Supporting Information

for

Enantio and diastereocontrol in intermolecular cyclopropanation reaction of styrene catalyzed by dirhodium(II) complexes with bulky *ortho*-metalated aryl phosphines. Catalysis in water as solvent. Study of a (+)-non-linear effect.

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Molecular modelling study.

The molecular structure determined for $Rh(O_2CMe)_2[p\text{-}Me_3SiC_6H_3)P(p\text{-}Me_3SiC_6H_4)_2]_2$, **5**, was used for this study. Considering that the only freedom degree is for the dihedral angle P-Rh-C(carbene)-C, Figure SI.1 shows the minimum in energy for molecular mechanic calculations in A_2 and A_3 intermediates that lead respectively, to the *cis* and *trans* cyclopropane products. With that model we only pretend to illustrate the steric effects for the intermediates in the cyclopropanation reaction of styrene with ethyl diazoacetate.

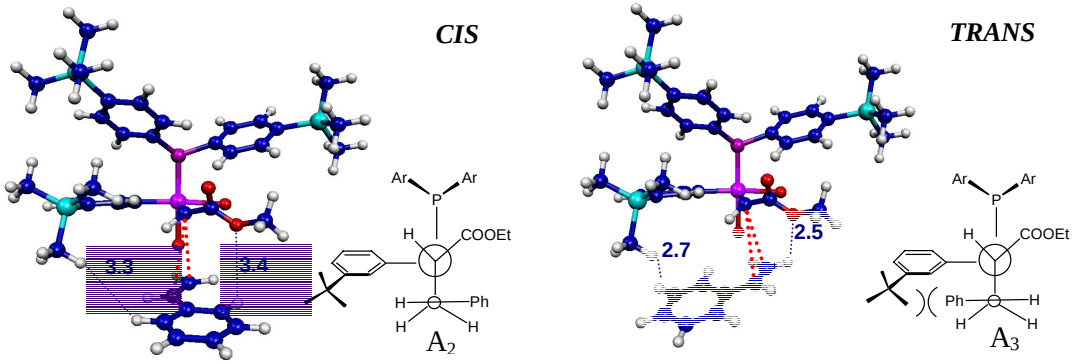

Figure SI.1. Representation of A_2 and A_3 transition states in the cyclopropanation of styrene with ethyl diazoacetate catalyzed by $Rh_2(O_2CCH_3)_2[(p\text{-}Me_3SiC_6H_4)P(p\text{-}Me_3SiC_6H_5)_2]_2$ compound.

In the A_2 intermediate, the approximate calculated distances between a hydrogen atom from Me_3Si - hydrogen in the phenyl ring of the approaching olefin, 3.3 Å, and between hydrogen in the phenyl ring of the approaching olefin - oxygen in the carbene, 3.4 Å, are bigger than in the intermediate A_3, 2.7 and 2.5 Å respectively. Sterically the intermediate A_2 is favoured versus A_3. The experimental results, high diastereoselectivity in *cis* isomer and high enantioselectivity for (1*S*, 2*R*) isomer support this model.

CD spectra of the selected dirhodium(II) compounds.

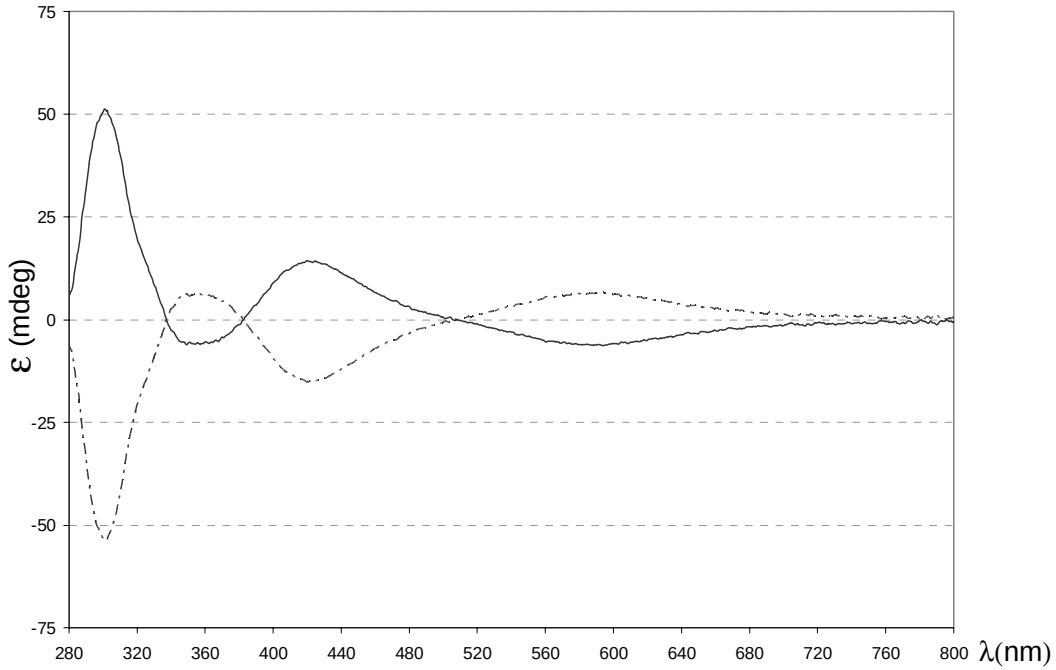

Figure SI.2. CD spectra of enantiomers **10(*M*)** (solid curve) and **10(*P*)** (dashed curve). $5 \cdot 10^{-5}$ M in $CDCl_3$.

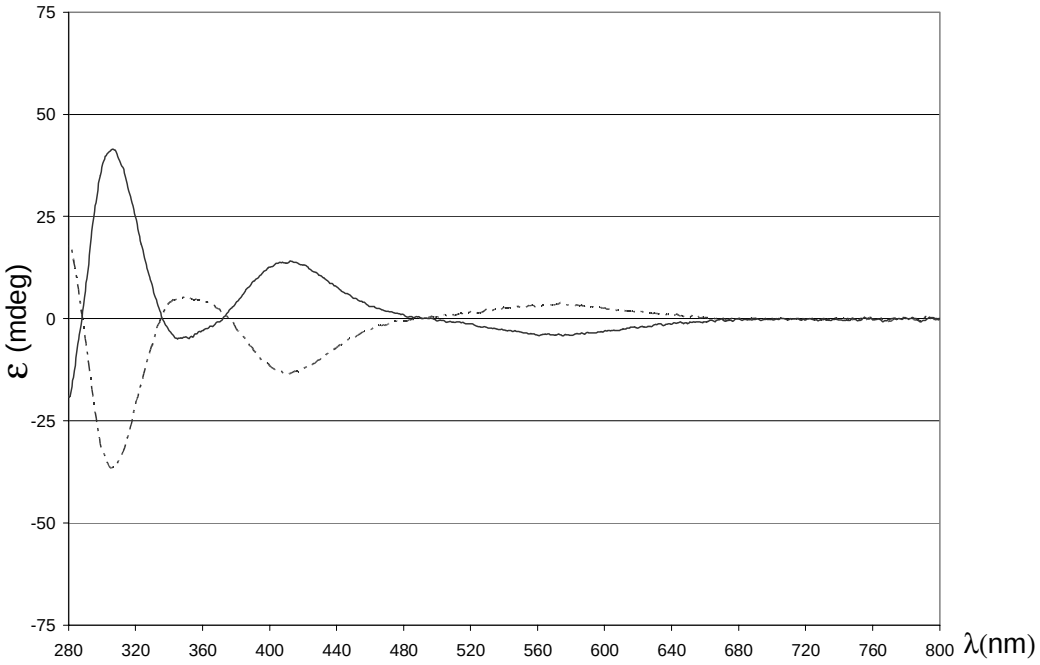

Figure SI.3. CD spectra of enantiomers **11(*M*)** (solid curve) and **11(*P*)** (dashed curve). $5 \cdot 10^{-5}$ M in $CDCl_3$

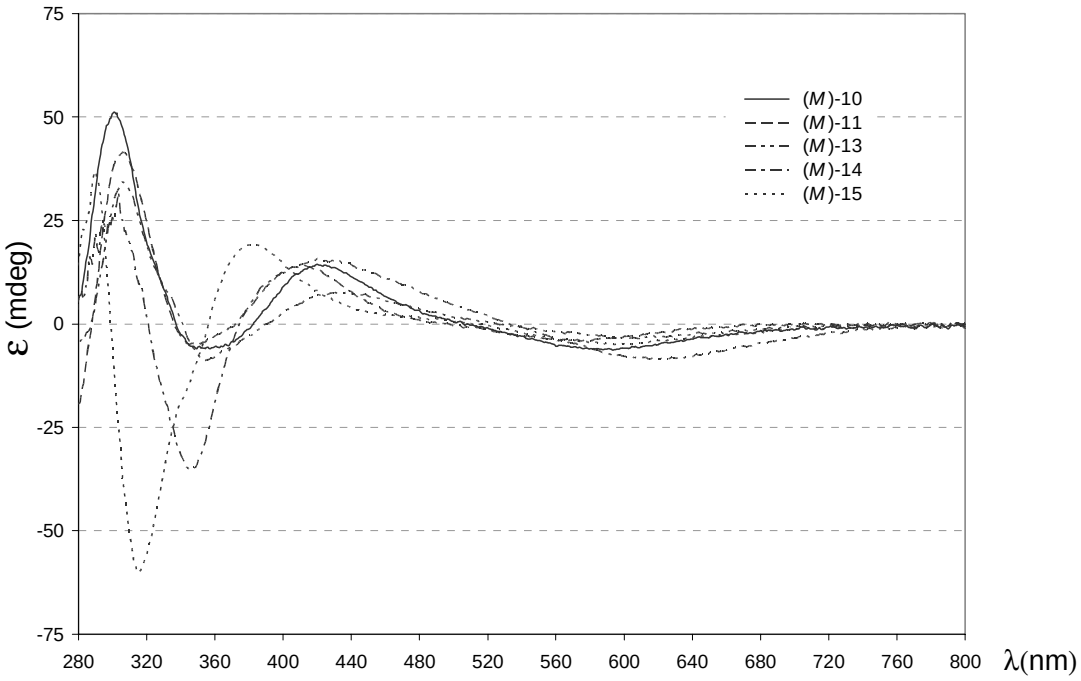

Figure SI.4. CD spectra of enantiomers **10(*M*), 11(*M*)** and **13(*M*)-15(*M*).** $5 \cdot 10^{-5}$ M in $CDCl_3$.

