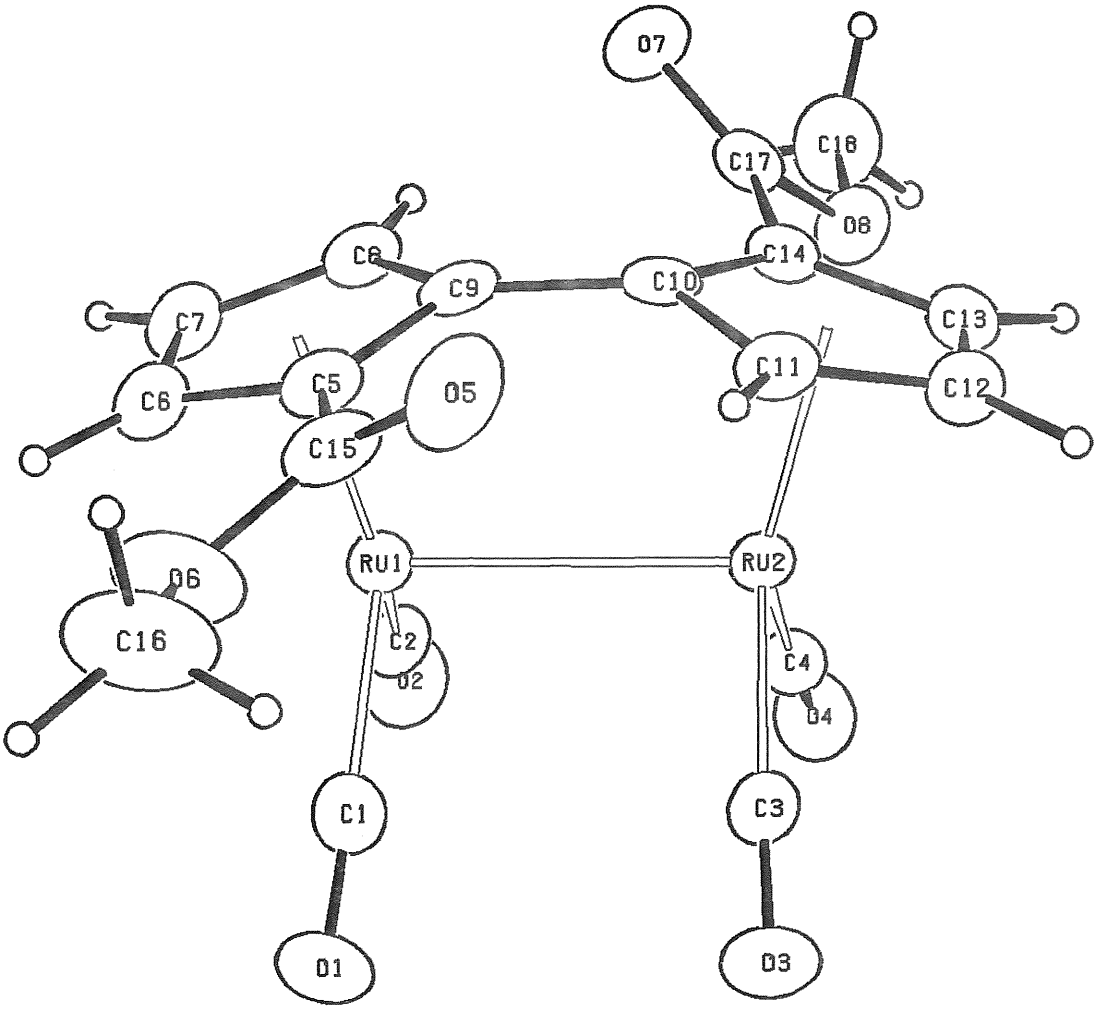
7) D. T. Cromer, ibid., Table 2.3.1.

