Experimental and Computational Investigation on the Formation Pathway of $[RuCl_2(CO)_2(ERR')_2]$ (E = S, Se, Te; R, R' = Me, Ph) from $[RuCl_2(CO)_3]_2$ and ERR'

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1. Synthetic Details

*1.1 [$RuCl_2(CO)_2(SMePh)_2$] (**2_{cct}**)*

SMePh (0.15 mL, 1.28 mmol) and $[RuCl_2(CO)_3]_2$ (0.164 g, 0.320 mmol). Light yellow crystals of $[RuCl_2(CO)_2(SMePh)_2]$ (**2_{cct}**). Yield 0.073 g (24%). Anal. calcd. for $C_{16}H_{16}Cl_2O_2RuS_2$: C, 40.34; H, 3.39; S, 13.46. Found: C, 40.15; H, 3.13; S, 13.59. NMR (δ, ppm; CH_2Cl_2): ^{13}C 21.9 (*C*H_3-), 129.1, 129.5, 130.3, 134.4 [*C*(arom)], 189.4 (*C*O).

*1.2 [$RuCl_2(CO)_2(SeMe_2)_2$] (**4_{cct}**) and [$RuCl_2(CO)_3(SeMe_2)$] (**10**)*

$SeMe_2$ (0.10 mL, 1.29 mmol) and $[RuCl_2(CO)_3]_2$ (0.164 g, 0.320 mmol). Yellow and colourless crystals of $[RuCl_2(CO)_2(SeMe_2)_2]$ (**4_{cct}**) (0.106 g, yield 37 %) and $[RuCl_2(CO)_3(SeMe_2)]$ (**10**) (0.044 g, yield 19 %), respectively. Anal. calcd. for $C_6H_{12}Cl_2O_2RuSe_2$: C, 16.16; H, 2.71. Found: C, 16.37; H, 2.65. NMR (δ, ppm; CH_2Cl_2): ^{13}C 14.4 (*C*H_3-), 191.6 (*C*O); ^{77}Se 88. Anal. calcd. for $C_5H_6Cl_2O_3RuSe$: C, 16.45; H, 1.66. Found: C, 16.75; H, 1.50. NMR (δ, ppm; CH_2Cl_2): ^{13}C 13.6 (*C*H_3-), 181.5(*1*), 185.3(*2*) (*C*O); ^{77}Se 55.

*1.3 [$RuCl_2(CO)_2(SeMePh)_2$] (**5_{cct}**) and $RuCl_2(CO)_3(SeMePh)$] (**11**)*

SeMePh (0.201 g, 1.17 mmol) and $[RuCl_2(CO)_3]_2$ (0.150 g, 0.293 mmol). Yellow and colourless crystals of $[RuCl_2(CO)_2(SeMePh)_2]$ (**5_{cct}**) (0.121 g, yield 36 %) and $[RuCl_2(CO)_3(SeMePh)]$ (**11**) (0.032 g, yield 13 %), respectively. Anal. Calcd. for $C_{16}H_{16}Cl_2O_2RuSe_2$: C, 33.70; H, 2.83. Found: C, 33.96; H, 2.86. NMR (δ, ppm; CH_2Cl_2): ^{13}C 15.0 and 15.1 (*C*H_3-), 129.2, 129.6, 130.0, 130.1 [*C*(arom)], 190.2 and 190.9, 190.9 and 191.7 (*C*O); ^{77}Se 225 and 227. Anal. Calcd. for $C_{10}H_8Cl_2O_3RuSe$: C, 28.12; H, 1.89. Found: C, 28.30; H, 1.75. NMR (δ, ppm; CH_2Cl_2): ^{13}C 14.1 (*C*H_3-), 127.7, 130.1, 130.4, 130.7 [*C*(arom)], 181.7(*1*), 184.5(*1*), 185.3(*1*) (*C*O); ^{77}Se 192.

*1.4 [$RuCl_2(CO)_2(SePh_2)_2$] (**6_{cct}**)*

$SePh_2$ (0.178 g, 0.764 mmol) and $[RuCl_2(CO)_3]_2$ (0.095 g, 0.186 mmol). Yellow crystals of $[RuCl_2(CO)_2(SePh_2)_2]$ (**6_{cct}**) (0.157 g, yield 42 %). Anal. Calcd. for $C_{26}H_{20}Cl_2O_2RuSe_2$: C, 44.97; H, 2.90. Found: C, 44.79, H, 2.81. NMR (δ, ppm; CH_2Cl_2): ^{77}Se 418.

*1.5 [$RuCl_2(CO)_2(TeMePh)_2$] (**8_{cct}**)*

TeMePh (0.308 g, 1.40 mmol) and $[RuCl_2(CO)_3]_2$ (0.179 g, 0.350 mmol). Orange-red crystals of $[RuCl_2(CO)_2(TeMePh)_2]$ (**8_{cct}**) (0.360 g, yield 77 %). Anal. Calcd. for $C_{16}H_{16}Cl_2O_2RuTe_2$: C, 28.79; H, 2.42. Found: C, 28.61; H, 2.36. NMR (δ, ppm; CH_2Cl_2): ^{13}C -3.7 and -3.6 (*C*H_3-), 114.2, 129.7, 130.1, 134.4 [*C*(arom)], 192. 3 and 192.9, 192.9 and 193.5 (*C*O); ^{125}Te 427 and 430.

2. Crystal Structure Determination of $\mathbf{2}_{cct}$, $\mathbf{4}_{cct}$, $\mathbf{5}_{cct}$, $\mathbf{6}_{cct}$, 10, and 11

2.1 Crystal data

Table S1. *Crystal data for the cct isomers of $[RuCl_2(CO)_2(SMePh)_2]$ ($\mathbf{2}_{cct}$), $[RuCl_2(CO)_2(SeMe_2)_2]$ ($\mathbf{4}_{cct}$), $[RuCl_2(CO)_2(SePh_2)_2]$ ($\mathbf{6}_{cct}$), $[RuCl_2(CO)_2(TeMePh)_2]$ ($\mathbf{8}_{cct}$), $[RuCl_2(CO)_3(SeMe_2)]$ (**10**), and $[RuCl_2(CO)_3(SeMePh)]$ (**11**).*

	$\mathbf{2}_{cct}$	$\mathbf{4}_{cct}$	$\mathbf{6}_{cct}$	$\mathbf{8}_{cct}$ [a]	**10**	**11**
Empirical formula	$C_{16}H_{16}O_2Cl_2S_2Ru$	$C_6H_{12}O_2Cl_2Se_2Ru$	$C_{26}H_{20}O_2Cl_2Se_2Ru$	$C_{32}H_{32}O_4Cl_4Te_4Ru_2$	$C_5H_6O_3Cl_2SeRu$	$C_{10}H_8O_3Cl_2SeRu$
Relative molecular mass	476.38	446.05	694.31	1334.91	365.03	427.09
Crystal system	orthorhombic	orthorhombic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	*Pbca*	$P2_12_12_1$	$P2_1$	$P2_1$	$P2_1/n$	$C2/c$
T (°C)	-153(2)	-153(2)	-173(2)	-153(2)	-123(2)	-153(2)
a (Å)	9.891(2)	6.9353(14)	6.4041(13)	11.917(2)	6.1101(12)	20.297(4)
b (Å)	12.172(2)	10.764(2)	17.358(4)	11.051(2)	16.755(3)	9.666(2)
c (Å)	30.653(6)	17.208(3)	11.699(2)	16.051(3)	10.176(2)	15.129(3)
β (°)			103.23(3)	110.59(3)	102.04(3)	112.81(3)
V (Å^3)	3690.4(12)	1284.7(4)	1265.9(5)	1978.8(4)	1018.9(4)	2735.9(11)
Z	8	4	2	2	4	8
ρ_{calc} (g/cm^3)	1.715	2.306	1.821	2.240	2.380	2.074
μ (mm^{-1})	1.370	7.273	3.727	3.957	5.600	4.188
F(000)	1904	840	676	1240	680	1632
Crystal size (mm^3)	0.25 x 0.15 x 0.15	0.20 x 0.15 x 0.10	0.40 x 0.20 x 0.10	0.20 x 0.17 x 0.10	0.35 x 0.15 x 0.15	0.25 x 0.15 x 0.10
θ range (°)	2.735-26.000	2.232-25.439	2.951-25.989	2.711-24.996	3.178-27.480	2.372-25.015
Refl. collected/unique	13561/3439	4657/2360	9429/4494	14979/6524	3882/2305	16318/2357
No of parameters/restraints	211	123	299	209/2	112	156
R_{INT}	0.0529	0.0259	0.0857	0.0853	0.0473	0.0361
R_1 [b] [I>2sσ(I)]	0.0399	0.0210	0.0551	0.0973	0.0379	0.0222
wR_2 [c] (all data)	0.1001	0.0508	0.1738	0.2534	0.0968	0.0565
GoF on F^2	1.051	1.046	1.065	1.073	1.036	1.112
$\Delta\rho_{max,min}$ (e Å−3)	1.940,-0.818	0.468,-0.508	1.103,-1.086	7.092,-1.521	0.892,-1.033	0.518,-0.570

[a] The structure determination and refinement is tentative. [b] $R_1 = \Sigma\,||F_o| - |F_c||/\Sigma|F_o|$. [c] $wR_2 = [\Sigma w(|F_o| - |F_c|)^2/\Sigma wF_o^2]^{½}$.

2.2 Selected bond lengths and angles cct-[$RuCl_2(CO)_2(ERR')_2$] (E = S, Se, Te; R, R' = Me, Ph)

Table S2. *Selected bond lengths (Å) and angles (°) of the cct-[$RuCl_2(CO)_2(ERR')_2$] (E = S, Se, Te; R, R' = Me, Ph) complexes.*[a]

	2$_{cct}$	**3**$_{cct}$ [b]	**4**$_{cct}$	**6**$_{cct}$	**9**$_{cct}$ [c]
Ru1-E1	2.4084(11)	2.388(1)	2.4908(7)	2.4922(16)	2.6478(7)
Ru1-E2	2.3774(12)	2.406(1)	2.5125(7)	2.5065(15)	2.6637(7)
Ru1-X1	2.4219(11)	2.435(1)	2.4267(13)	2.413(3)	2.436(2)
Ru1-X2	2.4186(10)	2.412(1)	2.4315(14)	2.438(3)	2.444(2)
Ru1-C1	1.877(4)	1.877(5)	1.870(6)	1.895(15)	1.871(7)
Ru1-C2	1.877(5)	1.883(5)	1.876(5)	1.867(12)	1.849(8)
C1-O1	1.133(5)	1.135(6)	1.142(7)	1.115(17)	1.130(9)
C2-O2	1.135(5)	1.126(6)	1.133(6)	1.152(16)	1.158(9)
E1-Ru1-E2	174.11(4)	166.19(4)	169.05(2)	164.01(6)	165.51(3)
E1-Ru1-X1	92.80(4)	84.08(5)	83.04(4)	88.81(8)	82.99(5)
E1-Ru1-X2	89.70(4)	89.28(5)	83.76(4)	83.66(8)	84.15(5)
E1-Ru1-C1	89.74(13)	94.3(2)	95.66(16)	90.2(4)	95.4(2)
E1-Ru1-C2	90.25(13)	90.4(2)	95.22(15)	94.4(4)	94.2(2)
E2-Ru1-X1	82.40(4)	84.21(5)	90.42(4)	83.89(8)	89.9(2)
E2-Ru1-X2	86.88(4)	83.86(5)	87.85(4)	82.36(8)	84.15(5)
E2-Ru1-C1	93.04(13)	92.7(2)	92.83(16)	103.4(4)	95.5(2)
E2-Ru1-C2	90.25(13)	101.1(2)	91.39(15)	93.1(4)	95.1(2)
X1-Ru1-X2	89.70(4)	92.14(4)	93.07(5)	91.64(10)	88.95(7)
X1-Ru1-C1	92.80(4)	88.1(2)	87.66(16)	86.3(4)	89.9(2)
X1-Ru1-C2	174.80(13)	174.2(2)	179.00(16)	173.6(4)	177.1(2)
X2-Ru1-C1	179.64(14)	176.5(2)	178.15(15)	176.8(4)	178.8(2)
X2-Ru1-C2	85.90(12)	86.0(2)	87.35(16)	89.1(4)	90.2(2)
C1-Ru1-C2	94.46(18)	94.1(2)	91.9(2)	93.4(5)	91.0(3)

[a] The tentative bond parameters of **8**$_{cct}$ are shown in Fig. S1. [b] Ref 1. [c] Ref. 2.

2.3 Selected bond lengths and angles of [$RuCl_2(CO)_3(SeRR')$] (R.R' = Me, Ph)

Table S3. *Selected bond lengths (Å) and angles (°) of [$RuCl_2(CO)_3(SeMe_2)$] (**10**) and [$RuCl_2(CO)_3(SeMePh)$] (**11**)*

	10	**11**
Ru1-Se1	2.5483(7)	2.5239(11)
Ru1-Cl1	2.4202(13)	2.4063(9)
Ru1-Cl2	2.4132(11)	2.4188(8)
Ru1-C1	1.895(4)	1.892(3)
Ru1-C2	1.903(5)	1.901(3)
Ru1-C3	1.944(5)	1.946(3)
C1-O1	1.141(5)	1.134(4)
C2-O2	1.133(6)	1.134(4)
C3-O3	1.130(5)	1.121(4)
Se1-Ru1-Cl1	92.30(13)	84.08(3)
Se1-Ru1-Cl2	89.63(3)	83.17(2)
Se1-Ru1-C1	92.3(13)	93.85(8)
Se1-Ru1-C2	86.29(12)	83.89(9)
Se1-Ru1-C3	174.71(13)	169.31(9)
Cl1-Ru1-Cl2	90.81(4)	89.99(3)
Cl1-Ru1-C1	86.27(13)	90.34(9)
Cl1-Ru1-C2	176.16(13)	176.92(9)
Cl1-Ru1-C3	91.59(11)	86.85(10)
Cl2-Ru1-C1	176.5(13)	176.95(9)
Cl2-Ru1-C2	89.16(14)	87.46(9)
Cl2-Ru1-C3	85.27(13)	91.21(9)
C1-Ru1-C2	93.88(19)	92.11(12)
C1-Ru1-C3	92.87(18)	91.83(12)
C2-Ru1-C3	92.23(13)	94.94(13)
C111-Se1-C121	96.4(2)	101.73(14)

3. Tentative Molecular Structure of $[RuCl_2(CO)_2(TeMePh)_2]$ (8_{cct}).

The crystals of *cct*-$[RuCl_2(CO)_2(TeMePh)_2]$ (**8_{cct}**) scattered X-rays only weakly. Therefore, the full anisotropic refinement of the non-hydrogen atoms was not possible. The anisotropic displacement of the carbon atoms in TeMePh ligands were therefore constrained to be equal within the given ligand. While the refinement must thus be considered only tentative, it provides unambiguous information about the identity of the complex (see Fig. S1).

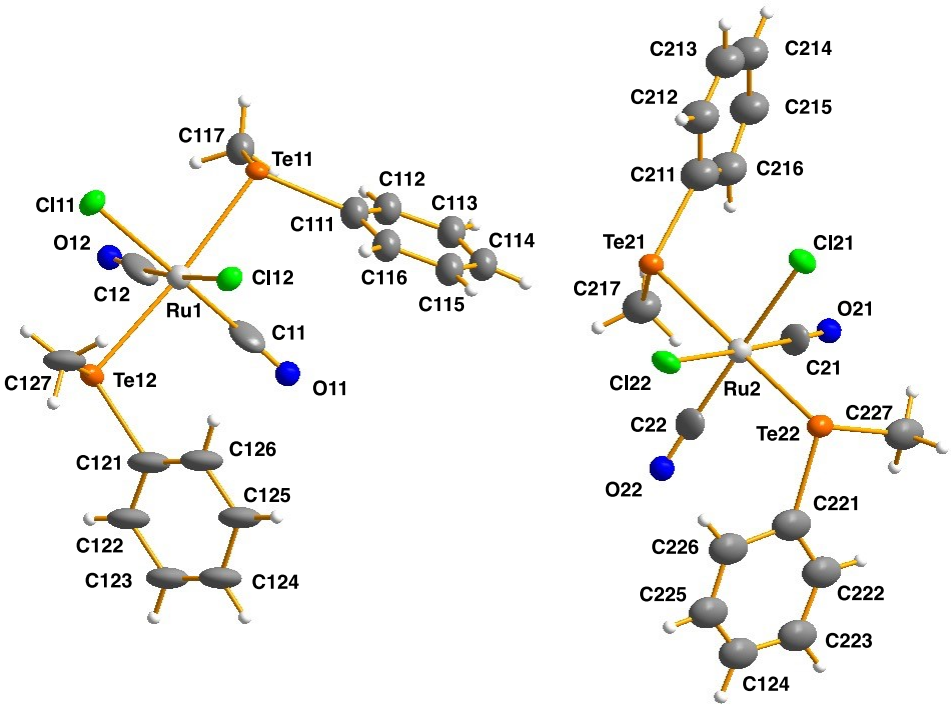


Fig. S1. Tentative molecular structure of *cct*-$[RuCl_2(CO)_2(TeMePh)_2$ (**8_{cct}**). The anisotropic displacement parameters are displayed in 50 % probability level. The selected bond lengths (Å) and angles (°): Ru-Te 2.624(4)-2.662(4), Ru-Cl 2.423(9)-2.447(10), Ru-C 1.82(4)-1.91(4), Te-C 2.067(16)-2.145(15), Te-Ru-Te 167.85(16)-174.63(14), Te-Ru-Cl 82.4(3)-95.6(2), Te-Ru-C 92.5(11)-98.1(12), Cl-Ru-Cl 88.7(3)-91.7(3), Cl-Ru-C(*trans*) 174.7(12)-178.9(12), Cl-Ru-C(*cis*) 85.9(11)-88.3(12), C-Ru-C 94.5(15)-96.6(17).

4. Assignment of NMR Spectra of $[RuCl_2(CO)_2(ERR')_2]$ and $[RuCl_2(CO)_3(ERR')]$ (E = S, Se, Te; R, R' = Me, Ph)

4.1 ^{77}Se and ^{125}Te NMR spectra

The ^{77}Se and ^{125}Te chemical shifts have been listed in Sections 1.2-1.5. The main features in the ^{77}Se and ^{125}Te NMR spectra of *cct*-$[RuCl_2(CO)_2(ERR')_2]$ (E = Se, Te) are exemplified in Fig. S2 by *cct*-$[RuCl_2(CO)_2(SeMe_2)_2]$ (**4**$_{cct}$), *cct*-$[RuCl_2(CO)_2(TePh_2)_2]$ (**9**$_{cct}$),[2] *cct*-$[RuCl_2(CO)_2(SeMePh)_2]$ (**5**$_{cct}$), and *cct*-$[RuCl_2(CO)_2(TeMePh)_2]$ (**8**$_{cct}$). Whereas there is no crystal structure available for **5**$_{cct}$, its identity can be verified by comparison of its ^{77}Se NMR resonance with the ^{125}Te NMR resonance of **8**$_{cct}$. The observed ^{77}Se chemical shifts of 225 and 227 ppm for **5**$_{cct}$ and ^{125}Te chemical shifts of 427 and 430 ppm for **8**$_{cct}$ are consistent with the reported relationship of $[\delta(Te) \sim (1.8)\cdot\delta(Se)]$ in analogous molecular species.[3]

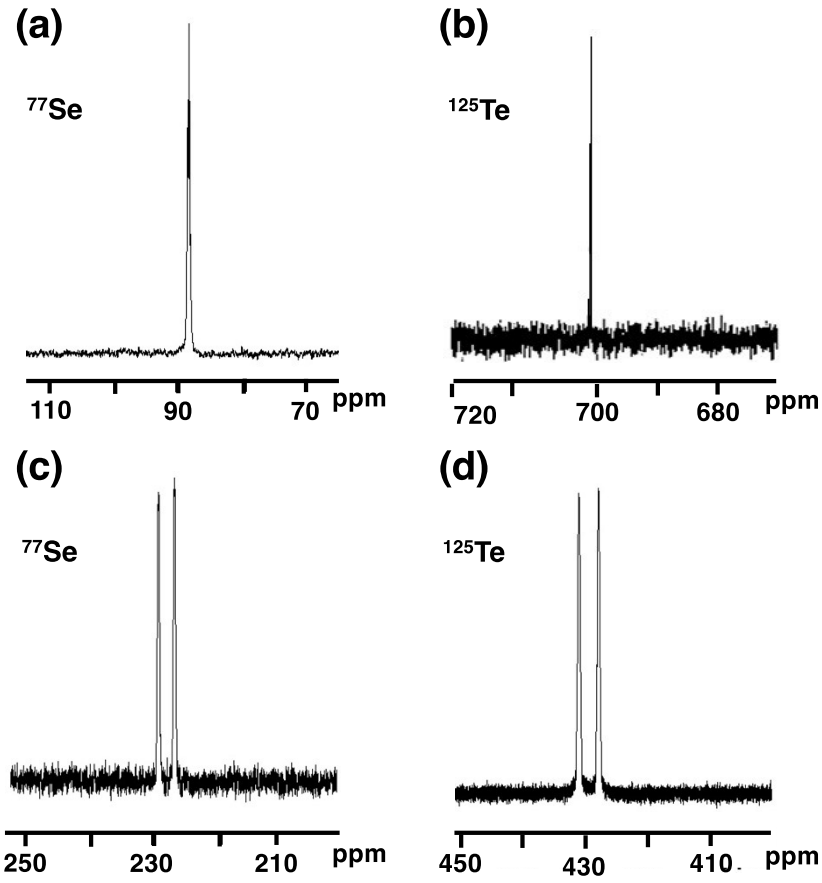


Fig. S2. (a) ^{77}Se NMR spectrum of *cct*-$[RuCl_2(CO)_2(SeMe_2)_2]$. (b) ^{125}Te NMR spectrum of *cct*-$[RuCl_2(CO)_2(TePh_2)_2]$.[2] (c) ^{77}Se NMR spectrum of *cct*-$[RuCl_2(CO)_2(SeMePh)_2]$. (d) ^{125}Te NMR spectrum of *cct*-$[RuCl_2(CO)_2(TeMePh)_2]$.

If free or relatively unrestricted rotation of the chalcogenoether ligand about the Ru-E bond is assumed, the complexes containing symmetrically substituted seleno- and telluroether ligands show expectedly only one resonance in their ^{77}Se or ^{125}Te NMR spectra [see Figs. S2(a) and S2(b)] indicating two chemically and magnetically equivalent nuclei in the complexes at NMR timescale. In case of complexes containing asymmetrically substituted chalcogenoethers, the NMR spectra show two close-lying resonances of equal intensity [see Fig. S2(c) and S2(d)]. They can be interpreted as the occurrence of two stereoisomers **A** and **B** with equal probability (the arrows in Fig. S3 indicate the possibility of the rotation of the ligand about the Ru-E bond), as shown in the Fig. S2.

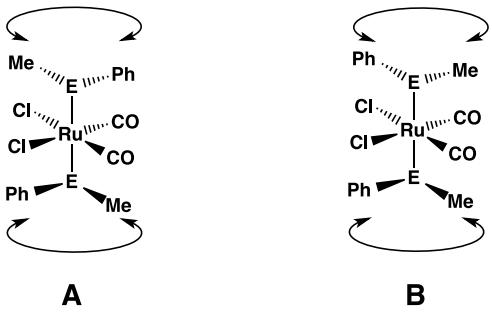


Fig. S3. The two possible stereoisomers of *cct*-$[RuCl_2(CO)_2(EMePh)_2]$ (E = S, Se, Te).

Similar situations of two very close-lying ^{77}Se or ^{125}Te NMR resonances due to the presence of two stereoisomers can also be exemplified by $[Co(dmgH)_2\{Te(Ph)(CH_2)_3SO_3Na\}_2][BF_4]$ ($dmgH^-$ = dimethylglyoximate) [4] and $Se[NH(mes)]_2$ (mes = mesityl, 2,4,6-trimethylphenyl).[5] The assignment in the latter case was verified by the PBE0/TZVP(P)//PBE0/TZVP computation of isotropic shielding tensors and consequently the ^{77}Se chemical shifts.

The nature of the rotamers and their impact on NMR spectra have been discussed in Section 4.2.

4.2 ^{13}C chemical shifts of $[RuCl_2(CO)_{4-n}(ERR')_n]$ (n = 1, 2; E = Se, Te; R, R' = Me, Ph)

The ^{13}C chemical shifts obtained from the $^{13}C\{^1H\}$ NMR spectra of the isolated products **2**$_{cct}$, 4$_{cct}$, **5**$_{cct}$, **8**$_{cct}$, **9**$_{cct}$,[2] and the related $[RuCl_2(CO)_2(Te(CH_2SiMe_3)_2\}_2]$ [6] are summarized in the Table S4. The $^{13}C\{^1H\}$ NMR spectra of the complexes recorded in this contribution are shown in Figs. S4-S10.

Table S4. ^{13}C chemical shifts (ppm) of the stoichiometrically pure $[RuCl_2(CO)_{4-n}(ERR')_n]$ (n = 1, 2; E = Se, Te; R, R' = Me, Ph), $[RuCl_2(CO)_2(TePh_2)_2]$, and $[RuCl_2(CO)_2\{Te(CH_2SiMe_3)_2\}_2]$.

***cct*-$[RuCl_2(CO)_2(ERR')_2]$**	**-CH_3**	**-CH_2-**	**C(arom.)**	**CO**
$[RuCl_2(CO)_3(ERR')]$				
$[RuCl_2(CO)_3(SeMe_2)]$ (**10**)	13.6		-	181.5(*1*) 185.3(*2*)
$[RuCl_2(CO)_3(SeMePh)]$ (**11**) [a]	14.1		127.7 130.1 130.2 130.7	181.7 184.5 185.3
***cct*-$[RuCl_2(CO)_2(ERR')_2]$**				
$[RuCl_2(CO)_2(SMePh)_2]$ (**2**$_{cct}$)	21.9		129.1 129.5 130.3 134.4	189.4
$[RuCl_2(CO)_2(SeMe_2)_2]$ (**4**$_{cct}$)	14.4		-	191.6
$[RuCl_2(CO)_2(SeMePh)_2]$ (**5**$_{cct}$) [a,b]	15.0/15.1		129.2 129.6 130.1 130.2	190.2/190.9 190.9/191.7
$[RuCl_2(CO)_2(TeMePh)_2]$ (**8**$_{cct}$) [a,b]	-3.6/-3.7		114.2 129.7 130.1 134.4	192.3/192.9 192.9/193.5
$[RuCl_2(CO)_2(TePh)_2]$ (**9**$_{cct}$) [c]			117.2 130.1 130.4 135.8	192.5
$[RuCl_2(CO)_2(Te(CH_2SiMe_3)_2\}_2]$ [d]	-0.1	0.7	-	194.5

[a] Restricted rotation of the ligand, see the text below. [b] Two stereoisomers, see 4.1 and the text below. [c] Ref. 2. [d] Ref. 6.