It is shown the same kind of Cotton effect for compounds that were eluted in the same order like diastereoisomers in the column chromatography.

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H40L H 0.4515 0.1188 0.0271 0.268 Uiso 1 1 calc R . .
C403 C 0.5577(10) 0.3014(13) 0.1239(12) 0.182(8) Uani 1 1 d . . .
H40D H 0.6162 0.2871 0.1060 0.273 Uiso 1 1 calc R . .
H40E H 0.5631 0.3557 0.1693 0.273 Uiso 1 1 calc R . .
H40F H 0.5222 0.3080 0.0761 0.273 Uiso 1 1 calc R . .
C501 C -0.1139(8) -0.0886(6) 0.0481(8) 0.116(4) Uani 1 1 d . . .
H50A H -0.0594 -0.0865 0.0192 0.173 Uiso 1 1 calc R . .
H50B H -0.1541 -0.1379 0.0156 0.173 Uiso 1 1 calc R . .
H50C H -0.1008 -0.0948 0.1043 0.173 Uiso 1 1 calc R . .
C502 C -0.2726(8) 0.0067(9) 0.1115(9) 0.136(5) Uani 1 1 d . . .
H50G H -0.3122 -0.0420 0.0770 0.204 Uiso 1 1 calc R . .
H50H H -0.3004 0.0604 0.1183 0.204 Uiso 1 1 calc R . .
H50I H -0.2603 -0.0019 0.1669 0.204 Uiso 1 1 calc R . .
C503 C -0.1844(11) 0.0301(9) -0.0497(8) 0.155(6) Uani 1 1 d . . .
H50D H -0.1279 0.0334 -0.0751 0.232 Uiso 1 1 calc R . .
H50E H -0.2114 0.0839 -0.0446 0.232 Uiso 1 1 calc R . .
H50F H -0.2232 -0.0186 -0.0854 0.232 Uiso 1 1 calc R . .
C601 C 0.071(3) 0.7696(13) 0.2189(17) 0.37(2) Uani 1 1 d . . .
H60D H 0.0656 0.8204 0.1986 0.562 Uiso 1 1 calc R . .
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H60E H 0.1235 0.7801 0.2577 0.562 Uiso 1 1 calc R . .
H60F H 0.0191 0.7586 0.2483 0.562 Uiso 1 1 calc R . .
C602 C 0.1776(19) 0.697(2) 0.079(3) 0.43(3) Uani 1 1 d . . .
H60A H 0.1704 0.7461 0.0565 0.652 Uiso 1 1 calc R . .
H60B H 0.1875 0.6463 0.0324 0.652 Uiso 1 1 calc R . .
H60C H 0.2280 0.7108 0.1199 0.652 Uiso 1 1 calc R . .
C603 C -0.0195(18) 0.6569(17) 0.064(2) 0.33(2) Uani 1 1 d . . .
H60G H -0.0246 0.7061 0.0409 0.502 Uiso 1 1 calc R . .
H60H H -0.0690 0.6516 0.0985 0.502 Uiso 1 1 calc R . .
H60I H -0.0202 0.6039 0.0173 0.502 Uiso 1 1 calc R . .

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O1 0.063(3) 0.049(2) 0.065(3) 0.019(2) 0.009(2) -0.002(2)
Si1 0.0511(10) 0.0606(11) 0.0964(17) 0.0284(11) 0.0007(10) -0.0055(9)
Rh2 0.0453(3) 0.0411(3) 0.0447(3) 0.0126(2) 0.0023(2) 0.00417(19)
P2 0.0489(8) 0.0489(8) 0.0451(9) 0.0157(7) -0.0003(7) 0.0064(6)
O2 0.061(3) 0.042(2) 0.074(3) 0.020(2) 0.012(2) 0.009(2)
C2 0.089(6) 0.060(5) 0.127(9) 0.037(5) 0.016(6) -0.007(4)
Si2 0.162(3) 0.1035(19) 0.0467(13) 0.0182(13) -0.0112(16) 0.0040(19)
Si3 0.0927(18) 0.0680(13) 0.0997(19) 0.0170(13) 0.0208(15) 0.0295(13)
O3 0.052(2) 0.058(2) 0.047(2) 0.005(2) 0.005(2) 0.005(2)
O4 0.053(2) 0.062(3) 0.043(2) 0.013(2) 0.005(2) 0.009(2)
Si4 0.0606(12) 0.1035(17) 0.0568(12) 0.0091(11) 0.0082(10) 0.0210(11)
O5 0.044(2) 0.085(3) 0.058(3) 0.012(2) -0.006(2) -0.008(2)
Si5 0.0755(15) 0.0844(15) 0.0757(16) 0.0073(12) -0.0152(12) -0.0119(12)
Si6 0.150(3) 0.105(2) 0.163(4) 0.093(2) -0.006(3) 0.013(2)
O6 0.045(2) 0.058(2) 0.065(3) 0.014(2) 0.004(2) 0.0127(19)
O7 0.075(4) 0.123(5) 0.074(4) 0.021(4) -0.006(3) -0.025(4)
O8 0.087(5) 0.203(9) 0.164(9) 0.109(7) 0.020(5) 0.005(5)
C10 0.082(5) 0.046(3) 0.057(4) 0.013(3) 0.001(4) 0.001(3)
C11 0.056(4) 0.045(3) 0.056(4) 0.021(3) -0.002(3) 0.001(3)
C12 0.048(3) 0.048(3) 0.047(3) 0.011(3) 0.000(3) 0.008(3)
C13 0.045(3) 0.056(3) 0.056(4) 0.018(3) -0.001(3) 0.002(3)
C14 0.059(4) 0.053(3) 0.065(4) 0.022(3) 0.003(3) -0.002(3)
C15 0.059(4) 0.051(4) 0.093(6) 0.038(4) -0.008(4) -0.011(3)
C16 0.063(4) 0.053(4) 0.086(5) 0.032(4) -0.009(4) 0.004(3)
C21 0.061(4) 0.053(3) 0.049(4) 0.020(3) -0.004(3) 0.005(3)
C22 0.062(4) 0.071(4) 0.057(4) 0.013(3) 0.001(3) 0.007(3)
C23 0.086(6) 0.083(5) 0.051(4) 0.015(4) -0.016(4) 0.010(4)
C24 0.105(7) 0.075(5) 0.046(4) 0.018(4) -0.008(4) 0.012(4)
C25 0.094(7) 0.099(6) 0.063(5) 0.025(5) 0.011(5) -0.005(5)
C26 0.069(5) 0.082(5) 0.058(4) 0.026(4) -0.001(4) -0.005(4)
C30 0.053(4) 0.055(3) 0.042(3) 0.006(3) -0.007(3) 0.001(3)
C31 0.058(4) 0.058(4) 0.050(4) 0.020(3) 0.001(3) 0.010(3)
C32 0.073(5) 0.065(4) 0.065(5) 0.007(4) -0.016(4) 0.014(4)
C34 0.081(5) 0.057(4) 0.078(5) 0.009(4) 0.007(4) 0.022(4)
C35 0.088(6) 0.082(5) 0.086(6) 0.009(4) -0.018(5) 0.039(5)
C36 0.075(5) 0.079(5) 0.065(5) 0.004(4) -0.013(4) 0.024(4)
C40 0.059(4) 0.129(8) 0.058(5) 0.006(5) 0.002(4) 0.009(5)
C41 0.053(3) 0.049(3) 0.038(3) 0.008(2) 0.005(3) 0.004(3)
C42 0.056(4) 0.050(3) 0.041(3) 0.009(3) 0.007(3) 0.007(3)
C43 0.047(3) 0.066(4) 0.038(3) 0.004(3) -0.001(3) -0.002(3)
C44 0.053(4) 0.065(4) 0.048(4) 0.015(3) 0.002(3) 0.003(3)
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C45 0.068(4) 0.073(4) 0.042(4) 0.008(3) 0.005(3) 0.017(4)
C46 0.057(4) 0.083(5) 0.052(4) 0.019(4) -0.003(3) 0.015(4)
C51 0.052(3) 0.059(4) 0.051(4) 0.014(3) -0.003(3) 0.005(3)
C52 0.072(5) 0.066(4) 0.082(6) 0.030(4) -0.018(4) 0.002(4)
C53 0.072(5) 0.083(5) 0.093(6) 0.031(5) -0.033(5) -0.004(4)
C54 0.063(4) 0.076(5) 0.059(4) 0.012(4) -0.005(4) -0.001(4)
C55 0.078(5) 0.057(4) 0.066(5) 0.010(3) -0.004(4) 0.007(4)
C56 0.070(4) 0.062(4) 0.058(4) 0.017(3) -0.015(4) 0.002(3)
C61 0.066(4) 0.058(4) 0.049(4) 0.022(3) -0.006(3) 0.004(3)
C62 0.078(5) 0.085(5) 0.099(7) 0.057(5) 0.022(5) 0.023(4)
C63 0.089(6) 0.081(5) 0.106(7) 0.045(5) -0.003(5) 0.023(5)
C64 0.091(6) 0.083(5) 0.091(6) 0.048(5) -0.004(5) 0.004(5)
C65 0.117(8) 0.092(6) 0.105(8) 0.058(6) 0.034(6) 0.021(6)
C66 0.089(6) 0.085(5) 0.074(5) 0.042(4) 0.021(5) 0.028(5)
C101 0.098(7) 0.090(6) 0.126(9) 0.047(6) 0.036(7) 0.013(5)
C102 0.080(6) 0.076(5) 0.128(9) 0.010(5) -0.019(6) -0.015(5)
C103 0.073(6) 0.111(7) 0.147(11) 0.056(7) -0.030(6) -0.006(5)
C201 0.202(18) 0.154(12) 0.098(10) -0.015(8) 0.020(10) 0.030(11)
C202 0.36(3) 0.194(16) 0.095(10) 0.083(11) -0.034(14) -0.088(17)
C203 0.194(17) 0.200(16) 0.073(8) 0.012(9) -0.055(9) 0.006(12)
C301 0.120(10) 0.074(6) 0.199(14) 0.041(7) 0.048(9) 0.023(6)
C302 0.090(8) 0.099(7) 0.208(15) 0.050(9) 0.042(9) 0.033(6)
C303 0.26(2) 0.143(11) 0.105(10) 0.008(8) 0.032(11) 0.102(13)
C330 0.085(6) 0.063(4) 0.080(6) 0.005(4) -0.018(5) 0.019(4)
C401 0.110(9) 0.227(16) 0.102(9) 0.016(9) -0.009(7) 0.099(10)
C402 0.108(10) 0.169(13) 0.189(16) -0.078(11) 0.009(10) 0.058(9)
C403 0.100(10) 0.27(2) 0.221(19) 0.146(17) 0.054(11) 0.010(12)
C501 0.127(10) 0.085(6) 0.109(9) -0.004(6) -0.029(7) -0.009(6)
C502 0.080(7) 0.136(10) 0.152(12) -0.015(9) -0.006(8) -0.015(7)
C503 0.191(15) 0.147(11) 0.100(9) 0.016(8) -0.079(10) -0.030(10)
C601 0.80(8) 0.116(15) 0.23(3) 0.076(16) 0.01(4) 0.09(3)
C602 0.33(4) 0.45(4) 0.80(8) 0.56(6) 0.31(5) 0.19(3)
C603 0.30(3) 0.30(3) 0.50(5) 0.31(3) -0.19(3) -0.04(2)

