# Crystallographic Data and Details of Refinement of **2**·0.5$C_6H_6$

*Experimental*

## Data Collection

An orange prismatic crystal of $C_{63}H_{52}O_2P_3SRu_2$ having approximate dimensions of 0.20 x 0.20 x 0.35 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7S diffractometer with graphite monochromated Mo-Kα radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range $26.08 < 2\theta < 31.07^o$ corresponded to atriclinic cell with dimensions:

| | |
|---|---|
| a = 14.174(2) Å | α = 98.509(9)° |
| b = 18.277(2) Å | β = 112.161(9)° |
| c = 11.229(1) Å | γ = 92.57(1)° |
| V = 2648.1(6) $Å^3$ | |

For Z = 2 and F.W. = 1168.22, the calculated density is 1.47 $g/cm^3$. Based on a statistical analysis of intensity distribution,and the successful solution and refinement of thestructure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of 23 ± 1°C using the ω-2θ scan technique to a maximum 2θ value of 55.0°.Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.36° with a take-off angle of 6.0°. Scans of $(1.78 + 0.30 \tan\theta)^o$ were made at a speed of 16.0°/min (in omega). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 5 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm and the crystal to detector distance was 235 mm, The computer-controlled slits were set to 9.0 mm (horizontal) and 13.0 mm (vertical).

## Data Reduction

Of the 12679 reflections which were collected, 12185 were unique ($R_{int} = 0.026$). The intensities of three representative reflection were measured after every 150 reflections. Over the course of data collection, the standards decreased by 0.4%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Mo-Kα radiation is 7.5 $cm^{-1}$. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.81 to 0.86.

## Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. The final cycle of full-matrix least-squares refinement[3] was

based on 12172 all reflections ($2\theta < 55.02$) and 649 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma (Fo^2 - Fc^2) / \Sigma Fo^2 = 0.089$$

$$R_w = [( \Sigma w (Fo^2 - Fc^2)^2 / \Sigma w (Fo^2)^2)]^{1/2} = 0.157$$

$$R1 = \Sigma ||Fo| - |Fc|| / \Sigma |Fo| = 0.044 \qquad \text{for } I > 2.0\sigma(I) \text{ data}$$

The standard deviation of an observation of unit weight[4] was 1.20. The weighting scheme was based on counting statistics and included a factor (p = 0.069) to downweight the intense reflections. Plots of $\Sigma$ w $(Fo^2 - Fc^2)^2$ versus $Fo^2$reflection order in data collection, sin $\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.62 and -1.11 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

*References*

(1) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G., (1994). J. Appl. Cryst. 27, 435.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma w(Fo^2-Fc^2)^2$ where

$w = 1/[\sigma^2(Fo^2)] = [\sigma^2_c(Fo^2) + (p\,(Max(Fo^2,0)+2Fc^2)/3)^2]^{-1}$

$\sigma_c(Fo^2)$ = e.s.d. based on counting statistics

$p$ = p-factor

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|Fo|-|Fc|)^2/(N_o-N_v)]^{1/2}$

where: $N_o$ = number of observations

$N_v$ = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch

Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1999).

*EXPERIMENTAL DETAILS*

A. Crystal Data

| | |
|---|---|
| Empirical Formula | $C_{63}H_{52}O_2P_3SRu_2$ |
| Formula Weight | 1168.22 |
| Crystal Color, Habit | orange, prismatic |
| Crystal Dimensions | 0.20 X 0.20 X 0.35 mm |
| Crystal System | triclinic |
| Lattice Type | Primitive |
| No. of Reflections Used for Unit Cell Determination (2θ range) | 25 ( 26.1 - 31.1° ) |
| Omega Scan Peak Width at Half-height | 0.36° |
| Lattice Parameters | a = 14.174(2) Å<br>b = 18.277(2) Å<br>c = 11.229(1) Å<br>α = 98.509(9)°<br>β = 112.161(9)°<br>γ = 92.57(1)°<br>V = 2648.1(6) Å$^3$ |
| Space Group | P-1 (#2) |
| Z value | 2 |
| $D_{calc}$ | 1.465 g/cm$^3$ |
| $F_{000}$ | 1190.00 |
| μ(MoKα) | 7.45 cm$^{-1}$ |

B. Intensity Measurements

| | |
|---|---|
| Diffractometer | Rigaku AFC7S (sealed tube) |

| | |
|---|---|
| Radiation | MoKα (λ = 0.71069 Å)<br>graphite monochromated |
| Attenuator | Zr foil (factor = 8.65) |
| Temperature | 23.0 °C |
| Collimator Size | 1.0 mm |
| Take-off Angle | 6.0° |
| Detector Aperture | 9.0 mm horizontal<br>13.0 mm vertical |
| Crystal to Detector Distance | 235 mm |
| Scan Type | ω-2θ |
| Scan Rate | 16.0°/min (in ω) (up to 5 scans) |
| Scan Width | (1.78 + 0.30 tan θ)° |
| $2\theta_{max}$ | 55.0° |
| No. of Reflections Measured | Total: 12679<br>Unique: 12185 ($R_{int}$ = 0.026) |
| Corrections | Lorentz-polarization<br>Absorption<br>(trans. factors: 0.8112 - 0.8616)<br>Decay (0.41% decline) |

C. Structure Solution and Refinement

| | |
|---|---|
| Structure Solution | Direct Methods (SIR92) |
| Refinement | Full-matrix least-squares |
| Function Minimized | $\Sigma w (Fo^2 - Fc^2)^2$ |
| Least Squares Weights | $1/\sigma^2(Fo^2)$ |
| p-factor | 0.0690 |
| Anomalous Dispersion | All non-hydrogen atoms |
| No. of Reflections (All, $2\sigma < 55.02°$) | 12172 |
| No. Variables | 649 |

| | |
|---|---|
| Reflection/Parameter Ratio | 18.76 |
| Residuals: R; Rw | 0.089 ; 0.157 |
| Residuals: R1 | 0.044 |
| No. of Reflections to calc R1 | 7579 |
| Goodness of Fit Indicator | 1.20 |
| Max Shift/Error in Final Cycle | 0.001 |
| Maximum peak in Final Diff. Map | 1.62 $e^-/Å^3$ |
| Minimum peak in Final Diff. Map | -1.11 $e^-/Å^3$ |

Table S1. Atomic coordinates and $B_{iso}/B_{eq}$ for **2**·0.5$C_6H_6$

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| Ru(1) | 0.68249(3) | 0.30512(2) | 0.70884(3) | 2.758(7) |
| Ru(2) | 0.89293(3) | 0.31572(2) | 0.80862(3) | 3.047(8) |
| S(1) | 0.78882(9) | 0.27348(7) | 0.5805(1) | 3.31(2) |
| P(1) | 0.78804(9) | 0.22484(6) | 0.8340(1) | 2.92(2) |
| P(2) | 0.51768(9) | 0.24334(7) | 0.5812(1) | 3.07(2) |
| P(3) | 1.04547(9) | 0.27301(8) | 0.8174(1) | 3.49(3) |
| O(1) | 0.6121(3) | 0.3593(2) | 0.9229(4) | 5.4(1) |
| O(2) | 0.9933(4) | 0.4058(3) | 1.0784(4) | 7.0(1) |
| C(1) | 0.6380(4) | 0.3382(3) | 0.8396(5) | 3.34(10) |
| C(2) | 0.9549(4) | 0.3679(3) | 0.9759(5) | 4.1(1) |
| C(3) | 0.8698(4) | 0.3582(3) | 0.6311(5) | 3.85(10) |
| C(4) | 0.8486(4) | 0.4172(3) | 0.7094(5) | 4.1(1) |
| C(5) | 0.7484(4) | 0.4215(3) | 0.7163(5) | 3.71(9) |
| C(6) | 0.6510(4) | 0.4095(3) | 0.6125(5) | 3.60(9) |
| C(7) | 0.6221(4) | 0.4080(3) | 0.4707(5) | 3.84(10) |
| C(8) | 0.5212(4) | 0.4216(3) | 0.3993(5) | 4.5(1) |
| C(9) | 0.4863(5) | 0.4231(4) | 0.2672(6) | 5.9(2) |
| C(10) | 0.5482(5) | 0.4120(4) | 0.2001(6) | 6.1(2) |
| C(11) | 0.6490(5) | 0.3999(4) | 0.2675(6) | 5.5(1) |
| C(12) | 0.6851(4) | 0.3990(3) | 0.3998(5) | 4.6(1) |
| C(13) | 0.7964(4) | 0.1310(2) | 0.7581(5) | 3.31(9) |
| C(14) | 0.8721(4) | 0.0880(3) | 0.8217(5) | 3.9(1) |
| C(15) | 0.8849(4) | 0.0207(3) | 0.7596(6) | 4.7(1) |
| C(16) | 0.8196(5) | -0.0067(3) | 0.6309(7) | 5.3(1) |
| C(17) | 0.7447(5) | 0.0332(3) | 0.5685(6) | 5.1(1) |
| C(18) | 0.7310(4) | 0.1019(3) | 0.6292(5) | 4.0(1) |
| C(19) | 0.7874(4) | 0.2099(3) | 0.9913(5) | 3.67(9) |
| C(20) | 0.8134(4) | 0.2679(3) | 1.0945(5) | 4.4(1) |
| C(21) | 0.8099(5) | 0.2581(4) | 1.2139(5) | 5.6(1) |
| C(22) | 0.7770(5) | 0.1912(4) | 1.2290(6) | 6.0(2) |
| C(23) | 0.7487(5) | 0.1318(4) | 1.1277(6) | 5.7(2) |
| C(24) | 0.7543(4) | 0.1407(3) | 1.0095(5) | 4.6(1) |
| C(25) | 0.4572(4) | 0.1896(3) | 0.6657(5) | 3.41(9) |
| C(26) | 0.5165(4) | 0.1647(3) | 0.7767(6) | 4.6(1) |
| C(27) | 0.4715(5) | 0.1254(4) | 0.8428(6) | 5.5(1) |
| C(28) | 0.3671(5) | 0.1098(4) | 0.7947(7) | 5.7(1) |
| C(29) | 0.3075(4) | 0.1342(3) | 0.6833(6) | 5.2(1) |
| C(30) | 0.3506(4) | 0.1751(3) | 0.6196(5) | 4.3(1) |
| C(31) | 0.4147(3) | 0.3019(3) | 0.5145(5) | 3.69(9) |
| C(32) | 0.4009(4) | 0.3583(3) | 0.6028(6) | 4.7(1) |
| C(33) | 0.3261(5) | 0.4047(3) | 0.5593(7) | 5.6(1) |
| C(34) | 0.2647(5) | 0.3970(4) | 0.4293(7) | 5.9(1) |
| C(35) | 0.2775(5) | 0.3419(4) | 0.3421(7) | 5.7(1) |
| C(36) | 0.3512(4) | 0.2933(3) | 0.3844(6) | 4.8(1) |
| C(37) | 0.5046(4) | 0.1765(3) | 0.4347(5) | 3.68(9) |
| C(38) | 0.5362(5) | 0.2017(3) | 0.3429(5) | 4.8(1) |
| C(39) | 0.5270(5) | 0.1544(4) | 0.2313(6) | 6.2(2) |
| C(40) | 0.4889(6) | 0.0819(4) | 0.2112(6) | 6.7(2) |
| C(41) | 0.4580(6) | 0.0558(4) | 0.2999(7) | 6.4(2) |