4.3 $^{13}C\{^1H\}$ NMR spectra of $[RuCl_2(CO)_{4-n}(ERR')_n]$ (n = 1, 2; E = Se, Te; R, R' = Me, Ph)

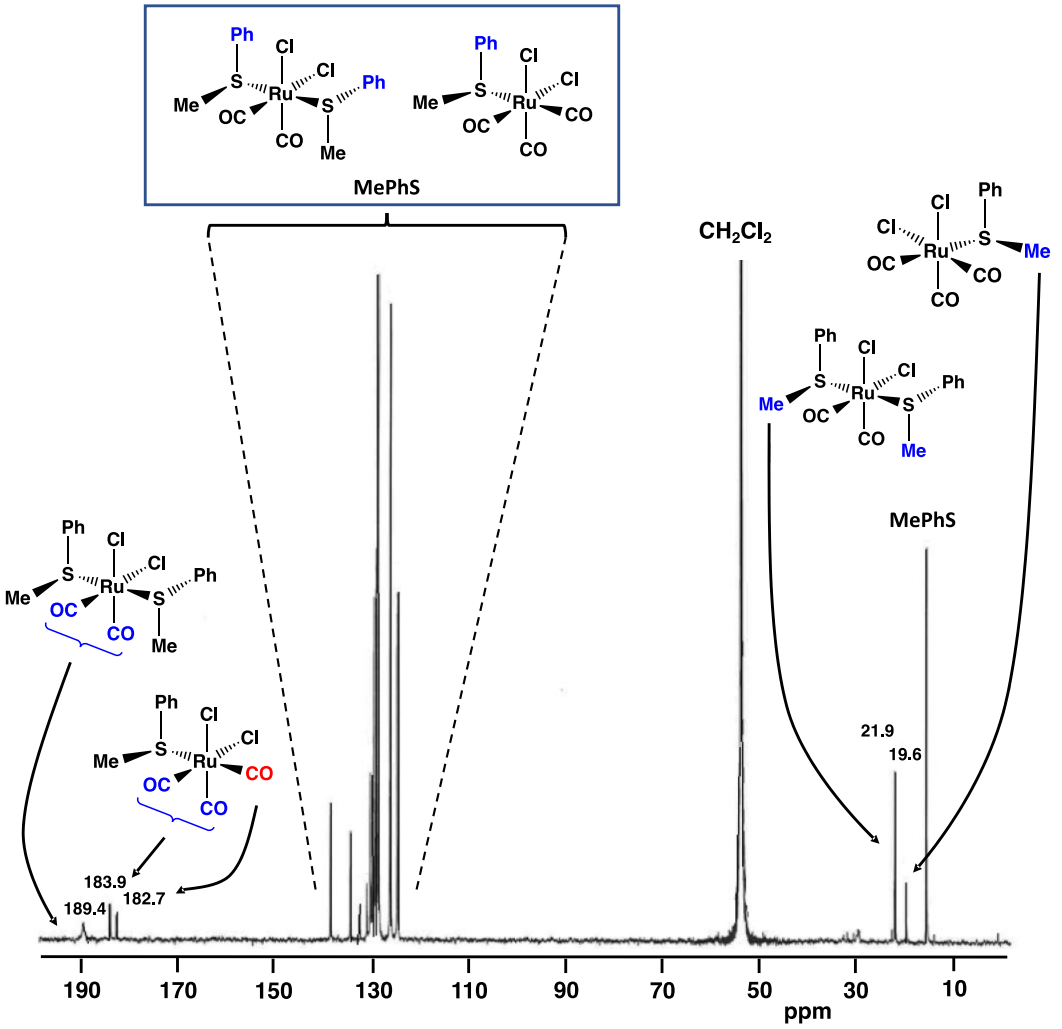


Fig. S4. $^{13}C\{^1H\}$ NMR spectrum of the reaction mixture of $[RuCl_2(CO)_3(SMePh)]$ and *cct*-$[RuCl_2(CO)_2(SMePh)_2]$ (**2**$_{cct}$) in CH_2Cl_2.

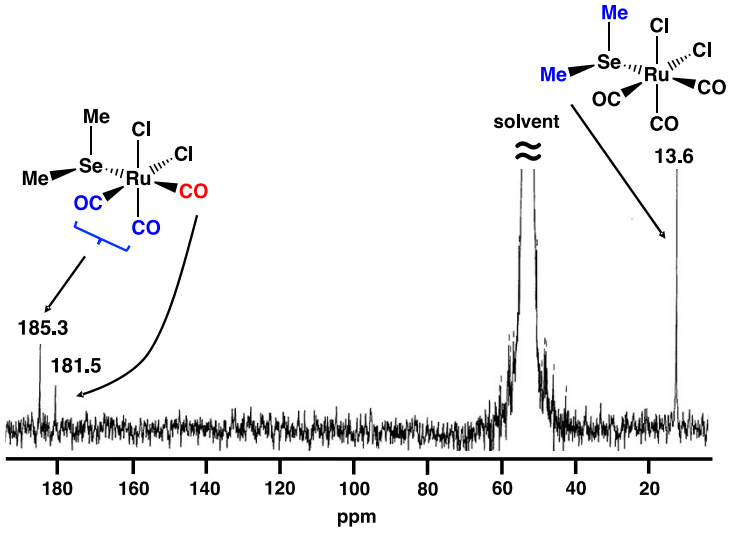


Fig. S5. $^{13}C\{^1H\}$ NMR spectrum of $[RuCl_2(CO)_3(SeMe_2)]$ (**10**) in CH_2Cl_2.

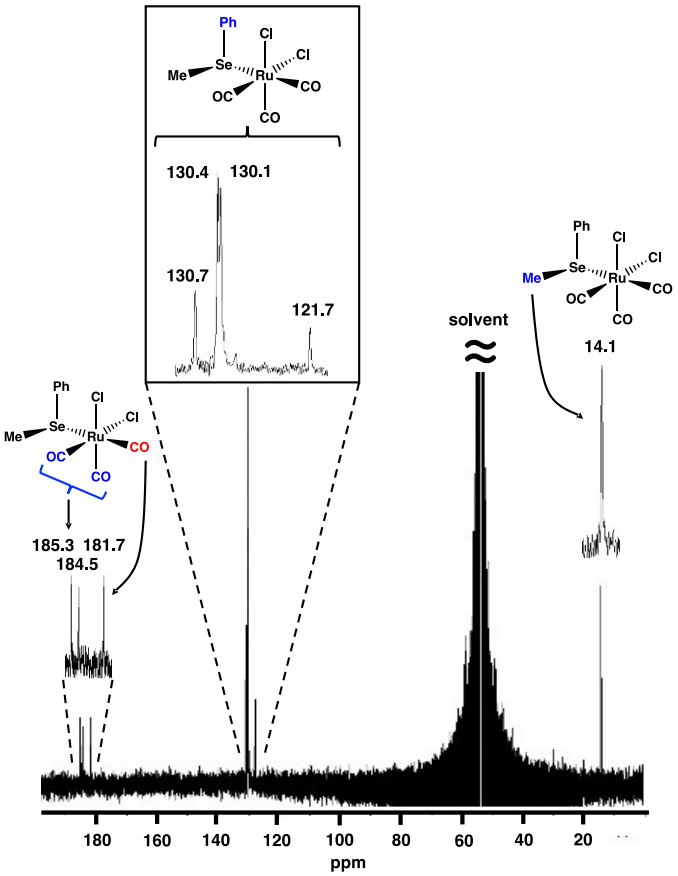


Fig. S6. $^{13}C\{^{1}H\}$ NMR spectrum of $[RuCl_2(CO)_3(SeMePh)]$ (**11**) in CH_2Cl_2.

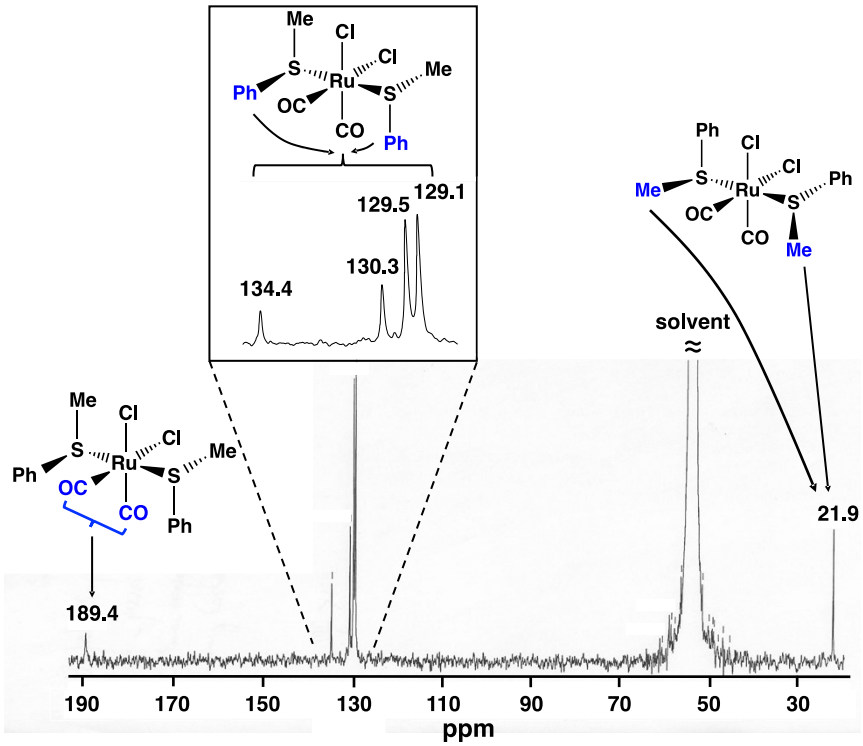


Fig. S7. $^{13}C\{^{1}H\}$ NMR spectrum of *cct*-$[RuCl_2(CO)_2(SMePh)_2]$ (**2**$_{cct}$) in CH_2Cl_2.

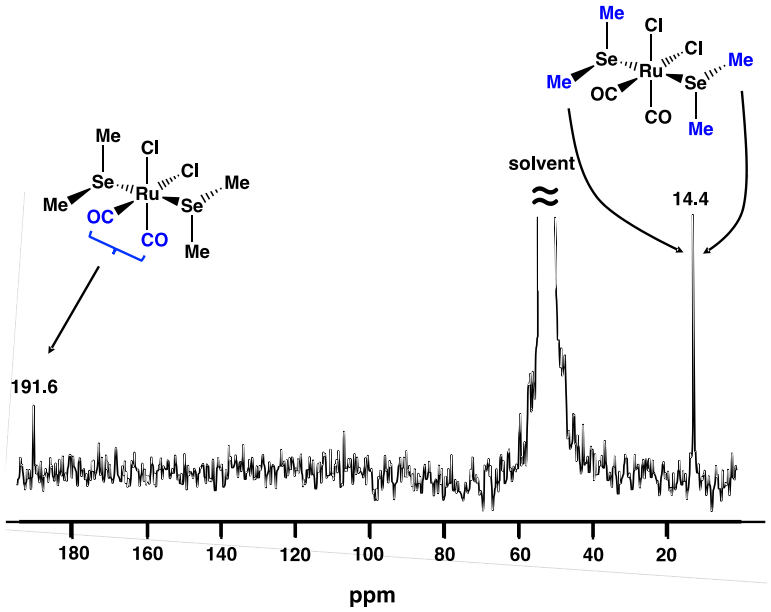


Fig S8. $^{13}C\{^{1}H\}$ NMR spectrum of *cct*-$[RuCl_2(CO)_2(SeMe_2)_2]$ (**4**$_{cct}$) in CH_2Cl_2.

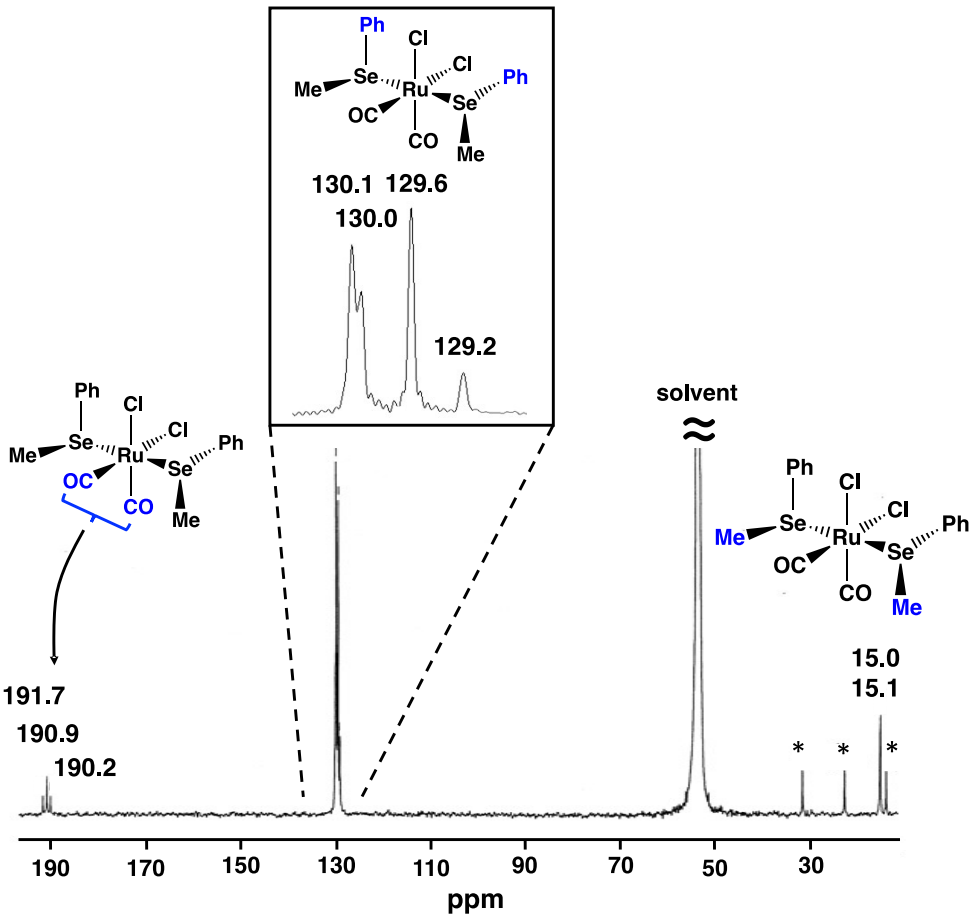


Fig. S9 $^{13}C\{^{1}H\}$ NMR spectrum of of *cct*-$[RuCl_2(CO)_2(SeMePh)_2]$ in CH_2Cl_2. The resonance marked with * are due to residual hexane.

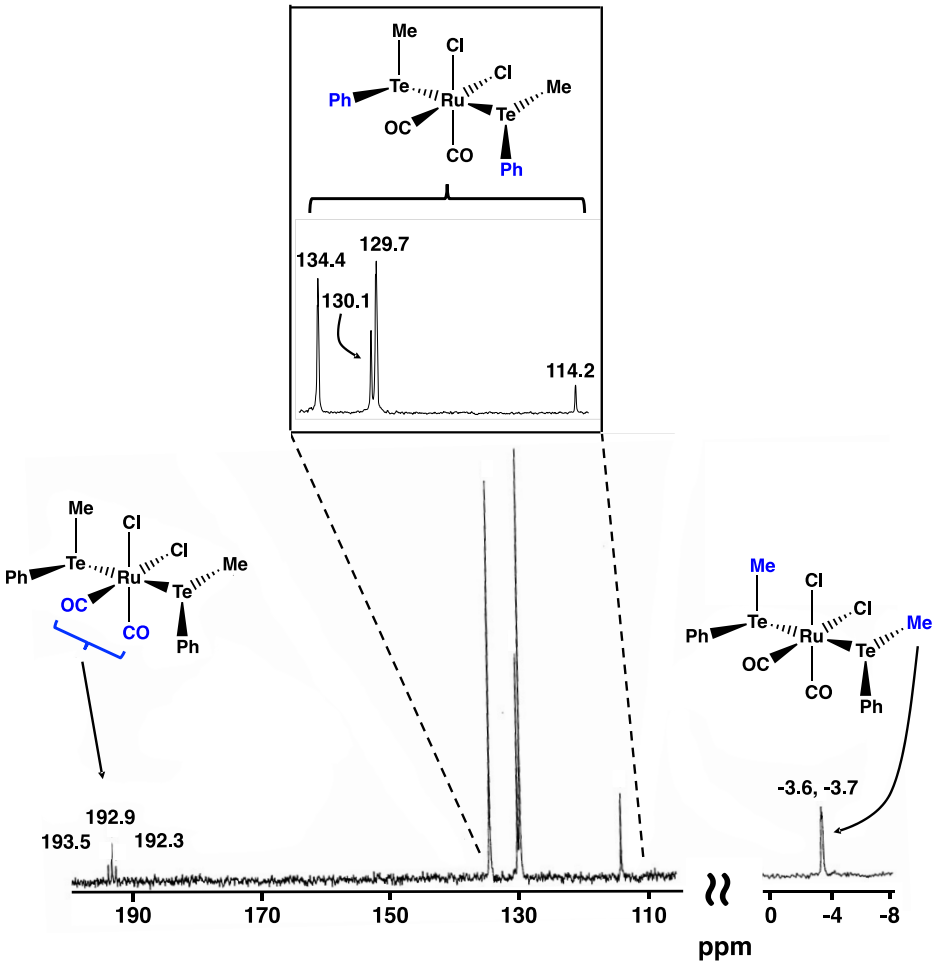


Fig. S10. $^{113}C\{^{1}H\}$ NMR spectrum of *cct*-$[RuCl_2(CO)_2(TeMePh)_2]$ in CH_2Cl_2..

4.4 Assignment of ^{13}C chemical shifts

If relatively free rotation of the chalcogenoether ligand about the Ru-E bond in $[RuCl_2(CO)_3(ERR')]$ is assumed in solution, the complex shows the virtual symmetry of C_s and the CO ligands should show two ^{13}C resonances in the intensity ratio of 2:1 for respective *cis*- and *trans*-positions with respect to the chalcogenoether ligand. For the same reason, all $[RuCl_2(CO)_2(ERR')_2]$ should show the virtual point group C_{2v} and the two CO ligands were expected to be equivalent and show only one ^{13}C resonance. Some spectra, however, turned out to be more complicated.

While $[RuCl_2(CO)_3(SeMe_2)]$ (**10**) exhibits the expected two ^{13}C resonances at 185.3 and 181.5 ppm in the intensity ratio of 2:1, there are three resonances of equal intensity observed at 185.3, 184.5, and 181.7 ppm for $[RuCl_2(CO)_3(SeMePh)]$ (**11**). This indicates that with bulkier organic substituents of the chalcogenoethers, the rotation may be restricted at least partially, or be slow at the NMR timescale, thus rendering all three CO ligands inequivalent.

The PBE0-D3/def2-TZVP calculations of the rotational barriers in $[RuCl_2(CO)_3(SeMe_2)]$ (**10**) are shown in Fig. S11. There are four local energy minima with the torsional angle of C3-Ru1-Se1-C111 at 32, 128, 248, and 272 ° (for the numbering of atoms, see Fig. 3 in the main text). The two first minimum-energy rotamers show the point group C_1 and are in fact mutual mirror images lying at global minima (denoted **I** and **II** in Fig. S11). The two last local minima are close to each other and are in fact a mirror-image pair with a very small barrier between them. The symmetry of this average rotamer (denoted **III**) is C_s and lies *ca.* 2 kJ mol^{-1} above the local minima **I** and **II** The rotational barrier **I** → **II** is *ca.* 10 kJ mol^{-1} and the barriers **II** → **III** and **III** → **I** are identical at about 8 kJ mol^{-1}.

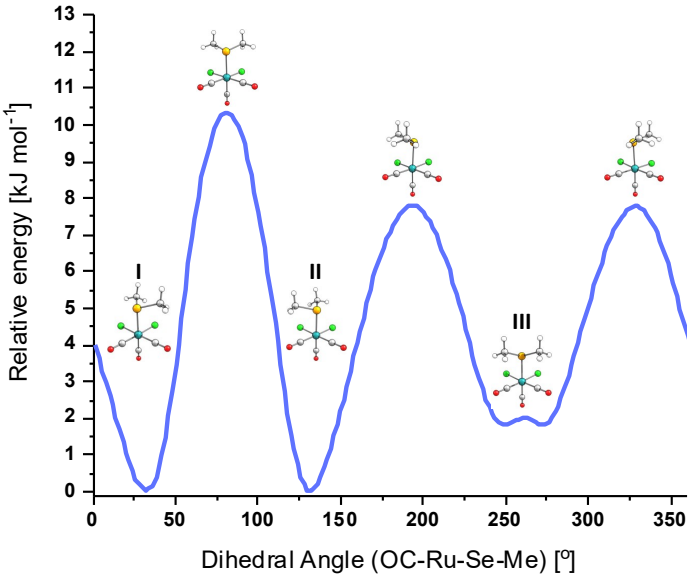


Fig. S11. Energy barriers of the rotation of $SeMe_2$ about the Ru-Se bond in $[RuCl_2(CO)_3(SeMe_2)]$.

All rotational barriers are very low and the rotamers **I**-**III** can therefore undergo rapid interconversion at NMR timescale. Thus, the two CO ligands *cis* to the $SeMe_2$ ligand appear equivalent but different from the CO-ligand *trans* to $SeMe_2$. Thus, the observed two resonances at 2:1 intensity ratio is quite expected.

The rotation scheme is analogous in case of $[RuCl_2(CO)_3(SeMePh)]$ (**11**), but while the geometries of rotamers in local energy minima **I**-**III** are rather similar to those of **10**, their relative energies differ significantly (see Fig. S12).

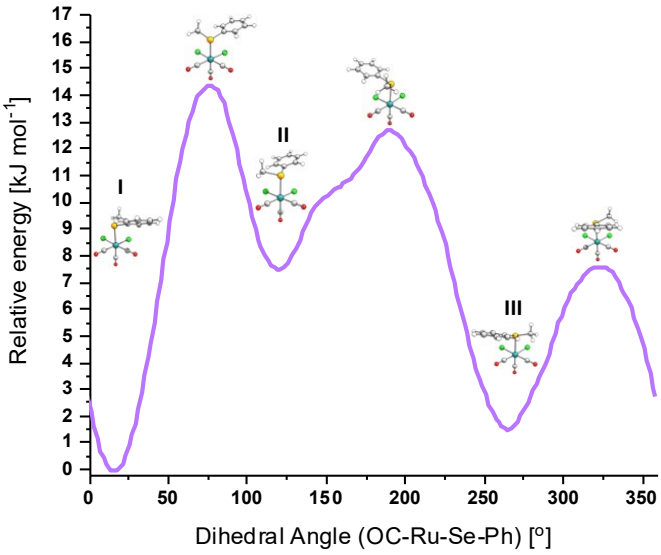


Fig. S12. Energy barriers of the rotation of SeMePh about the Ru-Se bond in $[RuCl_2(CO)_3(SeMePh)]$.

The rotamer **I** still lies in the global minimum, but **II** is *ca*. 7.5 kJ mol^{-1} and **III** *ca.* 1.5 kJ mol^{-1} higher in energy. One rotational barrier is also significantly higher in **11** than in **10**. The rotational barrier **I** → **II** is almost 15 kJ mol^{-1}. Those of **II** → **III** and **II** → **III** are only *ca.* 5 kJ mol^{-1} and *ca.* 6 kJ mol^{-1}, respectively. The SeMePh ligand is fluxional also in this complex. The most significant difference to the complex **10** is that regardless of the relative occurrence of the rotamers **I**-**III** in solution, the *cis*-CO ligands are always inequivalent and therefore, all three CO carbons should show separate resonances. This is consistent with the observation of three ^{13}C resonances of the relative intensity ratio of 1:1:1 in the NMR spectrum of **11** (see Fig. S6).

The analogous rotation barriers in $[RuCl_2(CO)_3(SePh_2)]$ are more irregular, though the general features are rather similar to those of $[RuCl_2(CO)_3(SeMe_2)]$ and $[RuCl_2(CO)_3(SeMePh)]$ (see Fig. S13).

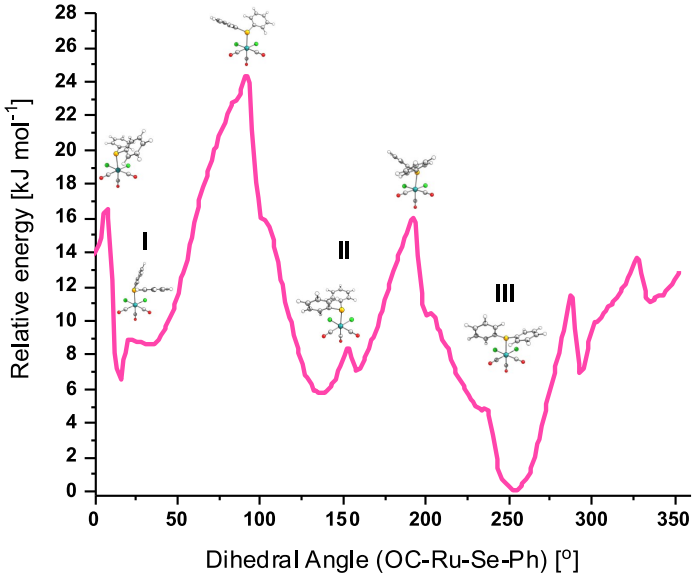


Fig. S13. Energy barriers of the rotation of $SePh_2$ about the Ru-Se bond in $[RuCl_2(CO)_3(SePh_2)]$.

The local minima in $[RuCl_2(CO)_3(SePh_2)]$ are similar to those in $[RuCl_2(CO)_3(SeMe_2)]$ and $[RuCl_2(CO)_3(SeMePh)]$ and the barriers between the minima **I**-**III** are 8-16 kJ mol^{-1}. Enabling

interconversion between them at ambient temperature. The *cis*-CO ligands therefore appear virtually identical at NMR timescale and two resonances at intensity ratio of 2:1 are observed.

The situation is quite similar in case of *cct*-$[RuCl_2(CO)_2(EMe_2)_2]$. The related DFT calculations of rotating two *trans*-$SeMe_2$ in $[RuCl_2(CO)_2(SeMe_2)_2]$ with respect to each other show three barriers of 6-13 kJ mol^{-1} (see Fig. S14). This again allows for relatively free rotation of both $SeMe_2$ ligands with apparent symmetry equivalence of the two *cis*-CO ligands. In case of unsymmetric chalcogenoether EMePh, the two CO ligands are again inequivalent showing two close-lying resonances.

Furthermore, the two ^{13}C resonances of the $[RuCl_2(CO)_2(EMePh)_2]$ complexes (**5**$_{cct}$ and **8**$_{cct}$) appear as pairs because of the presence of two stereoisomers in $[RuCl_2(CO)_2(EMePh)_2]$ (E = Se, Te; see Section 4.1). The chemical shifts of the two middle resonances almost coincide, and these four resonances appear as approximate 1:2:1 triplet in the case of both complexes **5**$_{cct}$ and **8**$_{cct}$ (see Figs. S9, S10, and S15).

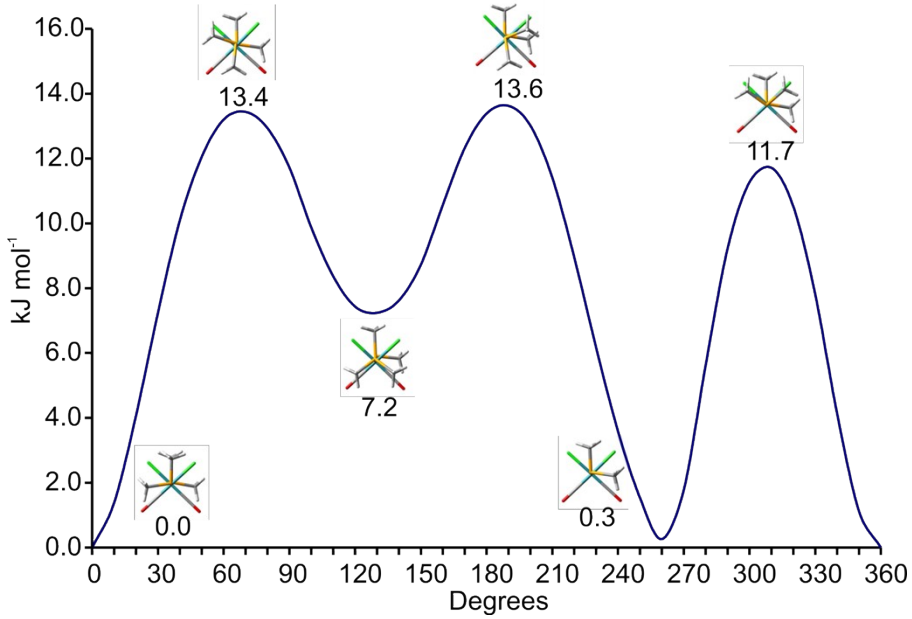


Fig. S14. Energy barriers of the rotation of $SeMe_2$ about the Ru-Se bond in *cct*-$[RuCl_2(CO)_2(SeMe_2)_2]$.