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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Rh1 O1 2.156(4) . ?
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Rh1 P1 2.2019(16) . ?
Rh1 O5 2.327(5) . ?
Rh1 Rh2 2.5116(6) . ?
P1 C11 1.782(7) . ?
P1 C21 1.824(7) . ?
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O1 C10 1.274(9) . ?
Si1 C103 1.854(9) . ?
Si1 C101 1.862(11) . ?
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Si1 C102 1.867(9) . ?
Si1 C14 1.873(7) . ?
Rh2 C12 2.004(6) . ?
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Rh2 O2 2.198(4) . ?
Rh2 P2 2.2078(17) . ?
Rh2 O6 2.326(4) . ?
P2 C41 1.803(6) . ?
P2 C51 1.826(7) . ?
P2 C61 1.835(6) . ?
O2 C10 1.254(9) . ?
C2 C10 1.497(10) . ?
C2 H2A 0.9600 . ?
C2 H2B 0.9600 . ?
C2 H2C 0.9600 . ?
Si2 C202 1.834(14) . ?
Si2 C201 1.871(14) . ?
Si2 C24 1.875(8) . ?
Si2 C203 1.912(17) . ?
Si3 C302 1.840(12) . ?
Si3 C34 1.868(7) . ?
Si3 C303 1.869(14) . ?
Si3 C301 1.873(11) . ?
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O4 C30 1.266(8) . ?
Si4 C401 1.838(11) . ?
Si4 C402 1.845(12) . ?
Si4 C44 1.868(7) . ?
Si4 C403 1.874(14) . ?
Si5 C501 1.840(11) . ?
Si5 C503 1.847(13) . ?
Si5 C502 1.849(13) . ?
Si5 C54 1.886(8) . ?
Si6 C602 1.72(2) . ?
Si6 C603 1.77(2) . ?
Si6 C601 1.83(2) . ?
Si6 C64 1.880(8) . ?
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C11 C12 1.408(8) . ?
C12 C13 1.406(9) . ?
C13 C14 1.385(9) . ?
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C14 C15 1.394(10) . ?
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C15 H15A 0.9300 . ?
C16 H16A 0.9300 . ?
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C21 C26 1.394(10) . ?
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C30 C40 1.499(10) . ?
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C31 C32 1.387(10) . ?
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C32 H32A 0.9300 . ?
C34 C35 1.381(12) . ?
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C41 C46 1.400(9) . ?
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C43 C44 1.378(9) . ?
C43 H43A 0.9300 . ?
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C45 C46 1.372(10) . ?
C45 H45A 0.9300 . ?
C46 H46A 0.9300 . ?
C51 C52 1.376(9) . ?
C51 C56 1.411(9) . ?
C52 C53 1.395(11) . ?
C52 H52A 0.9300 . ?
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C53 H53A 0.9300 . ?
C54 C55 1.384(10) . ?
C55 C56 1.362(10) . ?
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C42 Rh1 O3 175.9(2) . . ?
O1 Rh1 O3 85.19(18) . . ?
C42 Rh1 P1 89.85(18) . . ?
O1 Rh1 P1 175.36(14) . . ?
O3 Rh1 P1 93.97(13) . . ?
C42 Rh1 O5 94.1(2) . . ?
O1 Rh1 O5 89.23(18) . . ?
O3 Rh1 O5 84.07(18) . . ?
P1 Rh1 O5 95.22(14) . . ?
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O1 Rh1 Rh2 86.79(13) . . ?
O3 Rh1 Rh2 84.18(12) . . ?
P1 Rh1 Rh2 88.59(5) . . ?
O5 Rh1 Rh2 167.88(13) . . ?
C11 P1 C21 105.7(3) . . ?
C11 P1 C31 102.9(3) . . ?
C21 P1 C31 104.1(3) . . ?
C11 P1 Rh1 112.4(2) . . ?
C21 P1 Rh1 110.0(2) . . ?
C31 P1 Rh1 120.5(2) . . ?
C10 O1 Rh1 118.3(5) . . ?
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C103 Si1 C101 110.1(5) . . ?
C103 Si1 C102 110.6(5) . . ?
C101 Si1 C102 109.6(5) . . ?
C103 Si1 C14 109.5(4) . . ?
C101 Si1 C14 108.7(5) . . ?
C102 Si1 C14 108.2(4) . . ?
C12 Rh2 O4 92.7(2) . . ?
C12 Rh2 O2 175.1(2) . . ?
O4 Rh2 O2 82.48(17) . . ?
C12 Rh2 P2 90.63(19) . . ?
O4 Rh2 P2 174.27(13) . . ?
O2 Rh2 P2 94.26(14) . . ?
C12 Rh2 O6 90.8(2) . . ?
O4 Rh2 O6 86.72(16) . . ?
O2 Rh2 O6 88.00(16) . . ?
P2 Rh2 O6 97.91(13) . . ?
C12 Rh2 Rh1 97.05(18) . . ?
O4 Rh2 Rh1 87.04(12) . . ?
O2 Rh2 Rh1 83.71(12) . . ?
P2 Rh2 Rh1 87.92(5) . . ?
O6 Rh2 Rh1 170.21(12) . . ?
C41 P2 C51 103.1(3) . . ?
C41 P2 C61 104.7(3) . . ?
C51 P2 C61 103.7(3) . . ?
C41 P2 Rh2 112.7(2) . . ?
C51 P2 Rh2 120.0(2) . . ?
C61 P2 Rh2 111.2(2) . . ?
C10 O2 Rh2 120.6(4) . . ?
C10 C2 H2A 109.5 . . ?
C10 C2 H2B 109.5 . . ?
H2A C2 H2B 109.5 . . ?
C10 C2 H2C 109.5 . . ?
H2A C2 H2C 109.5 . . ?
H2B C2 H2C 109.5 . . ?
C202 Si2 C201 110.7(10) . . ?
C202 Si2 C24 109.2(6) . . ?
C201 Si2 C24 108.7(5) . . ?
C202 Si2 C203 110.2(8) . . ?
C201 Si2 C203 108.9(8) . . ?
C24 Si2 C203 109.2(6) . . ?
C302 Si3 C34 110.0(5) . . ?
C302 Si3 C303 109.8(8) . . ?
C34 Si3 C303 109.0(5) . . ?
C302 Si3 C301 108.4(6) . . ?
C34 Si3 C301 107.5(5) . . ?