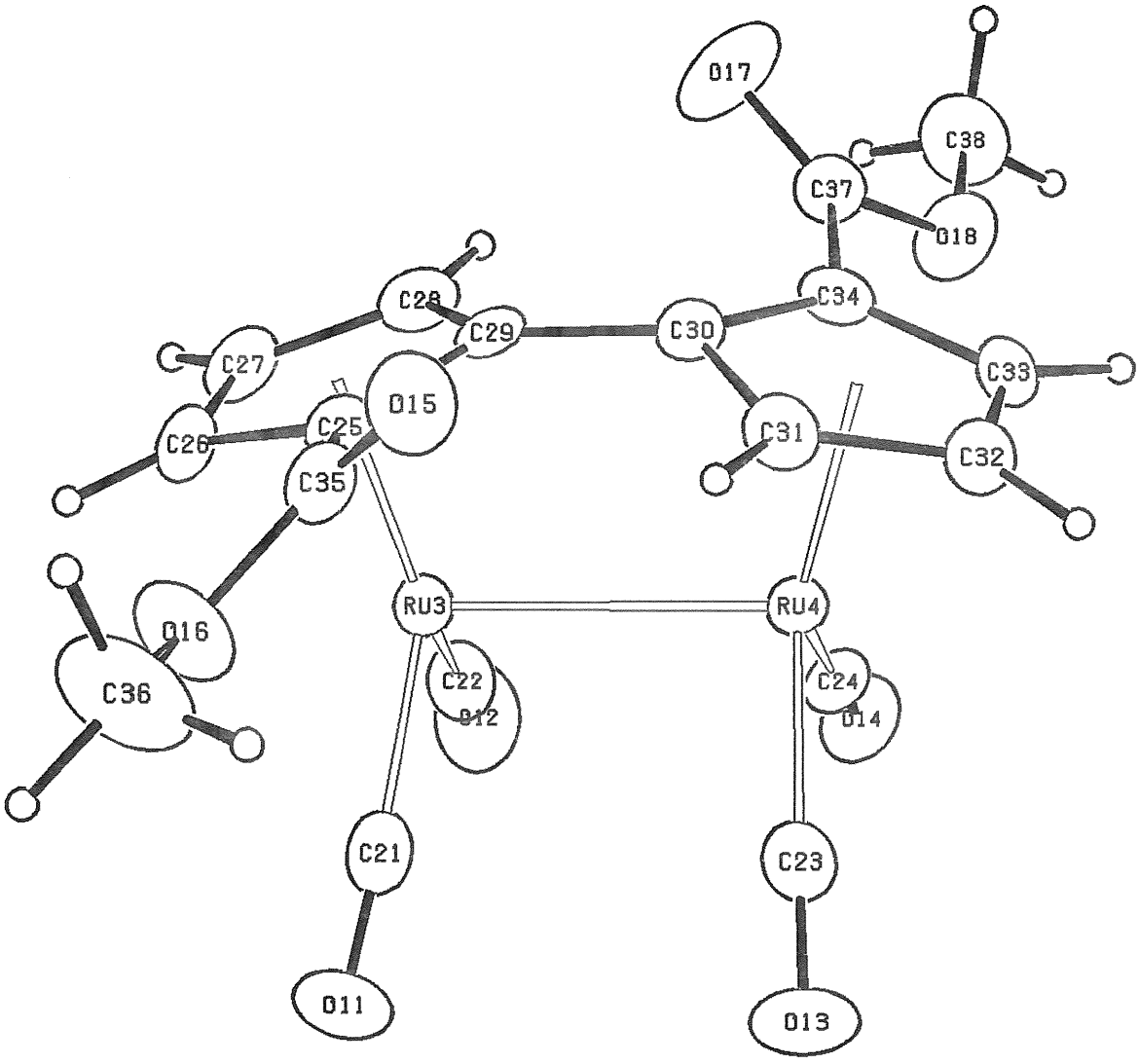
8) Instrumentation at the University of California Chemistry Department X-ray Crystallographic Facility (CHEXRAY) consists of two Enraf-Nonius CAD-4 diffractometers, one controlled by a DEC PDP 8/a with an RK05 disk and the other by a DEC PDP 8/e with an RL01 disk. Both use Enraf-Nonius software as described in the CAD4 Operation Manual, Enraf-Nonius, Delft, Nov. 1977, updated Jan. 1980.

9) C. K. Johnson, Report ORNL-3794, Oak Ridge National Laboratory, Oak Ridge, Tenn., 1965.

10) Zachariesen, W. H., Acta Crystallogr., 16, 1139 (1963).

11) Reflections used for azimuthal scans were located near x = 90° and the intensities were measured at 10° increments of rotation of the crystal about the diffraction vector.