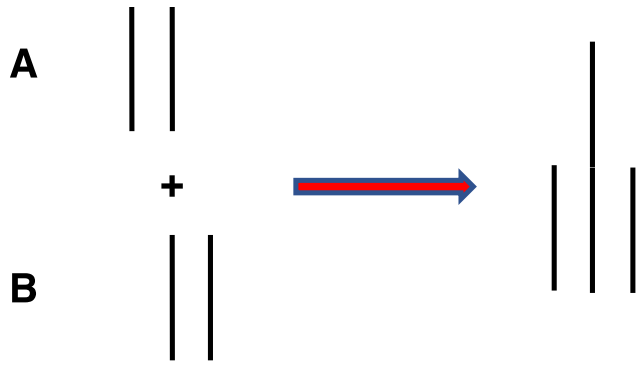
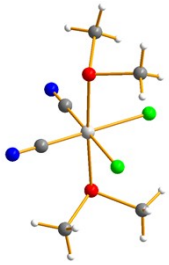
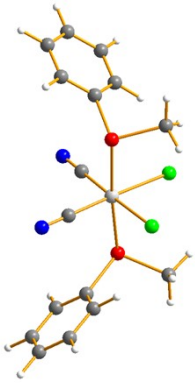
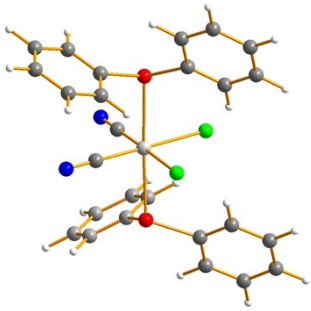
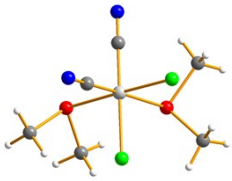
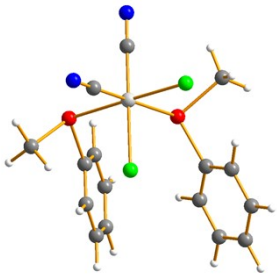
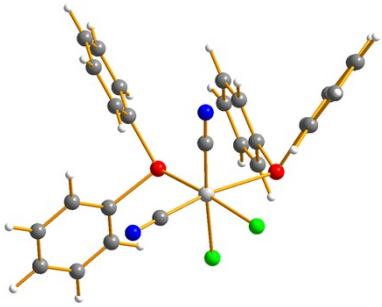
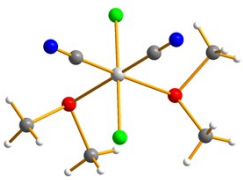
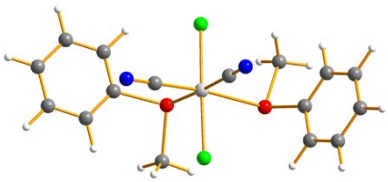
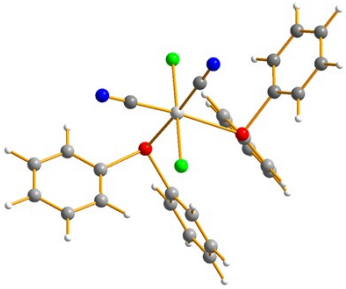


Fig. S15. The $^{13}C\{^1H\}$ NMR resonances of two inequivalent ^{13}C resonances in the two stereoisomers of *cct*-$[RuCl_2(CO)_2(EMePh)_2]$ (E = Se, Te). The designation of the two stereoisomers **A** and **B** (see Fig. S3) have been chosen arbitrarily.

5. Computational Results

Table S5. *Selected PBE0-D3/def2-TZVP optimized bond lengths of the five isomers of $[RuCl_2(CO)_2(ERR')_2]$ (E = S, Se, Te; R, R' = Me, Ph). Full atomic coordinates of all species are listed in Table S9.*

	$[RuCl_2(CO)_2(EMe_2)_2]$ E = S, Se, Te	$[RuCl_2(CO)_2(EMePh)_2]$ E = S, Se, Te	$[RuCl_2(CO)_2(EPh_2)_2]$ E = S, Se, Te
cct	 Ru-S: 2.399 Å Ru-Se: 2.512 Å Ru-Te: 2.663 Å Ru-Cl: 2.431-2.444 Å Ru-C: 1.844-1.852 Å	 Ru-S: 2.397 Å Ru-Se: 2.509 Å Ru-Te: 2.658 Å Ru-Cl: 2.433-2.448 Å Ru-C: 1.845-1.854 Å	 Ru-S: 2.395 Å Ru-Se: 2.500 Å Ru-Te: 2.643 Å Ru-Cl: 2.431-2.445 Å Ru-C: 1.847-1.855 Å
ccc	 Ru-S: 2.381-2.464 Å Ru-Se: 2.497-2.579 Å Ru-Te: 2.727 Å Ru-Cl: 2.405-2.432 Å Ru-C: 1.844-1.873 Å	 Ru-S: 2.393-2.465 Å Ru-Se: 2.504-2.573 Å Ru-Te: 2.644-2.710 Å Ru-Cl: 2.397-2.438 Å Ru-C: 1.843-1.875 Å	 Ru-S: 2.374-2.499 Å Ru-Se: 2.493-2.590 Å Ru-Te: 2.663 Å Ru-Cl: 2.400-2.425 Å Ru-C: 1.848-1.860 Å
tcc	 Ru-S: 2.457-2.471 Å Ru-Se: 2.572-2.583 Å Ru-Te: 2.719-2.728 Å Ru-Cl: 2.393-2.409 Å Ru-C: 1.855-1.863 Å	 Ru-S: 2.475 Å Ru-Se: 2.589 Å Ru-Te: 2.731 Å Ru-Cl: 2.393-2.401 Å Ru-C: 1.855-1.861 Å	 Ru-S: 2.362 Å Ru-Se: 2.481 Å Ru-Te: 2.617 Å Ru-Cl: 2.406-2.430 Å Ru-C: 1.924-1.937 Å

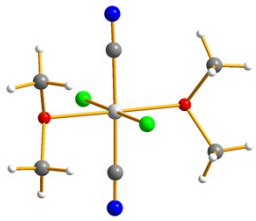
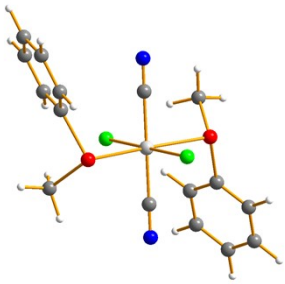
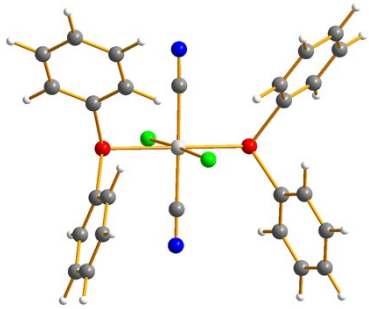
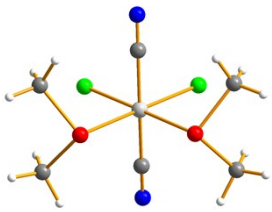
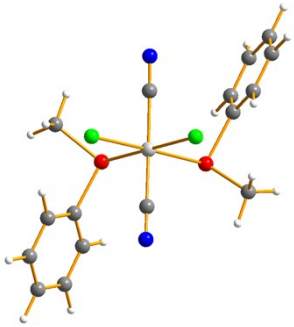
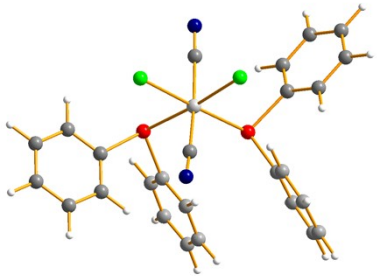
ttt	 Ru-S: 2.382 Å Ru-Se: 2.493 Å Ru-Te: 2.640 Å Ru-Cl: 2.406-2.418 Å Ru-C: 1.922-1.926 Å	 Ru-S: 2.382 Å Ru-Se: 2.494 Å Ru-Te: 2.641 Å Ru-Cl: 2.406-2.418 Å Ru-C: 1.925-1.934 Å	 Ru-S: 2.382 Å Ru-Se: 2.494 Å Ru-Te: 2.640 Å Ru-Cl: 2.406-2.418 Å Ru-C: 1.927-1.940 Å
ctc	 Ru-S: 2.355 Å Ru-Se: 2.475 Å Ru-Te: 2.624 Å Ru-Cl: 2.419-2.429 Å Ru-C: 1.924-1.932 Å	 Ru-S: 2.359 Å Ru-Se: 2.480 Å Ru-Te: 2.613-2.619 Å Ru-Cl: 2.417-2.436 Å Ru-C: 1.927-1.935 Å	 Ru-S: 2.362 Å Ru-Se: 2.483 Å Ru-Te: 2.618-2.624 Å Ru-Cl: 2.419-2.432 Å Ru-C: 1.925-1.937 Å

Table S6. Energies (kJ mol^{-1}) of $[RuCl_2(CO)_2(ERR')_2]$ (E= S, Se, Te; R, R' = Me, Ph) isomers relative to global minimum *cct* -isomer.

	ΔE				ΔH				ΔG_{298K}			
	tcc	*ccc*	*ttt*	*ctc*	*tcc*	*ccc*	*ttt*	*ctc*	*tcc*	*ccc*	*ttt*	*ctc*
S												
Me_2	31.8	17.1	66.8	64.3	31.4	16.9	66.0	62.7	26.5	15.4	63.4	58.2
MePh	32.6	14.1	66.3	65.4	32.2	14.8	65.3	64.4	29.8	19.5	64.3	64.3
Ph_2	19.0	11.8	59.9	59.3	18.0	11.6	58.2	57.8	18.4	14.3	54.9	57.9
Se												
Me_2	37.5	21.4	66.3	67.8	37.4	21.2	65.1	66.6	32.3	19.0	59.4	64.2
MePh	39.4	16.8	67.3	70.6	38.9	17.1	65.9	69.4	32.1	20.4	61.4	65.4
Ph_2	28.7	16.3	67.6	70.1	28.0	16.3	66.2	68.5	27.4	13.7	62.3	67.3
Te												
Me_2	51.0	29.2	64.6	68.7	50.4	28.9	63.4	67.5	43.8	26.8	60.0	65.3
MePh	55.0	24.1	67.2	73.7	54.5	24.2	66.0	72.8	53.2	26.3	63.7	71.2
Ph_2	44.3	17.3	73.7	66.9	43.7	17.5	72.6	65.8	46.9	21.1	70.1	69.8

Table S7. PBE0-D3/def2-TZVP energies (kJ mol^{-1}) of total reactions from $[RuCl_2(CO)_3]_2$ to $[RuCl_2(CO)_2(ER_2)_2]$ (E = S, Se, Te; R_2 = Me_2, MePh, Ph_2) in THF.

Reaction	ΔE	ΔH	ΔG_{298K}
$[RuCl_2(CO)_3]_2 + 4\ SMe_2 \rightleftarrows 2\ [RuCl_2(CO)_2(SMe_2)_2] + 2\ CO$	–112.1	–103.6	–38.8
$[RuCl_2(CO)_3]_2 + 4\ SMePh \rightleftarrows 2\ [RuCl_2(CO)_2(SMePh)_2] + 2\ CO$	–68.4	–61.7	–1.2
$[RuCl_2(CO)_3]_2 + 4\ SPh_2 \rightleftarrows 2\ [RuCl_2(CO)_2(SPh_2)_2] + 2\ CO$	–19.3	–10.8	+82.1
$[RuCl_2(CO)_3]_2 + 4\ SeMe_2 \rightleftarrows 2\ [RuCl_2(CO)_2(SeMe_2)_2] + 2\ CO$	–130.7	–124.6	–60.3
$[RuCl_2(CO)_3]_2 + 4\ SeMePh \rightleftarrows 2\ [RuCl_2(CO)_2(SeMePh)_2] + 2\ CO$	–100.1	–94.7	–27.1
$[RuCl_2(CO)_3]_2 + 4\ SePh_2 \rightleftarrows 2\ [RuCl_2(CO)_2(SePh_2)_2] + 2\ CO$	–67.5	–61.0	+33.3
$[RuCl_2(CO)_3]_2 + 4\ TeMe_2 \rightleftarrows 2\ [RuCl_2(CO)_2(TeMe_2)_2] + 2\ CO$	–196.4	–192.1	–129.4
$[RuCl_2(CO)_3]_2 + 4\ TeMePh \rightleftarrows 2\ [RuCl_2(CO)_2(TeMePh)_2] + 2\ CO$	–181.1	–176.8	–111.4
$[RuCl_2(CO)_3]_2 + 4\ TePh_2 \rightleftarrows 2\ [RuCl_2(CO)_2(TePh_2)_2] + 2\ CO$	–165.9	–160.9	–85.6

Table S8. PBE0-D3/def2-TZVP energy changes (kJ mol^{-1}) in individual reaction step **I3a,b** → **P** (see Fig. 4) along the reaction coordinate between $[RuCl_2(CO)_3]_2$ and different chalcogenoethers in THF.

Reaction	ΔE	ΔH	ΔG_{298K}
$[RuCl_2(CO)_3(SMe_2)] + SMe_2 \rightleftarrows [RuCl_2(CO)_2(SMe_2)_2] + CO$	–0.2	0.0	+9.8
$[RuCl_2(CO)_3(SMePh)] + SMePh \rightleftarrows [RuCl_2(CO)_2(SMePh)_2] + CO$	+10.8	+10.6	+19.0
$[RuCl_2(CO)_3(SPh_2)] + SPh_2 \rightleftarrows [RuCl_2(CO)_2(SPh_2)_2] + CO$	+21.9	+22.0	+37.8
$[RuCl_2(CO)_3(SeMe_2)] + SeMe_2 \rightleftarrows [RuCl_2(CO)_2(SeMe_2)_2] + CO$	–5.5	–5.8	+4.2
$[RuCl_2(CO)_3(SeMePh)] + SeMePh \rightleftarrows [RuCl_2(CO)_2(SeMePh)_2] + CO$	+1.8	+1.4	+14.0
$[RuCl_2(CO)_3(SePh_2)] + SePh_2 \rightleftarrows [RuCl_2(CO)_2(SePh_2)_2] + CO$	+8.8	+8.3	+24.0
$[RuCl_2(CO)_3(TeMe_2)] + TeMe_2 \rightleftarrows [RuCl_2(CO)_2(TeMe_2)_2] + CO$	–24.8	–25.5	–15.7
$[RuCl_2(CO)_3(TeMePh)] + TeMePh \rightleftarrows [RuCl_2(CO)_2(TeMePh)_2] + CO$	–22.2	–22.9	–12.5
$[RuCl_2(CO)_3(TePh_2)] + TePh_2 \rightleftarrows [RuCl_2(CO)_2(TePh_2)_2] + CO$	–18.9	–19.4	–7.9

Table S9. Total energies (a.u.) and optimized Cartesian coordinates (in Å) of the computed species.

```
9
SMe2 symmetry c2v (E= -477.821796008)
S         0.000000000      0.000000000      0.652220000
C         0.000000000      1.373724000     -0.505474000
H        -0.892318000      1.354082000     -1.133234000
H         0.000000000      2.292361000      0.081557000
H         0.892318000      1.354082000     -1.133234000
H         0.892318000     -1.354082000     -1.133234000
C         0.000000000     -1.373724000     -0.505474000
H        -0.892318000     -1.354082000     -1.133234000
H         0.000000000     -2.292361000      0.081557000

16
SMePh symmetry cs (E=-669.411295006)
S         1.882886120     -0.421813406      0.000000000
H         2.243210416      1.791509680      0.894868000
C         2.540727328      1.244349164      0.000000000
H         2.243210416      1.791509680     -0.894868000
H         3.624606408      1.129908701      0.000000000
C         0.144135593     -0.180072601      0.000000000
C        -0.648220743     -1.331243199      0.000000000
C        -0.472018081      1.068695422      0.000000000
C        -2.027755776     -1.229760417      0.000000000
C        -1.858107565      1.158752611      0.000000000
C        -2.643102005      0.016819838      0.000000000
H        -0.176344480     -2.308098493      0.000000000
H         0.116695743      1.976381362      0.000000000
H        -2.627291102     -2.133003908      0.000000000
H        -2.323197216      2.138174296      0.000000000
H        -3.723688617      0.094315139      0.000000000

23
SPh2 symmetry c2 (E=-860.998167289)
S         0.000000000      0.000000000     -1.580434996
C        -1.386041556     -0.017470716     -0.485957935
C        -2.475741637     -0.814509896     -0.822654095
C        -1.442346117      0.788863937      0.648700020
C        -3.616821555     -0.798990720     -0.032734874
C        -2.575797687      0.781028288      1.444133688
C        -3.668665913     -0.007850911      1.104981460
H        -2.425163070     -1.450784496     -1.698678931
H        -0.598013837      1.416003766      0.908458500
H        -4.461863878     -1.421560218     -0.303073765
H        -2.610011350      1.405139869      2.329782747
H        -4.555454548     -0.005608946      1.727587544
C         1.386041556      0.017470716     -0.485957935
C         1.442346117     -0.788863937      0.648700020
C         2.475741637      0.814509896     -0.822654095
C         2.575797687     -0.781028288      1.444133688
C         3.616821555      0.798990720     -0.032734874
C         3.668665913      0.007850911      1.104981460
H         0.598013837     -1.416003766      0.908458500
H         2.425163070      1.450784496     -1.698678931
H         2.610011350     -1.405139869      2.329782747
H         4.461863878      1.421560218     -0.303073765
H         4.555454548      0.005608946      1.727587544

9
SeMe2 symmetry c2v (E=-2481.02501944)
```

```
Se       0.000000000      0.000000000      0.470448000
C        0.000000000      1.454750000     -0.814003000
H       -0.894208000      1.406015000     -1.433757000
H        0.000000000      2.384050000     -0.246083000
H        0.894208000      1.406015000     -1.433757000
H        0.894208000     -1.406015000     -1.433757000
C        0.000000000     -1.454750000     -0.814003000
H       -0.894208000     -1.406015000     -1.433757000
H        0.000000000     -2.384050000     -0.246083000

16
SeMePh symmetry cs (E=-2672.61204693)
Se       1.463328845     -0.055423494      0.000000000
H        1.291961262      2.307821547      0.896725094
C        1.719395471      1.862914878      0.000000000
H        1.291961262      2.307821547     -0.896725094
H        2.798386988      2.011097992      0.000000000
C       -0.438345809     -0.158267665      0.000000000
C       -1.002658399     -1.433642040      0.000000000
C       -1.267018356      0.958117558      0.000000000
C       -2.379023145     -1.585396964      0.000000000
C       -2.646772380      0.795649837      0.000000000
C       -3.209520947     -0.471163582      0.000000000
H       -0.364053506     -2.310722359      0.000000000
H       -0.852206332      1.957690292      0.000000000
H       -2.805037088     -2.582301110      0.000000000
H       -3.282987804      1.673602089      0.000000000
H       -4.286242363     -0.591654114      0.000000000

23
SePh2 symmetry c1 (E=-2864.19773321)
Se       0.042719000     -1.493750000     -0.021935000
C        1.463556000     -0.215824000      0.053795000
C        2.705707000     -0.602082000     -0.439063000
C        1.301758000      1.042897000      0.621794000
C        3.783186000      0.268287000     -0.356770000
C        2.380425000      1.912255000      0.684628000
C        3.624236000      1.529205000      0.200308000
H        2.831953000     -1.578232000     -0.894328000
H        0.337334000      1.346396000      1.010693000
H        4.748092000     -0.039819000     -0.743006000
H        2.246919000      2.894633000      1.123443000
H        4.464195000      2.211462000      0.255110000
C       -1.459588000     -0.312291000     -0.067693000
C       -2.432156000     -0.413922000      0.919108000
C       -1.605302000      0.609122000     -1.100305000
C       -3.553973000      0.404008000      0.869623000
C       -2.716330000      1.436511000     -1.132085000
C       -3.694881000      1.332191000     -0.150705000
H       -2.309430000     -1.124172000      1.728119000
H       -0.848958000      0.680288000     -1.873138000
H       -4.312169000      0.320509000      1.639633000
H       -2.824016000      2.158560000     -1.933295000
H       -4.566192000      1.975726000     -0.183257000

9
TeMe2 symmetry c2v (E=-347.787073890)
Te       0.000000000      0.000000000      0.391545000
C        0.000000000      1.570486000     -1.055268000
H       -0.895304000      1.499424000     -1.669441000
H        0.000000000      2.513027000     -0.509683000
H        0.895304000      1.499424000     -1.669441000
```

```
H        0.895304000     -1.499424000     -1.669441000
C        0.000000000     -1.570486000     -1.055268000
H       -0.895304000     -1.499424000     -1.669441000
H        0.000000000     -2.513027000     -0.509683000

16
TeMePh symmetry cs (E=-539.372008116)
Te      -1.198571956     -0.190627981      0.000000000
H       -1.166787606      2.359251967     -0.897637004
C       -1.579688959      1.904306835      0.000000000
H       -1.166787606      2.359251967      0.897637004
H       -2.663771849      2.009547711      0.000000000
C        0.904291353     -0.078402825      0.000000000
C        1.590941229      1.131168200      0.000000000
C        1.621912057     -1.273577197      0.000000000
C        2.980149356      1.141729274      0.000000000
C        3.007975364     -1.255147931      0.000000000
C        3.693929504     -0.047273274      0.000000000
H        1.056917804      2.073371438      0.000000000
H        1.102647365     -2.226503810      0.000000000
H        3.504145179      2.091063928      0.000000000
H        3.554209498     -2.191741307      0.000000000
H        4.777426562     -0.034418582      0.000000000

23
TePh2 symmetry c1 (E=-730.956694172)
Te      -0.087350000     -1.439450000     -0.000080000
C       -1.558415000      0.077494000      0.000083000
C       -1.232264000      1.428521000      0.000447000
C       -2.896018000     -0.310314000     -0.000223000
C       -2.240816000      2.383207000      0.000568000
C       -3.897222000      0.649549000     -0.000124000
C       -3.574220000      2.000048000      0.000298000
H       -0.195503000      1.743529000      0.000625000
H       -3.166414000     -1.361173000     -0.000558000
H       -1.976957000      3.434997000      0.000848000
H       -4.935581000      0.337456000     -0.000345000
H       -4.357754000      2.748557000      0.000415000
C        1.579609000     -0.150103000     -0.000061000
C        2.129975000      0.278024000      1.204475000
C        2.129080000      0.279142000     -1.204622000
C        3.220303000      1.137265000      1.201796000
C        3.219399000      1.138386000     -1.201960000
C        3.764540000      1.567833000     -0.000084000
H        1.704835000     -0.054552000      2.144009000
H        1.703223000     -0.052565000     -2.144136000
H        3.644156000      1.470132000      2.142268000
H        3.642562000      1.472142000     -2.142428000
H        4.615914000      2.238571000     -0.000098000
```

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2
CO symmetry Cinfv (E=-113.231880415)
C         0.000000000      0.000000000      0.641707339
O         0.000000000      0.000000000     -0.481433661

13
THF symmetry c2 (E=-232.276490524)
H        -1.574349000     -1.091336000      0.469083000
O         0.000000000      0.000000000      1.243302000
C         0.478128000      1.063689000      0.423711000
C         0.000000000      0.761706000     -0.986037000
C         0.000000000     -0.761706000     -0.986037000
C        -0.478128000     -1.063689000      0.423711000
H         0.094632000      2.009464000      0.815175000
H         1.574349000      1.091336000      0.469083000
H         0.645406000      1.198158000     -1.748875000
H        -1.014297000      1.141489000     -1.134633000
H         1.014297000     -1.141489000     -1.134633000
H        -0.645406000     -1.198158000     -1.748875000
H        -0.094632000     -2.009464000      0.815175000

18
[Ru2Cl4(CO)6] symmetry c2h (E=-2710.01276904)
Ru        0.053592000      1.805601000      0.000000000
Cl        0.000000000      0.000000000      1.654308000
Cl        0.000000000      0.000000000     -1.654308000
Cl       -2.331049000      1.813817000      0.000000000
C         1.955393000      1.739280000      0.000000000
O         3.083622000      1.727078000      0.000000000
C         0.000000000      3.119878000     -1.339052000
O        -0.054729000      3.903792000     -2.149344000
O        -0.054729000      3.903792000      2.149344000
C         0.000000000      3.119878000      1.339052000
Ru       -0.053592000     -1.805601000      0.000000000
Cl        2.331049000     -1.813817000      0.000000000
C         0.000000000     -3.119878000     -1.339052000
C         0.000000000     -3.119878000      1.339052000
C        -1.955393000     -1.739280000      0.000000000
O         0.054729000     -3.903792000     -2.149344000
O         0.054729000     -3.903792000      2.149344000
O        -3.083622000     -1.727078000      0.000000000

18
I1b [Cl2(CO)3Ru-Cl-RuCl(CO)3] symmetry c1 (E=-2709.98550407)
Ru       -2.001086000     -0.121120000      0.005353000
Cl       -1.567455000      1.416636000     -1.780609000
Cl        0.129650000     -1.244018000     -0.504877000
Cl       -0.901309000      1.321133000      1.578149000
C        -2.834083000     -1.236051000     -1.271788000
O        -3.333042000     -1.891739000     -2.045405000
C        -2.261068000     -1.321076000      1.443491000
O        -2.404768000     -2.025121000      2.315868000
O        -4.543624000      1.360821000      0.576375000
C        -3.594050000      0.787156000      0.363292000
Ru        2.188825000     -0.014734000     -0.295649000
Cl        3.234088000     -2.111357000     -0.381705000
C         2.103099000      0.064631000      1.521318000
C         3.931094000      0.715825000     -0.214049000
C         1.441968000      1.762453000     -0.423942000
O         2.092320000      0.059626000      2.651351000
O         4.980167000      1.121156000     -0.136963000
O         1.184340000      2.855161000     -0.514122000
```

31
I1a [Cl2(CO)3Ru-Cl-RuCl(CO)3(THF)] symmetry c1 (E=-2942.29932941)
Ru 2.038211000 -0.559364000 0.116728000
Cl -2.367568000 1.702487000 1.475043000
Cl -0.146677000 -0.850189000 1.127932000
Cl 1.135811000 -0.796602000 -2.071445000
C 2.742749000 -0.375365000 1.872979000
O 3.168960000 -0.294178000 2.915267000
C 2.268530000 -2.418607000 0.152492000
O 2.381397000 -3.540676000 0.156079000
O 4.741768000 -0.250045000 -1.177462000
C 3.732087000 -0.349335000 -0.682624000
Ru -2.198319000 -0.135869000 -0.066383000
Cl -3.336465000 -1.577222000 1.483306000
C -2.046538000 -1.621531000 -1.224234000
C -3.871472000 0.324438000 -0.736067000
C -1.364981000 1.072030000 -1.256150000
O -1.986722000 -2.525305000 -1.900538000
O -4.899753000 0.602521000 -1.115065000
O -0.965989000 1.850608000 -1.973820000
H 1.939233000 1.938334000 -1.978324000
O 1.545595000 1.519257000 -0.017183000
C 1.311969000 2.332899000 1.154797000
C 0.803009000 3.633384000 0.578294000
C 1.518070000 3.751347000 -0.779145000
C 2.149120000 2.382529000 -1.008268000
H 0.587402000 1.807181000 1.772857000
H 2.259788000 2.457542000 1.688435000
H 1.020568000 4.470751000 1.240229000
H -0.277485000 3.572805000 0.448222000
H 2.289579000 4.520398000 -0.763906000
H 0.813067000 3.997589000 -1.571335000
H 3.228540000 2.403446000 -0.834222000

22
I2a [RuCl2(CO)3(THF)] symmetry c1 (E=-1587.28795185)
Ru -0.631932000 0.029269000 0.086137000
Cl -0.275869000 1.250456000 -1.940966000
Cl -0.653088000 -2.030618000 -1.136591000
C -0.658330000 1.679914000 1.007082000
O -0.712242000 2.673826000 1.544569000
C -2.469430000 0.105972000 -0.196340000
O -3.580021000 0.144216000 -0.402028000
O -0.976236000 -1.623847000 2.592465000
C -0.845132000 -0.997904000 1.660138000
H 2.165426000 -1.355491000 -1.226684000
O 1.516757000 -0.089325000 0.282198000
C 2.329071000 1.111968000 0.345734000
C 3.700898000 0.692242000 -0.140323000
C 3.728162000 -0.797969000 0.175250000
C 2.315992000 -1.213202000 -0.155004000
H 1.864702000 1.871809000 -0.281515000
H 2.336321000 1.436556000 1.388880000
H 4.493027000 1.252728000 0.355078000
H 3.785341000 0.852240000 -1.217206000
H 3.938278000 -0.966970000 1.233992000
H 4.459504000 -1.346977000 -0.417449000
H 1.961226000 -2.094045000 0.376505000

27
I2b [Cl2(CO)3Ru-Cl-RuCl(CO)3(SMe2)] symmetry c1 (E=-3187.86206413)