C303 Si3 C301 112.1(7) . . ?
C30 O3 Rh1 121.5(4) . . ?
C30 O4 Rh2 118.1(4) . . ?
C401 Si4 C402 113.0(8) . . ?
C401 Si4 C44 109.4(5) . . ?
C402 Si4 C44 108.7(5) . . ?
C401 Si4 C403 109.9(8) . . ?
C402 Si4 C403 107.8(9) . . ?
C44 Si4 C403 107.9(6) . . ?
C501 Si5 C503 109.4(6) . . ?
C501 Si5 C502 108.4(7) . . ?
C503 Si5 C502 112.3(7) . . ?
C501 Si5 C54 108.3(4) . . ?
C503 Si5 C54 108.5(5) . . ?
C502 Si5 C54 109.8(5) . . ?
C602 Si6 C603 115.8(17) . . ?
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C35 C36 H36A 119.5 . . ?
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H40B C40 H40C 109.5 . . ?
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Si1 C101 H10E 109.5 . . ?
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Si3 C303 H30H 109.5 . . ?
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Si3 C303 H30I 109.5 . . ?
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Si4 C402 H40J 109.5 . . ?
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Si4 C403 H40E 109.5 . . ?
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H50G C502 H50H 109.5 . . ?
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Si6 C601 H60E 109.5 . . ?
H60D C601 H60E 109.5 . . ?
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H60D C601 H60F 109.5 . . ?
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Si6 C602 H60B 109.5 . . ?
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Si6 C603 H60H 109.5 . . ?
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 '-x, -y, -z'
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 'x+1/2, -y+1/2, z-1/2'