| | | | | |
|---|---|---|---|---|
| C(42) | 0.4659(4) | 0.1022(3) | 0.4141(5) | 4.6(1) |
| C(43) | 1.0397(4) | 0.2260(3) | 0.6590(5) | 3.82(10) |
| C(44) | 0.9857(5) | 0.1565(3) | 0.6050(6) | 5.2(1) |
| C(45) | 0.9750(5) | 0.1206(4) | 0.4841(7) | 6.4(2) |
| C(46) | 1.0159(5) | 0.1559(4) | 0.4114(6) | 6.1(2) |
| C(47) | 1.0675(5) | 0.2252(4) | 0.4602(6) | 6.0(2) |
| C(48) | 1.0803(5) | 0.2597(3) | 0.5840(6) | 4.9(1) |
| C(49) | 1.1563(4) | 0.3429(3) | 0.8673(5) | 4.05(10) |
| C(50) | 1.1465(5) | 0.4186(4) | 0.8934(6) | 5.3(1) |
| C(51) | 1.2305(5) | 0.4717(4) | 0.9273(7) | 6.4(2) |
| C(52) | 1.3219(5) | 0.4495(5) | 0.9300(7) | 7.0(2) |
| C(53) | 1.3317(5) | 0.3760(5) | 0.9031(7) | 7.5(2) |
| C(54) | 1.2517(4) | 0.3209(4) | 0.8747(7) | 6.6(2) |
| C(55) | 1.1000(4) | 0.2076(3) | 0.9278(5) | 4.6(1) |
| C(56) | 1.1505(8) | 0.1490(5) | 0.8984(9) | 9.4(3) |
| C(57) | 1.1966(8) | 0.1027(6) | 0.9879(10) | 11.2(4) |
| C(58) | 1.1928(6) | 0.1159(5) | 1.1070(9) | 8.0(2) |
| C(59) | 1.1378(5) | 0.1700(4) | 1.1352(6) | 6.1(2) |
| C(60) | 1.0916(5) | 0.2161(3) | 1.0463(6) | 4.9(1) |
| C(61) | 1.0182(8) | 0.4373(4) | 0.433(1) | 7.8(3) |
| C(62) | 0.9479(7) | 0.4653(5) | 0.3721(7) | 7.5(2) |
| C(63) | 0.9210(7) | 0.5281(5) | 0.433(1) | 9.1(3) |
| H(1) | 0.9355 | 0.3648 | 0.6080 | 4.9 |
| H(2) | 0.898(4) | 0.460(3) | 0.748(5) | 5.0 |
| H(3) | 0.755(4) | 0.450(3) | 0.794(5) | 4.7 |
| H(4) | 0.596(4) | 0.433(3) | 0.645(5) | 4.2 |
| H(5) | 0.4765 | 0.4316 | 0.4426 | 5.8 |
| H(6) | 0.4183 | 0.4325 | 0.2213 | 7.2 |
| H(7) | 0.5232 | 0.4119 | 0.1089 | 7.7 |
| H(8) | 0.6919 | 0.3921 | 0.2215 | 7.0 |
| H(9) | 0.7550 | 0.3930 | 0.4441 | 5.8 |
| H(10) | 0.9162 | 0.1056 | 0.9094 | 4.6 |
| H(11) | 0.9381 | -0.0066 | 0.8049 | 5.6 |
| H(12) | 0.8277 | -0.0527 | 0.5892 | 6.3 |
| H(13) | 0.7009 | 0.0146 | 0.4810 | 6.1 |
| H(14) | 0.6782 | 0.1285 | 0.5846 | 4.7 |
| H(15) | 0.8343 | 0.3160 | 1.0846 | 5.3 |
| H(16) | 0.8262 | 0.2993 | 1.2804 | 6.8 |
| H(17) | 0.7742 | 0.1843 | 1.3086 | 7.1 |
| H(18) | 0.7276 | 0.0846 | 1.1378 | 6.8 |
| H(19) | 0.7345 | 0.0998 | 0.9405 | 5.4 |
| H(20) | 0.5877 | 0.1758 | 0.8101 | 5.3 |
| H(21) | 0.5128 | 0.1090 | 0.9186 | 6.6 |
| H(22) | 0.3376 | 0.0820 | 0.8387 | 6.7 |
| H(23) | 0.2368 | 0.1236 | 0.6529 | 6.0 |
| H(24) | 0.3089 | 0.1915 | 0.5448 | 5.1 |
| H(25) | 0.4426 | 0.3650 | 0.6921 | 5.3 |
| H(26) | 0.3178 | 0.4429 | 0.6186 | 6.7 |
| H(27) | 0.2130 | 0.4275 | 0.3999 | 7.2 |
| H(28) | 0.2356 | 0.3365 | 0.2515 | 6.6 |
| H(29) | 0.3580 | 0.2542 | 0.3227 | 5.7 |
| H(30) | 0.5645 | 0.2517 | 0.3589 | 5.6 |

| | | | | |
|---|---|---|---|---|
| H(31) | 0.5449 | 0.1728 | 0.1678 | 7.6 |
| H(32) | 0.4853 | 0.0496 | 0.1354 | 8.1 |
| H(33) | 0.4322 | 0.0053 | 0.2852 | 7.4 |
| H(34) | 0.4444 | 0.0855 | 0.4745 | 5.5 |
| H(35) | 0.9559 | 0.1325 | 0.6529 | 6.5 |
| H(36) | 0.9395 | 0.0722 | 0.4488 | 7.6 |
| H(37) | 1.0087 | 0.1321 | 0.3268 | 6.9 |
| H(38) | 1.0936 | 0.2501 | 0.4090 | 7.2 |
| H(39) | 1.1174 | 0.3072 | 0.6175 | 5.8 |
| H(40) | 1.0834 | 0.4331 | 0.8889 | 6.3 |
| H(41) | 1.2241 | 0.5221 | 0.9459 | 7.8 |
| H(42) | 1.3781 | 0.4851 | 0.9506 | 8.4 |
| H(43) | 1.3948 | 0.3610 | 0.9049 | 8.9 |
| H(44) | 1.2606 | 0.2707 | 0.8622 | 7.9 |
| H(45) | 1.1560 | 0.1427 | 0.8180 | 10.7 |
| H(46) | 1.2296 | 0.0639 | 0.9644 | 13.4 |
| H(47) | 1.2255 | 0.0882 | 1.1706 | 9.1 |
| H(48) | 1.1308 | 0.1772 | 1.2154 | 6.8 |
| H(49) | 1.0546 | 0.2533 | 1.0678 | 5.9 |
| H(50) | 1.0342 | 0.3922 | 0.3944 | 9.4 |
| H(51) | 0.9090 | 0.4464 | 0.2823 | 9.1 |
| H(52) | 0.8623 | 0.5490 | 0.3861 | 11.2 |

$B_{eq} = 8/3\ PI^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S2. Anisotropic Displacement Parameters for **2**·0.5$C_6H_6$

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| Ru(1) | 0.0344(2) | 0.0365(2) | 0.0360(2) | 0.0033(1) | 0.0175(1) | 0.0028(1) |
| Ru(2) | 0.0349(2) | 0.0418(2) | 0.0395(2) | -0.0018(2) | 0.0177(2) | 0.0020(2) |
| S(1) | 0.0464(6) | 0.0419(6) | 0.0415(6) | 0.0034(5) | 0.0233(5) | 0.0037(5) |
| P(1) | 0.0394(6) | 0.0357(6) | 0.0390(6) | 0.0033(5) | 0.0198(5) | 0.0047(5) |
| P(2) | 0.0361(6) | 0.0405(6) | 0.0401(6) | 0.0022(5) | 0.0175(5) | 0.0012(5) |
| P(3) | 0.0370(6) | 0.0533(8) | 0.0468(7) | 0.0034(5) | 0.0217(5) | 0.0087(5) |
| O(1) | 0.080(3) | 0.079(3) | 0.058(2) | 0.012(2) | 0.047(2) | -0.003(2) |
| O(2) | 0.082(3) | 0.105(4) | 0.054(2) | -0.024(3) | 0.018(2) | -0.031(2) |
| C(1) | 0.045(2) | 0.036(2) | 0.047(2) | 0.003(2) | 0.021(2) | 0.006(2) |
| C(2) | 0.048(3) | 0.054(3) | 0.048(2) | -0.003(2) | 0.017(2) | 0.003(2) |
| C(3) | 0.043(2) | 0.053(2) | 0.053(2) | -0.001(2) | 0.021(2) | 0.014(2) |
| C(4) | 0.055(3) | 0.048(3) | 0.054(3) | 0.006(2) | 0.020(2) | 0.017(2) |
| C(5) | 0.060(2) | 0.036(2) | 0.051(2) | 0.007(2) | 0.027(2) | 0.010(2) |
| C(6) | 0.052(2) | 0.040(2) | 0.053(2) | 0.005(2) | 0.029(2) | 0.010(2) |
| C(7) | 0.054(2) | 0.044(3) | 0.052(2) | 0.009(2) | 0.024(2) | 0.015(2) |
| C(8) | 0.051(3) | 0.067(4) | 0.062(3) | 0.012(3) | 0.026(2) | 0.021(3) |
| C(9) | 0.053(3) | 0.107(5) | 0.062(3) | 0.018(3) | 0.014(3) | 0.033(4) |
| C(10) | 0.067(3) | 0.113(6) | 0.052(3) | 0.002(4) | 0.021(3) | 0.021(3) |
| C(11) | 0.074(3) | 0.089(5) | 0.055(3) | 0.018(3) | 0.029(3) | 0.022(3) |
| C(12) | 0.056(3) | 0.071(4) | 0.056(3) | 0.014(3) | 0.029(2) | 0.022(3) |
| C(13) | 0.047(2) | 0.031(2) | 0.053(2) | -0.001(2) | 0.027(2) | 0.005(2) |
| C(14) | 0.049(3) | 0.040(2) | 0.062(3) | 0.005(2) | 0.024(2) | 0.015(2) |
| C(15) | 0.061(3) | 0.040(3) | 0.084(3) | 0.018(2) | 0.032(3) | 0.018(2) |
| C(16) | 0.075(4) | 0.038(3) | 0.088(3) | 0.009(2) | 0.038(3) | -0.005(3) |
| C(17) | 0.074(4) | 0.045(3) | 0.064(3) | 0.002(2) | 0.023(3) | -0.011(2) |
| C(18) | 0.053(3) | 0.045(3) | 0.053(2) | 0.006(2) | 0.022(2) | 0.003(2) |
| C(19) | 0.046(3) | 0.059(2) | 0.040(2) | 0.011(2) | 0.020(2) | 0.013(2) |
| C(20) | 0.062(3) | 0.061(3) | 0.049(3) | 0.007(3) | 0.027(3) | 0.006(2) |
| C(21) | 0.077(4) | 0.092(4) | 0.045(3) | 0.016(3) | 0.027(3) | 0.004(3) |
| C(22) | 0.082(4) | 0.106(4) | 0.052(3) | 0.024(4) | 0.034(3) | 0.031(3) |
| C(23) | 0.081(4) | 0.089(4) | 0.068(3) | 0.015(3) | 0.046(3) | 0.033(3) |
| C(24) | 0.062(3) | 0.060(3) | 0.062(3) | 0.006(3) | 0.032(3) | 0.017(3) |
| C(25) | 0.046(2) | 0.036(2) | 0.052(2) | -0.002(2) | 0.029(2) | -0.002(2) |
| C(26) | 0.044(3) | 0.072(4) | 0.062(3) | 0.003(2) | 0.023(2) | 0.018(3) |
| C(27) | 0.068(3) | 0.078(4) | 0.073(4) | 0.002(3) | 0.034(3) | 0.033(3) |
| C(28) | 0.070(3) | 0.079(4) | 0.086(4) | -0.005(3) | 0.052(3) | 0.017(3) |
| C(29) | 0.056(3) | 0.070(4) | 0.083(4) | -0.013(3) | 0.043(3) | 0.005(3) |
| C(30) | 0.045(2) | 0.059(3) | 0.060(3) | -0.004(2) | 0.023(2) | 0.003(2) |
| C(31) | 0.033(2) | 0.045(3) | 0.061(2) | 0.000(2) | 0.018(2) | 0.008(2) |
| C(32) | 0.056(3) | 0.050(3) | 0.073(4) | 0.008(2) | 0.030(3) | 0.002(2) |
| C(33) | 0.068(4) | 0.059(4) | 0.093(3) | 0.023(3) | 0.038(3) | 0.015(3) |
| C(34) | 0.055(3) | 0.059(4) | 0.103(4) | 0.017(3) | 0.019(3) | 0.022(3) |
| C(35) | 0.052(3) | 0.068(4) | 0.079(4) | 0.008(3) | 0.003(3) | 0.021(3) |
| C(36) | 0.052(3) | 0.051(3) | 0.063(3) | 0.002(2) | 0.010(2) | 0.000(3) |
| C(37) | 0.037(2) | 0.053(2) | 0.043(2) | 0.006(2) | 0.012(2) | -0.004(2) |
| C(38) | 0.063(3) | 0.072(4) | 0.048(3) | -0.004(3) | 0.027(3) | 0.001(2) |
| C(39) | 0.082(4) | 0.099(4) | 0.056(3) | -0.001(4) | 0.039(3) | -0.016(3) |
| C(40) | 0.088(5) | 0.096(4) | 0.062(4) | 0.007(4) | 0.033(3) | -0.029(3) |
| C(41) | 0.093(5) | 0.064(4) | 0.074(4) | -0.002(3) | 0.033(4) | -0.024(3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(42) | 0.057(3) | 0.055(3) | 0.058(3) | 0.005(2) | 0.020(3) | -0.003(2) |
| C(43) | 0.040(2) | 0.055(3) | 0.054(2) | 0.010(2) | 0.024(2) | 0.006(2) |
| C(44) | 0.076(4) | 0.054(3) | 0.087(4) | 0.002(2) | 0.058(4) | -0.001(3) |
| C(45) | 0.080(4) | 0.073(4) | 0.093(4) | -0.005(3) | 0.054(4) | -0.022(3) |
| C(46) | 0.075(4) | 0.094(4) | 0.057(3) | 0.023(3) | 0.029(3) | -0.013(3) |
| C(47) | 0.087(5) | 0.094(4) | 0.060(3) | 0.016(3) | 0.044(3) | 0.015(3) |
| C(48) | 0.071(4) | 0.061(4) | 0.060(3) | -0.002(3) | 0.038(3) | 0.006(2) |
| C(49) | 0.035(2) | 0.068(3) | 0.049(3) | -0.005(2) | 0.017(2) | 0.007(2) |
| C(50) | 0.055(3) | 0.069(3) | 0.077(4) | -0.002(2) | 0.022(3) | 0.022(3) |
| C(51) | 0.065(3) | 0.081(5) | 0.086(5) | -0.021(3) | 0.017(3) | 0.021(4) |
| C(52) | 0.051(3) | 0.136(5) | 0.065(4) | -0.039(3) | 0.009(3) | 0.025(4) |
| C(53) | 0.041(3) | 0.147(5) | 0.085(5) | -0.020(4) | 0.029(3) | -0.012(5) |
| C(54) | 0.038(3) | 0.115(5) | 0.087(5) | 0.006(3) | 0.023(3) | -0.006(4) |
| C(55) | 0.038(3) | 0.085(4) | 0.057(3) | 0.001(2) | 0.017(2) | 0.035(2) |
| C(56) | 0.169(8) | 0.130(7) | 0.151(7) | 0.111(6) | 0.135(7) | 0.084(6) |
| C(57) | 0.168(9) | 0.20(1) | 0.150(7) | 0.140(8) | 0.121(8) | 0.133(8) |
| C(58) | 0.075(5) | 0.129(7) | 0.132(6) | 0.042(4) | 0.051(5) | 0.087(6) |
| C(59) | 0.080(4) | 0.095(5) | 0.052(3) | -0.010(3) | 0.016(3) | 0.031(3) |
| C(60) | 0.069(4) | 0.064(4) | 0.055(3) | 0.003(3) | 0.026(3) | 0.007(2) |
| C(61) | 0.130(7) | 0.080(5) | 0.116(7) | 0.018(5) | 0.078(6) | 0.017(5) |
| C(62) | 0.095(6) | 0.110(6) | 0.072(5) | -0.030(4) | 0.031(4) | 0.009(4) |
| C(63) | 0.094(6) | 0.130(7) | 0.128(8) | 0.011(6) | 0.055(6) | 0.013(6) |