O7
C17
C18
O8
C14
C10
C9
C6
C7
C13
C11
C12
C5
C6
O5
C15
O6
C16
RU1
RU2
C2
O2
C4
O4
C1
C3
O1
O3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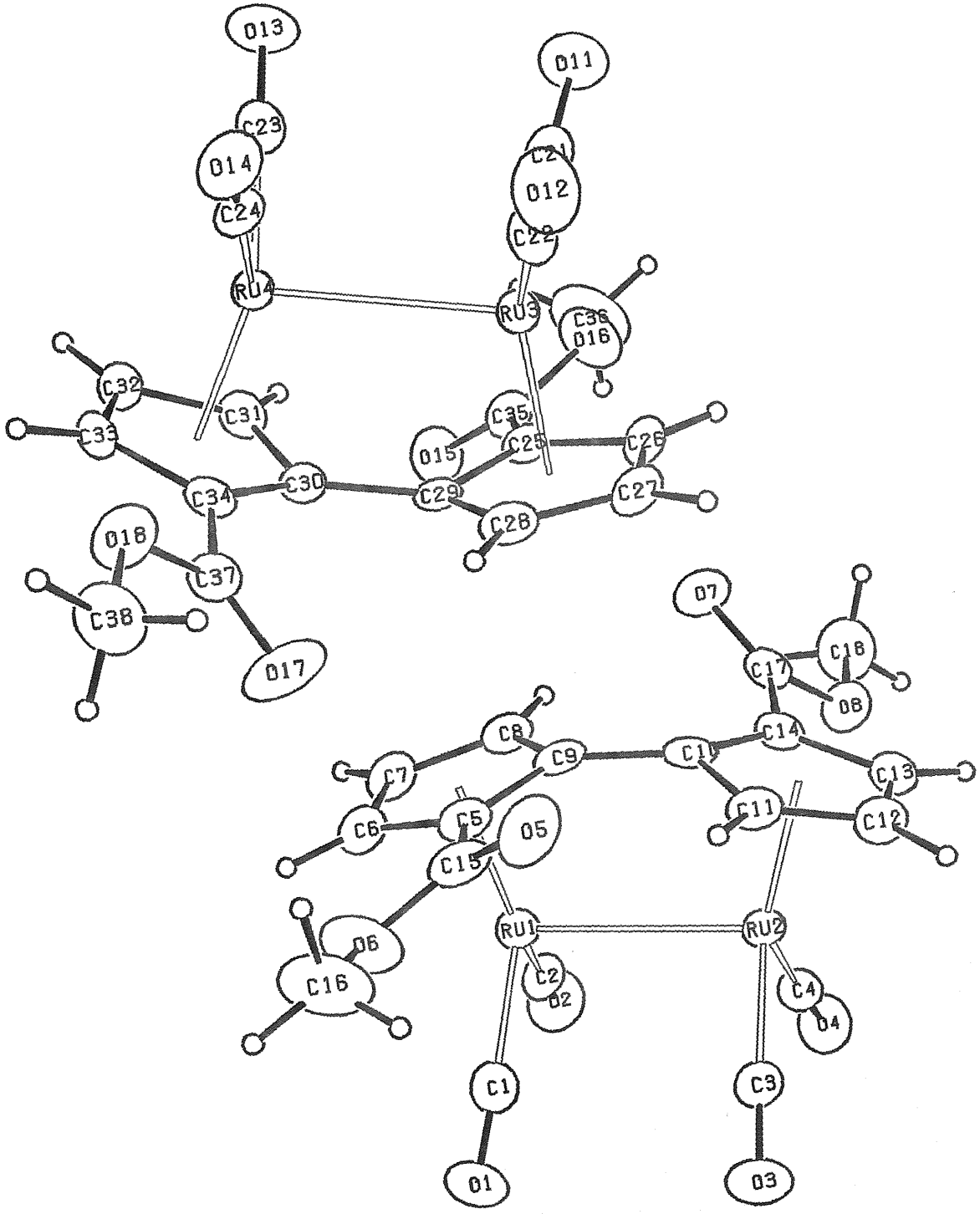
C38
C37
O18
C28
C34
C29
C30
C27
C33
O15
C25
C31
C26
C32
C35
RU3
RU4
O16
C36
C22
C24
O12
O14
C21
C23
O11
O13


O13
O11
C23
O14
C21
O12
C24
C22
RU4
RU3
C36
O16
C32
C31
C35
C33
O15
C25
C26
C34
C30
C29
C27
C28
O18
C37
C38
O17
O7
C17
C18
O8
C8
C14
C9
C1
C7
C13
C6
C5
C11
C12
O5
C15
O6
RU1
RU2
C16
C2
O2
C4
O4
C1
C3
O1
O3

RUFVCAR

Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
RU1	RU2	2.807(1)
RU1	C1	1.873(5)
RU1	C2	1.866(4)
RU2	C3	1.866(5)
RU2	C4	1.857(5)
RU1	C5	2.229(4)
RU1	C6	2.258(4)
RU1	C7	2.275(4)
RU1	C8	2.247(4)
RU1	C9	2.227(4)
RU1	CP1	1.894
RU2	C10	2.243(4)
RU2	C11	2.253(4)
RU2	C12	2.274(4)
RU2	C13	2.256(4)
RU2	C14	2.241(4)
RU2	CP2	1.900
C1	O1	1.136(5)
C2	O2	1.138(5)
C3	O3	1.136(5)
C4	O4	1.154(5)
C5	C6	1.425(6)
C5	C9	1.458(6)
C5	C15	1.490(6)
C6	C7	1.399(6)
C7	C8	1.401(6)
C8	C9	1.429(6)
C9	C10	1.451(6)
C10	C11	1.430(5)
C10	C14	1.457(6)
C11	C12	1.411(6)
C12	C13	1.400(6)
C13	C14	1.428(6)
C14	C17	1.487(6)
C15	O5	1.193(5)
C15	O6	1.338(6)
C16	O6	1.460(5)
C17	O7	1.195(5)
C17	O8	1.341(5)
C18	O8	1.447(5)

Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
RU3	RU4	2.788(1)
RU3	C21	1.866(5)
RU3	C22	1.859(5)
RU4	C23	1.868(5)
RU4	C24	1.869(5)
RU3	C25	2.243(4)
RU3	C26	2.241(4)
RU3	C27	2.256(4)
RU3	C28	2.244(4)
RU3	C29	2.253(4)
RU3	CP3	1.893
RU4	C30	2.239(4)
RU4	C31	2.243(4)
RU4	C32	2.271(4)
RU4	C33	2.257(4)
RU4	C34	2.233(4)
RU4	CP4	1.894
C21	O11	1.140(5)
C22	O12	1.142(5)
C23	O13	1.145(5)
C24	O14	1.139(5)
C25	C26	1.427(5)
C25	C29	1.455(5)
C25	C35	1.475(5)
C26	C27	1.404(6)
C27	C28	1.406(6)
C28	C29	1.430(5)
C29	C30	1.460(5)
C30	C31	1.431(6)
C30	C34	1.451(5)
C31	C32	1.412(6)
C32	C33	1.403(6)
C33	C34	1.423(6)
C34	C37	1.485(6)
C35	O15	1.199(5)
C35	O16	1.339(5)
C36	O16	1.447(5)
C37	O17	1.193(5)
C37	O18	1.320(5)
C38	O18	1.448(5)

Molecule 1
Intramolecular Angles

ATOM 1	ATOM 2	ATOM 3	ANGLE
CP1	RU1	RU2	105.88
CP1	RU1	C1	132.67
CP1	RU1	C2	130.73
C1	RU1	RU2	95.00(13)
C2	RU1	RU2	92.44(12)
C1	RU1	C2	89.00(18)
CP2	RU2	RU1	105.87
CP2	RU2	C3	130.98
CP2	RU2	C4	133.05
C3	RU2	RU1	91.04(13)
C4	RU2	RU1	95.18(13)
C3	RU2	C4	88.92(18)
RU1	C1	O1	177.4(4)
RU1	C2	O2	177.4(4)
RU2	C3	O3	177.7(4)
RU2	C4	O4	177.5(4)
C6	C5	C9	107.8(3)
C6	C5	C15	121.0(4)
C9	C5	C15	131.0(4)
C5	C6	C7	108.4(4)
C6	C7	C8	108.6(4)
C7	C8	C9	109.7(4)
C5	C9	C8	105.4(4)
C5	C9	C10	128.1(4)
C8	C9	C10	124.3(4)
C9	C10	C11	125.2(4)
C9	C10	C14	126.2(4)
C11	C10	C14	105.7(4)
C10	C11	C12	109.4(4)
C11	C12	C13	108.6(4)
C12	C13	C14	108.4(4)
C10	C14	C13	107.9(3)
C10	C14	C17	130.0(4)
C13	C14	C17	121.7(4)
O5	C15	O6	124.3(4)
O5	C15	C5	126.9(4)
O6	C15	C5	108.8(4)
C15	O6	C16	115.0(4)
O7	C17	O8	123.4(4)
O7	C17	C14	126.1(4)
O8	C17	C14	110.5(4)
C17	O8	C18	115.6(3)

Moleucule 2
Intramolecular Angles

ATOM 1	ATOM 2	ATOM 3	ANGLE
CP3	RU3	RU4	104.92
CP3	RU3	C21	132.49
CP3	RU3	C22	130.04
C21	RU3	RU4	96.00(14)
C22	RU3	RU4	93.27(13)
C21	RU3	C22	89.68(20)
CP4	RU4	RU3	107.32
CP4	RU4	C23	131.04
CP4	RU4	C24	132.88
C23	RU4	RU3	92.89(13)
C24	RU4	RU3	91.51(13)
C23	RU4	C24	88.98(18)
RU3	C21	O11	176.4(4)
RU3	C22	O12	176.8(4)
RU4	C23	O13	178.4(4)
RU4	C24	O14	177.9(4)
C26	C25	C29	107.7(3)
C26	C25	C35	122.1(4)
C29	C25	C35	129.8(4)
C25	C26	C27	108.6(4)
C26	C27	C28	108.3(3)
C27	C28	C29	109.6(3)
C25	C29	C28	105.7(3)
C25	C29	C30	126.5(3)
C28	C29	C30	125.1(4)
C29	C30	C31	124.4(4)
C29	C30	C34	126.6(4)
C31	C30	C34	105.5(3)
C30	C31	C32	109.7(3)
C31	C32	C33	108.0(4)
C32	C33	C34	108.6(3)
C30	C34	C33	108.2(4)
C30	C34	C37	129.8(4)
C33	C34	C37	121.5(4)
O15	C35	O16	123.8(4)
O15	C35	C25	125.9(4)
O16	C35	C25	110.2(4)
C35	O16	C36	115.2(4)
O17	C37	O18	122.6(4)
O17	C37	C34	125.8(4)
O18	C37	C34	111.5(4)
C37	O18	C38	116.4(4)