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_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
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 factors based on ALL data will be even larger.
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O1 O 0.5328(2) 0.2947(4) -0.1376(4) 0.100(3) Uani 1 1 d U . .
Rh1 Rh 0.53665(2) 0.26165(5) -0.05987(5) 0.0844(5) Uani 1 1 d . . .
Si1 Si 0.56209(10) -0.00101(17) -0.00649(18) 0.0921(15) Uani 1 1 d . . .
Rh2 Rh 0.56281(2) 0.19190(4) -0.08059(4) 0.0759(5) Uani 1 1 d . . .
Si2 Si 0.41307(9) 0.23311(19) 0.05112(17) 0.1013(17) Uani 1 1 d . . .
P2 P 0.61207(7) 0.21948(14) -0.01368(14) 0.0733(11) Uani 1 1 d . . .
O2 O 0.5605(2) 0.2362(4) -0.1517(4) 0.087(3) Uani 1 1 d U . .
C2 C 0.5443(4) 0.3032(6) -0.2182(7) 0.109(5) Uani 1 1 d U . .
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H2B H 0.5246 0.2949 -0.2577 0.164 Uiso 1 1 calc R . .
H2C H 0.5653 0.2995 -0.2182 0.164 Uiso 1 1 calc R . .
Si3 Si 0.65747(10) 0.3038(2) 0.2804(2) 0.118(2) Uani 1 1 d . . .
C3 C 0.4909(3) 0.1955(7) -0.1546(6) 0.092(4) Uani 1 1 d U . .
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C4 C 0.4576(3) 0.1810(6) -0.2113(6) 0.104(5) Uani 1 1 d U . .
H4A H 0.4576 0.1889 -0.2476 0.156 Uiso 1 1 calc R . .
H4B H 0.4381 0.1939 -0.2123 0.156 Uiso 1 1 calc R . .
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Si4 Si 0.59770(15) 0.4441(2) 0.0231(4) 0.174(4) Uani 1 1 d . . .
C5 C 0.5750(3) 0.1066(6) -0.1582(6) 0.082(4) Uani 1 1 d U . .
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Si5 Si 0.69629(11) 0.0960(2) 0.23472(18) 0.113(2) Uani 1 1 d . . .
O5 O 0.5046(3) 0.3227(6) -0.0548(8) 0.155(5) Uani 1 1 d U . .
Si6 Si 0.70540(12) 0.23743(18) -0.1340(2) 0.1018(16) Uani 1 1 d . . .
C6 C 0.5427(3) 0.0838(7) -0.1888(7) 0.113(6) Uani 1 1 d U . .
H6A H 0.5460 0.0568 -0.1690 0.170 Uiso 1 1 calc R . .
H6B H 0.5352 0.0795 -0.2314 0.170 Uiso 1 1 calc R . .
H6C H 0.5253 0.0996 -0.1865 0.170 Uiso 1 1 calc R . .
O6 O 0.58501(19) 0.1360(3) -0.1168(4) 0.082(3) Uani 1 1 d U . .
O7 O 0.4913(2) 0.2277(4) -0.1229(4) 0.097(3) Uani 1 1 d U . .
C7 C 0.6284(4) 0.1089(7) -0.1471(8) 0.120(6) Uani 1 1 d U . .
H7A H 0.6390 0.1059 -0.1027 0.144 Uiso 1 1 calc R . .
H7B H 0.6275 0.1387 -0.1567 0.144 Uiso 1 1 calc R . .
C8 C 0.6491(6) 0.0856(9) -0.1671(12) 0.174(10) Uani 1 1 d U . .
H8A H 0.6446 0.0558 -0.1683 0.261 Uiso 1 1 calc R . .
H8B H 0.6736 0.0908 -0.1384 0.261 Uiso 1 1 calc R . .
H8C H 0.6427 0.0950 -0.2077 0.261 Uiso 1 1 calc R . .
O9 O 0.5943(2) 0.0916(4) -0.1789(4) 0.093(3) Uani 1 1 d U . .
C9 C 0.4836(7) 0.3420(13) -0.0888(17) 0.209(9) Uani 1 1 d U . .
H9 H 0.4657 0.3207 -0.0981 0.251 Uiso 1 1 calc R . .
C10 C 0.4651(11) 0.3603(14) -0.1429(16) 0.32(2) Uani 1 1 d U . .
H10A H 0.4803 0.3749 -0.1523 0.486 Uiso 1 1 calc R . .
H10B H 0.4492 0.3801 -0.1420 0.486 Uiso 1 1 calc R . .
H10C H 0.4520 0.3392 -0.1740 0.486 Uiso 1 1 calc R . .
O11 O 0.4664(7) 0.3771(10) -0.0665(14) 0.261(11) Uani 1 1 d U . .
C11 C 0.5474(3) 0.1614(5) 0.0152(5) 0.083(3) Uani 1 1 d U . .
C12 C 0.5584(3) 0.1489(5) -0.0248(5) 0.079(3) Uani 1 1 d U . .
C13 C 0.5625(3) 0.0987(5) -0.0274(6) 0.084(3) Uani 1 1 d U . .
H13A H 0.5481 0.0918 -0.0711 0.101 Uiso 1 1 calc R . .
H13B H 0.5865 0.0949 -0.0164 0.101 Uiso 1 1 calc R . .
C14 C 0.5564(3) 0.0629(6) 0.0048(6) 0.087(3) Uani 1 1 d U . .
C15 C 0.5447(3) 0.0791(6) 0.0424(6) 0.090(4) Uani 1 1 d U . .
H15 H 0.5394 0.0603 0.0643 0.108 Uiso 1 1 calc R . .
C16 C 0.5407(3) 0.1256(6) 0.0482(6) 0.091(4) Uani 1 1 d U . .
H16 H 0.5334 0.1336 0.0746 0.109 Uiso 1 1 calc R . .
C20 C 0.4755(15) 0.3668(19) -0.018(3) 0.282(15) Uani 1 1 d U . .
H20A H 0.4545 0.3647 -0.0168 0.339 Uiso 1 1 calc R . .
H20B H 0.4839 0.3381 -0.0149 0.339 Uiso 1 1 calc R . .
C30 C 0.4950(17) 0.383(2) 0.025(2) 0.39(3) Uani 1 1 d U . .
H30A H 0.4956 0.3693 0.0594 0.579 Uiso 1 1 calc R . .
H30B H 0.4888 0.4119 0.0233 0.579 Uiso 1 1 calc R . .
H30C H 0.5176 0.3806 0.0302 0.579 Uiso 1 1 calc R . .
C21 C 0.5060(3) 0.2264(7) 0.0310(6) 0.105(5) Uani 1 1 d U . .
C22 C 0.5078(4) 0.2333(9) 0.0859(7) 0.150(7) Uani 1 1 d U . .
H22 H 0.5295 0.2393 0.1210 0.180 Uiso 1 1 calc R . .
C23 C 0.4806(4) 0.2320(9) 0.0917(7) 0.160(7) Uani 1 1 d U . .
H23 H 0.4838 0.2330 0.1308 0.192 Uiso 1 1 calc R . .
C24 C 0.4489(3) 0.2293(7) 0.0418(6) 0.113(6) Uani 1 1 d U . .
C25 C 0.4479(3) 0.2193(8) -0.0108(7) 0.135(6) Uani 1 1 d U . .
H25 H 0.4264 0.2117 -0.0451 0.162 Uiso 1 1 calc R . .
C26 C 0.4755(3) 0.2197(8) -0.0172(7) 0.140(7) Uani 1 1 d U . .
H26 H 0.4726 0.2150 -0.0557 0.169 Uiso 1 1 calc R . .
C31 C 0.5737(3) 0.2435(6) 0.0960(6) 0.087(4) Uani 1 1 d U . .
C32 C 0.5964(3) 0.2123(6) 0.1383(5) 0.081(3) Uani 1 1 d U . .
H32 H 0.5949 0.1836 0.1292 0.097 Uiso 1 1 calc R . .
C33 C 0.6209(3) 0.2299(6) 0.1946(6) 0.086(4) Uani 1 1 d U . .
H33 H 0.6377 0.2122 0.2250 0.104 Uiso 1 1 calc R . .
C34 C 0.6220(3) 0.2783(6) 0.2101(7) 0.094(4) Uani 1 1 d U . .
C35 C 0.5978(4) 0.3074(7) 0.1673(7) 0.112(5) Uani 1 1 d U . .
H35 H 0.5978 0.3359 0.1768 0.134 Uiso 1 1 calc R . .
C36 C 0.5746(3) 0.2910(6) 0.1119(7) 0.106(5) Uani 1 1 d U . .
H36 H 0.5582 0.3090 0.0813 0.127 Uiso 1 1 calc R . .
C41 C 0.6097(3) 0.2774(5) 0.0055(6) 0.082(3) Uani 1 1 d U . .
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C42 C 0.5780(3) 0.2974(5) -0.0133(6) 0.083(4) Uani 1 1 d U . .
C43 C 0.5769(4) 0.3445(6) -0.0024(8) 0.111(5) Uani 1 1 d U . .
H43 H 0.5548 0.3541 -0.0139 0.133 Uiso 1 1 calc R . .
C44 C 0.6036(4) 0.3782(7) 0.0225(9) 0.130(6) Uani 1 1 d U . .
C45 C 0.6347(4) 0.3599(6) 0.0377(8) 0.119(6) Uani 1 1 d U . .
H45 H 0.6544 0.3767 0.0515 0.143 Uiso 1 1 calc R . .
C46 C 0.6372(3) 0.3110(6) 0.0320(7) 0.096(4) Uani 1 1 d U . .
H46 H 0.6597 0.3010 0.0478 0.115 Uiso 1 1 calc R . .
C61 C 0.6396(3) 0.2242(5) -0.0456(5) 0.077(4) Uani 1 1 d U . .
C62 C 0.6326(3) 0.2566(7) -0.0907(7) 0.113(5) Uani 1 1 d U . .
H62 H 0.6149 0.2762 -0.1015 0.136 Uiso 1 1 calc R . .
C63 C 0.6513(3) 0.2587(6) -0.1174(6) 0.103(5) Uani 1 1 d U . .
H63 H 0.6457 0.2786 -0.1481 0.124 Uiso 1 1 calc R . .
C64 C 0.6792(4) 0.2309(6) -0.0988(6) 0.089(4) Uani 1 1 d U . .
C65 C 0.6864(3) 0.2004(5) -0.0522(6) 0.087(4) Uani 1 1 d U . .
H65 H 0.7055 0.1825 -0.0386 0.104 Uiso 1 1 calc R . .
C66 C 0.6667(3) 0.1965(5) -0.0268(5) 0.079(4) Uani 1 1 d U . .
H66 H 0.6715 0.1756 0.0024 0.095 Uiso 1 1 calc R . .
C51 C 0.6378(3) 0.1875(5) 0.0576(5) 0.070(3) Uani 1 1 d U . .
C56 C 0.6571(3) 0.2093(6) 0.1119(5) 0.080(3) Uani 1 1 d U . .
H56 H 0.6579 0.2388 0.1136 0.096 Uiso 1 1 calc R . .
C52 C 0.6386(3) 0.1367(5) 0.0548(5) 0.076(3) Uani 1 1 d U . .
H52 H 0.6256 0.1234 0.0165 0.092 Uiso 1 1 calc R . .
C53 C 0.6584(3) 0.1112(6) 0.1090(5) 0.088(4) Uani 1 1 d U . .
H53 H 0.6594 0.0818 0.1075 0.106 Uiso 1 1 calc R . .
C54 C 0.6762(3) 0.1343(6) 0.1648(5) 0.089(4) Uani 1 1 d U . .
C55 C 0.6760(3) 0.1834(6) 0.1663(5) 0.085(3) Uani 1 1 d U . .
H55 H 0.6889 0.1968 0.2046 0.102 Uiso 1 1 calc R . .
C111 C 0.69097(11) 0.3085(2) 0.2630(2) 0.126(6) Uani 1 1 d GU . .
C112 C 0.72251(10) 0.2880(3) 0.3020(3) 0.151(7) Uani 1 1 d GU . .
H112 H 0.7263 0.2744 0.3375 0.181 Uiso 1 1 calc R . .
C113 C 0.74837(11) 0.2879(3) 0.2882(3) 0.173(7) Uani 1 1 d GU . .
H113 H 0.7695 0.2742 0.3143 0.208 Uiso 1 1 calc R . .
C114 C 0.74269(12) 0.3082(3) 0.2352(3) 0.159(7) Uani 1 1 d GU . .
H114 H 0.7600 0.3081 0.2260 0.191 Uiso 1 1 calc R . .
C115 C 0.71115(13) 0.3287(3) 0.1962(3) 0.172(7) Uani 1 1 d GU . .
H115 H 0.7073 0.3423 0.1607 0.206 Uiso 1 1 calc R . .
C116 C 0.68529(12) 0.3288(3) 0.2100(3) 0.158(7) Uani 1 1 d GU . .
H116 H 0.6642 0.3425 0.1839 0.190 Uiso 1 1 calc R . .
C121 C 0.66099(13) 0.4034(2) 0.2874(3) 0.205(9) Uani 1 1 d GU . .
H121 H 0.6774 0.4016 0.2762 0.246 Uiso 1 1 calc R . .
C122 C 0.64630(11) 0.3668(2) 0.2941(3) 0.163(7) Uani 1 1 d GU . .
C123 C 0.62172(11) 0.3694(2) 0.3108(3) 0.186(8) Uani 1 1 d GU . .
H123 H 0.6119 0.3449 0.3153 0.223 Uiso 1 1 calc R . .
C124 C 0.61183(13) 0.4087(2) 0.3210(3) 0.244(11) Uani 1 1 d GU . .
H124 H 0.5954 0.4105 0.3322 0.293 Uiso 1 1 calc R . .
C125 C 0.62653(15) 0.4454(2) 0.3143(4) 0.260(13) Uani 1 1 d GU . .
H125 H 0.6199 0.4717 0.3211 0.312 Uiso 1 1 calc R . .
C126 C 0.65112(15) 0.4427(2) 0.2975(4) 0.260(12) Uani 1 1 d GU . .
H126 H 0.6610 0.4673 0.2931 0.312 Uiso 1 1 calc R . .
C131 C 0.66991(9) 0.2635(2) 0.3500(2) 0.131(6) Uani 1 1 d GU . .
C132 C 0.69521(10) 0.2820(3) 0.4055(2) 0.171(7) Uani 1 1 d GU . .
H132 H 0.7036 0.3089 0.4056 0.205 Uiso 1 1 calc R . .
C133 C 0.70791(10) 0.2603(3) 0.4609(2) 0.198(9) Uani 1 1 d GU . .
H133 H 0.7248 0.2727 0.4981 0.238 Uiso 1 1 calc R . .
C134 C 0.69533(11) 0.2202(3) 0.4608(2) 0.198(9) Uani 1 1 d GU . .
H134 H 0.7038 0.2057 0.4979 0.238 Uiso 1 1 calc R . .
C135 C 0.67004(11) 0.2017(3) 0.4052(2) 0.175(7) Uani 1 1 d GU . .
H135 H 0.6616 0.1748 0.4051 0.210 Uiso 1 1 calc R . .
C136 C 0.65734(10) 0.2233(2) 0.3498(2) 0.144(6) Uani 1 1 d GU . .
H136 H 0.6404 0.2110 0.3126 0.173 Uiso 1 1 calc R . .
C211 C 0.40293(11) 0.3245(2) -0.0033(3) 0.165(7) Uani 1 1 d GU . .
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H211 H 0.4175 0.3145 -0.0160 0.198 Uiso 1 1 calc R . .
C212 C 0.39540(10) 0.2990(2) 0.0325(3) 0.114(5) Uani 1 1 d GU . .
C213 C 0.37365(10) 0.3139(2) 0.0516(3) 0.147(6) Uani 1 1 d GU . .
H213 H 0.3686 0.2968 0.0756 0.176 Uiso 1 1 calc R . .
C214 C 0.35941(11) 0.3543(2) 0.0347(4) 0.197(9) Uani 1 1 d GU . .
H214 H 0.3449 0.3642 0.0474 0.236 Uiso 1 1 calc R . .
C215 C 0.36695(12) 0.3798(2) -0.0011(4) 0.205(11) Uani 1 1 d GU . .
H215 H 0.3574 0.4068 -0.0123 0.247 Uiso 1 1 calc R . .
C216 C 0.38870(12) 0.3649(2) -0.0201(3) 0.210(10) Uani 1 1 d GU . .
H216 H 0.3937 0.3820 -0.0441 0.252 Uiso 1 1 calc R . .
C221 C 0.42360(12) 0.1680(2) 0.1418(3) 0.251(11) Uani 1 1 d GU . .
H221 H 0.4192 0.1481 0.1116 0.301 Uiso 1 1 calc R . .
C222 C 0.42291(10) 0.2109(2) 0.1291(2) 0.167(8) Uani 1 1 d GU . .
C223 C 0.42951(10) 0.2407(2) 0.1742(2) 0.195(8) Uani 1 1 d GU . .
H223 H 0.4291 0.2694 0.1658 0.233 Uiso 1 1 calc R . .
C224 C 0.43678(11) 0.2276(3) 0.2319(3) 0.201(9) Uani 1 1 d GU . .
H224 H 0.4412 0.2475 0.2621 0.241 Uiso 1 1 calc R . .
C225 C 0.43746(13) 0.1847(3) 0.2446(3) 0.238(11) Uani 1 1 d GU . .
H225 H 0.4423 0.1759 0.2832 0.285 Uiso 1 1 calc R . .
C226 C 0.43087(13) 0.1549(3) 0.1995(3) 0.285(13) Uani 1 1 d GU . .
H226 H 0.4313 0.1262 0.2080 0.342 Uiso 1 1 calc R . .
C231 C 0.38255(11) 0.1892(2) -0.0041(3) 0.119(5) Uani 1 1 d GU . .
C232 C 0.34703(11) 0.1971(2) -0.0317(3) 0.152(7) Uani 1 1 d GU . .
H232 H 0.3395 0.2214 -0.0217 0.182 Uiso 1 1 calc R . .
C233 C 0.32272(12) 0.1685(3) -0.0743(3) 0.181(9) Uani 1 1 d GU . .
H233 H 0.2990 0.1738 -0.0928 0.217 Uiso 1 1 calc R . .
C234 C 0.33391(13) 0.1321(3) -0.0893(3) 0.183(8) Uani 1 1 d GU . .
H234 H 0.3176 0.1130 -0.1179 0.219 Uiso 1 1 calc R . .
C235 C 0.36942(14) 0.1243(2) -0.0617(3) 0.178(8) Uani 1 1 d GU . .
H235 H 0.3769 0.0999 -0.0717 0.214 Uiso 1 1 calc R . .
C236 C 0.39375(12) 0.1528(2) -0.0190(3) 0.183(9) Uani 1 1 d GU . .
H236 H 0.4175 0.1476 -0.0005 0.219 Uiso 1 1 calc R . .
C311 C 0.5677(4) -0.0382(7) 0.0597(7) 0.107(5) Uani 1 1 d U . .
C312 C 0.5907(4) -0.0218(8) 0.1190(8) 0.147(7) Uani 1 1 d U . .
H312 H 0.6029 0.0032 0.1245 0.176 Uiso 1 1 calc R . .
C313 C 0.5950(5) -0.0460(9) 0.1728(8) 0.160(8) Uani 1 1 d U . .
H313 H 0.6083 -0.0346 0.2124 0.192 Uiso 1 1 calc R . .
C314 C 0.5792(5) -0.0856(9) 0.1649(9) 0.150(7) Uani 1 1 d U . .
H314 H 0.5854 -0.1023 0.1994 0.180 Uiso 1 1 calc R . .
C315 C 0.5549(5) -0.1000(7) 0.1074(8) 0.117(5) Uani 1 1 d U . .
H315 H 0.5428 -0.1251 0.1020 0.140 Uiso 1 1 calc R . .
C316 C 0.5486(4) -0.0749(6) 0.0551(7) 0.104(5) Uani 1 1 d U . .
H316 H 0.5309 -0.0834 0.0158 0.125 Uiso 1 1 calc R . .
C321 C 0.5268(4) -0.0240(6) -0.0774(7) 0.092(4) Uani 1 1 d U . .
C322 C 0.5012(4) 0.0046(7) -0.1159(7) 0.106(4) Uani 1 1 d U . .
H322 H 0.5015 0.0323 -0.1035 0.128 Uiso 1 1 calc R . .
C323 C 0.4750(4) -0.0097(8) -0.1737(8) 0.127(5) Uani 1 1 d U . .
H323 H 0.4569 0.0082 -0.2009 0.152 Uiso 1 1 calc R . .
C324 C 0.5268(6) -0.0690(7) -0.0982(9) 0.143(7) Uani 1 1 d U . .
H324 H 0.5448 -0.0873 -0.0719 0.172 Uiso 1 1 calc R . .
C325 C 0.4763(6) -0.0547(9) -0.1917(9) 0.143(7) Uani 1 1 d U . .
H325 H 0.4588 -0.0630 -0.2312 0.172 Uiso 1 1 calc R . .
C326 C 0.5000(7) -0.0835(9) -0.1569(10) 0.154(7) Uani 1 1 d U . .
H326 H 0.4990 -0.1112 -0.1701 0.185 Uiso 1 1 calc R . .
C331 C 0.5993(4) -0.0056(7) -0.0142(8) 0.110(5) Uani 1 1 d U . .
C332 C 0.6300(4) -0.0007(7) 0.0345(10) 0.133(6) Uani 1 1 d U . .
H332 H 0.6329 0.0024 0.0733 0.159 Uiso 1 1 calc R . .
C333 C 0.6571(5) 0.0000(9) 0.0284(12) 0.158(7) Uani 1 1 d U . .
H333 H 0.6790 0.0047 0.0637 0.190 Uiso 1 1 calc R . .
C334 C 0.6553(7) -0.0056(12) -0.0239(15) 0.205(9) Uani 1 1 d U . .
H334 H 0.6757 -0.0068 -0.0245 0.246 Uiso 1 1 calc R . .
C335 C 0.6236(7) -0.0096(13) -0.0779(14) 0.222(10) Uani 1 1 d U . .
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H335 H 0.6205 -0.0099 -0.1170 0.266 Uiso 1 1 calc R . .
C336 C 0.5967(5) -0.0133(11) -0.0674(10) 0.188(8) Uani 1 1 d U . .
H336 H 0.5750 -0.0219 -0.1005 0.226 Uiso 1 1 calc R . .
C411 C 0.5631(3) 0.4447(5) -0.1080(6) 0.263(15) Uani 1 1 d GU . .
H411 H 0.5644 0.4154 -0.1039 0.316 Uiso 1 1 calc R . .
C412 C 0.5735(2) 0.4701(4) -0.0566(6) 0.186(10) Uani 1 1 d GU . .
C413 C 0.5716(2) 0.5139(4) -0.0627(7) 0.198(9) Uani 1 1 d GU . .
H413 H 0.5786 0.5310 -0.0283 0.238 Uiso 1 1 calc R . .
C414 C 0.5594(3) 0.5323(5) -0.1203(8) 0.229(11) Uani 1 1 d GU . .
H414 H 0.5582 0.5616 -0.1244 0.275 Uiso 1 1 calc R . .
C415 C 0.5491(4) 0.5068(7) -0.1717(7) 0.294(15) Uani 1 1 d GU . .
H415 H 0.5409 0.5191 -0.2102 0.352 Uiso 1 1 calc R . .
C416 C 0.5509(4) 0.4630(7) -0.1656(6) 0.310(16) Uani 1 1 d GU . .
H416 H 0.5440 0.4460 -0.2000 0.372 Uiso 1 1 calc R . .
C421 C 0.5470(4) 0.4940(6) 0.0443(8) 0.388(18) Uani 1 1 d GU . .
H421 H 0.5363 0.5105 0.0086 0.466 Uiso 1 1 calc R . .
C422 C 0.5372(5) 0.4983(8) 0.0873(10) 0.406(19) Uani 1 1 d GU . .
H422 H 0.5201 0.5177 0.0805 0.487 Uiso 1 1 calc R . .
C423 C 0.5532(6) 0.4736(8) 0.1406(10) 0.400(18) Uani 1 1 d GU . .
H423 H 0.5467 0.4765 0.1694 0.480 Uiso 1 1 calc R . .
C424 C 0.5788(6) 0.4446(7) 0.1508(8) 0.391(19) Uani 1 1 d GU . .
H424 H 0.5895 0.4280 0.1865 0.469 Uiso 1 1 calc R . .
C425 C 0.5885(5) 0.4403(6) 0.1078(7) 0.369(19) Uani 1 1 d GU . .
H425 H 0.6057 0.4208 0.1146 0.443 Uiso 1 1 calc R . .
C426 C 0.5726(4) 0.4650(5) 0.0545(7) 0.372(18) Uani 1 1 d GU . .
C431 C 0.6375(3) 0.4767(3) 0.0473(7) 0.346(17) Uani 1 1 d GU . .
C432 C 0.6499(2) 0.4877(4) 0.0095(8) 0.360(17) Uani 1 1 d GU . .
H432 H 0.6364 0.4823 -0.0328 0.432 Uiso 1 1 calc R . .
C433 C 0.6825(2) 0.5066(5) 0.0351(9) 0.357(16) Uani 1 1 d GU . .
H433 H 0.6907 0.5139 0.0098 0.429 Uiso 1 1 calc R . .
C434 C 0.7027(3) 0.5146(5) 0.0983(10) 0.344(17) Uani 1 1 d GU . .
H434 H 0.7245 0.5273 0.1154 0.413 Uiso 1 1 calc R . .
C435 C 0.6903(3) 0.5037(5) 0.1361(8) 0.338(16) Uani 1 1 d GU . .
H435 H 0.7038 0.5091 0.1784 0.406 Uiso 1 1 calc R . .
C436 C 0.6577(3) 0.4847(4) 0.1105(7) 0.358(16) Uani 1 1 d GU . .
H436 H 0.6494 0.4774 0.1358 0.429 Uiso 1 1 calc R . .
C511 C 0.7354(4) 0.1853(6) -0.1105(7) 0.095(4) Uani 1 1 d U . .
C512 C 0.7672(4) 0.1895(7) -0.0603(8) 0.109(4) Uani 1 1 d U . .
H512 H 0.7754 0.2146 -0.0380 0.131 Uiso 1 1 calc R . .
C513 C 0.7882(5) 0.1504(7) -0.0433(10) 0.124(5) Uani 1 1 d U . .
H513 H 0.8104 0.1531 -0.0079 0.149 Uiso 1 1 calc R . .
C514 C 0.7810(6) 0.1083(9) -0.0708(12) 0.153(7) Uani 1 1 d U . .
H514 H 0.7970 0.0862 -0.0544 0.184 Uiso 1 1 calc R . .
C515 C 0.7497(6) 0.1048(8) -0.1211(11) 0.143(7) Uani 1 1 d U . .
H515 H 0.7420 0.0802 -0.1448 0.172 Uiso 1 1 calc R . .
C516 C 0.7275(6) 0.1434(8) -0.1373(11) 0.140(6) Uani 1 1 d U . .
H516 H 0.7046 0.1399 -0.1703 0.168 Uiso 1 1 calc R . .
C521 C 0.7278(4) 0.2956(6) -0.1111(7) 0.093(4) Uani 1 1 d U . .
C522 C 0.7202(4) 0.3328(6) -0.0828(8) 0.108(5) Uani 1 1 d U . .
H522 H 0.7023 0.3283 -0.0757 0.130 Uiso 1 1 calc R . .
C523 C 0.7362(4) 0.3742(6) -0.0648(9) 0.115(5) Uani 1 1 d U . .
H523 H 0.7307 0.3940 -0.0444 0.138 Uiso 1 1 calc R . .
C524 C 0.7610(4) 0.3817(7) -0.0812(9) 0.119(5) Uani 1 1 d U . .
H524 H 0.7719 0.4079 -0.0741 0.142 Uiso 1 1 calc R . .
C525 C 0.7687(4) 0.3477(6) -0.1090(9) 0.109(5) Uani 1 1 d U . .
H525 H 0.7857 0.3525 -0.1185 0.131 Uiso 1 1 calc R . .
C526 C 0.7528(4) 0.3068(6) -0.1234(8) 0.105(5) Uani 1 1 d U . .
H526 H 0.7596 0.2870 -0.1419 0.126 Uiso 1 1 calc R . .
C531 C 0.6772(5) 0.2370(7) -0.2193(8) 0.127(6) Uani 1 1 d U . .
C532 C 0.6537(6) 0.2063(9) -0.2447(8) 0.171(8) Uani 1 1 d U . .
H532 H 0.6513 0.1858 -0.2210 0.206 Uiso 1 1 calc R . .
C533 C 0.6340(8) 0.2067(11) -0.3055(10) 0.212(11) Uani 1 1 d U . .
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H533 H 0.6140 0.1900 -0.3236 0.254 Uiso 1 1 calc R . .
C534 C 0.6400(8) 0.2292(11) -0.3447(11) 0.200(10) Uani 1 1 d U . .
H534 H 0.6276 0.2237 -0.3871 0.240 Uiso 1 1 calc R . .
C535 C 0.6663(7) 0.2618(10) -0.3177(10) 0.180(9) Uani 1 1 d U . .
H535 H 0.6696 0.2814 -0.3413 0.216 Uiso 1 1 calc R . .
C536 C 0.6859(6) 0.2615(8) -0.2544(9) 0.149(7) Uani 1 1 d U . .
H536 H 0.7059 0.2783 -0.2341 0.179 Uiso 1 1 calc R . .
C611 C 0.7305(3) 0.1302(6) 0.2993(6) 0.097(4) Uani 1 1 d U . .
C612 C 0.7251(4) 0.1565(9) 0.3362(8) 0.150(7) Uani 1 1 d U . .
H612 H 0.7029 0.1573 0.3301 0.180 Uiso 1 1 calc R . .
C613 C 0.7521(5) 0.1832(9) 0.3843(9) 0.165(8) Uani 1 1 d U . .
H613 H 0.7472 0.2048 0.4035 0.198 Uiso 1 1 calc R . .
C614 C 0.7817(4) 0.1752(8) 0.3975(8) 0.144(7) Uani 1 1 d U . .
H614 H 0.8009 0.1863 0.4333 0.173 Uiso 1 1 calc R . .
C615 C 0.7865(4) 0.1494(8) 0.3588(9) 0.132(6) Uani 1 1 d U . .
H615 H 0.8090 0.1480 0.3664 0.158 Uiso 1 1 calc R . .
C616 C 0.7616(4) 0.1260(6) 0.3109(7) 0.108(5) Uani 1 1 d U . .
H616 H 0.7668 0.1081 0.2880 0.130 Uiso 1 1 calc R . .
C626 C 0.7319(6) 0.0382(8) 0.1933(9) 0.141(6) Uani 1 1 d U . .
H626 H 0.7373 0.0639 0.1824 0.169 Uiso 1 1 calc R . .
C621 C 0.7116(6) 0.0380(7) 0.2195(8) 0.133(6) Uani 1 1 d U . .
C622 C 0.7017(8) -0.0035(9) 0.2338(10) 0.172(8) Uani 1 1 d U . .
H622 H 0.6881 -0.0030 0.2513 0.206 Uiso 1 1 calc R . .
C623 C 0.7105(11) -0.0402(12) 0.2237(15) 0.223(12) Uani 1 1 d U . .
H623 H 0.7008 -0.0641 0.2300 0.268 Uiso 1 1 calc R . .
C625 C 0.7452(8) -0.0014(9) 0.1825(11) 0.195(8) Uani 1 1 d U . .
H625 H 0.7587 -0.0011 0.1650 0.233 Uiso 1 1 calc R . .
C624 C 0.7351(10) -0.0466(11) 0.2027(15) 0.228(12) Uani 1 1 d U . .
H624 H 0.7439 -0.0729 0.2011 0.273 Uiso 1 1 calc R . .
C631 C 0.6648(4) 0.0814(11) 0.2556(8) 0.198(10) Uani 1 1 d U . .
C632 C 0.6753(6) 0.0619(13) 0.3127(11) 0.248(12) Uani 1 1 d U . .
H632 H 0.6989 0.0574 0.3412 0.298 Uiso 1 1 calc R . .
C633 C 0.6509(7) 0.0491(15) 0.3276(12) 0.282(13) Uani 1 1 d U . .
H633 H 0.6577 0.0396 0.3670 0.339 Uiso 1 1 calc R . .
C634 C 0.6186(7) 0.0512(15) 0.2831(13) 0.285(13) Uani 1 1 d U . .
H634 H 0.6016 0.0384 0.2877 0.342 Uiso 1 1 calc R . .
C635 C 0.6089(5) 0.0723(13) 0.2290(10) 0.248(12) Uani 1 1 d U . .
H635 H 0.5856 0.0794 0.2019 0.297 Uiso 1 1 calc R . .
C636 C 0.6324(5) 0.0826(11) 0.2150(9) 0.208(10) Uani 1 1 d U . .
H636 H 0.6249 0.0909 0.1748 0.249 Uiso 1 1 calc R . .