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table S3. Bond Lengths(Å) for **2**·0.5$C_6H_6$

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| Ru(1) | Ru(2) | 2.7481(7) | Ru(1) | S(1) | 2.480(1) |
| Ru(1) | P(1) | 2.364(1) | Ru(1) | P(2) | 2.355(1) |
| Ru(1) | C(1) | 1.841(5) | Ru(1) | C(5) | 2.261(5) |
| Ru(1) | C(6) | 2.309(5) | Ru(2) | S(1) | 2.407(1) |
| Ru(2) | P(1) | 2.300(1) | Ru(2) | P(3) | 2.304(1) |
| Ru(2) | C(2) | 1.833(6) | Ru(2) | C(3) | 2.162(5) |
| Ru(2) | C(4) | 2.294(6) | S(1) | C(3) | 1.768(6) |
| P(1) | C(13) | 1.829(5) | P(1) | C(19) | 1.830(5) |
| P(2) | C(25) | 1.848(5) | P(2) | C(31) | 1.842(5) |
| P(2) | C(37) | 1.840(5) | P(3) | C(43) | 1.827(6) |
| P(3) | C(49) | 1.833(5) | P(3) | C(55) | 1.834(6) |
| O(1) | C(1) | 1.150(6) | O(2) | C(2) | 1.166(7) |
| C(3) | C(4) | 1.405(8) | C(4) | C(5) | 1.457(8) |
| C(5) | C(6) | 1.413(8) | C(6) | C(7) | 1.482(7) |
| C(7) | C(8) | 1.405(8) | C(7) | C(12) | 1.403(8) |
| C(8) | C(9) | 1.380(9) | C(9) | C(10) | 1.359(10) |
| C(10) | C(11) | 1.388(10) | C(11) | C(12) | 1.380(8) |
| C(13) | C(14) | 1.393(8) | C(13) | C(18) | 1.397(8) |
| C(14) | C(15) | 1.377(8) | C(15) | C(16) | 1.389(9) |
| C(16) | C(17) | 1.346(9) | C(17) | C(18) | 1.395(8) |
| C(19) | C(20) | 1.372(8) | C(19) | C(24) | 1.397(8) |
| C(20) | C(21) | 1.396(8) | C(21) | C(22) | 1.35(1) |
| C(22) | C(23) | 1.37(1) | C(23) | C(24) | 1.392(8) |
| C(25) | C(26) | 1.371(8) | C(25) | C(30) | 1.398(7) |
| C(26) | C(27) | 1.395(8) | C(27) | C(28) | 1.370(10) |
| C(28) | C(29) | 1.370(10) | C(29) | C(30) | 1.374(8) |
| C(31) | C(32) | 1.394(8) | C(31) | C(36) | 1.377(8) |
| C(32) | C(33) | 1.376(9) | C(33) | C(34) | 1.37(1) |
| C(34) | C(35) | 1.36(1) | C(35) | C(36) | 1.393(9) |
| C(37) | C(38) | 1.395(8) | C(37) | C(42) | 1.394(8) |
| C(38) | C(39) | 1.371(8) | C(39) | C(40) | 1.36(1) |
| C(40) | C(41) | 1.37(1) | C(41) | C(42) | 1.392(8) |
| C(43) | C(44) | 1.380(8) | C(43) | C(48) | 1.381(8) |
| C(44) | C(45) | 1.367(9) | C(45) | C(46) | 1.38(1) |
| C(46) | C(47) | 1.36(1) | C(47) | C(48) | 1.380(9) |
| C(49) | C(50) | 1.395(9) | C(49) | C(54) | 1.403(8) |
| C(50) | C(51) | 1.396(9) | C(51) | C(52) | 1.37(1) |
| C(52) | C(53) | 1.36(1) | C(53) | C(54) | 1.39(1) |
| C(55) | C(56) | 1.383(9) | C(55) | C(60) | 1.367(8) |
| C(56) | C(57) | 1.40(1) | C(57) | C(58) | 1.35(1) |
| C(58) | C(59) | 1.36(1) | C(59) | C(60) | 1.393(9) |
| C(61) | C(62) | 1.17(1)* | C(61) | C(63)[1)] | 1.45(1) |
| C(62) | C(63) | 1.39(1)* | | | |

* restrained during refinement

Symmetry operations

(1) -X+2,-Y+1,-Z+1

Table S4. Bond Lengths(Å) for **2**·0.5$C_6H_6$

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| C(3) | H(1) | 1.06 | C(4) | H(2) | 0.95(6) |
| C(5) | H(3) | 0.91(6) | C(6) | H(4) | 1.07(6) |
| C(8) | H(5) | 0.94 | C(9) | H(6) | 0.94 |
| C(10) | H(7) | 0.95 | C(11) | H(8) | 0.94 |
| C(12) | H(9) | 0.95 | C(14) | H(10) | 0.94 |
| C(15) | H(11) | 0.95 | C(16) | H(12) | 0.93 |
| C(17) | H(13) | 0.94 | C(18) | H(14) | 0.93 |
| C(20) | H(15) | 0.95 | C(21) | H(16) | 0.93 |
| C(22) | H(17) | 0.94 | C(23) | H(18) | 0.94 |
| C(24) | H(19) | 0.94 | C(26) | H(20) | 0.93 |
| C(27) | H(21) | 0.93 | C(28) | H(22) | 0.94 |
| C(29) | H(23) | 0.93 | C(30) | H(24) | 0.93 |
| C(32) | H(25) | 0.94 | C(33) | H(26) | 0.93 |
| C(34) | H(27) | 0.93 | C(35) | H(28) | 0.95 |
| C(36) | H(29) | 0.95 | C(38) | H(30) | 0.94 |
| C(39) | H(31) | 0.94 | C(40) | H(32) | 0.94 |
| C(41) | H(33) | 0.94 | C(42) | H(34) | 0.92 |
| C(44) | H(35) | 0.94 | C(45) | H(36) | 0.95 |
| C(46) | H(37) | 0.95 | C(47) | H(38) | 0.95 |
| C(48) | H(39) | 0.94 | C(50) | H(40) | 0.93 |
| C(51) | H(41) | 0.93 | C(52) | H(42) | 0.94 |
| C(53) | H(43) | 0.94 | C(54) | H(44) | 0.93 |
| C(56) | H(45) | 0.93 | C(57) | H(46) | 0.93 |
| C(58) | H(47) | 0.93 | C(59) | H(48) | 0.93 |
| C(60) | H(49) | 0.93 | C(61) | H(50) | 0.95 |
| C(62) | H(51) | 0.95 | C(63) | H(52) | 0.93 |

