An experimental and DFT study of the Packing and Structure of Dithenoylmethane Monocarbonylphosphine Rhodium(I) complex [Rh((C$_4$H$_3$S)COCHCO(C$_4$H$_3$S))(CO)(PPh$_3$)].

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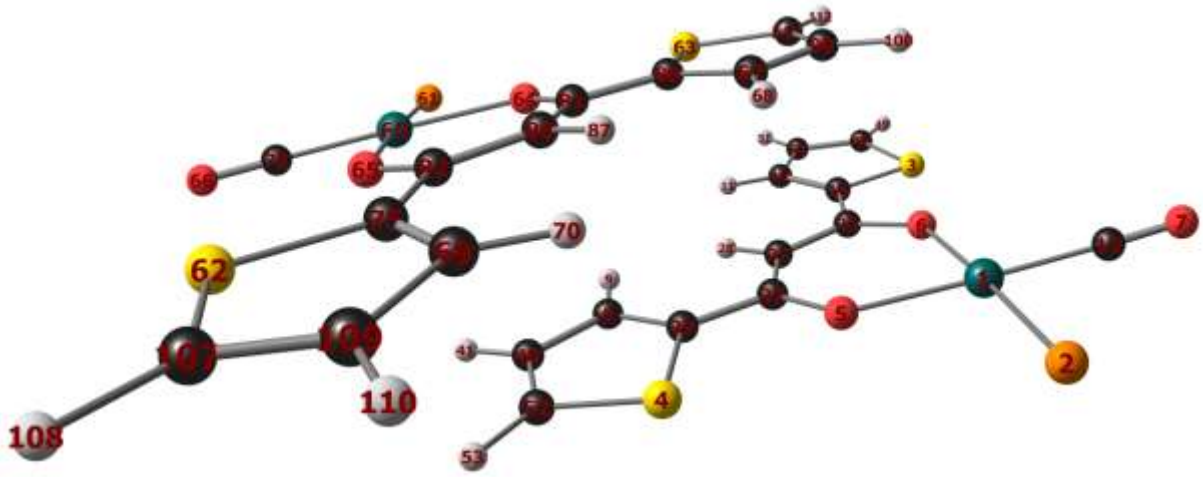

Figure S 1. Atom numbering used for two molecular units of [Rh((C$_4$H$_3$S)COCHCO(C$_4$H$_3$S))(CO)(PPh$_3$)]. Phenyl groups in P61 and P2 omitted for clarity.

Crystallographic data

Table 1. Crystal data and structure refinement for mo_rs02_0m_a.