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C1 0.047(7) 0.148(11) 0.049(7) -0.007(7) 0.023(5) -0.022(7)
O1 0.042(4) 0.181(10) 0.072(6) 0.002(6) 0.028(4) -0.004(5)
Rh1 0.0351(5) 0.1601(13) 0.0514(6) -0.0028(6) 0.0185(4) -0.0085(6)
Si1 0.066(2) 0.155(4) 0.056(2) -0.006(2) 0.0325(18) -0.038(2)
Rh2 0.0358(5) 0.1464(12) 0.0445(6) -0.0071(6) 0.0205(4) -0.0198(5)
Si2 0.0424(18) 0.209(6) 0.051(2) 0.031(3) 0.0238(16) 0.015(2)
P2 0.0376(15) 0.132(3) 0.0497(18) 0.0022(19) 0.0230(13) -0.0154(18)
O2 0.040(4) 0.165(9) 0.049(5) 0.002(5) 0.020(4) -0.007(5)
C2 0.069(9) 0.182(15) 0.077(9) 0.020(9) 0.040(7) -0.008(10)
Si3 0.051(2) 0.226(6) 0.071(3) -0.053(3) 0.0274(19) -0.022(3)
C3 0.033(5) 0.188(14) 0.044(7) 0.001(7) 0.014(5) -0.018(7)
O3 0.043(4) 0.200(10) 0.047(5) -0.011(6) 0.022(4) -0.024(5)
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C4 0.043(5) 0.198(16) 0.057(8) -0.003(8) 0.018(5) -0.033(8)
Si4 0.079(3) 0.128(5) 0.199(7) -0.043(5) -0.005(4) 0.012(3)
C5 0.044(5) 0.148(12) 0.048(7) 0.003(6) 0.022(5) -0.014(6)
Si5 0.071(2) 0.196(6) 0.048(2) 0.020(3) 0.0154(18) -0.044(3)
O5 0.061(7) 0.227(15) 0.168(13) 0.028(11) 0.055(8) 0.001(8)
Si6 0.087(3) 0.163(5) 0.083(3) -0.024(3) 0.064(2) -0.051(3)
C6 0.052(7) 0.197(17) 0.080(10) -0.037(10) 0.027(7) -0.026(8)
O6 0.044(4) 0.144(9) 0.062(5) -0.003(5) 0.031(4) -0.014(5)
O7 0.035(4) 0.193(11) 0.054(5) 0.000(6) 0.019(4) -0.015(5)
C7 0.074(8) 0.208(17) 0.108(11) -0.039(11) 0.069(8) -0.041(9)
C8 0.117(13) 0.26(3) 0.18(2) -0.011(19) 0.109(15) 0.014(16)
O9 0.060(4) 0.166(9) 0.055(5) -0.011(5) 0.032(4) -0.014(5)
C9 0.080(13) 0.29(2) 0.223(19) 0.032(15) 0.056(13) 0.041(13)
C10 0.28(4) 0.35(4) 0.160(18) -0.03(2) 0.00(2) 0.19(3)
O11 0.185(17) 0.32(2) 0.213(18) 0.02(2) 0.065(17) 0.096(15)
C11 0.034(5) 0.178(10) 0.035(6) -0.016(7) 0.018(4) -0.037(7)
C12 0.033(5) 0.156(9) 0.050(6) -0.021(7) 0.024(5) -0.035(7)
C13 0.046(6) 0.155(9) 0.049(6) -0.012(7) 0.024(5) -0.041(7)
C14 0.047(6) 0.156(10) 0.051(7) -0.009(7) 0.021(5) -0.036(7)
C15 0.050(6) 0.167(10) 0.051(7) -0.014(8) 0.025(5) -0.031(8)
C16 0.053(6) 0.169(10) 0.052(7) -0.016(8) 0.029(6) -0.033(8)
C20 0.23(3) 0.35(3) 0.22(2) 0.01(3) 0.09(3) 0.05(3)
C30 0.36(5) 0.42(5) 0.22(2) -0.03(4) 0.05(3) 0.09(4)
C21 0.040(5) 0.220(16) 0.044(6) -0.009(8) 0.016(5) -0.019(8)
C22 0.045(6) 0.34(2) 0.064(7) -0.048(12) 0.025(6) -0.021(11)
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C24 0.037(5) 0.263(18) 0.038(6) 0.000(9) 0.019(4) -0.011(9)
C25 0.043(6) 0.31(2) 0.064(7) -0.033(11) 0.036(6) -0.027(10)
C26 0.045(6) 0.31(2) 0.071(7) -0.044(11) 0.034(5) -0.045(10)
C31 0.030(5) 0.168(11) 0.053(6) -0.032(7) 0.016(5) -0.018(6)
C32 0.037(5) 0.171(10) 0.045(6) -0.017(6) 0.028(5) -0.017(6)
C33 0.039(5) 0.169(10) 0.053(6) -0.012(7) 0.025(4) -0.009(7)
C34 0.048(6) 0.170(11) 0.071(7) -0.023(7) 0.036(5) -0.018(7)
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C36 0.049(7) 0.170(10) 0.078(8) -0.036(8) 0.020(6) -0.005(8)
C41 0.042(6) 0.124(9) 0.070(8) 0.012(7) 0.024(6) -0.007(5)
C42 0.040(5) 0.133(9) 0.073(8) 0.000(8) 0.028(6) -0.008(6)
C43 0.052(6) 0.147(10) 0.108(11) -0.022(11) 0.025(7) 0.002(7)
C44 0.061(7) 0.144(11) 0.122(12) -0.028(11) 0.006(8) -0.001(7)
C45 0.053(6) 0.142(10) 0.116(12) -0.028(11) 0.015(8) -0.010(7)
C46 0.038(5) 0.138(9) 0.085(9) 0.001(9) 0.015(6) -0.009(6)
C61 0.039(5) 0.143(12) 0.052(7) 0.003(6) 0.025(5) -0.014(6)
C62 0.041(6) 0.209(14) 0.082(9) 0.052(9) 0.027(6) 0.002(7)
C63 0.044(6) 0.197(14) 0.054(7) 0.026(8) 0.017(5) -0.030(7)
C64 0.062(7) 0.144(13) 0.064(7) -0.020(7) 0.037(6) -0.046(7)
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C66 0.050(6) 0.146(11) 0.045(6) 0.000(6) 0.027(5) -0.008(6)
C51 0.045(6) 0.132(8) 0.038(5) 0.000(6) 0.027(4) -0.022(6)
C56 0.045(6) 0.151(9) 0.049(6) -0.017(6) 0.028(5) -0.018(6)
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C112 0.067(8) 0.28(2) 0.106(11) -0.029(11) 0.044(8) -0.018(10)
C113 0.065(8) 0.32(2) 0.131(13) -0.012(13) 0.052(9) -0.014(11)
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C115 0.088(9) 0.32(2) 0.112(12) -0.018(12) 0.059(9) -0.038(12)
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C123 0.152(16) 0.268(19) 0.172(17) -0.059(17) 0.110(13) 0.018(15)