* restrained during refinement

Table S5. Bond Angles(°) for **2**·0.5$C_6H_6$

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| Ru(2) | Ru(1) | S(1) | 54.53(3) | Ru(2) | Ru(1) | P(1) | 52.82(3) |
| Ru(2) | Ru(1) | P(2) | 153.53(4) | Ru(2) | Ru(1) | C(1) | 109.9(2) |
| Ru(2) | Ru(1) | C(5) | 69.7(1) | Ru(2) | Ru(1) | C(6) | 101.9(1) |
| S(1) | Ru(1) | P(1) | 79.81(4) | S(1) | Ru(1) | P(2) | 105.94(5) |
| S(1) | Ru(1) | C(1) | 164.3(2) | S(1) | Ru(1) | C(5) | 81.2(1) |
| S(1) | Ru(1) | C(6) | 86.7(1) | P(1) | Ru(1) | P(2) | 110.62(5) |
| P(1) | Ru(1) | C(1) | 92.0(2) | P(1) | Ru(1) | C(5) | 119.8(2) |
| P(1) | Ru(1) | C(6) | 154.6(1) | P(2) | Ru(1) | C(1) | 89.5(2) |
| P(2) | Ru(1) | C(5) | 129.5(2) | P(2) | Ru(1) | C(6) | 93.7(1) |
| C(1) | Ru(1) | C(5) | 91.5(2) | C(1) | Ru(1) | C(6) | 95.6(2) |
| C(5) | Ru(1) | C(6) | 36.0(2) | Ru(1) | Ru(2) | S(1) | 57.05(3) |
| Ru(1) | Ru(2) | P(1) | 54.98(3) | Ru(1) | Ru(2) | P(3) | 152.12(4) |
| Ru(1) | Ru(2) | C(2) | 114.4(2) | Ru(1) | Ru(2) | C(3) | 81.8(1) |
| Ru(1) | Ru(2) | C(4) | 73.8(2) | S(1) | Ru(2) | P(1) | 82.63(4) |
| S(1) | Ru(2) | P(3) | 99.95(5) | S(1) | Ru(2) | C(2) | 165.9(2) |
| S(1) | Ru(2) | C(3) | 45.1(1) | S(1) | Ru(2) | C(4) | 71.0(2) |
| P(1) | Ru(2) | P(3) | 111.03(5) | P(1) | Ru(2) | C(2) | 101.6(2) |
| P(1) | Ru(2) | C(3) | 126.4(1) | P(1) | Ru(2) | C(4) | 128.7(2) |
| P(3) | Ru(2) | C(2) | 91.1(2) | P(3) | Ru(2) | C(3) | 92.3(1) |
| P(3) | Ru(2) | C(4) | 116.3(2) | C(2) | Ru(2) | C(3) | 126.4(2) |
| C(2) | Ru(2) | C(4) | 96.4(2) | C(3) | Ru(2) | C(4) | 36.6(2) |
| Ru(1) | S(1) | Ru(2) | 68.42(3) | Ru(1) | S(1) | C(3) | 98.2(2) |
| Ru(2) | S(1) | C(3) | 60.1(2) | Ru(1) | P(1) | Ru(2) | 72.20(4) |
| Ru(1) | P(1) | C(13) | 120.7(2) | Ru(1) | P(1) | C(19) | 122.7(2) |
| Ru(2) | P(1) | C(13) | 113.8(2) | Ru(2) | P(1) | C(19) | 124.6(2) |
| C(13) | P(1) | C(19) | 102.2(2) | Ru(1) | P(2) | C(25) | 116.3(2) |
| Ru(1) | P(2) | C(31) | 117.0(2) | Ru(1) | P(2) | C(37) | 116.8(2) |
| C(25) | P(2) | C(31) | 98.7(2) | C(25) | P(2) | C(37) | 103.4(2) |
| C(31) | P(2) | C(37) | 102.1(2) | Ru(2) | P(3) | C(43) | 113.2(2) |
| Ru(2) | P(3) | C(49) | 117.0(2) | Ru(2) | P(3) | C(55) | 118.1(2) |
| C(43) | P(3) | C(49) | 101.7(2) | C(43) | P(3) | C(55) | 104.1(3) |
| C(49) | P(3) | C(55) | 100.5(3) | Ru(1) | C(1) | O(1) | 178.7(5) |
| Ru(2) | C(2) | O(2) | 175.0(6) | Ru(2) | C(3) | S(1) | 74.8(2) |
| Ru(2) | C(3) | C(4) | 76.8(3) | S(1) | C(3) | C(4) | 118.4(4) |
| Ru(2) | C(4) | C(3) | 66.6(3) | Ru(2) | C(4) | C(5) | 98.4(4) |
| C(3) | C(4) | C(5) | 122.7(5) | Ru(1) | C(5) | C(4) | 108.2(4) |
| Ru(1) | C(5) | C(6) | 73.8(3) | C(4) | C(5) | C(6) | 128.3(5) |
| Ru(1) | C(6) | C(5) | 70.2(3) | Ru(1) | C(6) | C(7) | 123.7(4) |
| C(5) | C(6) | C(7) | 130.4(5) | C(6) | C(7) | C(8) | 116.6(5) |
| C(6) | C(7) | C(12) | 127.8(5) | C(8) | C(7) | C(12) | 115.5(5) |
| C(7) | C(8) | C(9) | 121.7(6) | C(8) | C(9) | C(10) | 121.6(6) |
| C(9) | C(10) | C(11) | 118.6(6) | C(10) | C(11) | C(12) | 120.4(6) |
| C(7) | C(12) | C(11) | 122.2(6) | P(1) | C(13) | C(14) | 121.9(4) |
| P(1) | C(13) | C(18) | 120.5(4) | C(14) | C(13) | C(18) | 117.4(5) |
| C(13) | C(14) | C(15) | 121.8(5) | C(14) | C(15) | C(16) | 119.7(6) |
| C(15) | C(16) | C(17) | 119.4(5) | C(16) | C(17) | C(18) | 121.8(6) |
| C(13) | C(18) | C(17) | 119.9(5) | P(1) | C(19) | C(20) | 120.8(4) |
| P(1) | C(19) | C(24) | 122.0(4) | C(20) | C(19) | C(24) | 117.0(5) |
| C(19) | C(20) | C(21) | 121.7(6) | C(20) | C(21) | C(22) | 120.3(6) |
| C(21) | C(22) | C(23) | 120.0(6) | C(22) | C(23) | C(24) | 120.0(7) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C(19) | C(24) | C(23) | 121.0(6) | P(2) | C(25) | C(26) | 120.3(4) |
| P(2) | C(25) | C(30) | 120.8(4) | C(26) | C(25) | C(30) | 118.9(5) |
| C(25) | C(26) | C(27) | 120.7(5) | C(26) | C(27) | C(28) | 119.8(6) |
| C(27) | C(28) | C(29) | 119.7(6) | C(28) | C(29) | C(30) | 121.1(6) |
| C(25) | C(30) | C(29) | 119.7(6) | P(2) | C(31) | C(32) | 117.1(4) |
| P(2) | C(31) | C(36) | 124.2(4) | C(32) | C(31) | C(36) | 118.6(5) |
| C(31) | C(32) | C(33) | 120.2(6) | C(32) | C(33) | C(34) | 121.0(6) |
| C(33) | C(34) | C(35) | 119.3(6) | C(34) | C(35) | C(36) | 120.6(7) |
| C(31) | C(36) | C(35) | 120.2(6) | P(2) | C(37) | C(38) | 118.1(4) |
| P(2) | C(37) | C(42) | 122.3(4) | C(38) | C(37) | C(42) | 119.6(5) |
| C(37) | C(38) | C(39) | 120.4(6) | C(38) | C(39) | C(40) | 119.9(7) |
| C(39) | C(40) | C(41) | 120.7(6) | C(40) | C(41) | C(42) | 121.0(7) |
| C(37) | C(42) | C(41) | 118.4(6) | P(3) | C(43) | C(44) | 119.9(4) |
| P(3) | C(43) | C(48) | 122.7(5) | C(44) | C(43) | C(48) | 117.3(5) |
| C(43) | C(44) | C(45) | 122.0(6) | C(44) | C(45) | C(46) | 119.3(7) |
| C(45) | C(46) | C(47) | 120.3(6) | C(46) | C(47) | C(48) | 119.7(6) |
| C(43) | C(48) | C(47) | 121.4(6) | P(3) | C(49) | C(50) | 120.8(4) |
| P(3) | C(49) | C(54) | 120.1(5) | C(50) | C(49) | C(54) | 119.1(6) |
| C(49) | C(50) | C(51) | 120.5(6) | C(50) | C(51) | C(52) | 119.7(8) |
| C(51) | C(52) | C(53) | 120.1(7) | C(52) | C(53) | C(54) | 122.3(7) |
| C(49) | C(54) | C(53) | 118.2(8) | P(3) | C(55) | C(56) | 123.5(5) |
| P(3) | C(55) | C(60) | 119.5(5) | C(56) | C(55) | C(60) | 117.0(6) |
| C(55) | C(56) | C(57) | 122.2(8) | C(56) | C(57) | C(58) | 119.1(8) |
| C(57) | C(58) | C(59) | 119.8(7) | C(58) | C(59) | C(60) | 121.1(7) |
| C(55) | C(60) | C(59) | 120.6(7) | C(62) | C(61) | C(63)[1)] | 118.9(9) |
| C(61) | C(62) | C(63) | 119.0(9)* | C(61)[1)] | C(63) | C(62) | 121.9(8) |

* restrained during refinement

Symmetry operations

(1) -X+2,-Y+1,-Z+1

Table S 6. Bond Angles(°) for **2**·0.5$C_6H_6$

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| Ru(2) | C(3) | H(1) | 116.0 | S(1) | C(3) | H(1) | 122.2 |
| C(4) | C(3) | H(1) | 119.4 | Ru(2) | C(4) | H(2) | 113(3) |
| C(3) | C(4) | H(2) | 118(3) | C(5) | C(4) | H(2) | 118(3) |
| Ru(1) | C(5) | H(3) | 108(3) | C(4) | C(5) | H(3) | 109(3) |
| C(6) | C(5) | H(3) | 118(3) | Ru(1) | C(6) | H(4) | 102(2) |
| C(5) | C(6) | H(4) | 109(2) | C(7) | C(6) | H(4) | 111(2) |
| C(7) | C(8) | H(5) | 119.6 | C(9) | C(8) | H(5) | 118.7 |
| C(8) | C(9) | H(6) | 120.2 | C(10) | C(9) | H(6) | 118.2 |
| C(9) | C(10) | H(7) | 121.1 | C(11) | C(10) | H(7) | 120.3 |
| C(10) | C(11) | H(8) | 118.8 | C(12) | C(11) | H(8) | 120.8 |
| C(7) | C(12) | H(9) | 119.2 | C(11) | C(12) | H(9) | 118.5 |
| C(13) | C(14) | H(10) | 119.3 | C(15) | C(14) | H(10) | 118.9 |
| C(14) | C(15) | H(11) | 119.7 | C(16) | C(15) | H(11) | 120.5 |
| C(15) | C(16) | H(12) | 119.7 | C(17) | C(16) | H(12) | 120.9 |
| C(16) | C(17) | H(13) | 119.1 | C(18) | C(17) | H(13) | 119.1 |
| C(13) | C(18) | H(14) | 119.7 | C(17) | C(18) | H(14) | 120.5 |
| C(19) | C(20) | H(15) | 119.2 | C(21) | C(20) | H(15) | 119.1 |
| C(20) | C(21) | H(16) | 118.9 | C(22) | C(21) | H(16) | 120.7 |
| C(21) | C(22) | H(17) | 120.7 | C(23) | C(22) | H(17) | 119.2 |
| C(22) | C(23) | H(18) | 120.8 | C(24) | C(23) | H(18) | 119.2 |
| C(19) | C(24) | H(19) | 119.6 | C(23) | C(24) | H(19) | 119.4 |
| C(25) | C(26) | H(20) | 119.4 | C(27) | C(26) | H(20) | 119.8 |
| C(26) | C(27) | H(21) | 119.8 | C(28) | C(27) | H(21) | 120.4 |
| C(27) | C(28) | H(22) | 119.1 | C(29) | C(28) | H(22) | 121.2 |
| C(28) | C(29) | H(23) | 118.4 | C(30) | C(29) | H(23) | 120.5 |
| C(25) | C(30) | H(24) | 120.5 | C(29) | C(30) | H(24) | 119.8 |
| C(31) | C(32) | H(25) | 120.4 | C(33) | C(32) | H(25) | 119.4 |
| C(32) | C(33) | H(26) | 119.9 | C(34) | C(33) | H(26) | 119.1 |
| C(33) | C(34) | H(27) | 121.1 | C(35) | C(34) | H(27) | 119.5 |
| C(34) | C(35) | H(28) | 119.8 | C(36) | C(35) | H(28) | 119.5 |
| C(31) | C(36) | H(29) | 120.0 | C(35) | C(36) | H(29) | 119.8 |
| C(37) | C(38) | H(30) | 119.2 | C(39) | C(38) | H(30) | 120.4 |
| C(38) | C(39) | H(31) | 119.7 | C(40) | C(39) | H(31) | 120.4 |
| C(39) | C(40) | H(32) | 118.9 | C(41) | C(40) | H(32) | 120.4 |
| C(40) | C(41) | H(33) | 120.0 | C(42) | C(41) | H(33) | 119.0 |
| C(37) | C(42) | H(34) | 119.7 | C(41) | C(42) | H(34) | 121.9 |
| C(43) | C(44) | H(35) | 119.3 | C(45) | C(44) | H(35) | 118.6 |
| C(44) | C(45) | H(36) | 121.4 | C(46) | C(45) | H(36) | 119.3 |
| C(45) | C(46) | H(37) | 120.5 | C(47) | C(46) | H(37) | 119.2 |
| C(46) | C(47) | H(38) | 120.3 | C(48) | C(47) | H(38) | 119.9 |
| C(43) | C(48) | H(39) | 119.6 | C(47) | C(48) | H(39) | 119.0 |
| C(49) | C(50) | H(40) | 119.0 | C(51) | C(50) | H(40) | 120.5 |
| C(50) | C(51) | H(41) | 120.4 | C(52) | C(51) | H(41) | 119.9 |
| C(51) | C(52) | H(42) | 120.0 | C(53) | C(52) | H(42) | 119.8 |
| C(52) | C(53) | H(43) | 119.8 | C(54) | C(53) | H(43) | 117.9 |
| C(49) | C(54) | H(44) | 120.3 | C(53) | C(54) | H(44) | 121.5 |
| C(55) | C(56) | H(45) | 117.4 | C(57) | C(56) | H(45) | 120.4 |
| C(56) | C(57) | H(46) | 119.6 | C(58) | C(57) | H(46) | 121.3 |
| C(57) | C(58) | H(47) | 121.8 | C(59) | C(58) | H(47) | 118.4 |
| C(58) | C(59) | H(48) | 120.3 | C(60) | C(59) | H(48) | 118.7 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C(55) | C(60) | H(49) | 119.7 | C(59) | C(60) | H(49) | 119.8 |
| C(62) | C(61) | H(50) | 119.7 | C(63)[1)] | C(61) | H(50) | 121.4 |
| C(61) | C(62) | H(51) | 121.6 | C(63) | C(62) | H(51) | 119.4 |
| C(61)[1)] | C(63) | H(52) | 118.6 | C(62) | C(63) | H(52) | 119.5 |