Table of Torsion Angles in Degrees

Atom 1	Atom 2	Atom 3	Atom 4	Angle	
C1	RU1	RU2	C3	-5.19	(0.18)
C1	RU1	RU2	C4	83.82	(0.18)
C1	RU1	RU2	CP2	-138.59	(0.13)
C2	RU1	RU2	C3	-94.39	(0.18)
C2	RU1	RU2	C4	-5.39	(0.18)
C2	RU1	RU2	CP2	132.21	(0.13)
CP1	RU1	RU2	C3	131.88	(0.13)
CP1	RU1	RU2	C4	-139.11	(0.13)
CP1	RU1	RU2	CP2	-1.52	(0.02)
C5	C9	C10	C11	-1.48	(0.64)
C5	C9	C10	C14	156.10	(0.39)
C8	C9	C10	C11	-162.11	(0.39)
C8	C9	C10	C14	-4.53	(0.62)
C6	C5	C15	O5	-158.42	(0.42)
C6	C5	C15	O6	19.59	(0.51)
C9	C5	C15	O5	16.20	(0.71)
C9	C5	C15	O6	-165.79	(0.38)
C16	O6	C15	O5	7.91	(0.59)
C16	O6	C15	C5	-170.17	(0.34)
C10	C14	C17	O7	26.91	(0.68)
C10	C14	C17	O8	-155.69	(0.39)
C13	C14	C17	O7	-145.68	(0.42)
C13	C14	C17	O8	31.72	(0.52)
C18	O8	C17	O7	1.15	(0.56)
C18	O8	C17	C14	-176.33	(0.33)

Table of Torsion Angles in Degrees

Atom 1	Atom 2	Atom 3	Atom 4	Angle	
C21	RU3	RU4	C23	-1.37	(0.18)
C21	RU3	RU4	C24	-90.43	(0.19)
C21	RU3	RU4	CP4	133.41	(0.14)
C22	RU3	RU4	C23	88.66	(0.18)
C22	RU3	RU4	C24	-0.40	(0.18)
C22	RU3	RU4	CP4	-136.56	(0.13)
CP3	RU3	RU4	C23	-138.33	(0.12)
CP3	RU3	RU4	C24	132.61	(0.12)
CP3	RU3	RU4	CP4	-3.55	(0.02)
C25	C29	C30	C31	-2.90	(0.61)
C25	C29	C30	C34	-158.52	(0.39)
C28	C29	C30	C31	156.18	(0.39)
C28	C29	C30	C34	0.55	(0.62)
C26	C25	C35	O15	148.56	(0.42)
C26	C25	C35	O16	-29.42	(0.52)
C29	C25	C35	O15	-23.11	(0.68)
C29	C25	C35	O16	158.91	(0.38)
C36	O16	C35	O15	-5.48	(0.58)
C36	O16	C35	C25	172.55	(0.35)
C30	C34	C37	O17	-22.18	(0.71)
C30	C34	C37	O18	160.80	(0.39)
C33	C34	C37	O17	149.50	(0.44)
C33	C34	C37	O18	-27.51	(0.53)
C38	O18	C37	O17	-1.11	(0.59)
C38	O18	C37	C34	176.01	(0.34)