Identification code	shelx	
Empirical formula	C30 H22 O3 P Rh S2	
Formula weight	628.47	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.9164(5) Å	α= 83.584(3)°.
	b = 10.0741(6) Å	β= 83.702(3)°.
	c = 14.9025(9) Å	γ = 86.035(3)°.
Volume	1320.01(13) $Å^3$	
Z	2	
Density (calculated)	1.581 Mg/m^3	
Absorption coefficient	0.897 mm^{-1}	
F(000)	636	
Crystal size	0.240 x 0.160 x 0.100 mm^3	
Theta range for data collection	2.302 to 25.345°.	
Index ranges	-10<=h<=10, -12<=k<=12, -17<=l<=17	
Reflections collected	23014	
Independent reflections	4832 [R(int) = 0.0540]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4832 / 0 / 348	
Goodness-of-fit on F^2	1.089	
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0777	
R indices (all data)	R1 = 0.0396, wR2 = 0.0808	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.827 and -0.331 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_rs02_0m_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	7546(1)	5523(1)	7181(1)	19(1)
P(1)	6394(1)	7215(1)	6363(1)	17(1)
S(1)	4767(2)	7991(1)	9455(1)	35(1)
S(2)	10731(1)	1916(1)	8578(1)	29(1)
O(1)	6623(2)	6337(2)	8320(1)	25(1)
O(2)	8701(2)	4074(2)	7993(1)	22(1)
O(3)	8559(3)	4156(2)	5551(1)	34(1)
C(1)	6813(3)	5898(3)	9148(2)	22(1)
C(2)	5886(3)	6630(3)	9826(2)	23(1)
C(3)	5722(8)	6453(6)	10774(5)	26(2)
C(4)	4706(4)	7412(3)	11159(2)	32(1)
C(5)	4139(4)	8283(3)	10510(2)	36(1)
C(6)	7785(4)	4835(3)	9426(2)	25(1)
C(7)	8671(3)	4010(3)	8856(2)	22(1)
C(8)	9659(3)	2939(3)	9268(2)	23(1)
C(9)	9960(8)	2574(8)	10162(5)	29(1)
C(10)	11003(4)	1495(3)	10259(2)	36(1)
C(11)	11522(4)	1051(3)	9458(2)	36(1)
C(12)	8192(3)	4727(3)	6173(2)	23(1)
C(13)	6410(3)	7158(3)	5148(2)	18(1)
C(14)	7789(3)	6957(3)	4629(2)	22(1)
C(15)	7853(3)	6913(3)	3708(2)	25(1)
C(16)	6543(4)	7089(3)	3286(2)	30(1)
C(17)	5172(4)	7281(3)	3786(2)	33(1)
C(18)	5092(3)	7303(3)	4719(2)	27(1)
C(19)	4397(3)	7497(3)	6763(2)	21(1)
C(20)	3674(4)	8772(3)	6739(2)	31(1)
C(21)	2134(4)	8907(4)	6981(2)	40(1)
C(22)	1313(4)	7799(4)	7244(3)	45(1)
C(23)	2027(4)	6537(4)	7269(3)	44(1)
C(24)	3564(4)	6393(3)	7039(2)	33(1)
C(25)	7208(3)	8815(3)	6440(2)	19(1)
C(26)	7304(3)	9199(3)	7298(2)	24(1)
C(27)	7958(4)	10370(3)	7397(2)	27(1)

C(28)	8547(4)	11164(3)	6645(2)	28(1)
C(29)	8456(4)	10803(3)	5793(2)	31(1)
C(30)	7781(4)	9633(3)	5685(2)	25(1)
S(1A)	5939(13)	6225(10)	10917(7)	35(1)
S(2A)	9680(30)	2620(30)	10310(20)	29(1)
C(3A)	4980(30)	7680(20)	9601(19)	26(2)
C(9A)	10520(60)	2470(60)	8840(40)	29(1)

Table 3. Bond lengths [Å] and angles [°] for mo_rs02_0m_a.

Rh(1)-C(12)	1.802(3)
Rh(1)-O(1)	2.0355(19)
Rh(1)-O(2)	2.0798(18)
Rh(1)-P(1)	2.2393(7)
P(1)-C(13)	1.817(3)
P(1)-C(19)	1.828(3)
P(1)-C(25)	1.833(3)
S(1)-C(5)	1.661(4)
S(1)-C(2)	1.715(3)
S(2)-C(11)	1.685(3)
S(2)-C(8)	1.709(3)
O(1)-C(1)	1.289(3)
O(2)-C(7)	1.278(3)
O(3)-C(12)	1.151(4)
C(1)-C(6)	1.386(4)
C(1)-C(2)	1.465(4)
C(2)-C(3A)	1.32(2)
C(2)-C(3)	1.397(8)
C(2)-S(1A)	1.637(10)
C(3)-C(4)	1.405(8)
C(4)-C(5)	1.348(5)
C(4)-S(1A)	1.612(9)
C(5)-C(3A)	1.63(3)
C(6)-C(7)	1.399(4)
C(7)-C(8)	1.469(4)
C(8)-C(9A)	1.06(7)
C(8)-C(9)	1.391(8)
C(8)-S(2A)	1.55(3)
C(9)-C(10)	1.386(8)
C(10)-C(11)	1.345(5)
C(10)-S(2A)	1.58(3)
C(11)-C(9A)	1.84(5)
C(13)-C(18)	1.390(4)
C(13)-C(14)	1.393(4)
C(14)-C(15)	1.373(4)
C(15)-C(16)	1.378(4)
C(16)-C(17)	1.374(4)