```
Ru      -1.855228000     -0.451894000     -0.010084000
Cl       1.305780000      1.393929000     -1.650792000
Cl       0.172072000      0.077881000      1.267019000
Cl      -2.965601000     -0.044787000      2.079239000
C       -1.090771000     -0.724817000     -1.735612000
O       -0.821788000     -0.909857000     -2.816485000
C       -1.536341000     -2.263127000      0.515738000
O       -1.350378000     -3.323117000      0.849068000
O       -4.560958000     -1.161202000     -1.084903000
C       -3.533550000     -0.882881000     -0.701514000
Ru       2.320029000      0.085236000      0.092182000
Cl       1.712438000     -1.974040000     -0.986311000
C        3.049042000     -0.982241000      1.468143000
C        3.920063000      0.076998000     -0.877282000
C        2.741930000      1.720471000      0.933303000
O        3.478224000     -1.635473000      2.284787000
O        4.871760000      0.066166000     -1.486488000
O        2.985547000      2.708958000      1.425691000
S       -2.156294000      1.900857000     -0.641352000
C       -1.381353000      2.887639000      0.635103000
C       -3.880103000      2.285554000     -0.325973000
H       -0.306942000      2.797130000      0.497921000
H       -1.691403000      3.920262000      0.475848000
H       -1.678884000      2.533524000      1.620642000
H       -4.477131000      1.782694000     -1.085407000
H       -4.165507000      1.952631000      0.670691000
H       -4.003165000      3.362939000     -0.430820000

27
I2b [Cl2(CO)3Ru-Cl-RuCl(CO)3(SeMe2)] symmetry c1 (E=-5191.06751005)
Ru      -1.680790000     -0.718076000      0.002787000
Cl       1.292743000      1.469237000     -1.517309000
Cl       0.334623000     -0.172366000      1.294867000
Cl      -2.782246000     -0.505520000      2.127621000
C       -0.926969000     -0.835007000     -1.741303000
O       -0.658877000     -0.934078000     -2.834236000
C       -1.282210000     -2.547009000      0.400464000
O       -1.046054000     -3.619818000      0.651990000
O       -4.374910000     -1.420762000     -1.101861000
C       -3.350392000     -1.148558000     -0.705303000
Ru       2.449100000      0.112014000      0.097022000
Cl       1.993313000     -1.897539000     -1.137919000
C        3.293183000     -0.997965000      1.369083000
C        4.023589000      0.315593000     -0.893553000
C        2.751161000      1.702171000      1.066228000
O        3.792373000     -1.676498000      2.122860000
O        4.959531000      0.432344000     -1.515912000
O        2.921212000      2.663553000      1.637134000
Se      -2.101543000      1.770513000     -0.483539000
C       -1.349864000      2.673400000      1.049221000
C       -3.964034000      2.009649000     -0.006941000
H       -0.273363000      2.690681000      0.907260000
H       -1.753874000      3.684262000      1.044643000
H       -1.622520000      2.133324000      1.952803000
H       -4.566187000      1.572664000     -0.801053000
H       -4.155945000      1.521067000      0.945901000
H       -4.147631000      3.080924000      0.048557000

27
I2b [Cl2(CO)3Ru-Cl-RuCl(CO)3(TeMe2)] symmetry c1 (E=-3057.83632789)
Ru       1.517856000      0.973216000      0.002010000
Cl      -1.272492000     -1.499364000     -1.413575000
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Cl      -0.500840000      0.411665000      1.293654000
Cl       2.602222000      0.850527000      2.149447000
C        0.779179000      1.008691000     -1.745442000
O        0.502669000      1.059811000     -2.840729000
C        1.082621000      2.815946000      0.346298000
O        0.826513000      3.893568000      0.554820000
O        4.219931000      1.642566000     -1.098346000
C        3.190262000      1.384570000     -0.702693000
Ru      -2.563013000     -0.142548000      0.101799000
Cl      -2.275561000      1.810081000     -1.264367000
C       -3.517408000      0.973865000      1.285983000
C       -4.101458000     -0.552716000     -0.882690000
C       -2.738640000     -1.680621000      1.179972000
O       -4.083734000      1.657312000      1.985722000
O       -5.015802000     -0.794664000     -1.500954000
O       -2.833327000     -2.609923000      1.817819000
Te       2.022912000     -1.673490000     -0.412783000
C        1.252897000     -2.486905000      1.382194000
C        4.045975000     -1.768228000      0.234231000
H        0.180566000     -2.598566000      1.252310000
H        1.728361000     -3.456594000      1.517923000
H        1.487279000     -1.803150000      2.194558000
H        4.673729000     -1.369763000     -0.560588000
H        4.144294000     -1.180296000      1.144341000
H        4.284105000     -2.816014000      0.407078000

18
I3a,b [RuCl2(CO)3(SMe2)] symmetry c1 (E=-1832.84944921)
Ru      -0.404972000      0.083578000      0.073302000
C       -0.962351000     -0.253441000      1.841035000
O       -1.299024000     -0.469660000      2.899592000
C       -0.249226000      1.939938000      0.332073000
O       -0.175746000      3.061870000      0.468527000
Cl       0.348953000      0.444777000     -2.187208000
Cl      -0.624251000     -2.286342000     -0.316426000
S        1.918201000     -0.294981000      0.767463000
C        2.612364000     -1.469061000     -0.392880000
H        2.443747000     -1.123517000     -1.411321000
H        3.675337000     -1.557848000     -0.169825000
H        2.108472000     -2.418322000     -0.230526000
C        2.834661000      1.173600000      0.297468000
H        2.610447000      1.435852000     -0.735952000
H        2.548172000      1.979124000      0.971739000
H        3.895965000      0.961862000      0.422746000
C       -2.192946000      0.242542000     -0.566459000
O       -3.241420000      0.316569000     -0.975270000

25
I3a,b [RuCl2(CO)3(SMePh)] symmetry c1 (E=-2024.43484035)
Ru       1.077493000     -0.247641000     -0.004536000
C       -0.140428000     -1.582139000      0.532800000
O       -0.861929000     -2.385207000      0.871803000
C        1.345686000     -0.989279000     -1.714713000
O        1.516096000     -1.427714000     -2.744138000
Cl       2.583172000      1.518936000     -0.645937000
Cl       0.761921000      0.743431000      2.170903000
C        2.557457000     -1.179941000      0.741779000
O        3.445602000     -1.703613000      1.199538000
S       -0.696703000      1.148289000     -0.974531000
H       -0.572700000      2.642569000      0.907266000
C       -0.619519000      2.748773000     -0.173341000
H       -1.491346000      3.317565000     -0.492685000
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H        0.295761000      3.213678000     -0.534946000
C       -2.244767000      0.486283000     -0.418402000
C       -2.979013000     -0.241254000     -1.346610000
C       -2.694813000      0.638179000      0.887228000
C       -4.172922000     -0.831065000     -0.959591000
C       -3.896169000      0.055892000      1.258247000
C       -4.633385000     -0.680474000      0.340181000
H       -2.617061000     -0.344429000     -2.362855000
H       -2.106393000      1.183364000      1.613508000
H       -4.746493000     -1.401645000     -1.680070000
H       -4.252590000      0.171878000      2.274781000
H       -5.569113000     -1.137216000      0.639568000

32
I3a,b [RuCl2(CO)3(SPh2)] symmetry c1 (E=-2216.01656021)
Ru       1.459393000     -0.079146000      0.144593000
C        1.114754000      1.391103000      1.272929000
O        0.960757000      2.287673000      1.945271000
C        1.006741000     -1.337784000      1.472484000
O        0.756314000     -2.081612000      2.288164000
Cl       1.977044000     -1.871490000     -1.381184000
Cl       1.989340000      1.538422000     -1.558223000
C        3.293187000     -0.101655000      0.633638000
O        4.390908000     -0.122369000      0.891836000
S       -0.753706000     -0.029645000     -0.921983000
C       -1.842584000     -1.344823000     -0.409326000
C       -1.319288000     -2.627787000     -0.302769000
C       -3.205282000     -1.122120000     -0.253657000
C       -2.163695000     -3.685000000     -0.003218000
C       -4.037991000     -2.189214000      0.047007000
C       -3.521952000     -3.469840000      0.179355000
H       -0.263746000     -2.803233000     -0.472911000
H       -3.620053000     -0.129012000     -0.362194000
H       -1.751285000     -4.682919000      0.085853000
H       -5.099019000     -2.011713000      0.176152000
H       -4.177616000     -4.298691000      0.417416000
C       -1.574251000      1.438781000     -0.362310000
C       -2.052236000      1.576868000      0.936498000
C       -1.675723000      2.479082000     -1.275328000
C       -2.642711000      2.769084000      1.315675000
C       -2.256494000      3.675891000     -0.879171000
C       -2.741583000      3.819885000      0.411071000
H       -1.969971000      0.759833000      1.642948000
H       -1.297785000      2.353226000     -2.282062000
H       -3.019678000      2.881226000      2.325040000
H       -2.333041000      4.492672000     -1.586452000
H       -3.199521000      4.753106000      0.716339000

18
I3a,b [RuCl2(CO)3(SeMe2)] symmetry c1 (E=-3836.05421065)
Ru      -0.644973000      0.076679000      0.069035000
C       -1.004829000     -0.406729000      1.851143000
O       -1.225233000     -0.710167000      2.919529000
C       -0.549271000      1.914306000      0.448330000
O       -0.502273000      3.025856000      0.663105000
Cl      -0.140642000      0.633496000     -2.223774000
Cl      -0.732599000     -2.275870000     -0.461658000
Se       1.860644000     -0.220842000      0.533318000
C        2.471105000     -1.288201000     -0.956835000
H        2.089796000     -0.850294000     -1.876293000
H        3.559091000     -1.287971000     -0.921708000
H        2.074397000     -2.289034000     -0.813497000
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C        2.636083000      1.455795000     -0.045772000
H        2.215889000      1.718152000     -1.014875000
H        2.399771000      2.208754000      0.703092000
H        3.713571000      1.315704000     -0.104716000
C       -2.492887000      0.167738000     -0.393756000
O       -3.578954000      0.207103000     -0.696217000

25
I3a,b [RuCl2(CO)3(SeMePh)] symmetry c1 (E=-4027.63818258)
Ru      -1.201175000     -0.318349000      0.116710000
C       -0.033569000     -1.769415000      0.393033000
O        0.664976000     -2.646663000      0.547883000
C       -1.528213000     -0.062420000      1.950939000
O       -1.738166000      0.096777000      3.052150000
Cl      -2.602325000      1.599208000     -0.298236000
Cl      -0.820487000     -0.606526000     -2.250941000
C       -2.716357000     -1.450375000     -0.104295000
O       -3.620801000     -2.106203000     -0.261622000
Se       0.695271000      1.401264000      0.306130000
H        0.584612000      1.624988000     -2.198966000
C        0.661653000      2.338165000     -1.383437000
H        1.570320000      2.934145000     -1.433516000
H       -0.223737000      2.968295000     -1.349157000
C        2.317483000      0.398191000      0.105383000
C        3.136400000      0.292867000      1.220855000
C        2.648193000     -0.225094000     -1.089863000
C        4.303987000     -0.452688000      1.137451000
C        3.822783000     -0.957895000     -1.164125000
C        4.648550000     -1.074224000     -0.053721000
H        2.868528000      0.788615000      2.146655000
H        1.989320000     -0.162321000     -1.946710000
H        4.946432000     -0.540315000      2.005463000
H        4.088344000     -1.446612000     -2.094037000
H        5.562930000     -1.651956000     -0.117977000

32
I3a,b [RuCl2(CO)3(SePh2)] symmetry c1 (E=-4219.22031635)
Ru       1.567137000     -0.076783000      0.208838000
C        1.199751000      1.439436000      1.263390000
O        1.019247000      2.364426000      1.889719000
C        1.031567000     -1.276970000      1.556219000
O        0.725409000     -1.988979000      2.381848000
Cl       2.055101000     -1.939289000     -1.243868000
Cl       2.168662000      1.468834000     -1.540943000
C        3.385028000     -0.117863000      0.766756000
O        4.471767000     -0.149688000      1.067855000
Se      -0.686677000     -0.018189000     -0.999839000
C       -1.576361000      1.530195000     -0.299324000
C       -1.664059000      2.628710000     -1.141512000
C       -2.061358000      1.580341000      1.001150000
C       -2.243162000      3.799061000     -0.669391000
C       -2.649059000      2.748779000      1.456350000
C       -2.736914000      3.858279000      0.624531000
H       -1.282262000      2.575129000     -2.153822000
H       -1.986944000      0.719240000      1.654122000
H       -2.311204000      4.662022000     -1.320679000
H       -3.032145000      2.794383000      2.468756000
H       -3.192648000      4.771271000      0.988683000
C       -1.848797000     -1.414346000     -0.359015000
C       -1.320281000     -2.686176000     -0.188193000
C       -3.206772000     -1.177156000     -0.198072000
C       -2.161672000     -3.725073000      0.180945000
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C       -4.036570000     -2.224836000      0.173450000
C       -3.517161000     -3.496551000      0.368377000
H       -0.265082000     -2.870236000     -0.354483000
H       -3.621146000     -0.189509000     -0.354371000
H       -1.750076000     -4.717460000      0.321492000
H       -5.095908000     -2.040914000      0.307956000
H       -4.170014000     -4.310357000      0.660427000

18
I3a,b [RuCl2(CO)3(TeMe2)] symmetry c1 (E=-1702.82142056)]
Ru      -0.879492000      0.070796000      0.075474000
C       -1.145197000     -0.517561000      1.837809000
O       -1.311139000     -0.884159000      2.897497000
C       -0.802641000      1.883304000      0.550965000
O       -0.757489000      2.983255000      0.823047000
Cl      -0.485445000      0.780096000     -2.205033000
Cl      -0.865032000     -2.258501000     -0.580847000
Te       1.797949000     -0.201880000      0.420981000
C        2.321650000     -1.142530000     -1.400208000
H        1.810138000     -0.617148000     -2.203166000
H        3.404641000     -1.082824000     -1.491061000
H        1.987068000     -2.174277000     -1.335910000
C        2.477332000      1.716370000     -0.180601000
H        1.943924000      1.986185000     -1.090165000
H        2.266388000      2.419273000      0.622713000
H        3.549636000      1.651164000     -0.352314000
C       -2.755455000      0.123267000     -0.324027000
O       -3.853060000      0.145423000     -0.583746000

25
I3a,b [RuCl2(CO)3(TeMePh)] symmetry c1 (E=-1894.40442880)
Ru       1.346237000      0.394765000      0.155996000
C        0.241142000      1.826865000      0.661058000
O       -0.425718000      2.694240000      0.955578000
C        1.710128000     -0.110374000      1.925953000
O        1.944757000     -0.417625000      2.991455000
Cl       2.615458000     -1.537046000     -0.559947000
Cl       0.908448000      1.013550000     -2.144591000
C        2.915339000      1.487729000      0.017831000
O        3.841190000      2.123855000     -0.086441000
Te      -0.704745000     -1.377006000      0.166487000
H       -0.659049000     -1.108621000     -2.491556000
C       -0.722915000     -1.989577000     -1.859008000
H       -1.643152000     -2.548881000     -2.013259000
H        0.153461000     -2.619608000     -1.992006000
C       -2.428576000     -0.165821000      0.068522000
C       -2.598219000      0.754668000     -0.958622000
C       -3.384595000     -0.301532000      1.067197000
C       -3.741592000      1.539070000     -0.984792000
C       -4.522142000      0.494140000      1.036006000
C       -4.701515000      1.410702000      0.010550000
H       -1.838773000      0.876132000     -1.722809000
H       -3.251524000     -1.022380000      1.865967000
H       -3.878381000      2.258089000     -1.784045000
H       -5.269387000      0.391885000      1.814118000
H       -5.591478000      2.028501000     -0.013339000

32
I3a,b [RuCl2(CO)3(TePh2)] symmetry c1 (E=-2085.98748188)
Ru      -1.695546000     -0.037036000      0.291714000
C       -1.210679000     -1.530658000      1.321939000
O       -0.941045000     -2.444925000      1.933802000
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C       -1.140666000      1.184131000      1.605626000
O       -0.815472000      1.915199000      2.408199000
Cl      -2.247906000      1.819542000     -1.160473000
Cl      -2.284768000     -1.601195000     -1.458387000
C       -3.510114000     -0.062361000      0.912197000
O       -4.585171000     -0.072606000      1.254103000
Te       0.617111000      0.015365000     -1.077390000
C        1.754801000     -1.538430000     -0.218781000
C        2.163302000     -1.504724000      1.109674000
C        2.048927000     -2.631436000     -1.023798000
C        2.877248000     -2.572823000      1.628923000
C        2.755842000     -3.701674000     -0.491367000
C        3.170707000     -3.671532000      0.831114000
H        1.935682000     -0.653740000      1.740923000
H        1.732570000     -2.655512000     -2.060219000
H        3.199535000     -2.548390000      2.663196000
H        2.984413000     -4.556579000     -1.116561000
H        3.725179000     -4.506045000      1.243699000
C        1.747848000      1.624516000     -0.294042000
C        3.100576000      1.468949000     -0.020639000
C        1.132808000      2.862496000     -0.153261000
C        3.834955000      2.559731000      0.423360000
C        1.877210000      3.945999000      0.290034000
C        3.225442000      3.795977000      0.582228000
H        3.586644000      0.508899000     -0.143600000
H        0.080971000      2.986708000     -0.387540000
H        4.889091000      2.438387000      0.643778000
H        1.397148000      4.910469000      0.407236000
H        3.802765000      4.644215000      0.930522000

25
cct-[RuCl2(CO)2(SMe2)2] symmetry c2 (E=-2197.43944230)
Ru       0.000000000      0.000000000      0.218292000
Cl       1.758299000      0.021462000     -1.460082000
Cl      -1.758299000     -0.021462000     -1.460082000
C       -1.338976000     -0.061123000      1.496256000
O       -2.163466000     -0.120204000      2.279439000
S        0.000000000      2.398233000      0.153607000
S        0.000000000     -2.398233000      0.153607000
C        0.045697000      2.900915000     -1.565074000
C       -1.657946000      2.938415000      0.570189000
C        1.657946000     -2.938415000      0.570189000
C       -0.045697000     -2.900915000     -1.565074000
H       -0.058355000      3.985598000     -1.591981000
H        1.011696000      2.598983000     -1.961474000
H       -0.755070000      2.407556000     -2.112914000
H       -1.718778000      4.012359000      0.395792000
H       -2.384701000      2.402547000     -0.039398000
H       -1.820052000      2.735270000      1.627481000
H        1.820052000     -2.735270000      1.627481000
H        1.718778000     -4.012359000      0.395792000
H        2.384701000     -2.402547000     -0.039398000
H       -1.011696000     -2.598983000     -1.961474000
H        0.755070000     -2.407556000     -2.112914000
H        0.058355000     -3.985598000     -1.591981000
C        1.338976000      0.061123000      1.496256000
O        2.163466000      0.120204000      2.279439000

39
cct-[RuCl2(CO)2(SMePh)2] symmetry c2 (E=-2580.61012857)
Ru       0.000000000      0.000000000      0.347294000
Cl       1.359543000      1.102180000      2.036783000
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Cl      -1.359543000     -1.102180000      2.036783000
C       -1.014614000     -0.874818000     -0.934668000
O       -1.643718000     -1.402914000     -1.721977000
C        1.014614000      0.874818000     -0.934668000
O        1.643718000      1.402914000     -1.721977000
S       -1.674079000      1.713339000      0.424497000
H       -2.481083000      3.157385000      2.108206000
C       -1.790413000      2.315304000      2.109667000
H       -0.811572000      2.591242000      2.492238000
H       -2.190605000      1.486726000      2.690621000
C       -1.063807000      3.135860000     -0.441333000
C       -1.674611000      3.446578000     -1.649197000
C        0.000000000      3.892800000      0.035210000
C       -1.212851000      4.525101000     -2.389894000
C        0.444442000      4.975102000     -0.706008000
C       -0.157863000      5.291268000     -1.917484000
H       -2.505061000      2.848033000     -2.004819000
H        0.492047000      3.622559000      0.961330000
H       -1.685536000      4.768569000     -3.333844000
H        1.272954000      5.569236000     -0.339139000
H        0.198454000      6.136480000     -2.494281000
S        1.674079000     -1.713339000      0.424497000
H        2.481083000     -3.157385000      2.108206000
C        1.790413000     -2.315304000      2.109667000
H        0.811572000     -2.591242000      2.492238000
H        2.190605000     -1.486726000      2.690621000
C        1.063807000     -3.135860000     -0.441333000
C        1.674611000     -3.446578000     -1.649197000
C        0.000000000     -3.892800000      0.035210000
C        1.212851000     -4.525101000     -2.389894000
C       -0.444442000     -4.975102000     -0.706008000
C        0.157863000     -5.291268000     -1.917484000
H        2.505061000     -2.848033000     -2.004819000
H       -0.492047000     -3.622559000      0.961330000
H        1.685536000     -4.768569000     -3.333844000
H       -1.272954000     -5.569236000     -0.339139000
H       -0.198454000     -6.136480000     -2.494281000

53
cct-[RuCl2(CO)2(SPh2)2] symmetry c2 (E=-2963.77451335)
Ru      -0.000014000      0.000006000      0.492074000
Cl      -0.061793000      1.713421000      2.214888000
Cl       0.062855000     -1.717888000      2.210312000
C       -0.017505000     -1.311484000     -0.819756000
O       -0.049479000     -2.099044000     -1.640172000
C        0.016767000      1.315232000     -0.816022000
O        0.048078000      2.105353000     -1.633993000
S        2.372486000     -0.029403000      0.819361000
C        3.030436000     -1.438328000     -0.029669000
C        3.078635000     -1.516757000     -1.417157000
C        3.462795000     -2.494312000      0.760238000
C        3.572641000     -2.663315000     -2.012897000
C        3.944057000     -3.645478000      0.152181000
C        4.001947000     -3.728933000     -1.230119000
H        2.737791000     -0.687945000     -2.025729000
H        3.415808000     -2.415346000      1.839037000
H        3.614911000     -2.728845000     -3.093396000
H        4.278097000     -4.474238000      0.764506000
H        4.382370000     -4.626576000     -1.702833000
C        3.240158000      1.338582000      0.074208000
C        2.704778000      2.612667000      0.224088000
C        4.486346000      1.163096000     -0.515817000
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C        3.406772000      3.707998000     -0.252475000
C        5.177700000      2.268283000     -0.988540000
C        4.640208000      3.540792000     -0.865466000
H        1.752897000      2.747160000      0.723891000
H        4.920438000      0.177023000     -0.610293000
H        2.981934000      4.698485000     -0.140584000
H        6.145285000      2.126523000     -1.455238000
H        5.183675000      4.399840000     -1.240169000
S       -2.372455000      0.029087000      0.819741000
C       -3.029990000      1.437999000     -0.029704000
C       -3.459708000      2.495424000      0.759715000
C       -3.080005000      1.515041000     -1.417201000
C       -3.940133000      3.646652000      0.151110000
C       -3.573213000      2.661675000     -2.013449000
C       -3.999868000      3.728742000     -1.231196000
H       -3.411331000      2.417512000      1.838532000
H       -2.741128000      0.685125000     -2.025370000
H       -4.272142000      4.476527000      0.763030000
H       -3.616888000      2.726128000     -3.093957000
H       -4.379672000      4.626429000     -1.704325000
C       -3.240685000     -1.338595000      0.074647000
C       -4.488789000     -1.162762000     -0.511288000
C       -2.704146000     -2.612601000      0.220613000
C       -5.180943000     -2.267459000     -0.983912000
C       -3.406996000     -3.707493000     -0.255773000
C       -4.642352000     -3.539895000     -0.864727000
H       -4.923691000     -0.176744000     -0.602682000
H       -1.750794000     -2.747500000      0.717458000
H       -6.150017000     -2.125420000     -1.447422000
H       -2.981269000     -4.697935000     -0.146915000
H       -5.186470000     -4.398586000     -1.239310000

25
cct-[RuCl2(CO)2(SeMe2)2] symmetry c2(E=-6203.84944176)
Ru       0.000000000      0.000000000      0.224608000
Cl       1.760252000      0.036311000     -1.457261000
Cl      -1.760252000     -0.036311000     -1.457261000
C       -1.336571000     -0.030665000      1.500447000
O       -2.163229000     -0.058180000      2.284989000
Se       0.028574000      2.510126000      0.132657000
Se      -0.028574000     -2.510126000      0.132657000
C        0.000000000      2.935467000     -1.752580000
C       -1.800386000      3.021236000      0.506105000
C        1.800386000     -3.021236000      0.506105000
C        0.000000000     -2.935467000     -1.752580000
H       -0.174280000      4.006885000     -1.836971000
H        0.972652000      2.662893000     -2.152143000
H       -0.786713000      2.352898000     -2.226075000
H       -1.906263000      4.078240000      0.269263000
H       -2.462382000      2.408277000     -0.102576000
H       -1.980139000      2.856529000      1.566483000
H        1.980139000     -2.856529000      1.566483000
H        1.906263000     -4.078240000      0.269263000
H        2.462382000     -2.408277000     -0.102576000
H       -0.972652000     -2.662893000     -2.152143000
H        0.786713000     -2.352898000     -2.226075000
H        0.174280000     -4.006885000     -1.836971000
C        1.336571000      0.030665000      1.500447000
O        2.163229000      0.058180000      2.284989000