* restrained during refinement

Symmetry operations

(1) -X+2,-Y+1,-Z+1

## Crystallographic Data and Details of Refinement of **5**

*Experimental*

### Data Collection

An orange prismatic crystal of $C_{60}H_{49}O_2P_3Ru_2S$ having approximate dimensions of 0.20 x 0.08 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7S diffractometer with graphite monochromated Mo-Kα radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range $25.79 < 2\theta < 29.58^o$ corresponded to a primitive triclinic cell with dimensions:

| | | | |
|---|---|---|---|
| a = | 12.879(2) Å | α = | 97.72(1)° |
| b = | 19.454(4) Å | β = | 104.757(10)° |
| c = | 11.121(1) Å | γ = | 103.20(2)° |
| V = 2567.7(7) Å$^3$ | | | |

For Z = 2 and F.W. = 1129.17, the calculated density is 1.46 g/cm$^3$. Based on a statistical analysis of intensity distribution,and the successful solution and refinement of thestructure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of 23 ± 1°C using the ω-2θ scan technique to a maximum 2θ value of 55.0°.Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.27° with a take-off angle of 6.0°. Scans of $(0.84 + 0.30 \tan \theta)^o$ were made at a speed of 16.0°/min (in omega). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 5 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm and the crystal to detector distance was 235 mm, The computer-controlled slits were set to 9.0 mm (horizontal) and 13.0 mm (vertical).

### Data Reduction

Of the 12311 reflections which were collected, 11787 were unique ($R_{int}$ = 0.039). The intensities of three representative reflection were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 7.7 cm$^{-1}$. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.91 to 1.00.

### Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. The final cycle of full-matrix least-squares refinement[3] was based on 11787 all reflections ($2\theta < 54.99$) and 619 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma (Fo^2 - Fc^2) / \Sigma Fo^2 = 0.073$$

$$R_W = [( \Sigma w (Fo^2 - Fc^2)^2 / \Sigma w (Fo^2)^2)]^{1/2} = 0.107$$

$$R1 = \Sigma ||Fo| - |Fc|| / \Sigma |Fo| = 0.037 \quad \text{for } I > 2.0\sigma(I) \text{ data}$$

The standard deviation of an observation of unit weight[4] was 1.01. The weighting scheme was based on counting statistics and included a factor (p = 0.041) to downweight the intense reflections. Plots of $\Sigma$ w $(Fo^2 - Fc^2)^2$ versus $Fo^2$reflection order in data collection, sin $\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.88 and -0.96 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

*References*

(1) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G., (1994). J. Appl. Cryst. 27, 435.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma\, w(F_o^2-F_c^2)^2$ where

$w = 1/[\sigma^2(Fo^2)] = [\sigma^2_c(Fo^2) + (p\,(Max(Fo^2,0)+2Fc^2)/3)^2]^{-1}$

$\sigma_c(Fo^2)$ = e.s.d. based on counting statistics

$p$ = p-factor

(4) Standard deviation of an observation of unit weight:

$[\Sigma\, w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: $N_o$ = number of observations

$N_v$ = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1999).

*EXPERIMENTAL DETAILS*

A. Crystal Data

| | |
|---|---|
| Empirical Formula | $C_{60}H_{49}O_2P_3Ru_2S$ |
| Formula Weight | 1129.17 |
| Crystal Color, Habit | orange, prismatic |
| Crystal Dimensions | 0.20 X 0.08 X 0.20 mm |
| Crystal System | triclinic |
| Lattice Type | Primitive |
| No. of Reflections Used for Unit Cell Determination (2θ range) | 25 ( 25.8 - 29.6° ) |
| Omega Scan Peak Width at Half-height | 0.27° |
| Lattice Parameters | a = 12.879(2) Å<br>b = 19.454(4) Å<br>c = 11.121(1) Å<br>α = 97.72(1)°<br>β = 104.757(10)°<br>γ = 103.20(2)°<br>V = 2567.7(7) Å$^3$ |
| Space Group | P-1 (#2) |
| Z value | 2 |
| $D_{calc}$ | 1.460 g/cm$^3$ |
| $F_{000}$ | 1148.00 |
| μ(MoKα) | 7.66 cm$^{-1}$ |

B. Intensity Measurements

| | |
|---|---|
| Diffractometer | Rigaku AFC7S (sealed tube) |

| | |
|---|---|
| Radiation | MoKα (λ = 0.71069 Å)<br>graphite monochromated |
| Attenuator | Zr foil (factor = 8.58) |
| Temperature | 23.0 °C |
| Collimator Size | 1.0 mm |
| Take-off Angle | 6.0° |
| Detector Aperture | 9.0 mm horizontal<br>13.0 mm vertical |
| Crystal to Detector Distance | 235 mm |
| Scan Type | ω-2θ |
| Scan Rate | 16.0°/min (in ω) (up to 5 scans) |
| Scan Width | (0.84 + 0.30 tan θ)° |
| $2\theta_{max}$ | 55.0° |
| No. of Reflections Measured | Total: 12311<br>Unique: 11787 ($R_{int}$ = 0.039) |
| Corrections | Lorentz-polarization<br>Absorption<br>(trans. factors: 0.9121 - 0.9991) |

C. Structure Solution and Refinement

| | |
|---|---|
| Structure Solution | Direct Methods (SIR92) |
| Refinement | Full-matrix least-squares |
| Function Minimized | $\Sigma w (Fo^2 - Fc^2)^2$ |
| Least Squares Weights | $1/\sigma^2(Fo^2)$ |
| p-factor | 0.0410 |
| Anomalous Dispersion | All non-hydrogen atoms |
| No. of Reflections (All, $2\sigma < 54.99°$) | 11787 |
| No. Variables | 619 |
| Reflection/Parameter Ratio | 19.04 |

| | |
|---|---|
| Residuals: R; Rw | 0.073 ; 0.107 |
| Residuals: R1 | 0.037 |
| No. of Reflections to calc R1 | 7618 |
| Goodness of Fit Indicator | 1.01 |
| Max Shift/Error in Final Cycle | 0.003 |
| Maximum peak in Final Diff. Map | 0.88 $e^-/Å^3$ |
| Minimum peak in Final Diff. Map | -0.96 $e^-/Å^3$ |

Table S7. Atomic coordinates and $B_{iso}/B_{eq}$ for **5**

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| Ru(1) | 0.76248(2) | 0.34109(2) | 0.71960(3) | 2.257(6) |
| Ru(2) | 0.87187(2) | 0.23453(2) | 0.73915(3) | 2.494(6) |
| S(1) | 0.86077(8) | 0.31323(5) | 0.91928(9) | 2.87(2) |
| P(1) | 0.68149(8) | 0.21523(5) | 0.67052(9) | 2.42(2) |
| P(2) | 0.64647(8) | 0.40160(5) | 0.79636(10) | 2.62(2) |
| P(3) | 0.91269(8) | 0.13665(6) | 0.8175(1) | 2.92(2) |
| O(1) | 0.6491(3) | 0.3471(2) | 0.4523(3) | 5.22(9) |
| O(2) | 0.9366(3) | 0.1883(2) | 0.5069(3) | 5.7(1) |
| C(1) | 0.6944(3) | 0.3461(2) | 0.5557(4) | 3.23(9) |
| C(2) | 0.9077(3) | 0.2033(2) | 0.5944(4) | 3.38(9) |
| C(3) | 0.9913(3) | 0.3206(2) | 0.8925(4) | 3.50(9) |
| C(4) | 1.0053(3) | 0.3400(2) | 0.7836(5) | 3.50(9) |
| C(5) | 0.9369(3) | 0.3800(2) | 0.7111(4) | 3.1325 |
| C(6) | 0.9083(3) | 0.4400(2) | 0.7692(4) | 2.83(8) |
| C(7) | 0.9051(3) | 0.5038(2) | 0.7122(4) | 3.15(8) |
| C(8) | 0.9284(4) | 0.5706(2) | 0.7901(4) | 3.73(10) |
| C(9) | 0.9394(4) | 0.6336(2) | 0.7448(5) | 4.9(1) |
| C(10) | 0.9270(5) | 0.6316(3) | 0.6186(6) | 5.4(1) |
| C(11) | 0.9006(4) | 0.5663(3) | 0.5380(5) | 5.0(1) |
| C(12) | 0.8899(4) | 0.5030(2) | 0.5833(4) | 3.79(10) |
| C(13) | 0.5942(3) | 0.1718(2) | 0.5090(4) | 2.79(8) |
| C(14) | 0.4810(3) | 0.1398(2) | 0.4801(4) | 3.60(9) |
| C(15) | 0.4134(4) | 0.1130(3) | 0.3556(5) | 4.6(1) |
| C(16) | 0.4611(4) | 0.1187(3) | 0.2588(4) | 4.7(1) |
| C(17) | 0.5734(4) | 0.1505(3) | 0.2851(4) | 4.6(1) |
| C(18) | 0.6401(4) | 0.1770(2) | 0.4089(4) | 3.71(10) |
| C(19) | 0.6060(3) | 0.1691(2) | 0.7676(4) | 2.73(8) |
| C(20) | 0.5910(3) | 0.2075(2) | 0.8724(4) | 3.26(9) |
| C(21) | 0.5400(4) | 0.1742(3) | 0.9528(5) | 4.4(1) |
| C(22) | 0.5023(4) | 0.1010(3) | 0.9278(5) | 5.0(1) |
| C(23) | 0.5159(4) | 0.0608(3) | 0.8251(5) | 4.7(1) |
| C(24) | 0.5681(4) | 0.0941(2) | 0.7456(4) | 3.81(10) |
| C(25) | 0.4939(3) | 0.3645(2) | 0.7289(4) | 3.03(8) |
| C(26) | 0.4487(3) | 0.2991(2) | 0.6448(5) | 3.92(10) |
| C(27) | 0.3335(4) | 0.2715(3) | 0.5944(5) | 4.9(1) |
| C(28) | 0.2641(4) | 0.3087(3) | 0.6311(5) | 5.0(1) |
| C(29) | 0.3085(4) | 0.3744(3) | 0.7135(6) | 5.2(1) |
| C(30) | 0.4222(4) | 0.4019(3) | 0.7618(5) | 4.4(1) |
| C(31) | 0.6681(3) | 0.4108(2) | 0.9681(4) | 3.02(8) |
| C(32) | 0.7740(3) | 0.4462(3) | 1.0504(4) | 3.78(10) |
| C(33) | 0.7955(4) | 0.4541(3) | 1.1791(4) | 4.6(1) |
| C(34) | 0.7126(5) | 0.4263(3) | 1.2296(4) | 5.3(1) |
| C(35) | 0.6084(4) | 0.3890(3) | 1.1502(5) | 5.4(1) |
| C(36) | 0.5857(4) | 0.3823(3) | 1.0205(4) | 3.94(10) |
| C(37) | 0.6569(3) | 0.4948(2) | 0.7740(4) | 3.34(9) |
| C(38) | 0.6796(4) | 0.5523(2) | 0.8731(5) | 4.7(1) |
| C(39) | 0.6824(6) | 0.6208(3) | 0.8468(7) | 6.4(2) |
| C(40) | 0.6597(5) | 0.6308(3) | 0.7242(7) | 6.2(2) |
| C(41) | 0.6365(4) | 0.5739(3) | 0.6261(5) | 5.1(1) |
| C(42) | 0.6364(4) | 0.5062(2) | 0.6508(5) | 4.2(1) |