C(17)-C(18)	1.387(4)
C(19)-C(24)	1.379(4)
C(19)-C(20)	1.395(4)
C(20)-C(21)	1.382(5)
C(21)-C(22)	1.374(5)
C(22)-C(23)	1.380(5)
C(23)-C(24)	1.378(5)
C(25)-C(30)	1.389(4)
C(25)-C(26)	1.390(4)
C(26)-C(27)	1.380(4)
C(27)-C(28)	1.378(4)
C(28)-C(29)	1.372(4)
C(29)-C(30)	1.392(4)
S(2A)-C(9A)	2.25(6)

C(12)-Rh(1)-O(1)	174.44(11)
C(12)-Rh(1)-O(2)	91.91(10)
O(1)-Rh(1)-O(2)	89.11(7)
C(12)-Rh(1)-P(1)	91.24(9)
O(1)-Rh(1)-P(1)	88.12(6)
O(2)-Rh(1)-P(1)	175.10(6)
C(13)-P(1)-C(19)	104.32(13)
C(13)-P(1)-C(25)	103.21(13)
C(19)-P(1)-C(25)	104.09(13)
C(13)-P(1)-Rh(1)	118.87(9)
C(19)-P(1)-Rh(1)	113.05(9)
C(25)-P(1)-Rh(1)	111.82(9)
C(5)-S(1)-C(2)	92.07(16)
C(11)-S(2)-C(8)	92.47(16)
C(1)-O(1)-Rh(1)	126.94(18)
C(7)-O(2)-Rh(1)	125.47(17)
O(1)-C(1)-C(6)	126.0(3)
O(1)-C(1)-C(2)	114.1(2)
C(6)-C(1)-C(2)	119.9(3)
C(3A)-C(2)-C(1)	122.5(13)
C(3)-C(2)-C(1)	132.0(4)
C(3A)-C(2)-S(1A)	115.4(14)
C(1)-C(2)-S(1A)	122.0(4)
C(3)-C(2)-S(1)	109.5(3)

C(1)-C(2)-S(1)	118.5(2)
C(2)-C(3)-C(4)	112.9(4)
C(5)-C(4)-C(3)	111.0(4)
C(5)-C(4)-S(1A)	121.9(4)
C(4)-C(5)-C(3A)	100.3(9)
C(4)-C(5)-S(1)	114.5(2)
C(1)-C(6)-C(7)	125.7(3)
O(2)-C(7)-C(6)	126.5(3)
O(2)-C(7)-C(8)	115.1(2)
C(6)-C(7)-C(8)	118.4(3)
C(9A)-C(8)-C(7)	119(3)
C(9)-C(8)-C(7)	132.1(3)
C(9A)-C(8)-S(2A)	118(3)
C(7)-C(8)-S(2A)	122.9(10)
C(9)-C(8)-S(2)	109.1(3)
C(7)-C(8)-S(2)	118.7(2)
C(10)-C(9)-C(8)	113.6(4)
C(11)-C(10)-C(9)	112.1(4)
C(11)-C(10)-S(2A)	120.2(11)
C(10)-C(11)-S(2)	112.7(2)
C(10)-C(11)-C(9A)	91(2)
O(3)-C(12)-Rh(1)	176.0(3)
C(18)-C(13)-C(14)	119.0(3)
C(18)-C(13)-P(1)	122.1(2)
C(14)-C(13)-P(1)	118.9(2)
C(15)-C(14)-C(13)	120.8(3)
C(14)-C(15)-C(16)	119.8(3)
C(17)-C(16)-C(15)	120.2(3)
C(16)-C(17)-C(18)	120.4(3)
C(17)-C(18)-C(13)	119.7(3)
C(24)-C(19)-C(20)	119.4(3)
C(24)-C(19)-P(1)	118.0(2)
C(20)-C(19)-P(1)	122.5(2)
C(21)-C(20)-C(19)	119.5(3)
C(22)-C(21)-C(20)	120.6(3)
C(21)-C(22)-C(23)	120.0(3)
C(24)-C(23)-C(22)	119.8(3)
C(23)-C(24)-C(19)	120.7(3)
C(30)-C(25)-C(26)	118.7(3)