39
cct-[RuCl2(CO)2(SeMePh)2] symmetry c2 (E=-6587.01766694)
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Ru	0.000000000	0.000000000	0.230451000
Cl	1.340611000	1.120453000	1.929119000
Cl	-1.340611000	-1.120453000	1.929119000
C	-0.971710000	-0.912114000	-1.052580000
O	-1.571100000	-1.469998000	-1.844311000
C	0.971710000	0.912114000	-1.052580000
O	1.571100000	1.469998000	-1.844311000
Se	-1.821688000	1.721418000	0.336202000
H	-2.508938000	3.191585000	2.213467000
C	-1.833517000	2.339802000	2.169274000
H	-0.823051000	2.595090000	2.474416000
H	-2.206037000	1.505037000	2.758123000
C	-1.137299000	3.302760000	-0.508023000
C	-1.811020000	3.772108000	-1.626424000
C	0.000000000	3.943231000	-0.035009000
C	-1.337515000	4.901130000	-2.281229000
C	0.458270000	5.075237000	-0.690401000
C	-0.207350000	5.553704000	-1.811980000
H	-2.698963000	3.263733000	-1.983876000
H	0.536078000	3.548485000	0.820210000
H	-1.858417000	5.271276000	-3.156271000
H	1.345307000	5.580609000	-0.326967000
H	0.158639000	6.436854000	-2.322174000
Se	1.821688000	-1.721418000	0.336202000
H	2.508938000	-3.191585000	2.213467000
C	1.833517000	-2.339802000	2.169274000
H	0.823051000	-2.595090000	2.474416000
H	2.206037000	-1.505037000	2.758123000
C	1.137299000	-3.302760000	-0.508023000
C	1.811020000	-3.772108000	-1.626424000
C	0.000000000	-3.943231000	-0.035009000
C	1.337515000	-4.901130000	-2.281229000
C	-0.458270000	-5.075237000	-0.690401000
C	0.207350000	-5.553704000	-1.811980000
H	2.698963000	-3.263733000	-1.983876000
H	-0.536078000	-3.548485000	0.820210000
H	1.858417000	-5.271276000	-3.156271000
H	-1.345307000	-5.580609000	-0.326967000
H	-0.158639000	-6.436854000	-2.322174000

53
cct-[RuCl2(CO)2(SePh2)2] symmetry c2 (E=-6970.18282694)