C124 0.22(2) 0.28(2) 0.25(2) -0.07(2) 0.137(17) 0.034(18)
C125 0.22(2) 0.259(19) 0.26(2) -0.06(2) 0.109(19) 0.043(19)
C126 0.19(2) 0.267(19) 0.28(3) -0.06(2) 0.092(18) -0.011(19)
C131 0.044(7) 0.290(18) 0.062(7) -0.033(9) 0.031(6) 0.000(9)
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C211 0.172(17) 0.192(18) 0.140(16) 0.044(13) 0.089(13) 0.012(14)
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C213 0.080(11) 0.202(17) 0.146(15) 0.033(13) 0.052(9) 0.026(11)
C214 0.083(12) 0.194(19) 0.23(2) 0.010(15) 0.031(12) 0.026(12)
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C221 0.29(2) 0.35(2) 0.110(13) 0.077(14) 0.098(16) 0.10(2)
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C234 0.134(11) 0.204(19) 0.21(2) -0.017(15) 0.095(14) -0.033(14)
C235 0.153(13) 0.217(18) 0.20(2) -0.020(14) 0.115(15) -0.013(13)
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C311 0.071(8) 0.183(14) 0.067(7) 0.005(8) 0.037(6) -0.034(9)
C312 0.085(10) 0.243(17) 0.073(8) 0.013(9) 0.015(8) -0.067(11)
C313 0.105(12) 0.250(19) 0.066(7) 0.014(10) 0.007(9) -0.067(12)
C314 0.100(12) 0.236(18) 0.082(8) 0.036(11) 0.028(8) -0.044(12)
C315 0.108(11) 0.160(14) 0.088(8) 0.012(8) 0.055(8) -0.031(10)
C316 0.059(7) 0.181(14) 0.070(7) 0.015(8) 0.033(6) -0.026(8)
C321 0.085(8) 0.134(11) 0.063(8) -0.003(7) 0.044(6) -0.042(8)
C322 0.066(8) 0.167(12) 0.079(9) -0.011(8) 0.034(6) -0.034(7)
C323 0.063(8) 0.212(15) 0.088(9) -0.017(10) 0.029(6) -0.047(9)
C324 0.145(14) 0.149(12) 0.087(10) -0.028(10) 0.030(8) -0.033(11)
C325 0.102(12) 0.225(17) 0.079(11) -0.044(10) 0.033(8) -0.059(11)
C326 0.155(16) 0.196(15) 0.096(12) -0.055(11) 0.056(10) -0.047(12)
C331 0.073(7) 0.178(15) 0.087(9) 0.004(10) 0.048(6) -0.031(10)
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C333 0.081(8) 0.25(2) 0.158(13) -0.030(16) 0.072(9) -0.030(12)
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C336 0.090(9) 0.38(2) 0.105(10) -0.002(15) 0.061(9) 0.018(15)
C411 0.24(2) 0.194(18) 0.26(2) 0.039(15) 0.07(2) 0.03(2)
C412 0.084(11) 0.156(16) 0.26(2) 0.035(15) 0.049(14) -0.021(13)
C413 0.131(15) 0.169(15) 0.28(2) 0.058(16) 0.100(17) 0.016(15)
C414 0.21(2) 0.221(19) 0.32(3) 0.081(16) 0.18(2) 0.018(18)
C415 0.29(3) 0.25(2) 0.27(2) 0.071(19) 0.11(2) -0.02(3)
C416 0.31(3) 0.25(2) 0.26(2) 0.05(2) 0.07(2) 0.01(3)
C421 0.47(4) 0.39(3) 0.37(3) 0.01(3) 0.27(3) 0.19(2)
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C435 0.118(15) 0.27(2) 0.51(3) -0.25(2) 0.087(18) -0.002(15)