C(30)-C(25)-P(1)	123.2(2)
C(26)-C(25)-P(1)	118.0(2)
C(27)-C(26)-C(25)	120.5(3)
C(28)-C(27)-C(26)	120.4(3)
C(29)-C(28)-C(27)	119.8(3)
C(28)-C(29)-C(30)	120.2(3)
C(25)-C(30)-C(29)	120.3(3)
C(4)-S(1A)-C(2)	91.9(4)
C(8)-S(2A)-C(10)	95.7(14)
C(8)-S(2A)-C(9A)	24.7(15)
C(10)-S(2A)-C(9A)	71.2(17)
C(2)-C(3A)-C(5)	110.4(18)
C(8)-C(9A)-C(11)	113(4)
C(8)-C(9A)-S(2A)	38(2)
C(11)-C(9A)-S(2A)	76(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for mo_rs02_0m_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	19(1)	21(1)	16(1)	1(1)	-2(1)	4(1)
P(1)	15(1)	19(1)	15(1)	0(1)	-1(1)	1(1)
S(1)	42(1)	38(1)	21(1)	1(1)	3(1)	19(1)
S(2)	28(1)	32(1)	25(1)	1(1)	-5(1)	10(1)
O(1)	33(1)	23(1)	19(1)	1(1)	-4(1)	5(1)
O(2)	23(1)	25(1)	16(1)	2(1)	-2(1)	5(1)
O(3)	44(1)	28(1)	26(1)	-6(1)	3(1)	11(1)
C(1)	23(2)	23(1)	21(2)	-2(1)	-3(1)	-5(1)
C(2)	26(2)	22(1)	22(2)	-1(1)	-3(1)	-2(1)
C(3)	30(3)	18(3)	30(3)	0(2)	-5(2)	-5(2)
C(4)	30(2)	49(2)	18(2)	-8(1)	-1(1)	-1(2)
C(5)	36(2)	38(2)	33(2)	-6(2)	-1(2)	9(2)
C(6)	30(2)	26(2)	19(2)	1(1)	-7(1)	1(1)
C(7)	20(2)	20(1)	24(2)	2(1)	-3(1)	-4(1)
C(8)	21(2)	25(2)	24(2)	0(1)	-7(1)	0(1)
C(9)	29(4)	33(2)	26(3)	-4(2)	-3(2)	1(2)
C(10)	39(2)	35(2)	33(2)	12(2)	-20(2)	-1(2)
C(11)	28(2)	31(2)	46(2)	7(2)	-11(2)	6(1)
C(12)	20(2)	20(1)	26(2)	8(1)	-5(1)	3(1)
C(13)	19(2)	17(1)	18(1)	0(1)	-4(1)	1(1)
C(14)	19(2)	24(2)	22(2)	1(1)	-5(1)	-1(1)
C(15)	22(2)	29(2)	22(2)	-2(1)	2(1)	-4(1)
C(16)	32(2)	42(2)	18(2)	-2(1)	-4(1)	-3(2)
C(17)	23(2)	54(2)	24(2)	-4(2)	-9(1)	-2(2)
C(18)	19(2)	40(2)	21(2)	-4(1)	-2(1)	2(1)
C(19)	16(2)	31(2)	17(1)	-5(1)	-2(1)	4(1)
C(20)	26(2)	31(2)	33(2)	-3(1)	-2(1)	6(1)
C(21)	30(2)	46(2)	42(2)	-6(2)	-2(2)	17(2)
C(22)	20(2)	70(3)	44(2)	-7(2)	4(2)	8(2)
C(23)	26(2)	49(2)	55(2)	-4(2)	8(2)	-10(2)
C(24)	26(2)	31(2)	40(2)	-2(1)	3(2)	1(1)
C(25)	15(1)	19(1)	23(2)	0(1)	-1(1)	3(1)
C(26)	25(2)	25(2)	22(2)	1(1)	-2(1)	0(1)
C(27)	31(2)	26(2)	25(2)	-6(1)	-9(1)	3(1)