Ru	0.000000000	0.000000000	0.520533000
Cl	-1.665406000	0.445338000	2.239146000
Cl	1.665406000	-0.445338000	2.239146000
C	1.257087000	-0.385170000	-0.782399000
O	2.015111000	-0.631669000	-1.595558000
C	-1.257087000	0.385170000	-0.782399000
O	-2.015111000	0.631669000	-1.595558000
Se	0.740459000	2.361510000	0.876614000
C	2.263260000	2.591689000	-0.265381000
C	2.148446000	2.625331000	-1.648820000
C	3.501654000	2.668594000	0.354003000
C	3.293478000	2.748009000	-2.417707000
C	4.644476000	2.777748000	-0.427274000
C	4.540619000	2.820846000	-1.808949000
H	1.177314000	2.557917000	-2.124270000
H	3.575697000	2.640887000	1.434444000
H	3.211500000	2.777523000	-3.497667000
H	5.615343000	2.834750000	0.050062000
H	5.433334000	2.911039000	-2.416305000
C	-0.480613000	3.608844000	0.061121000

```
C       -1.843811000      3.400551000      0.216692000
C        0.000000000      4.757256000     -0.553515000
C       -2.734040000      4.341726000     -0.278589000
C       -0.901100000      5.689362000     -1.046617000
C       -2.266837000      5.482577000     -0.915007000
H       -2.208170000      2.517400000      0.728625000
H        1.063907000      4.928916000     -0.655162000
H       -3.798983000      4.177228000     -0.164411000
H       -0.528289000      6.582340000     -1.534337000
H       -2.966165000      6.213068000     -1.303938000
Se      -0.740459000     -2.361510000      0.876614000
C       -2.263260000     -2.591689000     -0.265381000
C       -3.501654000     -2.668594000      0.354003000
C       -2.148446000     -2.625331000     -1.648820000
C       -4.644476000     -2.777748000     -0.427274000
C       -3.293478000     -2.748009000     -2.417707000
C       -4.540619000     -2.820846000     -1.808949000
H       -3.575697000     -2.640887000      1.434444000
H       -1.177314000     -2.557917000     -2.124270000
H       -5.615343000     -2.834750000      0.050062000
H       -3.211500000     -2.777523000     -3.497667000
H       -5.433334000     -2.911039000     -2.416305000
C        0.480613000     -3.608844000      0.061121000
C        0.000000000     -4.757256000     -0.553515000
C        1.843811000     -3.400551000      0.216692000
C        0.901100000     -5.689362000     -1.046617000
C        2.734040000     -4.341726000     -0.278589000
C        2.266837000     -5.482577000     -0.915007000
H       -1.063907000     -4.928916000     -0.655162000
H        2.208170000     -2.517400000      0.728625000
H        0.528289000     -6.582340000     -1.534337000
H        3.798983000     -4.177228000     -0.164411000
H        2.966165000     -6.213068000     -1.303938000

25
cct-[RuCl2(CO)2(TeMe2)2] symmetry c2 (E=-1937.38606211)
Ru       0.000000000      0.000000000      0.252679000
Cl       1.514995000      0.900640000     -1.440413000
Cl      -1.514995000     -0.900640000     -1.440413000
C       -1.126563000     -0.714067000      1.526189000
O       -1.825385000     -1.159998000      2.311408000
Te      -1.467381000      2.217320000      0.109775000
Te       1.467381000     -2.217320000      0.109775000
C        0.000000000      3.709667000      0.464080000
C       -1.529456000      2.556122000     -1.979542000
C        1.529456000     -2.556122000     -1.979542000
C        0.000000000     -3.709667000      0.464080000
H       -0.416470000      4.672816000      0.176269000
H        0.238557000      3.703701000      1.525769000
H        0.874204000      3.457773000     -0.133568000
H       -1.889502000      3.571394000     -2.136040000
H       -0.523251000      2.411519000     -2.366333000
H       -2.214184000      1.825478000     -2.401923000
H        2.214184000     -1.825478000     -2.401923000
H        1.889502000     -3.571394000     -2.136040000
H        0.523251000     -2.411519000     -2.366333000
H       -0.238557000     -3.703701000      1.525769000
H       -0.874204000     -3.457773000     -0.133568000
H        0.416470000     -4.672816000      0.176269000
C        1.126563000      0.714067000      1.526189000
O        1.825385000      1.159998000      2.311408000
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39
cct-[RuCl2(CO)2(TeMePh)2] symmetry c2 (E=-2320.55300864)

Ru	0.000000000	0.000000000	0.108585000
Cl	-1.332934000	1.137501000	1.817795000
Cl	1.332934000	-1.137501000	1.817795000
C	0.927129000	-0.951144000	-1.172826000
O	1.495334000	-1.542684000	-1.965597000
C	-0.927129000	0.951144000	-1.172826000
O	-1.495334000	1.542684000	-1.965597000
Te	1.992430000	1.751112000	0.273675000
H	0.812980000	2.596951000	2.515614000
C	1.853626000	2.377403000	2.292890000
H	2.495751000	3.248116000	2.407135000
H	2.204034000	1.542029000	2.894568000
C	1.206856000	3.530017000	-0.547262000
C	0.000000000	4.048788000	-0.093172000
C	1.915631000	4.166721000	-1.558216000
C	-0.491764000	5.218596000	-0.652340000
C	1.411559000	5.333670000	-2.117952000
C	0.211503000	5.860236000	-1.663792000
H	-0.562970000	3.535786000	0.679191000
H	2.857884000	3.762212000	-1.910551000
H	-1.432277000	5.626148000	-0.300005000
H	1.962016000	5.831380000	-2.907777000
H	-0.178944000	6.772307000	-2.099870000
Te	-1.992430000	-1.751112000	0.273675000
H	-0.812980000	-2.596951000	2.515614000
C	-1.853626000	-2.377403000	2.292890000
H	-2.495751000	-3.248116000	2.407135000
H	-2.204034000	-1.542029000	2.894568000
C	-1.206856000	-3.530017000	-0.547262000
C	0.000000000	-4.048788000	-0.093172000
C	-1.915631000	-4.166721000	-1.558216000
C	0.491764000	-5.218596000	-0.652340000
C	-1.411559000	-5.333670000	-2.117952000
C	-0.211503000	-5.860236000	-1.663792000
H	0.562970000	-3.535786000	0.679191000
H	-2.857884000	-3.762212000	-1.910551000
H	1.432277000	-5.626148000	-0.300005000
H	-1.962016000	-5.831380000	-2.907777000
H	0.178944000	-6.772307000	-2.099870000

53
cct-[RuCl2(CO)2(TePh2)2] symmetry c2 (E=-2703.71949104)

Ru	0.000000000	0.000000000	0.578593000
Cl	-1.539436000	0.771508000	2.313848000
Cl	1.539436000	-0.771508000	2.313848000
C	1.167672000	-0.614994000	-0.713551000
O	1.880504000	-0.998176000	-1.516572000
C	-1.167672000	0.614994000	-0.713551000
O	-1.880504000	0.998176000	-1.516572000
Te	1.225382000	2.314063000	0.936170000
C	2.704086000	2.330262000	-0.567053000
C	2.363262000	2.283090000	-1.913933000
C	4.035649000	2.346699000	-0.173870000
C	3.365344000	2.260703000	-2.870298000
C	5.034228000	2.312640000	-1.139044000
C	4.699944000	2.272398000	-2.483865000
H	1.323975000	2.266150000	-2.221480000
H	4.300996000	2.386817000	0.876340000
H	3.102363000	2.226575000	-3.921033000
H	6.074162000	2.322786000	-0.834721000

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H        5.480302000      2.249675000     -3.235359000
C        0.000000000      3.793945000      0.046367000
C       -1.367283000      3.777611000      0.290885000
C        0.574415000      4.816703000     -0.698228000
C       -2.165316000      4.784110000     -0.234139000
C       -0.233473000      5.816598000     -1.220842000
C       -1.602150000      5.800874000     -0.992012000
H       -1.810388000      2.985392000      0.884489000
H        1.641765000      4.837882000     -0.882392000
H       -3.233241000      4.768359000     -0.049913000
H        0.212771000      6.610645000     -1.808240000
H       -2.229532000      6.583079000     -1.402922000
Te      -1.225382000     -2.314063000      0.936170000
C       -2.704086000     -2.330262000     -0.567053000
C       -4.035649000     -2.346699000     -0.173870000
C       -2.363262000     -2.283090000     -1.913933000
C       -5.034228000     -2.312640000     -1.139044000
C       -3.365344000     -2.260703000     -2.870298000
C       -4.699944000     -2.272398000     -2.483865000
H       -4.300996000     -2.386817000      0.876340000
H       -1.323975000     -2.266150000     -2.221480000
H       -6.074162000     -2.322786000     -0.834721000
H       -3.102363000     -2.226575000     -3.921033000
H       -5.480302000     -2.249675000     -3.235359000
C        0.000000000     -3.793945000      0.046367000
C       -0.574415000     -4.816703000     -0.698228000
C        1.367283000     -3.777611000      0.290885000
C        0.233473000     -5.816598000     -1.220842000
C        2.165316000     -4.784110000     -0.234139000
C        1.602150000     -5.800874000     -0.992012000
H       -1.641765000     -4.837882000     -0.882392000
H        1.810388000     -2.985392000      0.884489000
H       -0.212771000     -6.610645000     -1.808240000
H        3.233241000     -4.768359000     -0.049913000
H        2.229532000     -6.583079000     -1.402922000

25
ctc-[RuCl2(CO)2(SMe2)2] symmetry c1 (E=-2197.427326)
Ru      -0.035194000      0.449794000      0.075367000
S        1.630520000     -1.272229000     -0.468150000
C        2.156053000     -2.118955000      1.020043000
C        3.150555000     -0.437377000     -0.922539000
H        1.296076000     -2.658129000      1.410492000
H        2.947708000     -2.817845000      0.751319000
H        2.502810000     -1.406210000      1.766493000
H        2.901810000      0.243738000     -1.734244000
H        3.554097000      0.116180000     -0.075633000
H        3.866497000     -1.184829000     -1.261675000
S       -1.726795000     -0.986007000     -1.012285000
C       -3.275642000     -0.665789000     -0.164495000
C       -1.453802000     -2.671239000     -0.461059000
H       -3.605576000      0.334226000     -0.441416000
H       -3.127675000     -0.733466000      0.912966000
H       -4.011630000     -1.394140000     -0.503219000
H       -2.291587000     -3.279818000     -0.800377000
H       -1.367353000     -2.695907000      0.624733000
H       -0.537437000     -3.028682000     -0.927837000
C        1.267183000      1.514559000      0.860726000
O        2.058976000      2.162167000      1.358933000
Cl       0.418781000      1.301458000     -2.119088000
C       -1.302917000      1.777309000      0.380554000
Cl      -0.557242000     -0.579766000      2.170905000
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O       -2.050668000      2.611072000      0.577185000

39
ctc-[RuCl2(CO)2(SMePh)2] symmetry c2 (E=-2580.59773028)
Ru       0.000000000      0.000000000      0.396168000
S        0.485833000     -1.587888000     -1.439540000
C        2.015524000     -1.138709000     -2.252212000
H        1.794360000     -0.231291000     -2.813188000
H        2.802502000     -0.923499000     -1.534029000
H        2.290608000     -1.940080000     -2.936503000
S       -0.485833000      1.587888000     -1.439540000
C       -2.015524000      1.138709000     -2.252212000
H       -2.290608000      1.940080000     -2.936503000
H       -2.802502000      0.923499000     -1.534029000
H       -1.794360000      0.231291000     -2.813188000
C        0.860938000     -3.142921000     -0.677282000
C       -0.860938000      3.142921000     -0.677282000
C       -1.290472000      5.570920000      0.582339000
C        0.220295000      3.965774000     -0.380230000
C       -2.154827000      3.527323000     -0.352939000
C       -2.363127000      4.747799000      0.272481000
C        0.000000000      5.175689000      0.257687000
H        1.224367000      3.649924000     -0.635858000
H       -2.998111000      2.885790000     -0.571173000
H       -3.372828000      5.049793000      0.524255000
H        0.842334000      5.814870000      0.494053000
H       -1.460031000      6.520748000      1.075114000
C        1.290472000     -5.570920000      0.582339000
C       -0.220295000     -3.965774000     -0.380230000
C        2.154827000     -3.527323000     -0.352939000
C        2.363127000     -4.747799000      0.272481000
C        0.000000000     -5.175689000      0.257687000
H       -1.224367000     -3.649924000     -0.635858000
H        2.998111000     -2.885790000     -0.571173000
H        3.372828000     -5.049793000      0.524255000
H       -0.842334000     -5.814870000      0.494053000
H        1.460031000     -6.520748000      1.075114000
C        0.514829000     -1.203963000      1.712177000
Cl       2.201696000      0.935729000      0.324506000
O        0.829644000     -1.929565000      2.528194000
Cl      -2.201696000     -0.935729000      0.324506000
C       -0.514829000      1.203963000      1.712177000
O       -0.829644000      1.929565000      2.528194000

53
ctc-[RuCl2(CO)2(SPh2)2] symmetry c2 (E=-2963.76729129)
Ru       0.000000000      0.000000000      1.384875000
S       -1.013551000     -1.421866000     -0.366172000
S        1.013551000      1.421866000     -0.366172000
C       -0.057685000     -1.626648000     -1.852587000
C        1.122925000      3.080678000      0.267479000
C        1.423548000      5.610524000      1.337128000
C        2.392347000      3.541779000      0.590100000
C        0.000000000      3.871045000      0.475302000
C        0.158634000      5.140914000      1.005428000
C        2.537607000      4.810478000      1.133275000
H        3.256664000      2.911298000      0.419113000
H       -0.985880000      3.492126000      0.241334000
H       -0.712978000      5.763665000      1.168394000
H        3.525804000      5.173327000      1.389435000
H        1.538974000      6.603012000      1.756316000
C        1.279220000     -1.912238000     -4.255144000
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C       -0.781281000     -1.704157000     -3.037232000
C        1.329230000     -1.679852000     -1.859948000
C        1.992996000     -1.825667000     -3.068743000
C       -0.107113000     -1.849595000     -4.238742000
H       -1.862270000     -1.639859000     -3.015075000
H        1.880592000     -1.593213000     -0.932037000
H        3.075862000     -1.865318000     -3.079975000
H       -0.667846000     -1.903984000     -5.164156000
H        1.804415000     -2.020558000     -5.196861000
C       -0.595108000     -1.168177000      2.703750000
Cl       2.130391000     -1.113143000      1.438664000
O       -0.943927000     -1.877547000      3.518414000
Cl      -2.130391000      1.113143000      1.438664000
C        0.595108000      1.168177000      2.703750000
O        0.943927000      1.877547000      3.518414000
C        0.057685000      1.626648000     -1.852587000
C       -1.279220000      1.912238000     -4.255144000
C        0.781281000      1.704157000     -3.037232000
C       -1.329230000      1.679852000     -1.859948000
C       -1.992996000      1.825667000     -3.068743000
C        0.107113000      1.849595000     -4.238742000
H        1.862270000      1.639859000     -3.015075000
H       -1.880592000      1.593213000     -0.932037000
H       -3.075862000      1.865318000     -3.079975000
H        0.667846000      1.903984000     -5.164156000
H       -1.804415000      2.020558000     -5.196861000
C       -1.122925000     -3.080678000      0.267479000
C       -1.423548000     -5.610524000      1.337128000
C       -2.392347000     -3.541779000      0.590100000
C        0.000000000     -3.871045000      0.475302000
C       -0.158634000     -5.140914000      1.005428000
C       -2.537607000     -4.810478000      1.133275000
H       -3.256664000     -2.911298000      0.419113000
H        0.985880000     -3.492126000      0.241334000
H        0.712978000     -5.763665000      1.168394000
H       -3.525804000     -5.173327000      1.389435000
H       -1.538974000     -6.603012000      1.756316000

25
ctc-[RuCl2(CO)2(SeMe2)2] symmetry c1 (E=-6203.83515252)
Ru      -0.035384000      0.696645000      0.090214000
Se       1.707112000     -1.160499000     -0.269533000
C        2.441177000     -1.609630000      1.462512000
C        3.256974000     -0.253970000     -0.991946000
H        1.650605000     -2.094225000      2.029293000
H        3.275830000     -2.289717000      1.303799000
H        2.758974000     -0.703179000      1.972332000
H        2.917814000      0.268612000     -1.883504000
H        3.646339000      0.449234000     -0.258995000
H        4.002453000     -1.005838000     -1.241282000
Se      -1.849462000     -0.968957000     -0.690529000
C       -3.394857000     -0.485145000      0.372372000
C       -1.463933000     -2.617743000      0.249358000
H       -3.789562000      0.447217000     -0.026011000
H       -3.079961000     -0.363379000      1.407131000
H       -4.135554000     -1.275855000      0.271061000
H       -2.332534000     -3.266263000      0.152302000
H       -1.253048000     -2.383673000      1.291154000
H       -0.602800000     -3.078176000     -0.230530000
C        1.300000000      1.872773000      0.613906000
O        2.115325000      2.592762000      0.950409000
Cl       0.296052000      1.159819000     -2.240916000
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C       -1.315687000      2.034666000      0.244971000
Cl      -0.408446000     -0.003459000      2.348136000
O       -2.076968000      2.874805000      0.344109000

39
ctc-[RuCl2(CO)2(SeMePh)2] symmetry c2 (E=-6587.00265630)
Ru       0.000000000      0.000000000      0.567891000
Se       0.101903000     -1.740893000     -1.345323000
C        1.917488000     -1.799538000     -2.000017000
H        2.034837000     -0.909368000     -2.615163000
H        2.621240000     -1.761748000     -1.173390000
H        2.030063000     -2.696389000     -2.605542000
Se      -0.101903000      1.740893000     -1.345323000
C       -1.917488000      1.799538000     -2.000017000
H       -2.030063000      2.696389000     -2.605542000
H       -2.621240000      1.761748000     -1.173390000
H       -2.034837000      0.909368000     -2.615163000
C        0.000000000     -3.427087000     -0.438782000
C        0.000000000      3.427087000     -0.438782000
C        0.280862000      5.821469000      0.917972000
C        1.271224000      3.898333000     -0.135588000
C       -1.130918000      4.141444000     -0.073718000
C       -0.982748000      5.344441000      0.602740000
C        1.405470000      5.095642000      0.550115000
H        2.147121000      3.327892000     -0.420074000
H       -2.123239000      3.772889000     -0.297836000
H       -1.864804000      5.905118000      0.888939000
H        2.395608000      5.463323000      0.792262000
H        0.389661000      6.759062000      1.449903000
C       -0.280862000     -5.821469000      0.917972000
C       -1.271224000     -3.898333000     -0.135588000
C        1.130918000     -4.141444000     -0.073718000
C        0.982748000     -5.344441000      0.602740000
C       -1.405470000     -5.095642000      0.550115000
H       -2.147121000     -3.327892000     -0.420074000
H        2.123239000     -3.772889000     -0.297836000
H        1.864804000     -5.905118000      0.888939000
H       -2.395608000     -5.463323000      0.792262000
H       -0.389661000     -6.759062000      1.449903000
C        0.232817000     -1.295622000      1.874364000
Cl       2.353667000      0.425944000      0.466994000
O        0.380095000     -2.076116000      2.688360000
Cl      -2.353667000     -0.425944000      0.466994000
C       -0.232817000      1.295622000      1.874364000
O       -0.380095000      2.076116000      2.688360000

53
ctc-[RuCl2(CO)2(SePh2)2] symmetry c2 (E=-6970.17187690)
Ru       0.000000000      0.000000000      1.475836000
Se      -1.152880000     -1.427708000     -0.347028000
Se       1.152880000      1.427708000     -0.347028000
C       -0.059433000     -1.641536000     -1.912553000
C        1.143818000      3.225315000      0.336569000
C        1.255487000      5.763064000      1.421053000
C        2.342037000      3.693904000      0.857118000
C        0.000000000      4.008878000      0.350301000
C        0.064863000      5.284542000      0.890318000
C        2.391416000      4.967203000      1.406855000
H        3.230021000      3.072766000      0.835165000
H       -0.932929000      3.630851000     -0.044966000
H       -0.824348000      5.903808000      0.902102000
H        3.323703000      5.337106000      1.816824000
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H        1.297212000      6.759164000      1.845470000
C        1.373400000     -1.888843000     -4.261233000
C       -0.736920000     -1.726314000     -3.121800000
C        1.326523000     -1.671278000     -1.864228000
C        2.039502000     -1.798664000     -3.047849000
C       -0.013291000     -1.851664000     -4.297677000
H       -1.819072000     -1.683697000     -3.146325000
H        1.843059000     -1.589680000     -0.915261000
H        3.122532000     -1.821229000     -3.016868000
H       -0.536958000     -1.911470000     -5.244320000
H        1.936173000     -1.982004000     -5.182624000
C       -0.671979000     -1.133070000      2.786213000
Cl       2.045814000     -1.258852000      1.496269000
O       -1.064311000     -1.823729000      3.598283000
Cl      -2.045814000      1.258852000      1.496269000
C        0.671979000      1.133070000      2.786213000
O        1.064311000      1.823729000      3.598283000
C        0.059433000      1.641536000     -1.912553000
C       -1.373400000      1.888843000     -4.261233000
C        0.736920000      1.726314000     -3.121800000
C       -1.326523000      1.671278000     -1.864228000
C       -2.039502000      1.798664000     -3.047849000
C        0.013291000      1.851664000     -4.297677000
H        1.819072000      1.683697000     -3.146325000
H       -1.843059000      1.589680000     -0.915261000
H       -3.122532000      1.821229000     -3.016868000
H        0.536958000      1.911470000     -5.244320000
H       -1.936173000      1.982004000     -5.182624000
C       -1.143818000     -3.225315000      0.336569000
C       -1.255487000     -5.763064000      1.421053000
C       -2.342037000     -3.693904000      0.857118000
C        0.000000000     -4.008878000      0.350301000
C       -0.064863000     -5.284542000      0.890318000
C       -2.391416000     -4.967203000      1.406855000
H       -3.230021000     -3.072766000      0.835165000
H        0.932929000     -3.630851000     -0.044966000
H        0.824348000     -5.903808000      0.902102000
H       -3.323703000     -5.337106000      1.816824000
H       -1.297212000     -6.759164000      1.845470000

25
ctc-[RuCl2(CO)2(TeMe2)2] symmetry c1 (E=-1937.36663609)
Ru      -0.025550000      0.901890000      0.089165000
Te       1.816492000     -1.076638000     -0.201560000
C        2.654062000     -1.310574000      1.733962000
C        3.463502000     -0.007839000     -1.010038000
H        1.895558000     -1.774768000      2.359466000
H        3.531237000     -1.948552000      1.648898000
H        2.911214000     -0.329646000      2.126405000
H        3.093247000      0.504132000     -1.895876000
H        3.819125000      0.706803000     -0.271147000
H        4.242857000     -0.720878000     -1.267997000
Te      -1.994197000     -0.877359000     -0.545086000
C       -3.541699000     -0.230555000      0.757779000
C       -1.506674000     -2.556865000      0.662006000
H       -3.973072000      0.677643000      0.341649000
H       -3.091996000     -0.038213000      1.730102000
H       -4.293067000     -1.015477000      0.810374000
H       -2.400770000     -3.169819000      0.757794000
H       -1.170738000     -2.184588000      1.628152000
H       -0.722013000     -3.120192000      0.160418000
C        1.346715000      2.088632000      0.499445000
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O        2.177018000      2.821585000      0.768168000
Cl       0.279961000      1.160345000     -2.286410000
C       -1.312357000      2.246176000      0.169645000
Cl      -0.333200000      0.349679000      2.402681000
O       -2.076143000      3.090158000      0.221917000

39
ctc-[RuCl2(CO)2(TeMePh)2] symmetry c2 (E=-2320.53206424)
Ru       0.000000000      0.000000000      0.684441000
Te       0.711419000     -1.742085000     -1.294218000
C        2.724542000     -1.274648000     -1.758706000
H        2.687702000     -0.392712000     -2.395490000
H        3.263539000     -1.041901000     -0.844178000
H        3.159501000     -2.113688000     -2.297743000
Te      -0.711419000      1.742085000     -1.294218000
C       -2.724542000      1.274648000     -1.758706000
H       -3.159501000      2.113688000     -2.297743000
H       -3.263539000      1.041901000     -0.844178000
H       -2.687702000      0.392712000     -2.395490000
C        1.093090000     -3.491133000     -0.177246000
C       -1.093090000      3.491133000     -0.177246000
C       -1.488483000      5.782996000      1.329854000
C        0.000000000      4.255269000      0.215531000
C       -2.381235000      3.867788000      0.175574000
C       -2.573931000      5.018518000      0.928519000
C       -0.203066000      5.398682000      0.973794000
H        1.006521000      3.954961000     -0.051704000
H       -3.238816000      3.275757000     -0.117762000
H       -3.580047000      5.311682000      1.205160000
H        0.649314000      5.991484000      1.284712000
H       -1.643798000      6.678160000      1.920362000
C        1.488483000     -5.782996000      1.329854000
C        0.000000000     -4.255269000      0.215531000
C        2.381235000     -3.867788000      0.175574000
C        2.573931000     -5.018518000      0.928519000
C        0.203066000     -5.398682000      0.973794000
H       -1.006521000     -3.954961000     -0.051704000
H        3.238816000     -3.275757000     -0.117762000
H        3.580047000     -5.311682000      1.205160000
H       -0.649314000     -5.991484000      1.284712000
H        1.643798000     -6.678160000      1.920362000
C        0.674099000     -1.152132000      1.980417000
Cl       2.075711000      1.198870000      0.540048000
O        1.090673000     -1.830898000      2.793880000
Cl      -2.075711000     -1.198870000      0.540048000
C       -0.674099000      1.152132000      1.980417000
O       -1.090673000      1.830898000      2.793880000

53
ctc-[RuCl2(CO)2(TePh2)2] symmetry c2 (E=-2703.70261027)
Ru       0.000000000      0.000000000      1.582528000
Te      -1.304676000     -1.451355000     -0.323197000
Te       1.304676000      1.451355000     -0.323197000
C       -0.031467000     -1.661472000     -1.992752000
C        1.144542000      3.430336000      0.403837000
C        1.029211000      5.988674000      1.456712000
C        2.232764000      3.937099000      1.104097000
C        0.000000000      4.194019000      0.224284000
C       -0.050163000      5.477499000      0.749404000
C        2.168709000      5.217694000      1.635331000
H        3.130569000      3.343829000      1.239413000
H       -0.850385000      3.799098000     -0.315747000
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H       -0.942126000      6.076923000      0.608457000
H        3.015732000      5.612844000      2.183860000
H        0.982451000      6.990207000      1.867852000
C        1.527226000     -1.849439000     -4.272892000
C       -0.640777000     -1.721836000     -3.240213000
C        1.352886000     -1.692056000     -1.877366000
C        2.128910000     -1.788018000     -3.024308000
C        0.144356000     -1.817174000     -4.379953000
H       -1.720135000     -1.683119000     -3.329314000
H        1.823841000     -1.646199000     -0.901344000
H        3.208958000     -1.811226000     -2.936898000
H       -0.328794000     -1.857152000     -5.354002000
H        2.137527000     -1.918585000     -5.165735000
C       -0.751546000     -1.104597000      2.882053000
Cl       1.960735000     -1.395278000      1.562077000
O       -1.186303000     -1.775019000      3.691172000
Cl      -1.960735000      1.395278000      1.562077000
C        0.751546000      1.104597000      2.882053000
O        1.186303000      1.775019000      3.691172000
C        0.031467000      1.661472000     -1.992752000
C       -1.527226000      1.849439000     -4.272892000
C        0.640777000      1.721836000     -3.240213000
C       -1.352886000      1.692056000     -1.877366000
C       -2.128910000      1.788018000     -3.024308000
C       -0.144356000      1.817174000     -4.379953000
H        1.720135000      1.683119000     -3.329314000
H       -1.823841000      1.646199000     -0.901344000
H       -3.208958000      1.811226000     -2.936898000
H        0.328794000      1.857152000     -5.354002000
H       -2.137527000      1.918585000     -5.165735000
C       -1.144542000     -3.430336000      0.403837000
C       -1.029211000     -5.988674000      1.456712000
C       -2.232764000     -3.937099000      1.104097000
C        0.000000000     -4.194019000      0.224284000
C        0.050163000     -5.477499000      0.749404000
C       -2.168709000     -5.217694000      1.635331000
H       -3.130569000     -3.343829000      1.239413000
H        0.850385000     -3.799098000     -0.315747000
H        0.942126000     -6.076923000      0.608457000
H       -3.015732000     -5.612844000      2.183860000
H       -0.982451000     -6.990207000      1.867852000

25
ccc-[RuCl2(CO)2(SMe2)2] symmetry c1 (E=-2197.43293862)
Ru       0.067232000      0.394195000      0.033802000
S       -1.577326000     -1.416666000      0.328614000
C       -2.365549000     -1.667563000     -1.259297000
C       -2.947596000     -0.712486000      1.245523000
H       -1.612393000     -2.073065000     -1.930517000
H       -3.179419000     -2.379059000     -1.122140000
H       -2.726195000     -0.713265000     -1.640359000
H       -2.617315000     -0.557204000      2.271445000
H       -3.245339000      0.232614000      0.792586000
H       -3.769594000     -1.427301000      1.235968000
S        1.751600000     -0.976078000      1.010221000
C        3.293921000     -0.566672000      0.192438000
C        1.554060000     -2.654132000      0.409134000
H        3.584518000      0.431905000      0.514655000
H        3.156626000     -0.597468000     -0.887796000
H        4.048460000     -1.284016000      0.514021000
H        2.424918000     -3.223940000      0.732819000
H        1.464959000     -2.648298000     -0.676285000
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H        0.656411000     -3.067201000      0.863852000
C        1.260758000      1.794765000     -0.296694000
O        1.944173000      2.671294000     -0.526806000
Cl      -1.672528000      1.721386000     -0.963152000
Cl       0.661431000     -0.508048000     -2.142749000
C       -0.359432000      1.100347000      1.685665000
O       -0.614244000      1.560373000      2.697156000

39
ccc-[RuCl2(CO)2(SMePh)2] symmetry c1 (E=-2580.60473914)
Ru      -1.350237000      0.018673000      0.330003000
S       -0.564567000      2.266083000      0.086498000
C       -0.976730000      2.884357000     -1.540304000
H       -2.058026000      2.992262000     -1.550661000
H       -0.493761000      3.853317000     -1.661162000
H       -0.681760000      2.187933000     -2.322574000
Cl      -2.162363000     -2.225310000      0.552407000
C       -0.103739000     -0.411835000      1.632983000
S        0.164311000     -0.676260000     -1.486749000
O        0.619571000     -0.729650000      2.452756000
C       -0.739440000     -1.801155000     -2.548207000
H       -1.286373000     -2.531507000     -1.956229000
H       -0.029577000     -2.271462000     -3.226837000
H       -1.444653000     -1.181841000     -3.098295000
C        1.209420000      2.276546000      0.063355000
C        1.398491000     -1.715646000     -0.750518000
C        3.376471000     -3.196593000      0.500146000
C        1.163011000     -3.048992000     -0.439069000
C        2.616823000     -1.121289000     -0.444979000
C        3.600965000     -1.863563000      0.188921000
C        2.160501000     -3.785666000      0.180706000
H        0.206801000     -3.505113000     -0.654765000
H        2.793153000     -0.083587000     -0.698091000
H        4.547941000     -1.395846000      0.431311000
H        1.979440000     -4.826084000      0.423492000
H        4.148387000     -3.778026000      0.990141000
C        3.979888000      2.332039000      0.199825000
C        1.846602000      2.167984000      1.296180000
C        1.953550000      2.425258000     -1.099714000
C        3.339575000      2.460314000     -1.022920000
C        3.229241000      2.182856000      1.358825000
H        1.263205000      2.079775000      2.205301000
H        1.473254000      2.510129000     -2.064187000
H        3.917261000      2.578318000     -1.931848000
H        3.720425000      2.089946000      2.319818000
H        5.061693000      2.351616000      0.251660000
C       -2.572979000      0.573514000      1.625772000
Cl      -3.041872000      0.417142000     -1.355470000
O       -3.334671000      0.887336000      2.406348000

53
ccc-[RuCl2(CO)2(SPh2)2] symmetry c1 (E=-2963.77000594)
Ru      -0.137190000      1.382947000      0.037069000
S        1.264193000     -0.533544000      0.000408000
Cl      -1.573194000      3.292937000     -0.183897000
C       -0.848690000      1.023915000      1.712217000
S       -1.930945000      0.173817000     -1.213951000
O       -1.292258000      0.826515000      2.742202000
C        2.908907000     -0.134687000     -0.546192000
C       -3.440698000     -0.127299000     -0.317299000
C       -5.890496000     -0.488657000      0.935047000
C       -3.871519000      0.788294000      0.633097000
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C       -4.245165000     -1.207188000     -0.668066000
C       -5.462873000     -1.387175000     -0.032743000
C       -5.095872000      0.600623000      1.257465000
H       -3.270281000      1.657793000      0.863883000
H       -3.923698000     -1.908229000     -1.427359000
H       -6.081292000     -2.235093000     -0.302566000
H       -5.424826000      1.315608000      2.002257000
H       -6.843284000     -0.634325000      1.429784000
C        5.425801000      0.409885000     -1.547740000
C        3.217463000     -0.487652000     -1.853330000
C        3.849191000      0.479960000      0.268132000
C        5.110409000      0.749136000     -0.238589000
C        4.480190000     -0.208395000     -2.352671000
H        2.471271000     -0.972256000     -2.470431000
H        3.613007000      0.739184000      1.291749000
H        5.848562000      1.227345000      0.394034000
H        4.724161000     -0.479357000     -3.372851000
H        6.413201000      0.624707000     -1.938762000
C        1.161291000      2.498257000      0.752975000
Cl       0.699734000      1.802566000     -2.187690000
O        1.927796000      3.219942000      1.178732000
C        1.571932000     -1.219453000      1.609497000
C       -1.334826000     -1.459725000     -1.545948000
C       -0.177623000     -3.905514000     -2.117849000
C       -0.741413000     -1.664390000     -2.783408000
C       -1.353506000     -2.467717000     -0.588888000
C       -0.785925000     -3.694426000     -0.886203000
C       -0.152148000     -2.890091000     -3.061457000
H       -0.727341000     -0.864784000     -3.513579000
H       -1.802949000     -2.293575000      0.381165000
H       -0.804092000     -4.484666000     -0.144945000
H        0.318881000     -3.050532000     -4.023849000
H        0.274872000     -4.864458000     -2.340536000
C        2.075035000     -2.456219000      4.033717000
C        1.676196000     -2.604628000      1.668953000
C        1.715852000     -0.450793000      2.756783000
C        1.968865000     -1.074017000      3.968538000
C        1.929237000     -3.220279000      2.884585000
H        1.556195000     -3.191011000      0.766262000
H        1.631678000      0.626983000      2.716869000
H        2.080825000     -0.474546000      4.863774000
H        2.007652000     -4.299720000      2.932371000
H        2.268689000     -2.938876000      4.984198000

25
ccc-[RuCl2(CO)2(SeMe2)2] symmetry c1 (E=-6203.84128413)
Ru       0.069572000      0.635180000      0.021041000
Se      -1.672032000     -1.262968000      0.139401000
C       -2.650040000     -1.101345000     -1.518948000
C       -3.044615000     -0.552316000      1.303529000
H       -1.976941000     -1.411629000     -2.313409000
H       -3.514191000     -1.759971000     -1.456017000
H       -2.935371000     -0.059588000     -1.647494000
H       -2.662381000     -0.584816000      2.321774000
H       -3.258808000      0.470609000      0.999613000
H       -3.923149000     -1.188058000      1.214911000
Se       1.864090000     -0.971049000      0.678880000
C        3.400272000     -0.405076000     -0.353286000
C        1.526675000     -2.596177000     -0.317736000
H        3.768027000      0.519560000      0.086578000
H        3.086450000     -0.251965000     -1.383882000
H        4.157412000     -1.182929000     -0.273762000
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H        2.425290000     -3.206856000     -0.249474000
H        1.295169000     -2.330180000     -1.347031000
H        0.690167000     -3.106213000      0.153767000
C        1.289021000      2.037279000     -0.158483000
O        1.997107000      2.916692000     -0.284119000
Cl      -1.696050000      2.132833000     -0.634413000
Cl       0.466089000      0.060560000     -2.308447000
C       -0.241715000      1.063823000      1.787173000
O       -0.435989000      1.350298000      2.874391000

39
ccc-[RuCl2(CO)2(SeMePh)2] symmetry c1 (E=-6587.01127711)
Ru       1.367071000      0.267486000      0.431319000
Se       0.889295000     -2.175746000      0.159369000
C        1.302914000     -2.647469000     -1.666505000
H        2.386284000     -2.616113000     -1.736627000
H        0.928442000     -3.655199000     -1.835985000
H        0.870623000     -1.928363000     -2.357761000
Cl       1.866496000      2.603738000      0.673721000
C        0.082679000      0.488949000      1.743786000
Se      -0.314595000      0.771718000     -1.449278000
O       -0.684084000      0.675237000      2.566010000
C        0.449508000      2.253614000     -2.425421000
H        0.865978000      2.973577000     -1.726072000
H       -0.334531000      2.678813000     -3.048076000
H        1.242181000      1.821779000     -3.031658000
C       -1.022346000     -2.360989000      0.118111000
C       -1.769828000      1.650359000     -0.562858000
C       -3.888208000      2.778272000      0.810888000
C       -2.915245000      0.901111000     -0.333907000
C       -1.670739000      2.959313000     -0.112486000
C       -2.739952000      3.520800000      0.569606000
C       -3.972641000      1.468433000      0.362084000
H       -2.982990000     -0.119725000     -0.689199000
H       -0.764329000      3.529973000     -0.265331000
H       -2.668294000      4.542775000      0.922947000
H       -4.865240000      0.882269000      0.547103000
H       -4.716623000      3.221888000      1.350413000
C       -3.772137000     -2.688847000      0.215215000
C       -1.680982000     -2.312879000      1.341452000
C       -1.728755000     -2.578582000     -1.055982000
C       -3.106427000     -2.748730000     -0.999324000
C       -3.056949000     -2.466997000      1.384592000
H       -1.126474000     -2.162148000      2.260401000
H       -1.229085000     -2.617843000     -2.013958000
H       -3.657482000     -2.920578000     -1.916294000
H       -3.569085000     -2.422078000      2.338170000
H       -4.847367000     -2.815517000      0.252032000
C        2.674755000     -0.121357000      1.703984000
Cl       3.032416000      0.116823000     -1.324255000
O        3.481791000     -0.330919000      2.475042000

53
ccc-[RuCl2(CO)2(SePh2)2] symmetry c1 (E=-6970.17660244)
Ru      -0.022336000      1.404048000      0.283708000
Se       1.381794000     -0.564308000     -0.324466000
Cl      -1.362164000      3.383505000      0.521703000
C       -0.697733000      0.740358000      1.870703000
Se      -2.023621000      0.546626000     -1.118515000
O       -1.137414000      0.356490000      2.849934000
C        3.202271000      0.057178000     -0.462801000
C       -3.538886000      0.098221000     -0.015748000
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C       -5.821329000     -0.418350000      1.464113000
C       -3.853289000      0.909966000      1.064434000
C       -4.370033000     -0.953279000     -0.380241000
C       -5.507354000     -1.211961000      0.369650000
C       -4.996884000      0.643913000      1.803810000
H       -3.220975000      1.751813000      1.319278000
H       -4.136285000     -1.572700000     -1.236852000
H       -6.151469000     -2.037575000      0.090624000
H       -5.239365000      1.274153000      2.651352000
H       -6.710887000     -0.624921000      2.047219000
C        5.794138000      0.946269000     -0.822719000
C        3.640009000      0.390879000     -1.737381000
C        4.048495000      0.150934000      0.630897000
C        5.348501000      0.597460000      0.444268000
C        4.940182000      0.841181000     -1.911180000
H        2.970976000      0.308401000     -2.584027000
H        3.712885000     -0.124917000      1.621799000
H        6.012819000      0.672825000      1.296966000
H        5.285009000      1.105601000     -2.903745000
H        6.810195000      1.295831000     -0.962260000
C        1.379909000      2.259598000      1.157251000
Cl       0.721834000      2.182502000     -1.888887000
O        2.210189000      2.814479000      1.698097000
C        1.588333000     -1.761620000      1.161933000
C       -1.525028000     -1.207002000     -1.708830000
C       -0.638657000     -3.656423000     -2.632165000
C       -1.122451000     -1.334174000     -3.029794000
C       -1.484844000     -2.290816000     -0.840901000
C       -1.051267000     -3.519067000     -1.312825000
C       -0.670112000     -2.564887000     -3.486636000
H       -1.154282000     -0.479950000     -3.695338000
H       -1.788183000     -2.181528000      0.193376000
H       -1.022657000     -4.368657000     -0.640961000
H       -0.349307000     -2.667987000     -4.516318000
H       -0.292395000     -4.617500000     -2.993217000
C        1.903612000     -3.613836000      3.190948000
C        1.707138000     -3.109426000      0.849074000
C        1.630884000     -1.332739000      2.480446000
C        1.790255000     -2.264683000      3.495136000
C        1.864333000     -4.035269000      1.869428000
H        1.671708000     -3.433371000     -0.183966000
H        1.549363000     -0.282195000      2.725753000
H        1.823864000     -1.931778000      4.525502000
H        1.953284000     -5.087863000      1.628592000
H        2.022884000     -4.339041000      3.987075000

25
ccc-[RuCl2(CO)2(TeMe2)2] symmetry c1 (E=-1937.37495054)
Ru       0.064629000      0.835562000      0.023071000
Te      -1.795540000     -1.157524000      0.075188000
C       -2.923769000     -0.690649000     -1.654575000
C       -3.210546000     -0.349516000      1.435337000
H       -2.313687000     -0.956422000     -2.513881000
H       -3.838929000     -1.278401000     -1.622038000
H       -3.117067000      0.379508000     -1.637004000
H       -2.812384000     -0.461569000      2.441899000
H       -3.342840000      0.700788000      1.182193000
H       -4.138900000     -0.907097000      1.332444000
Te       2.006019000     -0.878023000      0.538532000
C        3.527742000     -0.156805000     -0.751568000
C        1.554091000     -2.541431000     -0.700278000
H        3.938674000      0.749781000     -0.312032000
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H        3.067221000      0.047710000     -1.716029000
H        4.296442000     -0.923563000     -0.824006000
H        2.470503000     -3.118060000     -0.813458000
H        1.198821000     -2.157515000     -1.654518000
H        0.793068000     -3.139837000     -0.204179000
C        1.297000000      2.237891000     -0.125292000
O        2.015303000      3.113851000     -0.221855000
Cl      -1.728203000      2.382452000     -0.491753000
Cl       0.348295000      0.347487000     -2.352062000
C       -0.196016000      1.151731000      1.816856000
O       -0.368057000      1.365159000      2.926104000

39
ccc-[RuCl2(CO)2(TeMePh)2] symmetry c1 (E=-2320.54384165)
Ru       1.363841000      0.641864000      0.482853000
Te       1.364650000     -1.990742000      0.237333000
C        1.746136000     -2.350749000     -1.813818000
H        2.797727000     -2.122063000     -1.966120000
H        1.542812000     -3.402348000     -2.007207000
H        1.134274000     -1.696038000     -2.429618000
Cl       1.387685000      3.049400000      0.705271000
C        0.173739000      0.580182000      1.889335000
Te      -0.582647000      0.781886000     -1.397047000
O       -0.549683000      0.579271000      2.772322000
C       -0.268969000      2.696367000     -2.248176000
H       -0.174846000      3.423134000     -1.446244000
H       -1.109725000      2.906073000     -2.905548000
H        0.662626000      2.627976000     -2.806057000
C       -0.695298000     -2.468657000      0.190528000
C       -2.318006000      1.284084000     -0.309730000
C       -4.594323000      1.870648000      1.152638000
C       -3.431873000      0.461873000     -0.411520000
C       -2.332230000      2.398146000      0.521368000
C       -3.477407000      2.691374000      1.246352000
C       -4.569871000      0.755833000      0.327954000
H       -3.416093000     -0.409194000     -1.055371000
H       -1.450333000      3.022135000      0.619799000
H       -3.492574000      3.559623000      1.894974000
H       -5.437791000      0.110681000      0.255024000
H       -5.484334000      2.100699000      1.726669000
C       -3.387178000     -3.138902000      0.251371000
C       -1.384903000     -2.462652000      1.398855000
C       -1.347578000     -2.813554000     -0.986419000
C       -2.694457000     -3.152723000     -0.949159000
C       -2.731349000     -2.790398000      1.424159000
H       -0.881666000     -2.208200000      2.324647000
H       -0.825490000     -2.828156000     -1.934215000
H       -3.200364000     -3.423191000     -1.868631000
H       -3.266670000     -2.777630000      2.366132000
H       -4.438917000     -3.398133000      0.274329000
C        2.839784000      0.550063000      1.636170000
Cl       2.831611000      0.810444000     -1.456169000
O        3.735038000      0.526999000      2.335529000

53
ccc-[RuCl2(CO)2(TePh2)2] symmetry c1 (E=-2703.71288416)
Ru       0.054570000      1.450045000      0.354043000
Te       1.480462000     -0.548180000     -0.573778000
Cl      -1.322008000      3.379866000      0.848384000
C       -0.467198000      0.595546000      1.898990000
Te      -2.171341000      0.726532000     -1.007616000
O       -0.797198000      0.073851000      2.858758000
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C        3.493179000      0.116738000     -0.422178000
C       -3.615912000      0.090280000      0.402521000
C       -5.608066000     -0.636375000      2.186720000
C       -3.772181000      0.800111000      1.585932000
C       -4.464919000     -0.966263000      0.094970000
C       -5.455754000     -1.331159000      0.994921000
C       -4.770015000      0.430441000      2.476930000
H       -3.126502000      1.641307000      1.811462000
H       -4.357596000     -1.512067000     -0.834790000
H       -6.112277000     -2.160520000      0.758563000
H       -4.888130000      0.980888000      3.403060000
H       -6.383408000     -0.924247000      2.886920000
C        6.142033000      0.927360000     -0.342299000
C        3.844725000      1.367291000     -0.913508000
C        4.459458000     -0.737994000      0.092810000
C        5.784111000     -0.325447000      0.134212000
C        5.171985000      1.769362000     -0.866949000
H        3.089936000      2.028115000     -1.324412000
H        4.191966000     -1.716952000      0.471018000
H        6.536458000     -0.989752000      0.543384000
H        5.444707000      2.748891000     -1.242277000
H        7.176885000      1.246776000     -0.305647000
C        1.517182000      2.231534000      1.225477000
Cl       0.610744000      2.401448000     -1.835412000
O        2.363385000      2.729498000      1.797507000
C        1.658404000     -1.937944000      1.005059000
C       -1.729440000     -1.192569000     -1.769532000
C       -1.013551000     -3.645640000     -2.841552000
C       -1.450196000     -1.297676000     -3.126565000
C       -1.644799000     -2.307537000     -0.942993000
C       -1.299166000     -3.535556000     -1.487046000
C       -1.083742000     -2.527006000     -3.658236000
H       -1.513409000     -0.428531000     -3.771361000
H       -1.851597000     -2.226970000      0.117850000
H       -1.244973000     -4.407550000     -0.845756000
H       -0.861081000     -2.608353000     -4.715558000
H       -0.736573000     -4.605997000     -3.259918000
C        1.907381000     -3.825676000      3.015378000
C        1.469831000     -3.282516000      0.715004000
C        1.983519000     -1.532761000      2.294040000
C        2.108572000     -2.480252000      3.297329000
C        1.590765000     -4.226540000      1.726458000
H        1.230987000     -3.598172000     -0.293398000
H        2.149954000     -0.486579000      2.520925000
H        2.361393000     -2.165513000      4.302910000
H        1.440602000     -5.275919000      1.501578000
H        2.001984000     -4.562806000      3.804005000

25
ttt-[RuCl2(CO)2(SMe2)2] symmetry c2v (E=-2197.41399505 )
Ru       0.000000000      0.000000000      0.191003000
C        0.000000000     -1.928981000      0.245206000
O        0.000000000     -3.059605000      0.312809000
S       -2.381536000      0.000000000      0.241431000
S        2.381536000      0.000000000      0.241431000
C       -2.943138000      1.359647000     -0.787225000
C       -2.943138000     -1.359647000     -0.787225000
C        2.943138000      1.359647000     -0.787225000
C        2.943138000     -1.359647000     -0.787225000
H       -4.019663000      1.260259000     -0.923971000
H       -2.733824000      2.287094000     -0.256765000
H       -2.423200000      1.340357000     -1.744180000
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H       -4.019663000     -1.260259000     -0.923971000
H       -2.423200000     -1.340357000     -1.744180000
H       -2.733824000     -2.287094000     -0.256765000
H        2.733824000      2.287094000     -0.256765000
H        4.019663000      1.260259000     -0.923971000
H        2.423200000      1.340357000     -1.744180000
H        2.733824000     -2.287094000     -0.256765000
H        2.423200000     -1.340357000     -1.744180000
H        4.019663000     -1.260259000     -0.923971000
Cl       0.000000000      0.000000000     -2.215107000
Cl       0.000000000      0.000000000      2.598383000
C        0.000000000      1.928981000      0.245206000
O        0.000000000      3.059605000      0.312809000

39
ttt-[RuCl2(CO)2(SMePh)2] symmetry c2 (E=-2580.58488248)
Ru       0.000000000      0.000000000      0.294615000
Cl      -0.000001000      0.000005000     -2.115745000
C       -1.196418000      1.519351000      0.311487000
O       -1.889339000      2.413633000      0.336251000
S        1.837531000      1.510213000      0.418254000
S       -1.837531000     -1.510215000      0.418248000
C        3.311117000      0.636064000     -0.041678000
C       -3.311117000     -0.636064000     -0.041680000
C        5.608433000     -0.794989000     -0.608069000
C        3.549743000      0.212814000     -1.343761000
C        4.210100000      0.348820000      0.977268000
C        5.357969000     -0.375556000      0.689892000
C        4.706049000     -0.497569000     -1.621697000
H        2.826506000      0.411377000     -2.124548000
H        4.009041000      0.687575000      1.986720000
H        6.059143000     -0.604888000      1.483322000
H        4.897770000     -0.829460000     -2.635234000
H        6.507842000     -1.356197000     -0.832036000
C       -5.608433000      0.794991000     -0.608065000
C       -4.210100000     -0.348824000      0.977267000
C       -3.549743000     -0.212809000     -1.343762000
C       -4.706049000      0.497575000     -1.621694000
C       -5.357970000      0.375552000      0.689893000
H       -4.009042000     -0.687584000      1.986718000
H       -2.826505000     -0.411369000     -2.124549000
H       -4.897770000      0.829471000     -2.635231000
H       -6.059143000      0.604881000      1.483325000
H       -6.507843000      1.356200000     -0.832031000
C        1.196418000     -1.519352000      0.311479000
Cl       0.000001000     -0.000006000      2.700333000
O        1.889339000     -2.413634000      0.336238000
C       -1.697960000     -2.713381000     -0.908328000
C        1.697961000      2.713385000     -0.908318000
H       -0.893930000     -3.392108000     -0.624787000
H       -1.454036000     -2.227358000     -1.849891000
H       -2.636651000     -3.262158000     -0.966770000
H        2.636652000      3.262162000     -0.966758000
H        0.893930000      3.392110000     -0.624774000
H        1.454036000      2.227366000     -1.849882000

53
ttt-[RuCl2(CO)2(SPh2)2] symmetry cs (E=-2963.75171683)
Ru      -0.008697819      0.629624383      0.000000000
Cl      -0.136217013     -1.776110051      0.000000000
C       -1.948616789      0.619859119      0.000000000
O       -3.078572271      0.610015163      0.000000000
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S       -0.021302290      0.803211237     -2.375609054
S       -0.021302290      0.803211237      2.375609054
C        1.402265195      0.058306278     -3.135890555
C       -1.361867202     -0.147052183     -3.056810002
C       -1.361867202     -0.147052183      3.056810002
C        1.402265195      0.058306278      3.135890555
C        3.621325592     -0.967726848     -4.427206060
C        2.051390776     -1.048281131     -2.605000035
C        1.856641465      0.659030506     -4.304933578
C        2.967589803      0.139306327     -4.950598079
C        3.163752671     -1.557766199     -3.257456039
H        1.680475226     -1.508517651     -1.696436518
H        1.344780171      1.528099992     -4.700720594
H        3.326159242      0.606256859     -5.860053596
H        3.673369527     -2.421434002     -2.847058024
H        4.492627058     -1.369223096     -4.931053562
C       -3.559082642     -1.481792221     -4.073184438
C       -2.522571327      0.560429666     -3.346223535
C       -1.286483157     -1.514971235     -3.277955938
C       -2.389691147     -2.176565964     -3.793304407
C       -3.625112236     -0.114563303     -3.847541503
H       -2.561071308      1.630914244     -3.180285587
H       -0.380371726     -2.058033594     -3.047969412
H       -2.335467251     -3.244145728     -3.970625856
H       -4.532130562      0.433928314     -4.071686528
H       -4.418530979     -2.007237464     -4.472303413
C       -3.559082642     -1.481792221      4.073184438
C       -2.522571327      0.560429666      3.346223535
C       -1.286483157     -1.514971235      3.277955938
C       -2.389691147     -2.176565964      3.793304407
C       -3.625112236     -0.114563303      3.847541503
H       -2.561071308      1.630914244      3.180285587
H       -0.380371726     -2.058033594      3.047969412
H       -2.335467251     -3.244145728      3.970625856
H       -4.532130562      0.433928314      4.071686528
H       -4.418530979     -2.007237464      4.472303413
C        3.621325592     -0.967726848      4.427206060
C        2.051390776     -1.048281131      2.605000035
C        1.856641465      0.659030506      4.304933578
C        2.967589803      0.139306327      4.950598079
C        3.163752671     -1.557766199      3.257456039
H        1.680475226     -1.508517651      1.696436518
H        1.344780171      1.528099992      4.700720594
H        3.326159242      0.606256859      5.860053596
H        3.673369527     -2.421434002      2.847058024
H        4.492627058     -1.369223096      4.931053562
C        1.922337532      0.722373269      0.000000000
Cl      -0.010650091      3.035984026      0.000000000
O        3.046038148      0.857018031      0.000000000

25
ttt-[RuCl2(CO)2(SeMe2)2] symmetry cs (E=-6203.82418568)
Ru       0.137339000      0.113262000      0.000000000
C        1.394302000     -1.345935000      0.000000000
O        2.147630000     -2.193290000      0.000000000
Se       0.185174000      0.152043000      2.491991000
Se       0.185174000      0.152043000     -2.491991000
C       -1.646885000      0.507163000      3.012861000
C        0.185174000     -1.714067000      3.011978000
C       -1.646885000      0.507163000     -3.012861000
C        0.185174000     -1.714067000     -3.011978000
H       -1.737395000      0.301312000      4.077808000
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H       -1.845204000      1.559603000      2.819996000
H       -2.305762000     -0.127985000      2.424240000
H       -0.035767000     -1.764736000      4.076536000
H       -0.562311000     -2.239752000      2.421370000
H        1.181226000     -2.107779000      2.820110000
H       -1.845204000      1.559603000     -2.819996000
H       -1.737395000      0.301312000     -4.077808000
H       -2.305762000     -0.127985000     -2.424240000
H        1.181226000     -2.107779000     -2.820110000
H       -0.562311000     -2.239752000     -2.421370000
H       -0.035767000     -1.764736000     -4.076536000
Cl      -1.711629000     -1.429929000      0.000000000
Cl       1.985775000      1.659349000      0.000000000
C       -1.076920000      1.608357000      0.000000000
O       -1.778699000      2.498838000      0.000000000

39
ttt-[RuCl2(CO)2(SeMePh)2] symmetry c2 (E=-6586.99203641)
Ru       0.000000000      0.000000000      0.316682000
Cl       0.000000000      0.000000000     -2.094795000
C       -1.697008000     -0.918697000      0.319165000
O       -2.696223000     -1.452159000      0.326318000
Se      -1.221833000      2.169536000      0.461575000
Se       1.221833000     -2.169536000      0.461575000
C        0.000000000      3.515526000     -0.153710000
C        0.000000000     -3.515526000     -0.153710000
C        1.803303000      5.465295000     -0.915529000
C        0.474692000      3.532171000     -1.458128000
C        0.418493000      4.459436000      0.773211000
C        1.328974000      5.433849000      0.387305000
C        1.374500000      4.516876000     -1.835423000
H        0.168631000      2.769378000     -2.163537000
H        0.038958000      4.435889000      1.788084000
H        1.661771000      6.171356000      1.107981000
H        1.748975000      4.536632000     -2.852194000
H        2.510737000      6.229181000     -1.215863000
C       -1.803303000     -5.465295000     -0.915529000
C       -0.418493000     -4.459436000      0.773211000
C       -0.474692000     -3.532171000     -1.458128000
C       -1.374500000     -4.516876000     -1.835423000
C       -1.328974000     -5.433849000      0.387305000
H       -0.038958000     -4.435889000      1.788084000
H       -0.168631000     -2.769378000     -2.163537000
H       -1.748975000     -4.536632000     -2.852194000
H       -1.661771000     -6.171356000      1.107981000
H       -2.510737000     -6.229181000     -1.215863000
C        1.697008000      0.918697000      0.319165000
Cl       0.000000000      0.000000000      2.725418000
O        2.696223000      1.452159000      0.326318000
C        2.460575000     -2.194403000     -1.028963000
C       -2.460575000      2.194403000     -1.028963000
H        3.287701000     -1.543048000     -0.750990000
H        1.965518000     -1.817454000     -1.919905000
H        2.809196000     -3.217358000     -1.152559000
H       -2.809196000      3.217358000     -1.152559000
H       -3.287701000      1.543048000     -0.750990000
H       -1.965518000      1.817454000     -1.919905000

53
ttt-[RuCl2(CO)2(SePh2)2] symmetry cs (E=-6970.15708578)
Ru      -0.016805000      0.698009000      0.000000000
Cl       0.225601000     -1.698194000      0.000000000
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C        1.916627000      0.783259000      0.000000000
O        3.047201000      0.822996000      0.000000000
Se      -0.007231000      0.889049000      2.486415000
Se      -0.007231000      0.889049000     -2.486415000
C       -1.483431000     -0.085732000      3.234294000
C        1.454812000     -0.179420000      3.135130000
C        1.454812000     -0.179420000     -3.135130000
C       -1.483431000     -0.085732000     -3.234294000
C       -3.622882000     -1.365640000      4.423265000
C       -2.042889000     -1.193707000      2.614965000
C       -1.982966000      0.391687000      4.439418000
C       -3.056171000     -0.255399000      5.033608000
C       -3.116786000     -1.832386000      3.218327000
H       -1.633648000     -1.560438000      1.680470000
H       -1.540657000      1.262612000      4.908612000
H       -3.451631000      0.113845000      5.972321000
H       -3.557743000     -2.699705000      2.741243000
H       -4.463519000     -1.867438000      4.887829000
C        3.658873000     -1.582124000      4.031264000
C        2.641390000      0.497125000      3.383928000
C        1.353830000     -1.547155000      3.334178000
C        2.463003000     -2.244509000      3.789284000
C        3.747847000     -0.212696000      3.826963000
H        2.704705000      1.569319000      3.235902000
H        0.426464000     -2.066628000      3.134841000
H        2.391020000     -3.313927000      3.949017000
H        4.676848000      0.310302000      4.020469000
H        4.522126000     -2.134451000      4.383155000
C        3.658873000     -1.582124000     -4.031264000
C        2.641390000      0.497125000     -3.383928000
C        1.353830000     -1.547155000     -3.334178000
C        2.463003000     -2.244509000     -3.789284000
C        3.747847000     -0.212696000     -3.826963000
H        2.704705000      1.569319000     -3.235902000
H        0.426464000     -2.066628000     -3.134841000
H        2.391020000     -3.313927000     -3.949017000
H        4.676848000      0.310302000     -4.020469000
H        4.522126000     -2.134451000     -4.383155000
C       -3.622882000     -1.365640000     -4.423265000
C       -2.042889000     -1.193707000     -2.614965000
C       -1.982966000      0.391687000     -4.439418000
C       -3.056171000     -0.255399000     -5.033608000
C       -3.116786000     -1.832386000     -3.218327000
H       -1.633648000     -1.560438000     -1.680470000
H       -1.540657000      1.262612000     -4.908612000
H       -3.451631000      0.113845000     -5.972321000
H       -3.557743000     -2.699705000     -2.741243000
H       -4.463519000     -1.867438000     -4.887829000
C       -1.946020000      0.667872000      0.000000000
Cl      -0.147465000      3.103765000      0.000000000
O       -3.077741000      0.717411000      0.000000000

25
ttt-[RuCl2(CO)2(TeMe2)2] symmetry c2v (E=-1937.36145321)
Ru       0.000000000      0.000000000      0.180800000
C        0.000000000      1.921981000      0.184858000
O        0.000000000      3.057751000      0.187014000
Te       2.639085000      0.000000000      0.234825000
Te      -2.639085000      0.000000000      0.234825000
C        3.103742000     -1.546116000     -1.145495000
C        3.103742000      1.546116000     -1.145495000
C       -3.103742000     -1.546116000     -1.145495000
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C       -3.103742000      1.546116000     -1.145495000
H        4.150476000     -1.446214000     -1.425938000
H        2.936274000     -2.500841000     -0.650727000
H        2.444514000     -1.430535000     -2.003595000
H        4.150476000      1.446214000     -1.425938000
H        2.444514000      1.430535000     -2.003595000
H        2.936274000      2.500841000     -0.650727000
H       -2.936274000     -2.500841000     -0.650727000
H       -4.150476000     -1.446214000     -1.425938000
H       -2.444514000     -1.430535000     -2.003595000
H       -2.936274000      2.500841000     -0.650727000
H       -2.444514000      1.430535000     -2.003595000
H       -4.150476000      1.446214000     -1.425938000
Cl       0.000000000      0.000000000     -2.232169000
Cl       0.000000000      0.000000000      2.598367000
C        0.000000000     -1.921981000      0.184858000
O        0.000000000     -3.057751000      0.187014000

39
ttt-[RuCl2(CO)2(TeMePh)2] symmetry c2 (E=-2320.52740534)
Ru       0.000000000      0.000000000      0.344815000
Cl       0.000000000      0.000000000     -2.070582000
C       -1.673924000     -0.950334000      0.328977000
O       -2.663001000     -1.506076000      0.313038000
Te      -1.326092000      2.277670000      0.508840000
Te       1.326092000     -2.277670000      0.508840000
C        0.000000000      3.709246000     -0.295076000
C        0.000000000     -3.709246000     -0.295076000
C        1.751671000      5.616921000     -1.273512000
C        0.541202000      3.556478000     -1.565878000
C        0.331560000      4.806340000      0.489771000
C        1.213985000      5.759023000     -0.003003000
C        1.413919000      4.517964000     -2.052968000
H        0.303420000      2.682867000     -2.162441000
H       -0.092734000      4.924590000      1.480487000
H        1.476668000      6.614185000      0.608726000
H        1.837656000      4.402810000     -3.043978000
H        2.437808000      6.362691000     -1.657607000
C       -1.751671000     -5.616921000     -1.273512000
C       -0.331560000     -4.806340000      0.489771000
C       -0.541202000     -3.556478000     -1.565878000
C       -1.413919000     -4.517964000     -2.052968000
C       -1.213985000     -5.759023000     -0.003003000
H        0.092734000     -4.924590000      1.480487000
H       -0.303420000     -2.682867000     -2.162441000
H       -1.837656000     -4.402810000     -3.043978000
H       -1.476668000     -6.614185000      0.608726000
H       -2.437808000     -6.362691000     -1.657607000
C        1.673924000      0.950334000      0.328977000
Cl       0.000000000      0.000000000      2.762303000
O        2.663001000      1.506076000      0.313038000
C        2.609083000     -2.214618000     -1.183272000
C       -2.609083000      2.214618000     -1.183272000
H        3.435158000     -1.551026000     -0.932067000
H        2.045074000     -1.819974000     -2.024991000
H        2.971152000     -3.223584000     -1.367893000
H       -2.971152000      3.223584000     -1.367893000
H       -3.435158000      1.551026000     -0.932067000
H       -2.045074000      1.819974000     -2.024991000

53
ttt-[RuCl2(CO)2(TePh2)2] symmetry c2 (E=-2703.69140606)
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```
Ru       0.000000000      0.000000000      0.733535000
Cl       0.000000000      0.000000000     -1.676007000
C       -1.496556000      1.213535000      0.734317000
O       -2.368387000      1.938670000      0.743713000
Te       1.615668000      2.077354000      0.939017000
Te      -1.615668000     -2.077354000      0.939017000
C        3.395358000      1.593385000     -0.085092000
C        0.867913000      3.453398000     -0.480896000
C       -3.395358000     -1.593385000     -0.085092000
C       -0.867913000     -3.453398000     -0.480896000
C        5.799353000      1.044684000     -1.342495000
C        3.426098000      0.693704000     -1.142817000
C        4.559161000      2.217804000      0.350358000
C        5.762212000      1.940354000     -0.283200000
C        4.634021000      0.424432000     -1.770774000
H        2.513584000      0.216729000     -1.482968000
H        4.534159000      2.916329000      1.179064000
H        6.670764000      2.424521000      0.055075000
H        4.661182000     -0.274906000     -2.598341000
H        6.740273000      0.828327000     -1.834792000
C       -0.217817000      5.282237000     -2.253043000
C        0.000000000      4.433486000     -0.014120000
C        1.201014000      3.383945000     -1.826018000
C        0.657557000      4.306069000     -2.708971000
C       -0.547018000      5.344691000     -0.906653000
H       -0.252720000      4.495948000      1.038933000
H        1.874573000      2.619137000     -2.190130000
H        0.917032000      4.255508000     -3.760118000
H       -1.225869000      6.107918000     -0.544561000
H       -0.641843000      5.997249000     -2.948253000
C       -5.799353000     -1.044684000     -1.342495000
C       -4.559161000     -2.217804000      0.350358000
C       -3.426098000     -0.693704000     -1.142817000
C       -4.634021000     -0.424432000     -1.770774000
C       -5.762212000     -1.940354000     -0.283200000
H       -4.534159000     -2.916329000      1.179064000
H       -2.513584000     -0.216729000     -1.482968000
H       -4.661182000      0.274906000     -2.598341000
H       -6.670764000     -2.424521000      0.055075000
H       -6.740273000     -0.828327000     -1.834792000
C        0.217817000     -5.282237000     -2.253043000
C       -1.201014000     -3.383945000     -1.826018000
C        0.000000000     -4.433486000     -0.014120000
C        0.547018000     -5.344691000     -0.906653000
C       -0.657557000     -4.306069000     -2.708971000
H       -1.874573000     -2.619137000     -2.190130000
H        0.252720000     -4.495948000      1.038933000
H        1.225869000     -6.107918000     -0.544561000
H       -0.917032000     -4.255508000     -3.760118000
H        0.641843000     -5.997249000     -2.948253000
C        1.496556000     -1.213535000      0.734317000
Cl       0.000000000      0.000000000      3.152024000
O        2.368387000     -1.938670000      0.743713000

25
tcc-[RuCl2(CO)2(SMe2)2] symmetry c2v (E=-2197.41495783)
Ru       0.000000000      0.000000000      0.219754000
Cl       0.000000000      1.730358000      1.910998000
C       -1.925380000      0.000000000      0.376616000
O       -3.041987000      0.000000000      0.560718000
S        0.000000000      1.636621000     -1.473272000
C        1.363329000      2.758319000     -1.155074000
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```
C       -1.363329000      2.758319000     -1.155074000
H        2.286718000      2.224045000     -1.373838000
H        1.270422000      3.609266000     -1.829506000
H        1.342339000      3.076608000     -0.113535000
H       -2.286718000      2.224045000     -1.373838000
H       -1.342339000      3.076608000     -0.113535000
H       -1.270422000      3.609266000     -1.829506000
Cl       0.000000000     -1.730358000      1.910998000
C        1.925380000      0.000000000      0.376616000
S        0.000000000     -1.636621000     -1.473272000
O        3.041987000      0.000000000      0.560718000
C       -1.363329000     -2.758319000     -1.155074000
C        1.363329000     -2.758319000     -1.155074000
H       -2.286718000     -2.224045000     -1.373838000
H       -1.342339000     -3.076608000     -0.113535000
H       -1.270422000     -3.609266000     -1.829506000
H        1.270422000     -3.609266000     -1.829506000
H        1.342339000     -3.076608000     -0.113535000
H        2.286718000     -2.224045000     -1.373838000

39
tcc-[RuCl2(CO)2(SMePh)2] symmetry c2 (E=-2580.58521109)
Ru       0.000000000      0.000000000      0.706022000
Cl      -1.309821000     -1.090354000      2.420077000
C        1.230618000     -1.487659000      0.838468000
O        1.942619000     -2.353157000      0.990247000
S       -1.256241000     -1.002279000     -1.020361000
C       -2.983536000     -1.061227000     -0.538862000
H       -3.355388000     -0.039603000     -0.614376000
H       -3.511519000     -1.698448000     -1.246638000
H       -3.085997000     -1.415501000      0.484115000
Cl       1.309821000      1.090354000      2.420077000
C       -1.230618000      1.487659000      0.838468000
S        1.256241000      1.002279000     -1.020361000
O       -1.942619000      2.353157000      0.990247000
C        2.983536000      1.061227000     -0.538862000
H        3.085997000      1.415501000      0.484115000
H        3.511519000      1.698448000     -1.246638000
H        3.355388000      0.039603000     -0.614376000
C       -0.823722000     -2.720780000     -1.094139000
C        0.823722000      2.720780000     -1.094139000
C       -0.013280000      5.349935000     -1.274834000
C        1.234762000      3.636261000     -0.133169000
C        0.000000000      3.109239000     -2.143297000
C       -0.423943000      4.427376000     -2.225754000
C        0.816929000      4.953435000     -0.234129000
H        1.848441000      3.317872000      0.699525000
H       -0.307250000      2.382983000     -2.886838000
H       -1.069619000      4.732698000     -3.040430000
H        1.134543000      5.672006000      0.512100000
H       -0.340539000      6.380578000     -1.343175000
C        0.013280000     -5.349935000     -1.274834000
C        0.000000000     -3.109239000     -2.143297000
C       -1.234762000     -3.636261000     -0.133169000
C       -0.816929000     -4.953435000     -0.234129000
C        0.423943000     -4.427376000     -2.225754000
H        0.307250000     -2.382983000     -2.886838000
H       -1.848441000     -3.317872000      0.699525000
H       -1.134543000     -5.672006000      0.512100000
H        1.069619000     -4.732698000     -3.040430000
H        0.340539000     -6.380578000     -1.343175000
```