RUFVCAR -- Molecule 1

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(Å²)
RU1	0.25610(2)	-0.15519(2)	0.09728(2)	1.552(6)
RU2	0.36358(2)	-0.15428(2)	0.25749(2)	1.674(6)
O1	0.1656(2)	-0.3271(2)	0.1412(2)	3.49(7)
O2	0.3555(2)	-0.2851(2)	0.0100(2)	3.12(7)
O3	0.2798(2)	-0.3153(2)	0.3297(2)	3.42(7)
O4	0.4725(2)	-0.3002(2)	0.2030(2)	3.22(7)
O5	0.1445(2)	0.0113(2)	0.2639(2)	3.05(7)
O6	0.0714(2)	-0.0780(2)	0.1584(2)	3.48(7)
O7	0.4493(2)	0.0739(2)	0.1119(2)	2.78(6)
O8	0.5286(2)	-0.0372(2)	0.1862(2)	2.59(6)
C1	0.2013(2)	-0.2635(3)	0.1250(3)	2.28(9)
C2	0.3178(2)	-0.2375(3)	0.0445(2)	2.07(9)
C3	0.3106(2)	-0.2547(3)	0.3007(3)	2.24(9)
C4	0.4294(2)	-0.2455(3)	0.2229(3)	2.19(9)
C5	0.1894(2)	-0.0280(3)	0.1311(3)	1.93(8)
C6	0.1623(2)	-0.0484(3)	0.0401(3)	2.32(9)
C7	0.2240(2)	-0.0351(3)	-0.0039(3)	2.23(9)
C8	0.2899(2)	-0.0072(3)	0.0576(3)	2.04(8)
C9	0.2715(2)	-0.0024(3)	0.1434(3)	1.89(8)
C10	0.3287(2)	-0.0003(3)	0.2248(3)	1.84(8)
C11	0.3135(2)	-0.0216(3)	0.3101(2)	2.09(9)
C12	0.3840(3)	-0.0433(3)	0.3681(3)	2.47(9)
C13	0.4446(2)	-0.0368(3)	0.3216(3)	2.33(9)
C14	0.4126(2)	-0.0093(3)	0.2331(3)	2.00(8)
C15	0.1352(2)	-0.0282(3)	0.1940(3)	2.42(9)
C16	0.0073(3)	-0.0709(4)	0.2057(3)	4.4(1)
C17	0.4628(2)	0.0147(3)	0.1691(3)	2.12(9)
C18	0.5845(2)	-0.0158(4)	0.1314(3)	3.5(1)
H6	0.1110	-0.0675	0.0137	2.6*
H7	0.2215	-0.0436	-0.0652	2.5*
H8	0.3393	0.0064	0.0442	2.3*
H11	0.2636	-0.0213	0.3254	2.4*
H12	0.3893	-0.0596	0.4286	2.8*
H13	0.4980	-0.0487	0.3450	2.7*
H16A	-0.0353	-0.1081	0.1760	5.0*
H16B	0.0237	-0.0946	0.2639	5.0*
H16C	-0.0079	-0.0050	0.2078	5.0*
H18A	0.6288	-0.0558	0.1483	4.0*
H18B	0.5617	-0.0277	0.0715	4.0*
H18C	0.5995	0.0502	0.1385	4.0*

Starred atoms were included with isotropic thermal parameters.
The thermal parameter given for anisotropically refined atoms is the isotropic equivalent thermal parameter defined as:
$(4/3) * [a^2*\beta(1,1) + b^2*\beta(2,2) + c^2*\beta(3,3) + ab(\cos\gamma)*\beta(1,2) + ac(\cos\beta)*\beta(1,3) + bc(\cos\alpha)*\beta(2,3)]$
where a,b,c are real cell parameters, and $\beta(i,j)$ are anisotropic betas.

RUFVCAR -- Molecule 2

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(Å²)
RU3	0.25059(2)	0.36445(2)	0.15867(2)	1.610(6)
RU4	0.12596(2)	0.39438(2)	0.01912(2)	1.536(6)
O11	0.3467(2)	0.5341(3)	0.1222(3)	5.35(9)
O12	0.1806(2)	0.4815(3)	0.2866(2)	4.00(8)
O13	0.1954(2)	0.5757(2)	-0.0414(2)	3.13(7)
O14	0.0417(2)	0.5143(2)	0.1327(2)	2.87(6)
O15	0.3238(2)	0.2027(2)	-0.0482(2)	2.61(6)
O16	0.4083(2)	0.2932(2)	0.0452(2)	3.08(7)
O17	0.0455(2)	0.1421(2)	0.1341(2)	4.84(8)
O18	-0.0370(2)	0.2592(2)	0.0849(2)	3.10(7)
C21	0.3082(2)	0.4715(3)	0.1353(3)	3.0(1)
C22	0.2067(2)	0.4391(3)	0.2362(3)	2.56(9)
C23	0.1697(2)	0.5069(3)	-0.0172(3)	2.12(9)
C24	0.0745(2)	0.4704(3)	0.0895(3)	2.16(9)
C25	0.2997(2)	0.2398(3)	0.0945(2)	1.71(8)
C26	0.3382(2)	0.2446(3)	0.1845(3)	2.02(8)
C27	0.2833(2)	0.2283(3)	0.2378(3)	2.24(9)
C28	0.2103(2)	0.2144(3)	0.1827(3)	2.11(9)
C29	0.2178(2)	0.2209(3)	0.0926(2)	1.62(8)
C30	0.1537(2)	0.2362(3)	0.0182(2)	1.76(8)
C31	0.1620(2)	0.2769(3)	-0.0645(3)	2.06(9)
C32	0.0895(2)	0.3123(3)	-0.1094(3)	2.06(9)
C33	0.0346(2)	0.2950(3)	-0.0565(3)	2.15(9)
C34	0.0723(2)	0.2481(3)	0.0221(3)	1.96(8)
C35	0.3426(2)	0.2423(3)	0.0216(3)	2.04(8)
C36	0.4602(3)	0.2905(4)	-0.0167(3)	4.6(1)
C37	0.0280(2)	0.2103(3)	0.0873(3)	2.33(9)
C38	-0.0877(2)	0.2245(4)	0.1416(3)	3.6(1)
H26	0.3919	0.2568	0.2049	2.3*
H27	0.2936	0.2269	0.3003	2.6*
H28	0.1631	0.2024	0.2023	2.4*
H31	0.2090	0.2796	-0.0858	2.4*
H32	0.0796	0.3424	-0.1656	2.4*
H33	-0.0189	0.3118	-0.0707	2.5*
H36A	0.5049	0.3282	0.0053	5.3*
H36B	0.4751	0.2254	-0.0242	5.3*
H36C	0.4343	0.3159	-0.0715	5.3*
H38A	-0.1324	0.2646	0.1347	4.1*
H38B	-0.1029	0.1598	0.1260	4.1*
H38C	-0.0608	0.2264	0.2011	4.1*