| | | | | |
|---|---|---|---|---|
| C(43) | 0.8490(3) | 0.1029(2) | 0.9358(4) | 3.30(9) |
| C(44) | 0.8199(4) | 0.0307(3) | 0.9417(5) | 4.3(1) |
| C(45) | 0.7842(4) | 0.0092(3) | 1.0415(5) | 5.0(1) |
| C(46) | 0.7782(5) | 0.0585(3) | 1.1360(6) | 5.5(1) |
| C(47) | 0.8066(5) | 0.1304(3) | 1.1330(5) | 5.3(1) |
| C(48) | 0.8407(4) | 0.1524(3) | 1.0325(5) | 4.6(1) |
| C(49) | 1.0622(3) | 0.1566(2) | 0.9036(4) | 3.24(9) |
| C(50) | 1.1009(4) | 0.1539(3) | 1.0300(5) | 4.3(1) |
| C(51) | 1.2147(5) | 0.1750(3) | 1.0916(5) | 5.3(1) |
| C(52) | 1.2894(4) | 0.1970(3) | 1.0283(6) | 5.3(1) |
| C(53) | 1.2527(4) | 0.1997(3) | 0.9032(6) | 5.1(1) |
| C(54) | 1.1397(4) | 0.1800(3) | 0.8405(5) | 4.3(1) |
| C(55) | 0.8881(4) | 0.0547(2) | 0.6968(4) | 3.9(1) |
| C(56) | 0.8018(4) | 0.0393(3) | 0.5867(5) | 4.4(1) |
| C(57) | 0.7837(5) | -0.0205(3) | 0.4931(5) | 5.6(1) |
| C(58) | 0.8525(6) | -0.0648(3) | 0.5107(7) | 7.1(2) |
| C(59) | 0.9376(6) | -0.0515(3) | 0.6218(8) | 7.0(2) |
| C(60) | 0.9555(5) | 0.0080(3) | 0.7137(6) | 5.4(1) |
| H(1) | 1.047(4) | 0.310(2) | 0.951(4) | 4.1 |
| H(2) | 1.071(4) | 0.338(2) | 0.765(4) | 4.3 |
| H(3) | 0.934(3) | 0.377(2) | 0.627(4) | 3.8 |
| H(4) | 0.937(3) | 0.452(2) | 0.850(4) | 3.3 |
| H(5) | 0.9369 | 0.5730 | 0.8803 | 4.4 |
| H(6) | 0.9562 | 0.6797 | 0.8021 | 5.6 |
| H(7) | 0.9365 | 0.6762 | 0.5867 | 6.0 |
| H(8) | 0.8894 | 0.5650 | 0.4476 | 5.7 |
| H(9) | 0.8705 | 0.4573 | 0.5245 | 4.5 |
| H(10) | 0.4470 | 0.1355 | 0.5491 | 4.2 |
| H(11) | 0.3344 | 0.0897 | 0.3365 | 5.3 |
| H(12) | 0.4159 | 0.0992 | 0.1713 | 5.3 |
| H(13) | 0.6053 | 0.1558 | 0.2154 | 5.3 |
| H(14) | 0.7193 | 0.1996 | 0.4258 | 4.3 |
| H(15) | 0.6183 | 0.2602 | 0.8914 | 3.8 |
| H(16) | 0.5309 | 0.2024 | 1.0263 | 5.2 |
| H(17) | 0.4661 | 0.0765 | 0.9826 | 5.7 |
| H(18) | 0.4872 | 0.0078 | 0.8064 | 5.4 |
| H(19) | 0.5778 | 0.0653 | 0.6722 | 4.4 |
| H(20) | 0.4976 | 0.2725 | 0.6189 | 4.5 |
| H(21) | 0.3016 | 0.2259 | 0.5315 | 5.7 |
| H(22) | 0.1837 | 0.2878 | 0.5991 | 5.9 |
| H(23) | 0.2581 | 0.4008 | 0.7386 | 6.0 |
| H(24) | 0.4535 | 0.4491 | 0.8199 | 5.2 |
| H(25) | 0.8343 | 0.4664 | 1.0161 | 4.4 |
| H(26) | 0.8698 | 0.4800 | 1.2365 | 5.1 |
| H(27) | 0.7287 | 0.4319 | 1.3208 | 5.9 |
| H(28) | 0.5508 | 0.3679 | 1.1859 | 6.0 |
| H(29) | 0.5111 | 0.3562 | 0.9657 | 4.5 |
| H(30) | 0.6957 | 0.5455 | 0.9609 | 5.6 |
| H(31) | 0.6986 | 0.6622 | 0.9145 | 7.4 |
| H(32) | 0.6606 | 0.6785 | 0.7072 | 6.8 |
| H(33) | 0.6220 | 0.5816 | 0.5390 | 5.8 |
| H(34) | 0.6206 | 0.4660 | 0.5800 | 4.9 |
| H(35) | 0.8246 | -0.0059 | 0.8759 | 5.2 |

| | | | | |
|---|---|---|---|---|
| H(36) | 0.7616 | -0.0415 | 1.0436 | 5.6 |
| H(37) | 0.7548 | 0.0429 | 1.2076 | 6.2 |
| H(38) | 0.8017 | 0.1660 | 1.2010 | 6.1 |
| H(39) | 0.8596 | 0.2030 | 1.0313 | 5.3 |
| H(40) | 1.0479 | 0.1360 | 1.0760 | 5.1 |
| H(41) | 1.2418 | 0.1748 | 1.1817 | 6.0 |
| H(42) | 1.3689 | 0.2120 | 1.0758 | 6.1 |
| H(43) | 1.3076 | 0.2156 | 0.8592 | 6.0 |
| H(44) | 1.1144 | 0.1820 | 0.7499 | 5.2 |
| H(45) | 0.7513 | 0.0697 | 0.5739 | 5.1 |
| H(46) | 0.7207 | -0.0303 | 0.4147 | 6.5 |
| H(47) | 0.8395 | -0.1059 | 0.4423 | 8.1 |
| H(48) | 0.9828 | -0.0850 | 0.6315 | 7.7 |
| H(49) | 1.0154 | 0.0167 | 0.7926 | 6.3 |

$B_{eq} = 8/3\ PI^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S8. Anisotropic Displacement Parameters for **5**

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| Ru(1) | 0.0261(1) | 0.0312(2) | 0.0285(2) | 0.0071(1) | 0.0085(1) | 0.0067(1) |
| Ru(2) | 0.0285(2) | 0.0340(2) | 0.0334(2) | 0.0104(1) | 0.0101(1) | 0.0056(1) |
| S(1) | 0.0372(5) | 0.0389(5) | 0.0316(5) | 0.0140(4) | 0.0056(4) | 0.0051(4) |
| P(1) | 0.0287(5) | 0.0334(5) | 0.0284(5) | 0.0059(4) | 0.0086(4) | 0.0053(4) |
| P(2) | 0.0296(5) | 0.0351(5) | 0.0360(5) | 0.0105(4) | 0.0101(4) | 0.0074(4) |
| P(3) | 0.0361(5) | 0.0364(5) | 0.0407(6) | 0.0134(4) | 0.0124(4) | 0.0072(4) |
| O(1) | 0.081(2) | 0.066(2) | 0.041(2) | 0.015(2) | 0.001(2) | 0.020(2) |
| O(2) | 0.090(3) | 0.086(3) | 0.063(2) | 0.034(2) | 0.051(2) | 0.015(2) |
| C(1) | 0.045(2) | 0.042(2) | 0.037(2) | 0.009(2) | 0.013(2) | 0.013(2) |
| C(2) | 0.043(2) | 0.047(2) | 0.046(2) | 0.016(2) | 0.021(2) | 0.014(2) |
| C(3) | 0.032(2) | 0.045(2) | 0.049(3) | 0.012(2) | 0.003(2) | 0.002(2) |
| C(4) | 0.026(2) | 0.040(2) | 0.067(3) | 0.008(2) | 0.017(2) | 0.008(2) |
| C(5) | 0.0307 | 0.0395 | 0.0487 | 0.0023 | 0.0163 | 0.0128 |
| C(6) | 0.030(2) | 0.036(2) | 0.035(2) | 0.002(2) | 0.007(2) | 0.003(2) |
| C(7) | 0.028(2) | 0.045(2) | 0.045(2) | 0.005(2) | 0.010(2) | 0.011(2) |
| C(8) | 0.052(3) | 0.036(2) | 0.045(2) | 0.008(2) | 0.004(2) | 0.008(2) |
| C(9) | 0.071(3) | 0.038(2) | 0.062(3) | 0.009(2) | 0.003(3) | 0.009(2) |
| C(10) | 0.075(4) | 0.046(3) | 0.076(4) | 0.005(3) | 0.008(3) | 0.030(3) |
| C(11) | 0.066(3) | 0.072(3) | 0.053(3) | 0.013(3) | 0.018(2) | 0.029(3) |
| C(12) | 0.049(2) | 0.050(3) | 0.044(2) | 0.008(2) | 0.016(2) | 0.008(2) |
| C(13) | 0.034(2) | 0.033(2) | 0.037(2) | 0.009(2) | 0.008(2) | 0.006(2) |
| C(14) | 0.037(2) | 0.052(3) | 0.041(2) | 0.004(2) | 0.008(2) | 0.002(2) |
| C(15) | 0.041(2) | 0.070(3) | 0.045(3) | 0.000(2) | -0.003(2) | 0.002(2) |
| C(16) | 0.056(3) | 0.071(3) | 0.035(2) | 0.013(2) | -0.002(2) | -0.007(2) |
| C(17) | 0.059(3) | 0.086(4) | 0.031(2) | 0.019(3) | 0.015(2) | 0.009(2) |
| C(18) | 0.042(2) | 0.059(3) | 0.039(2) | 0.013(2) | 0.012(2) | 0.008(2) |
| C(19) | 0.031(2) | 0.040(2) | 0.035(2) | 0.010(2) | 0.010(2) | 0.015(2) |
| C(20) | 0.042(2) | 0.048(2) | 0.040(2) | 0.017(2) | 0.016(2) | 0.013(2) |
| C(21) | 0.053(3) | 0.069(3) | 0.054(3) | 0.017(2) | 0.030(2) | 0.021(2) |
| C(22) | 0.062(3) | 0.078(4) | 0.061(3) | 0.012(3) | 0.036(3) | 0.033(3) |
| C(23) | 0.056(3) | 0.045(3) | 0.072(3) | 0.000(2) | 0.019(3) | 0.023(2) |
| C(24) | 0.048(2) | 0.042(2) | 0.056(3) | 0.009(2) | 0.020(2) | 0.011(2) |
| C(25) | 0.034(2) | 0.042(2) | 0.041(2) | 0.012(2) | 0.010(2) | 0.013(2) |
| C(26) | 0.037(2) | 0.046(2) | 0.063(3) | 0.011(2) | 0.011(2) | 0.008(2) |
| C(27) | 0.039(2) | 0.059(3) | 0.074(3) | 0.004(2) | 0.001(2) | 0.013(3) |
| C(28) | 0.028(2) | 0.077(4) | 0.087(4) | 0.016(2) | 0.008(2) | 0.035(3) |
| C(29) | 0.041(3) | 0.079(4) | 0.088(4) | 0.028(3) | 0.025(3) | 0.024(3) |
| C(30) | 0.041(2) | 0.059(3) | 0.069(3) | 0.021(2) | 0.015(2) | 0.011(2) |
| C(31) | 0.039(2) | 0.043(2) | 0.039(2) | 0.016(2) | 0.016(2) | 0.008(2) |
| C(32) | 0.037(2) | 0.059(3) | 0.045(2) | 0.012(2) | 0.013(2) | 0.001(2) |
| C(33) | 0.042(2) | 0.082(4) | 0.043(3) | 0.015(2) | 0.009(2) | -0.001(2) |
| C(34) | 0.069(3) | 0.098(4) | 0.036(2) | 0.024(3) | 0.015(2) | 0.016(3) |
| C(35) | 0.058(3) | 0.091(4) | 0.052(3) | 0.002(3) | 0.026(2) | 0.018(3) |
| C(36) | 0.042(2) | 0.061(3) | 0.044(2) | 0.009(2) | 0.012(2) | 0.010(2) |
| C(37) | 0.036(2) | 0.039(2) | 0.056(3) | 0.015(2) | 0.016(2) | 0.012(2) |
| C(38) | 0.078(4) | 0.041(3) | 0.065(3) | 0.022(2) | 0.026(3) | 0.007(2) |
| C(39) | 0.102(5) | 0.044(3) | 0.099(5) | 0.028(3) | 0.034(4) | 0.004(3) |
| C(40) | 0.096(5) | 0.045(3) | 0.109(5) | 0.028(3) | 0.041(4) | 0.032(3) |
| C(41) | 0.063(3) | 0.063(3) | 0.078(4) | 0.028(3) | 0.021(3) | 0.038(3) |
| C(42) | 0.053(3) | 0.048(3) | 0.062(3) | 0.017(2) | 0.016(2) | 0.016(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(43) | 0.036(2) | 0.045(2) | 0.045(2) | 0.012(2) | 0.010(2) | 0.016(2) |
| C(44) | 0.048(3) | 0.050(3) | 0.061(3) | 0.009(2) | 0.009(2) | 0.017(2) |
| C(45) | 0.059(3) | 0.054(3) | 0.073(4) | 0.002(2) | 0.020(3) | 0.028(3) |
| C(46) | 0.070(4) | 0.081(4) | 0.080(4) | 0.026(3) | 0.038(3) | 0.046(3) |
| C(47) | 0.088(4) | 0.071(4) | 0.070(3) | 0.041(3) | 0.047(3) | 0.027(3) |
| C(48) | 0.076(3) | 0.058(3) | 0.062(3) | 0.032(3) | 0.037(3) | 0.026(2) |
| C(49) | 0.036(2) | 0.037(2) | 0.052(2) | 0.014(2) | 0.013(2) | 0.007(2) |
| C(50) | 0.045(3) | 0.060(3) | 0.056(3) | 0.018(2) | 0.007(2) | 0.014(2) |
| C(51) | 0.059(3) | 0.074(4) | 0.060(3) | 0.027(3) | 0.001(3) | 0.008(3) |
| C(52) | 0.042(3) | 0.053(3) | 0.097(4) | 0.018(2) | 0.001(3) | 0.004(3) |
| C(53) | 0.042(3) | 0.066(3) | 0.091(4) | 0.018(2) | 0.023(3) | 0.023(3) |
| C(54) | 0.047(3) | 0.056(3) | 0.065(3) | 0.022(2) | 0.018(2) | 0.016(2) |
| C(55) | 0.053(3) | 0.039(2) | 0.056(3) | 0.010(2) | 0.022(2) | 0.003(2) |
| C(56) | 0.057(3) | 0.048(3) | 0.055(3) | 0.003(2) | 0.019(2) | 0.002(2) |
| C(57) | 0.081(4) | 0.058(3) | 0.057(3) | -0.007(3) | 0.024(3) | -0.009(3) |
| C(58) | 0.114(6) | 0.045(3) | 0.108(5) | 0.000(3) | 0.064(5) | -0.015(3) |
| C(59) | 0.091(5) | 0.050(3) | 0.134(6) | 0.029(3) | 0.052(5) | -0.004(4) |
| C(60) | 0.069(3) | 0.048(3) | 0.093(4) | 0.027(3) | 0.026(3) | 0.002(3) |