C(28)	26(2)	21(2)	38(2)	-2(1)	-8(1)	0(1)
C(29)	31(2)	27(2)	31(2)	5(1)	3(1)	-3(1)
C(30)	30(2)	25(2)	19(2)	1(1)	-1(1)	-1(1)
S(1A)	42(1)	38(1)	21(1)	1(1)	3(1)	19(1)
S(2A)	28(1)	32(1)	25(1)	1(1)	-5(1)	10(1)
C(3A)	30(3)	18(3)	30(3)	0(2)	-5(2)	-5(2)
C(9A)	29(4)	33(2)	26(3)	-4(2)	-3(2)	1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_rs02_0m_a.

	x	y	z	U(eq)
H(3)	6243	5757	11122	31
H(4)	4452	7443	11793	39
H(5)	3438	9005	10645	43
H(6)	7857	4651	10060	30
H(9)	9496	3022	10657	35
H(10)	11314	1114	10826	43
H(11)	12255	328	9395	43
H(14)	8696	6850	4917	26
H(15)	8798	6761	3363	30
H(16)	6588	7077	2647	36
H(17)	4273	7401	3491	40
H(18)	4139	7416	5064	32
H(20)	4236	9542	6558	37
H(21)	1638	9773	6965	48
H(22)	255	7901	7409	55
H(23)	1459	5769	7445	53
H(24)	4056	5524	7071	39
H(26)	6915	8652	7821	29
H(27)	8001	10630	7986	32
H(28)	9016	11958	6717	34
H(29)	8854	11353	5274	37
H(30)	7712	9394	5093	30
H(3A)	4830	8024	8996	31
H(9A)	10745	2743	8215	35

Table 6. Torsion angles [°] for mo_rs02_0m_a.

Rh(1)-O(1)-C(1)-C(6)	5.5(4)
Rh(1)-O(1)-C(1)-C(2)	-174.59(19)
O(1)-C(1)-C(2)-C(3A)	-2.1(14)
C(6)-C(1)-C(2)-C(3A)	177.8(14)
O(1)-C(1)-C(2)-C(3)	177.8(5)
C(6)-C(1)-C(2)-C(3)	-2.3(6)
O(1)-C(1)-C(2)-S(1A)	179.3(6)
C(6)-C(1)-C(2)-S(1A)	-0.8(7)
O(1)-C(1)-C(2)-S(1)	-3.2(4)
C(6)-C(1)-C(2)-S(1)	176.8(2)
C(5)-S(1)-C(2)-C(3)	0.1(4)
C(5)-S(1)-C(2)-C(1)	-179.2(3)
C(1)-C(2)-C(3)-C(4)	179.3(4)
S(1)-C(2)-C(3)-C(4)	0.2(6)
C(2)-C(3)-C(4)-C(5)	-0.4(7)
S(1A)-C(4)-C(5)-C(3A)	2.9(10)
C(3)-C(4)-C(5)-S(1)	0.4(5)
C(2)-S(1)-C(5)-C(4)	-0.3(3)
O(1)-C(1)-C(6)-C(7)	-3.6(5)
C(2)-C(1)-C(6)-C(7)	176.4(3)
Rh(1)-O(2)-C(7)-C(6)	4.7(4)
Rh(1)-O(2)-C(7)-C(8)	-176.34(19)
C(1)-C(6)-C(7)-O(2)	-2.0(5)
C(1)-C(6)-C(7)-C(8)	179.1(3)
O(2)-C(7)-C(8)-C(9A)	16(4)
C(6)-C(7)-C(8)-C(9A)	-165(4)
O(2)-C(7)-C(8)-C(9)	178.3(5)
C(6)-C(7)-C(8)-C(9)	-2.7(6)
O(2)-C(7)-C(8)-S(2A)	-174.4(16)
C(6)-C(7)-C(8)-S(2A)	4.6(16)
O(2)-C(7)-C(8)-S(2)	0.3(4)
C(6)-C(7)-C(8)-S(2)	179.3(2)
C(11)-S(2)-C(8)-C(9)	0.2(4)
C(11)-S(2)-C(8)-C(7)	178.6(3)
C(7)-C(8)-C(9)-C(10)	-179.0(4)
S(2)-C(8)-C(9)-C(10)	-0.9(7)
C(8)-C(9)-C(10)-C(11)	1.3(7)