Starred atoms were included with isotropic thermal parameters.
The thermal parameter given for anisotropically refined atoms is the isotropic equivalent thermal parameter defined as:
$(4/3) * [a^2*\beta(1,1) + b^2*\beta(2,2) + c^2*\beta(3,3) + ab(\cos \gamma)*\beta(1,2)$
$+ ac(\cos \beta)*\beta(1,3) + bc(\cos \alpha)*\beta(2,3)]$
where a,b,c are real cell parameters, and $\beta(i,j)$ are anisotropic betas.

RUFVCAR -- Molecule 1

Table of Anisotropic Thermal Parameters - B's

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
RU1	1.70(1)	1.55(1)	1.51(1)	0.13(1)	0.58(1)	-0.11(1)	1.552(6)
RU2	1.98(1)	1.50(1)	1.57(1)	-0.10(1)	0.43(1)	0.18(1)	1.674(6)
O1	3.2(1)	2.7(1)	4.6(2)	-1.1(1)	0.7(1)	0.4(1)	3.49(7)
O2	3.2(1)	3.6(1)	2.9(1)	1.1(1)	1.39(9)	-0.6(1)	3.12(7)
O3	4.2(1)	2.9(1)	3.3(1)	-1.1(1)	1.1(1)	0.7(1)	3.42(7)
O4	2.4(1)	3.2(1)	4.0(1)	0.8(1)	0.4(1)	-0.4(1)	3.22(7)
O5	3.4(1)	3.9(1)	2.1(1)	1.3(1)	1.24(9)	0.2(1)	3.05(7)
O6	3.3(1)	2.8(1)	5.2(1)	-0.4(1)	2.97(9)	-1.0(1)	3.48(7)
O7	2.9(1)	2.7(1)	3.0(1)	-0.0(1)	1.2(1)	1.0(1)	2.78(6)
O8	2.2(1)	3.1(1)	2.6(1)	0.1(1)	0.70(9)	0.5(1)	2.59(6)
C1	2.0(2)	2.3(2)	2.5(2)	0.4(2)	0.4(1)	-0.2(2)	2.28(9)
C2	2.2(2)	2.3(2)	1.7(2)	0.3(2)	0.3(1)	0.3(1)	2.07(9)
C3	2.9(2)	2.1(2)	1.7(2)	-0.1(2)	0.3(1)	0.1(1)	2.24(9)
C4	2.2(2)	2.1(2)	2.2(2)	-0.3(2)	0.3(1)	0.2(2)	2.19(9)
C5	2.2(2)	1.4(2)	2.4(2)	0.7(1)	1.0(1)	0.1(1)	1.93(8)
C6	2.1(2)	2.2(2)	2.6(2)	0.5(2)	0.4(1)	0.4(2)	2.32(9)
C7	2.7(2)	2.5(2)	1.7(1)	0.4(2)	0.8(1)	0.4(1)	2.23(9)
C8	2.4(2)	1.7(2)	2.2(2)	0.2(1)	0.9(1)	0.5(1)	2.04(8)
C9	2.7(2)	1.0(2)	2.2(2)	0.4(1)	0.8(1)	0.3(1)	1.89(8)
C10	2.7(2)	0.8(1)	2.1(2)	-0.2(1)	0.8(1)	-0.1(1)	1.84(8)
C11	3.0(2)	1.5(2)	1.9(2)	0.0(1)	1.0(1)	-0.1(1)	2.09(9)
C12	3.8(2)	2.3(2)	1.4(1)	-0.5(2)	0.7(1)	0.0(1)	2.47(9)
C13	2.8(2)	1.9(2)	2.2(2)	-0.6(2)	0.2(1)	-0.1(2)	2.33(9)
C14	2.2(2)	1.5(2)	2.3(2)	-0.4(1)	0.5(1)	-0.2(1)	2.00(8)
C15	2.9(2)	1.7(2)	3.0(2)	0.8(1)	1.3(1)	0.6(1)	2.42(9)
C16	3.5(2)	3.3(2)	7.6(2)	-0.1(2)	3.9(2)	-0.3(2)	4.4(1)
C17	2.5(2)	1.7(2)	2.2(2)	-0.5(1)	0.3(1)	-0.5(1)	2.12(9)
C18	2.4(2)	4.9(3)	3.6(2)	0.1(2)	1.6(1)	0.2(2)	3.5(1)

The form of the anisotropic temperature factor is:
$\exp[-\frac{1}{4}\{h^2a^{*2}B(1,1) + k^2b^{*2}B(2,2) + l^2c^{*2}B(3,3) + 2hka^*b^*B(1,2) + 2hla^*c^*B(1,3) + 2klb^*c^*B(2,3)\}]$ where a*, b*, and c* are reciprocal lattice constants.