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S9. Bond Lengths(Å) for **5**

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| Ru(1) | Ru(2) | 2.7620(4) | Ru(1) | S(1) | 2.456(1) |
| Ru(1) | P(1) | 2.359(1) | Ru(1) | P(2) | 2.352(1) |
| Ru(1) | C(1) | 1.837(4) | Ru(1) | C(5) | 2.232(4) |
| Ru(1) | C(6) | 2.252(4) | Ru(2) | S(1) | 2.408(1) |
| Ru(2) | P(1) | 2.299(1) | Ru(2) | P(3) | 2.309(1) |
| Ru(2) | C(2) | 1.848(4) | Ru(2) | C(3) | 2.191(4) |
| Ru(2) | C(4) | 2.257(4) | S(1) | C(3) | 1.758(4) |
| P(1) | C(13) | 1.826(4) | P(1) | C(19) | 1.821(4) |
| P(2) | C(25) | 1.844(4) | P(2) | C(31) | 1.836(4) |
| P(2) | C(37) | 1.842(4) | P(3) | C(43) | 1.836(4) |
| P(3) | C(49) | 1.842(4) | P(3) | C(55) | 1.850(4) |
| O(1) | C(1) | 1.153(5) | O(2) | C(2) | 1.153(5) |
| C(3) | C(4) | 1.358(6) | C(4) | C(5) | 1.466(6) |
| C(5) | C(6) | 1.425(6) | C(6) | C(7) | 1.471(5) |
| C(7) | C(8) | 1.385(6) | C(7) | C(12) | 1.395(6) |
| C(8) | C(9) | 1.378(6) | C(9) | C(10) | 1.365(7) |
| C(10) | C(11) | 1.369(7) | C(11) | C(12) | 1.382(6) |
| C(13) | C(14) | 1.382(5) | C(13) | C(18) | 1.391(6) |
| C(14) | C(15) | 1.389(6) | C(15) | C(16) | 1.374(7) |
| C(16) | C(17) | 1.373(7) | C(17) | C(18) | 1.380(6) |
| C(19) | C(20) | 1.378(5) | C(19) | C(24) | 1.394(6) |
| C(20) | C(21) | 1.383(6) | C(21) | C(22) | 1.360(7) |
| C(22) | C(23) | 1.368(7) | C(23) | C(24) | 1.383(6) |
| C(25) | C(26) | 1.378(6) | C(25) | C(30) | 1.388(6) |
| C(26) | C(27) | 1.391(6) | C(27) | C(28) | 1.376(7) |
| C(28) | C(29) | 1.372(7) | C(29) | C(30) | 1.372(6) |
| C(31) | C(32) | 1.392(6) | C(31) | C(36) | 1.381(6) |
| C(32) | C(33) | 1.367(6) | C(33) | C(34) | 1.368(7) |
| C(34) | C(35) | 1.374(7) | C(35) | C(36) | 1.379(6) |
| C(37) | C(38) | 1.381(6) | C(37) | C(42) | 1.386(6) |
| C(38) | C(39) | 1.396(7) | C(39) | C(40) | 1.369(9) |
| C(40) | C(41) | 1.366(8) | C(41) | C(42) | 1.380(6) |
| C(43) | C(44) | 1.384(6) | C(43) | C(48) | 1.387(6) |
| C(44) | C(45) | 1.383(7) | C(45) | C(46) | 1.354(8) |
| C(46) | C(47) | 1.371(7) | C(47) | C(48) | 1.385(6) |
| C(49) | C(50) | 1.379(6) | C(49) | C(54) | 1.390(6) |
| C(50) | C(51) | 1.387(7) | C(51) | C(52) | 1.358(8) |
| C(52) | C(53) | 1.363(8) | C(53) | C(54) | 1.382(6) |
| C(55) | C(56) | 1.372(6) | C(55) | C(60) | 1.392(6) |
| C(56) | C(57) | 1.384(7) | C(57) | C(58) | 1.370(9) |
| C(58) | C(59) | 1.374(9) | C(59) | C(60) | 1.370(7) |

Table S10. Bond Lengths(Å) for **5**

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| C(3) | H(1) | 0.92(4) | C(4) | H(2) | 0.92(4) |
| C(5) | H(3) | 0.92(4) | C(6) | H(4) | 0.85(4) |
| C(8) | H(5) | 0.97 | C(9) | H(6) | 0.97 |
| C(10) | H(7) | 0.97 | C(11) | H(8) | 0.97 |
| C(12) | H(9) | 0.97 | C(14) | H(10) | 0.98 |
| C(15) | H(11) | 0.97 | C(16) | H(12) | 0.97 |
| C(17) | H(13) | 0.97 | C(18) | H(14) | 0.97 |
| C(20) | H(15) | 0.98 | C(21) | H(16) | 0.97 |
| C(22) | H(17) | 0.97 | C(23) | H(18) | 0.99 |
| C(24) | H(19) | 0.98 | C(26) | H(20) | 0.97 |
| C(27) | H(21) | 0.98 | C(28) | H(22) | 0.97 |
| C(29) | H(23) | 0.98 | C(30) | H(24) | 0.98 |
| C(32) | H(25) | 0.98 | C(33) | H(26) | 0.98 |
| C(34) | H(27) | 0.97 | C(35) | H(28) | 0.97 |
| C(36) | H(29) | 0.97 | C(38) | H(30) | 0.98 |
| C(39) | H(31) | 0.97 | C(40) | H(32) | 0.97 |
| C(41) | H(33) | 0.98 | C(42) | H(34) | 0.98 |
| C(44) | H(35) | 0.97 | C(45) | H(36) | 0.97 |
| C(46) | H(37) | 0.98 | C(47) | H(38) | 0.98 |
| C(48) | H(39) | 0.96 | C(50) | H(40) | 0.98 |
| C(51) | H(41) | 0.97 | C(52) | H(42) | 0.98 |
| C(53) | H(43) | 0.98 | C(54) | H(44) | 0.99 |
| C(56) | H(45) | 0.97 | C(57) | H(46) | 0.99 |
| C(58) | H(47) | 0.98 | C(59) | H(48) | 0.97 |
| C(60) | H(49) | 0.97 | | | |