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C436 0.126(17) 0.31(3) 0.49(3) -0.20(3) 0.066(19) -0.004(18)
C511 0.086(7) 0.142(11) 0.093(9) -0.025(8) 0.072(6) -0.025(8)
C512 0.087(8) 0.163(12) 0.098(10) -0.011(9) 0.064(7) -0.014(8)
C513 0.104(10) 0.151(13) 0.139(13) -0.020(10) 0.079(9) -0.014(8)
C514 0.128(12) 0.176(14) 0.152(16) -0.047(13) 0.073(10) -0.008(12)
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C525 0.070(8) 0.136(12) 0.131(13) 0.008(10) 0.061(8) -0.020(8)
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C615 0.057(7) 0.210(18) 0.102(12) -0.019(10) 0.024(7) -0.007(9)
C616 0.061(7) 0.163(14) 0.079(9) -0.004(8) 0.023(7) -0.002(8)
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C621 0.140(15) 0.124(12) 0.061(10) 0.010(9) 0.005(8) -0.042(11)
C622 0.222(19) 0.130(15) 0.093(12) 0.009(13) 0.036(12) -0.060(15)
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C632 0.117(11) 0.49(3) 0.106(12) 0.107(16) 0.039(9) -0.082(18)
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C634 0.121(10) 0.57(3) 0.123(15) 0.095(19) 0.039(10) -0.12(2)
C635 0.089(9) 0.50(3) 0.106(13) 0.069(16) 0.020(9) -0.128(16)
C636 0.080(8) 0.42(3) 0.087(11) 0.058(14) 0.020(7) -0.084(15)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)

 treatment of cell esds is used for estimating esds involving l.s. planes.
;

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Rh1 Rh2 2.6833(19) . ?
Si1 C331 1.801(16) . ?
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C3 O7 1.29(2) . ?
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Si4 C44 2.10(2) . ?
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O1 Rh1 P1 177.4(3) . . ?
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O7 Rh1 O5 94.5(5) . . ?
O1 Rh1 O5 84.6(5) . . ?
P1 Rh1 O5 97.9(4) . . ?
C42 Rh1 Rh2 102.4(5) . . ?
O7 Rh1 Rh2 77.5(3) . . ?
O1 Rh1 Rh2 92.6(3) . . ?
P1 Rh1 Rh2 84.80(12) . . ?
O5 Rh1 Rh2 171.6(4) . . ?
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C321 Si1 C14 114.9(7) . . ?
C311 Si1 C14 115.6(7) . . ?
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O3 Rh2 P2 173.6(4) . . ?
C12 Rh2 P2 99.3(3) . . ?
O3 Rh2 O2 86.2(4) . . ?
C12 Rh2 O2 172.4(4) . . ?
P2 Rh2 O2 88.3(2) . . ?
O3 Rh2 O6 85.7(4) . . ?
C12 Rh2 O6 89.7(5) . . ?
P2 Rh2 O6 97.6(2) . . ?
O2 Rh2 O6 89.8(4) . . ?
O3 Rh2 Rh1 92.1(3) . . ?
C12 Rh2 Rh1 101.0(4) . . ?
P2 Rh2 Rh1 83.65(12) . . ?
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C15 C16 C11 126.9(13) . . ?
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C634 C633 C632 116(2) . . ?
C633 C634 C635 121(2) . . ?
C636 C635 C634 121(2) . . ?
C631 C636 C635 121(2) . . ?

_diffrn_measured_fraction_theta_max    0.775
_diffrn_reflns_theta_full              23.55
_diffrn_measured_fraction_theta_full   0.775
_refine_diff_density_max    1.198
_refine_diff_density_min   -0.602
_refine_diff_density_rms    0.142
```