53
tcc-[RuCl2(CO)2(SPh2)2] symmetry c2 (E=-2963.75193985)

Ru	0.000000000	0.000000000	0.864005000
Cl	-1.129867000	1.254305000	2.585100000
C	-1.494839000	-1.222715000	1.017521000
O	-2.375242000	-1.908347000	1.197055000
S	-1.051371000	1.179520000	-0.891370000
Cl	1.129867000	-1.254305000	2.585100000
C	1.494839000	1.222715000	1.017521000
S	1.051371000	-1.179520000	-0.891370000
O	2.375242000	1.908347000	1.197055000
C	-2.810598000	1.225448000	-0.638961000
C	0.606486000	-2.897734000	-0.958979000
C	-0.104253000	-5.554626000	-1.234343000
C	0.500943000	-3.453010000	-2.229489000
C	0.355577000	-3.658584000	0.175120000
C	0.000000000	-4.990796000	0.029696000
C	0.146406000	-4.786413000	-2.362854000
H	0.692129000	-2.842166000	-3.103683000
H	0.448295000	-3.211025000	1.158133000
H	-0.195969000	-5.589440000	0.911265000
H	0.060409000	-5.222238000	-3.350966000
H	-0.385201000	-6.595761000	-1.340707000
C	-5.552171000	1.110892000	-0.305238000
C	-3.537328000	0.217476000	-1.261609000
C	-3.442123000	2.181642000	0.142830000
C	-4.817928000	2.121823000	0.300314000
C	-4.910874000	0.158143000	-1.083821000
H	-3.030886000	-0.514458000	-1.880744000
H	-2.869494000	2.960710000	0.626462000
H	-5.316829000	2.867389000	0.907989000
H	-5.479575000	-0.628373000	-1.565207000
H	-6.626734000	1.068543000	-0.172987000
C	-0.606486000	2.897734000	-0.958979000
C	2.810598000	-1.225448000	-0.638961000
C	5.552171000	-1.110892000	-0.305238000
C	3.537328000	-0.217476000	-1.261609000
C	3.442123000	-2.181642000	0.142830000
C	4.817928000	-2.121823000	0.300314000
C	4.910874000	-0.158143000	-1.083821000
H	3.030886000	0.514458000	-1.880744000
H	2.869494000	-2.960710000	0.626462000
H	5.316829000	-2.867389000	0.907989000
H	5.479575000	0.628373000	-1.565207000
H	6.626734000	-1.068543000	-0.172987000
C	0.104253000	5.554626000	-1.234343000
C	-0.500943000	3.453010000	-2.229489000
C	-0.355577000	3.658584000	0.175120000
C	0.000000000	4.990796000	0.029696000
C	-0.146406000	4.786413000	-2.362854000
H	-0.692129000	2.842166000	-3.103683000
H	-0.448295000	3.211025000	1.158133000
H	0.195969000	5.589440000	0.911265000
H	-0.060409000	5.222238000	-3.350966000
H	0.385201000	6.595761000	-1.340707000

25
tcc-[RuCl2(CO)2(SeMe2)2] symmetry c2v (E=-6203.82361531)