Table S11. Bond Angles(°) for **5**

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| Ru(2) | Ru(1) | S(1) | 54.59(2) | Ru(2) | Ru(1) | P(1) | 52.63(2) |
| Ru(2) | Ru(1) | P(2) | 147.31(3) | Ru(2) | Ru(1) | C(1) | 114.3(1) |
| Ru(2) | Ru(1) | C(5) | 68.5(1) | Ru(2) | Ru(1) | C(6) | 100.7(1) |
| S(1) | Ru(1) | P(1) | 81.76(3) | S(1) | Ru(1) | P(2) | 98.75(3) |
| S(1) | Ru(1) | C(1) | 168.8(1) | S(1) | Ru(1) | C(5) | 81.5(1) |
| S(1) | Ru(1) | C(6) | 85.2(1) | P(1) | Ru(1) | P(2) | 110.67(4) |
| P(1) | Ru(1) | C(1) | 90.0(1) | P(1) | Ru(1) | C(5) | 117.1(1) |
| P(1) | Ru(1) | C(6) | 153.0(1) | P(2) | Ru(1) | C(1) | 91.2(1) |
| P(2) | Ru(1) | C(5) | 131.7(1) | P(2) | Ru(1) | C(6) | 94.6(1) |
| C(1) | Ru(1) | C(5) | 95.8(2) | C(1) | Ru(1) | C(6) | 99.2(2) |
| C(5) | Ru(1) | C(6) | 37.1(1) | Ru(1) | Ru(2) | S(1) | 56.22(2) |
| Ru(1) | Ru(2) | P(1) | 54.64(3) | Ru(1) | Ru(2) | P(3) | 153.26(3) |
| Ru(1) | Ru(2) | C(2) | 114.2(1) | Ru(1) | Ru(2) | C(3) | 80.3(1) |
| Ru(1) | Ru(2) | C(4) | 73.5(1) | S(1) | Ru(2) | P(1) | 84.05(3) |
| S(1) | Ru(2) | P(3) | 104.52(4) | S(1) | Ru(2) | C(2) | 160.7(1) |
| S(1) | Ru(2) | C(3) | 44.7(1) | S(1) | Ru(2) | C(4) | 70.2(1) |
| P(1) | Ru(2) | P(3) | 109.43(4) | P(1) | Ru(2) | C(2) | 104.1(1) |
| P(1) | Ru(2) | C(3) | 126.7(1) | P(1) | Ru(2) | C(4) | 127.9(1) |
| P(3) | Ru(2) | C(2) | 89.4(1) | P(3) | Ru(2) | C(3) | 98.6(1) |
| P(3) | Ru(2) | C(4) | 120.4(1) | C(2) | Ru(2) | C(3) | 121.0(2) |
| C(2) | Ru(2) | C(4) | 91.3(2) | C(3) | Ru(2) | C(4) | 35.5(2) |
| Ru(1) | S(1) | Ru(2) | 69.19(3) | Ru(1) | S(1) | C(3) | 98.5(2) |
| Ru(2) | S(1) | C(3) | 61.1(1) | Ru(1) | P(1) | Ru(2) | 72.72(3) |
| Ru(1) | P(1) | C(13) | 119.3(1) | Ru(1) | P(1) | C(19) | 122.5(1) |
| Ru(2) | P(1) | C(13) | 124.2(1) | Ru(2) | P(1) | C(19) | 114.9(1) |
| C(13) | P(1) | C(19) | 102.8(2) | Ru(1) | P(2) | C(25) | 118.5(1) |
| Ru(1) | P(2) | C(31) | 114.0(1) | Ru(1) | P(2) | C(37) | 117.7(1) |
| C(25) | P(2) | C(31) | 103.2(2) | C(25) | P(2) | C(37) | 98.3(2) |
| C(31) | P(2) | C(37) | 102.7(2) | Ru(2) | P(3) | C(43) | 119.8(1) |
| Ru(2) | P(3) | C(49) | 111.3(1) | Ru(2) | P(3) | C(55) | 115.6(2) |
| C(43) | P(3) | C(49) | 101.0(2) | C(43) | P(3) | C(55) | 103.9(2) |
| C(49) | P(3) | C(55) | 103.1(2) | Ru(1) | C(1) | O(1) | 177.6(4) |
| Ru(2) | C(2) | O(2) | 174.9(4) | Ru(2) | C(3) | S(1) | 74.2(1) |
| Ru(2) | C(3) | C(4) | 74.9(3) | S(1) | C(3) | C(4) | 118.5(3) |
| Ru(2) | C(4) | C(3) | 69.6(2) | Ru(2) | C(4) | C(5) | 97.4(2) |
| C(3) | C(4) | C(5) | 123.1(4) | Ru(1) | C(5) | C(4) | 108.3(3) |
| Ru(1) | C(5) | C(6) | 72.2(2) | C(4) | C(5) | C(6) | 123.0(4) |
| Ru(1) | C(6) | C(5) | 70.7(2) | Ru(1) | C(6) | C(7) | 123.5(3) |
| C(5) | C(6) | C(7) | 121.9(4) | C(6) | C(7) | C(8) | 119.5(4) |
| C(6) | C(7) | C(12) | 123.9(4) | C(8) | C(7) | C(12) | 116.3(4) |
| C(7) | C(8) | C(9) | 122.5(4) | C(8) | C(9) | C(10) | 120.0(5) |
| C(9) | C(10) | C(11) | 119.2(4) | C(10) | C(11) | C(12) | 120.9(5) |
| C(7) | C(12) | C(11) | 121.0(4) | P(1) | C(13) | C(14) | 122.5(3) |
| P(1) | C(13) | C(18) | 119.2(3) | C(14) | C(13) | C(18) | 118.0(4) |
| C(13) | C(14) | C(15) | 122.0(4) | C(14) | C(15) | C(16) | 118.7(4) |
| C(15) | C(16) | C(17) | 120.4(4) | C(16) | C(17) | C(18) | 120.7(4) |
| C(13) | C(18) | C(17) | 120.2(4) | P(1) | C(19) | C(20) | 120.5(3) |
| P(1) | C(19) | C(24) | 122.1(3) | C(20) | C(19) | C(24) | 117.2(4) |
| C(19) | C(20) | C(21) | 122.3(4) | C(20) | C(21) | C(22) | 119.3(4) |
| C(21) | C(22) | C(23) | 120.3(4) | C(22) | C(23) | C(24) | 120.3(4) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C(19) | C(24) | C(23) | 120.6(4) | P(2) | C(25) | C(26) | 120.8(3) |
| P(2) | C(25) | C(30) | 120.7(3) | C(26) | C(25) | C(30) | 118.6(4) |
| C(25) | C(26) | C(27) | 120.3(4) | C(26) | C(27) | C(28) | 120.0(5) |
| C(27) | C(28) | C(29) | 120.0(4) | C(28) | C(29) | C(30) | 119.9(4) |
| C(25) | C(30) | C(29) | 121.2(5) | P(2) | C(31) | C(32) | 118.6(3) |
| P(2) | C(31) | C(36) | 123.5(3) | C(32) | C(31) | C(36) | 117.8(4) |
| C(31) | C(32) | C(33) | 121.3(4) | C(32) | C(33) | C(34) | 120.2(4) |
| C(33) | C(34) | C(35) | 119.6(4) | C(34) | C(35) | C(36) | 120.4(4) |
| C(31) | C(36) | C(35) | 120.7(4) | P(2) | C(37) | C(38) | 123.1(4) |
| P(2) | C(37) | C(42) | 117.6(3) | C(38) | C(37) | C(42) | 119.3(4) |
| C(37) | C(38) | C(39) | 119.1(5) | C(38) | C(39) | C(40) | 120.8(5) |
| C(39) | C(40) | C(41) | 120.1(5) | C(40) | C(41) | C(42) | 119.9(5) |
| C(37) | C(42) | C(41) | 120.8(5) | P(3) | C(43) | C(44) | 123.2(4) |
| P(3) | C(43) | C(48) | 118.6(3) | C(44) | C(43) | C(48) | 117.8(4) |
| C(43) | C(44) | C(45) | 120.7(5) | C(44) | C(45) | C(46) | 120.7(5) |
| C(45) | C(46) | C(47) | 120.1(5) | C(46) | C(47) | C(48) | 119.7(5) |
| C(43) | C(48) | C(47) | 121.1(5) | P(3) | C(49) | C(50) | 123.1(3) |
| P(3) | C(49) | C(54) | 118.3(3) | C(50) | C(49) | C(54) | 118.4(4) |
| C(49) | C(50) | C(51) | 120.1(5) | C(50) | C(51) | C(52) | 120.8(5) |
| C(51) | C(52) | C(53) | 119.9(5) | C(52) | C(53) | C(54) | 120.2(5) |
| C(49) | C(54) | C(53) | 120.5(5) | P(3) | C(55) | C(56) | 119.6(4) |
| P(3) | C(55) | C(60) | 121.9(4) | C(56) | C(55) | C(60) | 118.5(4) |
| C(55) | C(56) | C(57) | 120.7(5) | C(56) | C(57) | C(58) | 119.7(5) |
| C(57) | C(58) | C(59) | 120.5(5) | C(58) | C(59) | C(60) | 119.5(6) |
| C(55) | C(60) | C(59) | 121.0(6) | | | | |

Table S12. Bond Angles(°) for **5**

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| Ru(2) | C(3) | H(1) | 119(2) | S(1) | C(3) | H(1) | 119(2) |
| C(4) | C(3) | H(1) | 122(2) | Ru(2) | C(4) | H(2) | 116(2) |
| C(3) | C(4) | H(2) | 117(2) | C(5) | C(4) | H(2) | 117(2) |
| Ru(1) | C(5) | H(3) | 107(2) | C(4) | C(5) | H(3) | 116(2) |
| C(6) | C(5) | H(3) | 116(2) | Ru(1) | C(6) | H(4) | 110(2) |
| C(5) | C(6) | H(4) | 114(2) | C(7) | C(6) | H(4) | 110(2) |
| C(7) | C(8) | H(5) | 118.5 | C(9) | C(8) | H(5) | 119.0 |
| C(8) | C(9) | H(6) | 120.5 | C(10) | C(9) | H(6) | 119.5 |
| C(9) | C(10) | H(7) | 120.1 | C(11) | C(10) | H(7) | 120.7 |
| C(10) | C(11) | H(8) | 118.8 | C(12) | C(11) | H(8) | 120.3 |
| C(7) | C(12) | H(9) | 119.3 | C(11) | C(12) | H(9) | 119.7 |
| C(13) | C(14) | H(10) | 119.3 | C(15) | C(14) | H(10) | 118.7 |
| C(14) | C(15) | H(11) | 121.3 | C(16) | C(15) | H(11) | 120.0 |
| C(15) | C(16) | H(12) | 120.1 | C(17) | C(16) | H(12) | 119.5 |
| C(16) | C(17) | H(13) | 119.4 | C(18) | C(17) | H(13) | 119.9 |
| C(13) | C(18) | H(14) | 120.2 | C(17) | C(18) | H(14) | 119.6 |
| C(19) | C(20) | H(15) | 119.0 | C(21) | C(20) | H(15) | 118.7 |
| C(20) | C(21) | H(16) | 120.8 | C(22) | C(21) | H(16) | 120.0 |
| C(21) | C(22) | H(17) | 120.8 | C(23) | C(22) | H(17) | 118.9 |
| C(22) | C(23) | H(18) | 120.1 | C(24) | C(23) | H(18) | 119.6 |
| C(19) | C(24) | H(19) | 119.2 | C(23) | C(24) | H(19) | 120.2 |
| C(25) | C(26) | H(20) | 119.9 | C(27) | C(26) | H(20) | 119.8 |
| C(26) | C(27) | H(21) | 120.1 | C(28) | C(27) | H(21) | 119.9 |
| C(27) | C(28) | H(22) | 119.4 | C(29) | C(28) | H(22) | 120.6 |
| C(28) | C(29) | H(23) | 119.4 | C(30) | C(29) | H(23) | 120.7 |
| C(25) | C(30) | H(24) | 119.3 | C(29) | C(30) | H(24) | 119.6 |
| C(31) | C(32) | H(25) | 119.8 | C(33) | C(32) | H(25) | 118.9 |
| C(32) | C(33) | H(26) | 120.9 | C(34) | C(33) | H(26) | 119.0 |
| C(33) | C(34) | H(27) | 119.6 | C(35) | C(34) | H(27) | 120.7 |
| C(34) | C(35) | H(28) | 119.5 | C(36) | C(35) | H(28) | 120.1 |
| C(31) | C(36) | H(29) | 120.1 | C(35) | C(36) | H(29) | 119.3 |
| C(37) | C(38) | H(30) | 120.5 | C(39) | C(38) | H(30) | 120.3 |
| C(38) | C(39) | H(31) | 120.9 | C(40) | C(39) | H(31) | 118.2 |
| C(39) | C(40) | H(32) | 119.9 | C(41) | C(40) | H(32) | 120.0 |
| C(40) | C(41) | H(33) | 119.7 | C(42) | C(41) | H(33) | 120.5 |
| C(37) | C(42) | H(34) | 120.1 | C(41) | C(42) | H(34) | 119.1 |
| C(43) | C(44) | H(35) | 120.5 | C(45) | C(44) | H(35) | 118.8 |
| C(44) | C(45) | H(36) | 120.2 | C(46) | C(45) | H(36) | 119.0 |
| C(45) | C(46) | H(37) | 120.2 | C(47) | C(46) | H(37) | 119.8 |
| C(46) | C(47) | H(38) | 120.1 | C(48) | C(47) | H(38) | 120.2 |
| C(43) | C(48) | H(39) | 120.1 | C(47) | C(48) | H(39) | 118.8 |
| C(49) | C(50) | H(40) | 119.9 | C(51) | C(50) | H(40) | 120.0 |
| C(50) | C(51) | H(41) | 119.9 | C(52) | C(51) | H(41) | 119.2 |
| C(51) | C(52) | H(42) | 118.0 | C(53) | C(52) | H(42) | 122.0 |
| C(52) | C(53) | H(43) | 118.8 | C(54) | C(53) | H(43) | 121.1 |
| C(49) | C(54) | H(44) | 120.2 | C(53) | C(54) | H(44) | 119.3 |
| C(55) | C(56) | H(45) | 120.3 | C(57) | C(56) | H(45) | 118.9 |
| C(56) | C(57) | H(46) | 119.0 | C(58) | C(57) | H(46) | 121.3 |
| C(57) | C(58) | H(47) | 118.3 | C(59) | C(58) | H(47) | 121.2 |
| C(58) | C(59) | H(48) | 117.9 | C(60) | C(59) | H(48) | 122.6 |
| C(55) | C(60) | H(49) | 120.1 | C(59) | C(60) | H(49) | 118.9 |