RUFVCAR -- Molecule 2

Table of Anisotropic Thermal Parameters - B's (Continued)

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
RU3	1.61(1)	1.55(1)	1.64(1)	0.07(1)	0.22(1)	-0.12(1)	1.610(6)
RU4	1.47(1)	1.40(1)	1.73(1)	-0.00(1)	0.30(1)	0.16(1)	1.536(6)
O11	4.1(2)	3.5(2)	7.8(2)	-2.0(1)	-0.6(2)	2.0(2)	5.35(9)
O12	4.3(1)	4.7(2)	2.9(1)	1.2(1)	0.5(1)	-1.8(1)	4.00(8)
O13	4.6(1)	2.2(1)	2.9(1)	-0.9(1)	1.6(1)	0.2(1)	3.13(7)
O14	2.9(1)	3.2(1)	2.8(1)	1.0(1)	1.26(9)	0.2(1)	2.87(6)
O15	2.4(1)	3.3(1)	2.3(1)	0.2(1)	1.01(9)	-0.3(1)	2.61(6)
O16	2.1(1)	3.7(1)	3.9(1)	-0.7(1)	1.53(9)	-1.0(1)	3.08(7)
O17	3.0(1)	4.0(2)	8.1(2)	1.0(1)	2.5(1)	3.8(1)	4.84(8)
O18	2.3(1)	3.4(1)	3.9(1)	0.7(1)	1.4(1)	1.0(1)	3.10(7)
C21	2.3(2)	2.8(2)	3.5(2)	0.2(2)	-0.3(2)	0.5(2)	3.0(1)
C22	2.8(2)	2.5(2)	2.1(2)	0.2(2)	-0.2(1)	-0.7(2)	2.56(9)
C23	2.2(2)	2.5(2)	1.7(2)	-0.1(2)	0.4(1)	-0.3(1)	2.12(9)
C24	2.0(2)	1.9(2)	2.5(2)	0.1(1)	0.3(1)	0.8(1)	2.16(9)
C25	1.7(1)	1.3(2)	2.2(2)	0.3(1)	0.6(1)	0.1(1)	1.71(8)
C26	2.0(2)	1.9(2)	2.0(2)	0.7(1)	-0.0(1)	0.0(1)	2.02(8)
C27	2.9(2)	2.0(2)	1.8(2)	0.6(2)	0.5(1)	0.4(1)	2.24(9)
C28	2.5(2)	1.7(2)	2.4(2)	0.0(1)	1.2(1)	0.4(1)	2.11(9)
C29	2.0(2)	0.7(1)	2.2(2)	0.3(1)	0.5(1)	-0.0(1)	1.62(8)
C30	2.0(2)	1.3(2)	1.9(2)	0.1(1)	0.4(1)	-0.1(1)	1.76(8)
C31	2.0(2)	2.0(2)	2.2(2)	-0.1(1)	0.4(1)	-0.4(1)	2.06(9)
C32	2.4(2)	2.1(2)	1.6(2)	-0.1(2)	0.1(1)	-0.0(1)	2.06(9)
C33	1.7(2)	1.9(2)	2.5(2)	-0.1(1)	-0.4(1)	-0.3(2)	2.15(9)
C34	1.8(1)	1.4(2)	2.7(2)	-0.3(1)	0.6(1)	-0.4(1)	1.96(8)
C35	1.6(1)	2.1(2)	2.6(2)	0.6(1)	0.6(1)	0.3(1)	2.04(8)
C36	3.3(2)	5.0(3)	6.4(2)	-1.4(2)	3.2(2)	-1.3(2)	4.6(1)
C37	1.8(2)	2.1(2)	3.1(2)	-0.1(1)	0.5(1)	0.2(2)	2.33(9)
C38	2.3(2)	4.4(2)	4.4(2)	-0.5(2)	1.7(1)	0.3(2)	3.6(1)

The form of the anisotropic temperature factor is:
$\exp[-\frac{1}{4}\{h^2a^{*2}B(1,1) + k^2b^{*2}B(2,2) + l^2c^{*2}B(3,3) + 2hka^*b^*B(1,2) + 2hla^*c^*B(1,3) + 2klb^*c^*B(2,3)\}]$ where a*, b*, and c* are reciprocal lattice constants.