Ru	0.000000000	0.000000000	0.486232000
Cl	0.000000000	1.722015000	2.185693000
C	-1.924706000	0.000000000	0.600070000
O	-3.049153000	0.000000000	0.737835000

```
Se       0.000000000      1.736976000     -1.277246000
C        1.443924000      2.935165000     -0.798909000
C       -1.443924000      2.935165000     -0.798909000
H        2.378628000      2.432340000     -1.038928000
H        1.341824000      3.837572000     -1.398882000
H        1.376197000      3.148341000      0.265958000
H       -2.378628000      2.432340000     -1.038928000
H       -1.376197000      3.148341000      0.265958000
H       -1.341824000      3.837572000     -1.398882000
Cl       0.000000000     -1.722015000      2.185693000
C        1.924706000      0.000000000      0.600070000
Se       0.000000000     -1.736976000     -1.277246000
O        3.049153000      0.000000000      0.737835000
C       -1.443924000     -2.935165000     -0.798909000
C        1.443924000     -2.935165000     -0.798909000
H       -2.378628000     -2.432340000     -1.038928000
H       -1.376197000     -3.148341000      0.265958000
H       -1.341824000     -3.837572000     -1.398882000
H        1.341824000     -3.837572000     -1.398882000
H        1.376197000     -3.148341000      0.265958000
H        2.378628000     -2.432340000     -1.038928000

39
tcc-[RuCl2(CO)2(SeMePh)2] symmetry c2 (E=-6586.99077168)
Ru       0.000000000      0.000000000      0.831381000
Cl      -1.120529000     -1.269057000      2.555834000
C        1.451234000     -1.270144000      0.933400000
O        2.300912000     -2.008402000      1.053559000
Se      -1.142078000     -1.254164000     -0.977326000
C       -2.927440000     -1.644481000     -0.336630000
H       -3.489314000     -0.715262000     -0.416627000
H       -3.352457000     -2.403338000     -0.989907000
H       -2.876001000     -1.969016000      0.699257000
Cl       1.120529000      1.269057000      2.555834000
C       -1.451234000      1.270144000      0.933400000
Se       1.142078000      1.254164000     -0.977326000
O       -2.300912000      2.008402000      1.053559000
C        2.927440000      1.644481000     -0.336630000
H        2.876001000      1.969016000      0.699257000
H        3.352457000      2.403338000     -0.989907000
H        3.489314000      0.715262000     -0.416627000
C       -0.407308000     -3.026546000     -0.950185000
C        0.407308000      3.026546000     -0.950185000
C       -0.749209000      5.534306000     -0.991939000
C        0.578289000      3.872483000      0.136801000
C       -0.335035000      3.418237000     -2.055170000
C       -0.919519000      4.677338000     -2.069094000
C        0.000000000      5.132065000      0.106420000
H        1.129850000      3.541174000      1.008097000
H       -0.456684000      2.748353000     -2.898534000
H       -1.503287000      4.987716000     -2.927548000
H        0.128689000      5.798778000      0.950971000
H       -1.202634000      6.518359000     -1.006266000
C        0.749209000     -5.534306000     -0.991939000
C        0.335035000     -3.418237000     -2.055170000
C       -0.578289000     -3.872483000      0.136801000
C        0.000000000     -5.132065000      0.106420000
C        0.919519000     -4.677338000     -2.069094000
H        0.456684000     -2.748353000     -2.898534000
H       -1.129850000     -3.541174000      1.008097000
H       -0.128689000     -5.798778000      0.950971000
H        1.503287000     -4.987716000     -2.927548000
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H        1.202634000     -6.518359000     -1.006266000

53
tcc-[RuCl2(CO)2(SePh2)2] symmetry c1 (E=-6970.15613177)
Ru       0.000098000      1.375620000     -0.000285000
Cl      -1.523831000      3.087778000      0.730819000
C        0.810405000      1.554304000      1.740427000
O        1.277449000      1.775795000      2.747902000
Se      -1.617800000     -0.319739000      0.816081000
Cl       1.524236000      3.087205000     -0.732265000
C       -0.811017000      1.553749000     -1.740709000
Se       1.618172000     -0.319755000     -0.816110000
O       -1.279462000      1.774913000     -2.747601000
C       -3.395378000      0.294627000      0.405332000
C        1.577770000     -1.884939000      0.300789000
C        1.523484000     -4.229999000      1.767854000
C        1.838827000     -3.094810000     -0.327932000
C        1.285578000     -1.840701000      1.655899000
C        1.262805000     -3.017622000      2.389103000
C        1.810358000     -4.267647000      0.410954000
H        2.051505000     -3.121983000     -1.389784000
H        1.067795000     -0.903582000      2.149301000
H        1.033679000     -2.982486000      3.447370000
H        2.004996000     -5.213687000     -0.079867000
H        1.496550000     -5.148738000      2.341532000
C       -5.955234000      1.232094000     -0.041371000
C       -4.104734000      0.868414000      1.450160000
C       -3.951809000      0.177592000     -0.858064000
C       -5.238141000      0.648508000     -1.076577000
C       -5.388336000      1.340714000      1.220253000
H       -3.659298000      0.952492000      2.433921000
H       -3.403008000     -0.283150000     -1.669008000
H       -5.678521000      0.558084000     -2.062513000
H       -5.945205000      1.792740000      2.032389000
H       -6.958953000      1.599967000     -0.218161000
C       -1.577870000     -1.884993000     -0.300709000
C        3.395719000      0.294435000     -0.404934000
C        5.955695000      1.231378000      0.042224000
C        4.105955000      0.866678000     -1.450000000
C        3.951346000      0.178649000      0.858934000
C        5.237726000      0.649300000      1.077681000
C        5.389617000      1.338725000     -1.219871000
H        3.661151000      0.949781000     -2.434127000
H        3.401888000     -0.280922000      1.670091000
H        5.677468000      0.559866000      2.063992000
H        5.947164000      1.789542000     -2.032214000
H        6.959452000      1.599055000      0.219204000
C       -1.524348000     -4.230311000     -1.767400000
C       -1.839577000     -3.094657000      0.328147000
C       -1.285410000     -1.841094000     -1.655771000
C       -1.263024000     -3.018139000     -2.388783000
C       -1.811506000     -4.267624000     -0.410553000
H       -2.052491000     -3.121576000      1.389960000
H       -1.067206000     -0.904151000     -2.149319000
H       -1.033711000     -2.983261000     -3.447017000
H       -2.006675000     -5.213496000      0.080379000
H       -1.497692000     -5.149149000     -2.340932000

25
tcc-[RuCl2(CO)2(TeMe2)2] symmetry c2v (E=-1937.35988137)
Ru       0.000000000      0.000000000      0.684927000
Cl       0.000000000      1.714695000      2.405479000
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C       -1.923155000      0.000000000      0.744001000
O       -3.054993000      0.000000000      0.823049000
Te       0.000000000      1.883365000     -1.141958000
C        1.555824000      3.155039000     -0.458575000
C       -1.555824000      3.155039000     -0.458575000
H        2.505113000      2.684761000     -0.707876000
H        1.461253000      4.109353000     -0.972995000
H        1.440869000      3.260509000      0.618274000
H       -2.505113000      2.684761000     -0.707876000
H       -1.440869000      3.260509000      0.618274000
H       -1.461253000      4.109353000     -0.972995000
Cl       0.000000000     -1.714695000      2.405479000
C        1.923155000      0.000000000      0.744001000
Te       0.000000000     -1.883365000     -1.141958000
O        3.054993000      0.000000000      0.823049000
C       -1.555824000     -3.155039000     -0.458575000
C        1.555824000     -3.155039000     -0.458575000
H       -2.505113000     -2.684761000     -0.707876000
H       -1.440869000     -3.260509000      0.618274000
H       -1.461253000     -4.109353000     -0.972995000
H        1.461253000     -4.109353000     -0.972995000
H        1.440869000     -3.260509000      0.618274000
H        2.505113000     -2.684761000     -0.707876000

39
tcc-[RuCl2(CO)2(TeMePh)2] symmetry c1 (E=-2320.52494078)
Ru      -0.019512000      0.951190000     -0.024880000
Cl       1.244673000      2.646588000      1.161721000
C        1.207032000      1.118408000     -1.501767000
O        1.926823000      1.254196000     -2.366863000
Te       1.383034000     -0.992101000      1.015731000
C        1.877804000     -0.272874000      2.951178000
H        0.995080000     -0.402823000      3.575155000
H        2.702751000     -0.876224000      3.323871000
H        2.137696000      0.779290000      2.866630000
Cl      -1.417339000      2.679864000     -1.020485000
C       -1.208447000      0.884918000      1.491070000
Te      -1.587648000     -0.553280000     -1.485835000
O       -1.887217000      0.889022000      2.398703000
C       -0.989026000     -2.583990000     -1.290078000
H       -1.772403000     -3.206313000     -1.718665000
H       -0.806331000     -2.844668000     -0.250640000
H       -0.070200000     -2.688860000     -1.865750000
C        3.308723000     -0.748807000      0.188892000
C       -3.305151000     -0.696042000     -0.265804000
C       -5.559242000     -0.738985000      1.345433000
C       -4.225028000      0.343907000     -0.338501000
C       -3.508906000     -1.758802000      0.603319000
C       -4.640928000     -1.776991000      1.406822000
C       -5.349348000      0.320197000      0.473466000
H       -4.059306000      1.178355000     -1.010097000
H       -2.796962000     -2.571393000      0.672990000
H       -4.799574000     -2.606140000      2.086549000
H       -6.063645000      1.133523000      0.421093000
H       -6.439313000     -0.755519000      1.977377000
C        5.821559000     -0.500236000     -0.941621000
C        3.868892000     -1.826639000     -0.484770000
C        3.993705000      0.454733000      0.300799000
C        5.255219000      0.571506000     -0.263512000
C        5.128508000     -1.696328000     -1.054987000
H        3.332535000     -2.765426000     -0.567684000
H        3.537377000      1.301024000      0.802411000
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H        5.794141000      1.508088000     -0.178940000
H        5.567339000     -2.533724000     -1.584776000
H        6.805550000     -0.401014000     -1.384764000

53
tcc-[RuCl2(CO)2(TePh2)2] symmetry c1 (E=-2703.69401729)
Ru       0.012051000      1.489719000      0.219927000
Cl      -1.480335000      3.226222000     -0.562227000
C       -1.054182000      1.405107000      1.823510000
O       -1.696507000      1.452565000      2.755810000
Te      -1.508325000     -0.242279000     -1.020591000
Cl       1.296871000      3.151096000      1.441439000
C        0.977526000      1.778544000     -1.419526000
Te       1.806580000     -0.202385000      1.095669000
O        1.489724000      1.995491000     -2.407477000
C       -1.661588000     -1.982085000      0.167450000
C        3.637867000      0.337267000      0.160180000
C        6.091419000      0.930842000     -0.983006000
C        3.962066000      1.655734000     -0.121026000
C        4.539190000     -0.686575000     -0.110210000
C        5.763984000     -0.385292000     -0.686468000
C        5.191975000      1.946628000     -0.697183000
H        3.268018000      2.453823000      0.113822000
H        4.291342000     -1.718147000      0.111253000
H        6.462633000     -1.184804000     -0.904074000
H        5.442105000      2.976719000     -0.923339000
H        7.048572000      1.163122000     -1.434963000
C       -1.969260000     -4.335683000      1.600000000
C       -2.016617000     -3.151669000     -0.492629000
C       -1.452812000     -1.989112000      1.539801000
C       -1.609856000     -3.166622000      2.255177000
C       -2.170414000     -4.327691000      0.227965000
H       -2.168633000     -3.153629000     -1.565852000
H       -1.164347000     -1.088517000      2.065377000
H       -1.446098000     -3.167160000      3.326289000
H       -2.442067000     -5.240382000     -0.289154000
H       -2.087706000     -5.255804000      2.159890000
C       -3.482402000      0.409039000     -0.621563000
C        1.611994000     -1.935400000     -0.102246000
C        1.327382000     -4.226795000     -1.630728000
C        1.525757000     -3.172108000      0.521342000
C        1.569276000     -1.839104000     -1.488050000
C        1.425772000     -2.988409000     -2.250574000
C        1.380218000     -4.318237000     -0.248128000
H        1.560705000     -3.247827000      1.601547000
H        1.664414000     -0.878866000     -1.981094000
H        1.390362000     -2.913511000     -3.331029000
H        1.302631000     -5.283314000      0.238137000
H        1.208790000     -5.122686000     -2.228582000
C       -6.066908000      1.310437000     -0.206361000
C       -4.116148000      1.158237000     -1.604455000
C       -4.133938000      0.100596000      0.563464000
C       -5.429412000      0.555154000      0.767621000
C       -5.410402000      1.609904000     -1.391667000
H       -3.607582000      1.398546000     -2.530695000
H       -3.649893000     -0.495056000      1.327499000
H       -5.939347000      0.316219000      1.693652000
H       -5.905037000      2.197165000     -2.156447000
H       -7.078104000      1.663872000     -0.042468000

31
TS1a to [Ru2Cl4(CO)6] + THF symmetry c1 (E=-2942.27773709)
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Ru      -2.284624000      0.208139000     -0.115136000
Cl      -0.414826000      1.276435000      0.938651000
Cl      -0.739838000     -1.573406000     -0.760242000
Cl      -2.757951000     -0.970281000      1.917477000
C       -1.824676000      1.121072000     -1.706351000
O       -1.528193000      1.667581000     -2.650331000
C       -3.723786000     -0.723356000     -0.903820000
O       -4.589193000     -1.289705000     -1.359335000
O       -4.081251000      2.407938000      0.854487000
C       -3.412388000      1.579894000      0.475235000
Ru       1.541856000     -1.036806000      0.000330000
Cl       2.110865000     -0.780873000     -2.276857000
C        1.844163000     -2.830047000     -0.046858000
C        3.353212000     -0.743385000      0.433784000
C        1.012886000     -1.136340000      1.836254000
O        2.031005000     -3.945495000     -0.093231000
O        4.450509000     -0.648601000      0.678796000
O        0.753380000     -1.247132000      2.928259000
H        3.792256000      2.246342000      1.599279000
O        2.574110000      1.563930000      0.084082000
C        2.368945000      2.418853000     -1.049300000
C        2.820940000      3.791400000     -0.596915000
C        2.429247000      3.777189000      0.875049000
C        2.752227000      2.349463000      1.272039000
H        2.935888000      2.014006000     -1.886352000
H        1.304468000      2.410713000     -1.304036000
H        2.342097000      4.589577000     -1.164639000
H        3.904052000      3.891590000     -0.705306000
H        1.358405000      3.964309000      0.983217000
H        2.971919000      4.505677000      1.477543000
H        2.094858000      1.960666000      2.051715000

44
TS2a to 2x [RuCl2(CO)3(THF)] symmetry c1 (E= -3174.56760121)
Ru       2.761622000     -0.011354000     -0.429815000
Cl      -3.178877000     -0.862339000      1.963270000
Cl       0.710384000      1.134297000     -0.886666000
Cl       3.512771000      1.836457000      0.904792000
C        2.130671000     -1.438919000     -1.502019000
O        1.788612000     -2.263148000     -2.195840000
C        3.486780000      0.824160000     -1.925484000
O        3.913083000      1.360972000     -2.824532000
O        5.416341000     -1.311310000      0.191138000
C        4.411065000     -0.843850000     -0.033453000
Ru      -2.617882000     -0.655469000     -0.325677000
Cl      -0.885213000     -2.259407000     -0.041036000
C       -2.029973000     -0.427123000     -2.122198000
C       -3.738656000     -1.976794000     -0.847859000
C       -4.012569000      0.634508000     -0.466121000
O       -1.700115000     -0.324997000     -3.197367000
O       -4.431512000     -2.821630000     -1.148652000
O       -4.896784000      1.330064000     -0.562800000
H       -0.030487000     -0.151229000      1.713280000
O        1.894284000     -0.807447000      1.359033000
C        2.101403000     -2.155267000      1.834948000
C        1.159990000     -2.310424000      3.012459000
C        0.976088000     -0.874869000      3.492668000
C        0.946515000     -0.105748000      2.194994000
H        1.886503000     -2.847260000      1.019765000
H        3.150905000     -2.245268000      2.126563000
H        1.574509000     -2.969115000      3.775072000
H        0.206006000     -2.717761000      2.674801000
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H        1.822097000     -0.557262000      4.106772000
H        0.057582000     -0.735475000      4.062744000
H        1.287154000      0.924725000      2.266111000
H       -0.726858000      2.122860000      1.753038000
O       -2.211315000      2.258439000      0.327465000
C       -1.977495000      3.305301000     -0.621276000
C       -1.106065000      4.326568000      0.088390000
C       -1.506468000      4.129128000      1.545446000
C       -1.686869000      2.626270000      1.604832000
H       -1.499060000      2.879652000     -1.505631000
H       -2.944756000      3.730988000     -0.910953000
H       -1.274906000      5.339940000     -0.276545000
H       -0.051291000      4.077361000     -0.048671000
H       -2.450922000      4.637031000      1.758289000
H       -0.755427000      4.484625000      2.251569000
H       -2.386942000      2.288088000      2.369836000

31
TS3a to [RuCl2(CO)3(SMe2)] + THF symmetry c1 (E=-2065.09736216)
Ru       0.894805000     -0.487098000      0.016411000
Cl      -0.416492000     -2.365862000      0.763854000
Cl       0.432201000     -0.951098000     -2.268640000
C        1.165712000     -0.080746000      1.845455000
O        1.325168000      0.154307000      2.940118000
C        2.290688000     -1.656631000      0.000334000
O        3.155290000     -2.388228000     -0.020904000
O        2.663661000      1.727746000     -1.025747000
C        1.965310000      0.936186000     -0.613783000
H       -2.323061000     -1.499533000     -1.274715000
O       -1.980643000      0.182354000     -0.132851000
C       -2.675893000      0.151091000      1.119410000
C       -3.881679000     -0.747894000      0.915173000
C       -4.155058000     -0.573931000     -0.572809000
C       -2.746800000     -0.502134000     -1.126108000
H       -1.997804000     -0.221203000      1.889421000
H       -2.971183000      1.174917000      1.372756000
H       -4.721514000     -0.464673000      1.550391000
H       -3.617223000     -1.785840000      1.130113000
H       -4.689115000      0.362170000     -0.758367000
H       -4.730756000     -1.391816000     -1.007466000
H       -2.665998000      0.052619000     -2.062691000
S       -0.365669000      2.420101000      0.377324000
C        0.803309000      3.720797000      0.781303000
H        0.296022000      4.685972000      0.761547000
H        1.168394000      3.530216000      1.790423000
H        1.643563000      3.735489000      0.086772000
H        0.143047000      2.893704000     -1.929446000
C       -0.756804000      2.865954000     -1.314185000
H       -1.247645000      3.839250000     -1.332648000
H       -1.435011000      2.102158000     -1.687668000

31
TS3a to [RuCl2(CO)3(SeMe2)] + THF symmetry c1 (E=-4068.30284386)
Ru      -1.138297000      0.286561000      0.040526000
Cl      -0.699832000      2.640052000      0.398630000
Cl      -0.990936000      0.550693000     -2.312271000
C       -1.093957000      0.079841000      1.920701000
O       -1.061227000     -0.034205000      3.045613000
C       -2.889417000      0.789218000      0.073272000
O       -3.979223000      1.099537000      0.080810000
O       -1.974261000     -2.554383000     -0.537963000
C       -1.578949000     -1.518726000     -0.296378000
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H        1.316970000      2.039556000     -1.700324000
O        1.745481000      0.809948000     -0.108779000
C        2.348025000      1.212742000      1.123673000
C        3.542132000      2.058368000      0.733357000
C        3.016317000      2.758532000     -0.512947000
C        2.191984000      1.665814000     -1.169345000
H        1.623480000      1.798634000      1.699147000
H        2.607287000      0.311495000      1.683324000
H        4.396615000      1.422394000      0.486341000
H        3.840727000      2.746145000      1.525130000
H        3.804198000      3.131883000     -1.167805000
H        2.372851000      3.595214000     -0.231412000
H        2.797803000      1.067240000     -1.859225000
Se       1.288127000     -1.938816000      0.277803000
C        0.754058000     -3.778237000      0.580151000
H        1.605811000     -4.427929000      0.384841000
H        0.459191000     -3.861305000      1.625088000
H       -0.080678000     -4.047560000     -0.064583000
H        0.726952000     -2.484205000     -2.118893000
C        1.613368000     -2.092493000     -1.623143000
H        2.465612000     -2.749703000     -1.785324000
H        1.827466000     -1.090989000     -1.986360000

31
TS3a to [RuCl2(CO)3(TeMe2)] + THF symmetry c1 (E=-1935.06932658)
Ru      -1.191208000     -0.631730000     -0.047692000
Cl      -1.233247000     -0.466495000      2.320779000
Cl      -2.743952000      1.225368000     -0.247635000
C       -0.055470000     -2.129297000      0.160667000
O        0.453485000     -3.132616000      0.325754000
C       -2.683768000     -1.678203000     -0.076496000
O       -3.607488000     -2.335445000     -0.082723000
O       -1.012865000     -0.630526000     -3.064091000
C       -1.073950000     -0.636149000     -1.933871000
H       -0.673184000      2.418477000     -1.648510000
O        0.278150000      1.808258000      0.078753000
C        0.009876000      2.685564000      1.186888000
C       -0.316634000      4.037877000      0.582328000
C        0.469514000      4.004138000     -0.721650000
C        0.285504000      2.561842000     -1.141028000
H       -0.803961000      2.256289000      1.769884000
H        0.911492000      2.732313000      1.806539000
H       -0.034139000      4.860999000      1.239115000
H       -1.386771000      4.107741000      0.375764000
H        1.526289000      4.218370000     -0.540918000
H        0.097735000      4.702953000     -1.471433000
H        1.090104000      2.177899000     -1.772410000
Te       2.261873000     -0.215093000     -0.254475000
C        2.407831000     -0.142463000      1.864024000
H        3.421171000      0.142352000      2.137599000
H        1.688643000      0.591670000      2.217185000
H        2.158552000     -1.123255000      2.263708000
H        2.924697000     -2.805217000      0.134815000
C        3.410292000     -2.003345000     -0.418601000
H        4.407448000     -1.816935000     -0.023823000
H        3.470635000     -2.260754000     -1.474950000

18
TS1b to [Cl2(CO)3Ru-Cl-RuCl(CO)3] symmetry c1 (E=-2709.98493804)
Ru       1.993512000      0.116273000     -0.008603000
Cl       1.043623000     -0.830770000     -2.004239000
Cl      -0.111121000      1.321859000      0.313782000
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Cl       1.130254000     -1.666010000      1.349640000
C        2.612683000      1.535066000     -1.092193000
O        2.976449000      2.379038000     -1.749903000
C        2.671225000      0.850793000      1.593882000
O        3.070260000      1.274283000      2.562641000
O        4.462966000     -1.524297000     -0.474832000
C        3.544873000     -0.891254000     -0.294935000
Ru      -2.114358000      0.068096000     -0.186739000
Cl      -3.177793000      2.162863000     -0.197174000
C       -2.313619000     -0.333163000      1.573751000
C       -3.829500000     -0.638156000     -0.541579000
C       -1.357974000     -1.690717000     -0.472934000
O       -2.429503000     -0.550454000      2.677551000
O       -4.872285000     -1.029274000     -0.716529000
O       -1.169547000     -2.787129000     -0.655808000

36
TS2b to 2 x [RuCl2(CO)3(SMe2)] symmetry c1 (E=-3665.67053312)
Ru      -2.458878000      0.290223000     -0.387105000
Cl       3.845343000      0.519368000     -1.346244000
Cl      -0.393728000      0.510202000      0.854538000
Cl      -2.235789000     -2.096924000     -0.526943000
C       -2.633186000      2.160997000     -0.215084000
O       -2.726541000      3.282987000     -0.104293000
C       -1.433593000      0.436057000     -1.993971000
O       -0.819279000      0.513664000     -2.935113000
O       -5.012386000     -0.015114000     -1.951071000
C       -4.059659000      0.105961000     -1.352436000
Ru       2.428849000     -0.834593000      0.003576000
Cl       1.654578000     -1.929248000     -1.956323000
C        1.256352000     -1.947466000      1.005682000
C        3.774774000     -2.031307000      0.193669000
C        3.034164000      0.106550000      1.547562000
O        0.624894000     -2.670583000      1.600864000
O        4.621164000     -2.779598000      0.284277000
O        3.468185000      0.538640000      2.498379000
S       -3.618306000      0.022243000      1.758966000
C       -2.622609000     -1.098063000      2.740391000
C       -5.032748000     -1.033120000      1.439855000
H       -1.710246000     -0.572065000      3.008817000
H       -3.196312000     -1.341012000      3.634497000
H       -2.388993000     -1.988806000      2.159914000
H       -5.763783000     -0.453973000      0.878051000
H       -4.720260000     -1.912843000      0.878371000
H       -5.461513000     -1.317304000      2.400137000
S        2.004154000      3.021065000      0.841188000
C        3.678271000      3.649462000      0.685609000
C        1.433732000      3.256830000     -0.841925000
H        4.158715000      3.536817000      1.657993000
H        4.227186000      3.067538000     -0.056187000
H        3.675910000      4.705453000      0.410965000
H        0.408788000      2.891281000     -0.882201000
H        1.450376000      4.313587000     -1.112376000
H        2.049686000      2.677544000     -1.531093000

36
TS2b to 2 x [RuCl2(CO)3(SeMe2)] symmetry c1 (E=-7672.08024812)
Ru       2.431776000      0.032294000      0.697112000
Cl      -3.914202000     -0.126576000      1.581092000
Cl       0.298160000      0.408478000     -0.386123000
Cl       2.482861000     -2.272182000      0.009518000
C        2.389688000      1.853157000      1.174233000
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O        2.351772000      2.948701000      1.457210000
C        1.535549000     -0.495312000      2.304254000
O        1.034778000     -0.797223000      3.267294000
O        5.123664000     -0.450592000      1.949771000
C        4.113511000     -0.259438000      1.475362000
Ru      -2.552971000     -1.038603000     -0.148619000
Cl      -1.444274000     -2.369323000      1.481268000
C       -1.385473000     -1.776179000     -1.450014000
C       -3.757826000     -2.359319000     -0.447601000
C       -3.440272000      0.076089000     -1.413058000
O       -0.736763000     -2.271604000     -2.231856000
O       -4.515169000     -3.186948000     -0.611954000
O       -4.058266000      0.582829000     -2.217127000
Se       3.506508000      0.692844000     -1.539553000
C        2.489009000     -0.302769000     -2.846542000
C        5.109091000     -0.389945000     -1.613284000
H        1.518196000      0.177165000     -2.928183000
H        3.035854000     -0.238682000     -3.785684000
H        2.386745000     -1.328681000     -2.500872000
H        5.832970000      0.039839000     -0.924234000
H        4.854786000     -1.410438000     -1.333435000
H        5.490613000     -0.340197000     -2.631070000
Se      -2.237450000      2.683335000     -0.373673000
C       -4.080404000      3.233757000     -0.130675000
C       -1.734723000      2.736075000      1.494206000
H       -4.550606000      3.242613000     -1.112734000
H       -4.580128000      2.515148000      0.518069000
H       -4.113256000      4.232856000      0.300843000
H       -0.700516000      2.405181000      1.551130000
H       -1.826793000      3.754973000      1.866667000
H       -2.375501000      2.052968000      2.049635000

36
TS2b to 2 x [RuCl2(CO)3(TeMe2)] symmetry c1 (E=-3405.61202713)
Ru       2.355768000     -0.250357000      0.902679000
Cl      -4.012044000     -0.780916000      1.395443000
Cl       0.143776000      0.336367000      0.066126000
Cl       2.442273000     -2.285924000     -0.386365000
C        2.293520000      1.368420000      1.855153000
O        2.243952000      2.344345000      2.429096000
C        1.592807000     -1.252308000      2.360240000
O        1.192432000     -1.832410000      3.239339000
O        5.160692000     -0.900959000      1.760799000
C        4.103502000     -0.646192000      1.442122000
Ru      -2.424789000     -1.307772000     -0.326035000
Cl      -1.364148000     -2.831826000      1.177516000
C       -1.149971000     -1.769823000     -1.643042000
C       -3.530000000     -2.637001000     -0.880195000
C       -3.312856000     -0.074570000     -1.477443000
O       -0.436641000     -2.092432000     -2.458764000
O       -4.225419000     -3.470976000     -1.206474000
O       -3.939736000      0.457980000     -2.260779000
Te       3.292486000      1.093037000     -1.267186000
C        2.096518000      0.236213000     -2.788010000
C        5.005033000     -0.068152000     -1.736682000
H        1.108429000      0.681953000     -2.713942000
H        2.566920000      0.481587000     -3.738381000
H        2.056858000     -0.836140000     -2.613455000
H        5.795934000      0.190670000     -1.035875000
H        4.726364000     -1.116737000     -1.650242000
H        5.304038000      0.182747000     -2.752153000
Te      -2.398865000      2.565527000      0.005531000
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C       -4.498738000      2.872388000      0.198189000
C       -2.086245000      2.273984000      2.087443000
H       -4.909530000      2.987435000     -0.803648000
H       -4.924140000      1.995094000      0.682936000
H       -4.684292000      3.771443000      0.782223000
H       -1.020189000      2.114035000      2.232050000
H       -2.414366000      3.163333000      2.621705000
H       -2.648683000      1.393826000      2.393905000

27
TS4a,b to [RuCl2(CO)2(SMe2)2] + CO symmetry c1 (E=-2310.62946087)
Ru      -0.313514000     -0.009024000      0.151824000
C        0.211553000     -0.785610000      1.753568000
O        0.531672000     -1.266591000      2.733242000
C        1.168598000      2.399069000     -0.227227000
O        1.230408000      3.507721000     -0.404540000
C        0.432798000     -1.386115000     -0.839496000
O        0.883402000     -2.237416000     -1.448006000
Cl      -0.942509000      1.028888000     -1.944657000
Cl      -1.193780000      1.817531000      1.485208000
S       -2.349995000     -1.062179000      0.313440000
C       -3.634187000      0.141482000     -0.023040000
H       -3.445252000      0.627262000     -0.977666000
H       -4.577988000     -0.404845000     -0.027139000
H       -3.613082000      0.867721000      0.784704000
C       -2.546500000     -2.092776000     -1.138562000
H       -2.338864000     -1.512286000     -2.036316000
H       -1.861679000     -2.933863000     -1.049838000
H       -3.572748000     -2.460237000     -1.139320000
S        2.962698000     -0.032753000      0.276102000
C        3.714616000     -1.618844000      0.648906000
H        3.495859000     -1.843605000      1.692574000
H        3.297498000     -2.401845000      0.013991000
H        4.795238000     -1.567907000      0.511886000
C        3.404080000      0.117075000     -1.456846000
H        4.480632000      0.254580000     -1.559009000
H        3.087733000     -0.766474000     -2.011764000
H        2.891358000      0.992950000     -1.853773000

27
TS4a,b to [RuCl2(CO)2(SeMe2)2] + CO symmetry c1 (E=-6317.03964385)
Ru       0.342305000      0.074752000     -0.027728000
Cl       0.626005000      1.731062000      1.711564000
Cl       1.359244000      1.496365000     -1.725119000
C        0.041428000     -1.168743000     -1.367878000
O       -0.154874000     -1.931665000     -2.190504000
Se      -3.012260000     -0.233035000     -0.354433000
Se       2.509216000     -0.848093000      0.517511000
C       -3.833713000     -1.958292000     -0.026776000
C       -3.406525000      0.551084000      1.374772000
C        3.687024000      0.675326000      0.689432000
C        3.218836000     -1.489652000     -1.162670000
H       -4.897291000     -1.829162000      0.166478000
H       -3.690162000     -2.556525000     -0.924942000
H       -3.347533000     -2.438695000      0.821468000
H       -4.468643000      0.778571000      1.437839000
H       -3.117221000     -0.143737000      2.161332000
H       -2.822975000      1.466247000      1.462101000
H        3.397558000      1.197592000      1.596511000
H        4.697207000      0.275072000      0.766962000
H        3.561621000      1.310924000     -0.183049000
H        2.683453000     -2.399749000     -1.423509000
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H        3.080308000     -0.716689000     -1.915447000
H        4.273124000     -1.708148000     -1.000515000
C       -0.422971000     -1.025515000      1.248180000
O       -0.848617000     -1.718530000      2.046818000
C       -1.264795000      2.304112000     -0.637564000
O       -1.393048000      3.404870000     -0.826863000

27
TS4a,b to [RuCl2(CO)2(TeMe2)2] + CO symmetry c1 (E=-2050.57510062)
Ru       0.372551000      0.134074000     -0.063370000
Cl       0.721922000      1.772682000      1.690070000
Cl       1.273772000      1.598410000     -1.787204000
C        0.092737000     -1.116034000     -1.397121000
O       -0.065956000     -1.888826000     -2.220362000
Te      -3.148679000     -0.202719000     -0.294985000
Te       2.742553000     -0.722759000      0.443754000
C       -4.402564000     -1.866695000      0.170158000
C       -3.218189000      0.573393000      1.690097000
C        3.895134000      1.052254000      0.436158000
C        3.404884000     -1.352204000     -1.468025000
H       -5.369602000     -1.504688000      0.513863000
H       -4.524366000     -2.451602000     -0.739940000
H       -3.921301000     -2.467749000      0.939750000
H       -4.190140000      1.028686000      1.863555000
H       -3.047775000     -0.248395000      2.382977000
H       -2.426442000      1.313962000      1.793756000
H        3.639162000      1.602949000      1.337168000
H        4.940961000      0.748374000      0.439322000
H        3.631415000      1.616245000     -0.454505000
H        2.913534000     -2.293390000     -1.705327000
H        3.138948000     -0.575287000     -2.181768000
H        4.483023000     -1.491812000     -1.410487000
C       -0.297509000     -1.005136000      1.230301000
O       -0.654318000     -1.720787000      2.044279000
C       -1.334982000      2.281173000     -0.528697000
O       -1.442850000      3.389520000     -0.682926000
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6. References

1. M. Taimisto, R. Oilunkaniemi, R. S. Laitinen, and M. Ahlgrén, *Z. Naturforsch.* 2003, **58b**, 959–964.
2. R. Oilunkaniemi, R. S. Laitinen, and M. Ahlgrén, *Inorg. Chem. Commun.* 2000, **3**, 8–10.
3. H. C. E. McFarlane and W. McFarlane, *J. Chem. Soc., Dalton Trans.* 1973, 2416–2418.
4. G. Garcia-Herbosa, W. R. McNamara, W. W. Brennessel, J. V. Cuevas, S. Sur, and R. Eisenberg, *Polyhedron* 2013, **58**, 39–46.
5. T. Maaninen, H. M. Tuononen, K. Kosunen, R. Oilunkaniemi, J. Hiitola, R. Laitinen, and T. Chivers, *Z. Anorg. Allg. Chem.* 2004, **630**, 1947–1954.
6. L. Vigo, M. J. Poropudas, R. Oilunkaniemi, and R. S. Laitinen, *J. Organomet. Chem.* 2008, **693**, 557–563.