C(9)-C(10)-C(11)-S(2)	-1.1(5)
S(2A)-C(10)-C(11)-C(9A)	13(2)
C(8)-S(2)-C(11)-C(10)	0.5(3)
C(19)-P(1)-C(13)-C(18)	-0.5(3)
C(25)-P(1)-C(13)-C(18)	-109.0(2)
Rh(1)-P(1)-C(13)-C(18)	126.6(2)
C(19)-P(1)-C(13)-C(14)	179.7(2)
C(25)-P(1)-C(13)-C(14)	71.2(2)
Rh(1)-P(1)-C(13)-C(14)	-53.2(2)
C(18)-C(13)-C(14)-C(15)	0.5(4)
P(1)-C(13)-C(14)-C(15)	-179.7(2)
C(13)-C(14)-C(15)-C(16)	1.0(4)
C(14)-C(15)-C(16)-C(17)	-1.3(5)
C(15)-C(16)-C(17)-C(18)	0.1(5)
C(16)-C(17)-C(18)-C(13)	1.4(5)
C(14)-C(13)-C(18)-C(17)	-1.7(4)
P(1)-C(13)-C(18)-C(17)	178.5(2)
C(13)-P(1)-C(19)-C(24)	90.7(3)
C(25)-P(1)-C(19)-C(24)	-161.4(2)
Rh(1)-P(1)-C(19)-C(24)	-39.8(3)
C(13)-P(1)-C(19)-C(20)	-84.7(3)
C(25)-P(1)-C(19)-C(20)	23.2(3)
Rh(1)-P(1)-C(19)-C(20)	144.7(2)
C(24)-C(19)-C(20)-C(21)	-0.8(5)
P(1)-C(19)-C(20)-C(21)	174.6(3)
C(19)-C(20)-C(21)-C(22)	0.1(5)
C(20)-C(21)-C(22)-C(23)	0.0(6)
C(21)-C(22)-C(23)-C(24)	0.7(6)
C(22)-C(23)-C(24)-C(19)	-1.5(6)
C(20)-C(19)-C(24)-C(23)	1.5(5)
P(1)-C(19)-C(24)-C(23)	-174.1(3)
C(13)-P(1)-C(25)-C(30)	-4.9(3)
C(19)-P(1)-C(25)-C(30)	-113.6(2)
Rh(1)-P(1)-C(25)-C(30)	124.0(2)
C(13)-P(1)-C(25)-C(26)	177.5(2)
C(19)-P(1)-C(25)-C(26)	68.7(2)
Rh(1)-P(1)-C(25)-C(26)	-53.6(2)
C(30)-C(25)-C(26)-C(27)	-0.1(4)
P(1)-C(25)-C(26)-C(27)	177.6(2)

C(25)-C(26)-C(27)-C(28)	-1.0(5)
C(26)-C(27)-C(28)-C(29)	1.4(5)
C(27)-C(28)-C(29)-C(30)	-0.5(5)
C(26)-C(25)-C(30)-C(29)	1.0(4)
P(1)-C(25)-C(30)-C(29)	-176.6(2)
C(28)-C(29)-C(30)-C(25)	-0.6(5)
C(5)-C(4)-S(1A)-C(2)	-2.8(8)
C(3A)-C(2)-S(1A)-C(4)	1.3(16)
C(1)-C(2)-S(1A)-C(4)	180.0(3)
C(9A)-C(8)-S(2A)-C(10)	-6(4)
C(7)-C(8)-S(2A)-C(10)	-176.4(7)
C(7)-C(8)-S(2A)-C(9A)	-170(4)
C(11)-C(10)-S(2A)-C(8)	-9(2)
C(11)-C(10)-S(2A)-C(9A)	-11(2)
C(1)-C(2)-C(3A)-C(5)	-178.6(7)
S(1A)-C(2)-C(3A)-C(5)	0(2)
C(4)-C(5)-C(3A)-C(2)	-1.7(18)
C(7)-C(8)-C(9A)-C(11)	-174.6(15)
S(2A)-C(8)-C(9A)-C(11)	15(5)
C(7)-C(8)-C(9A)-S(2A)	171(4)
C(10)-C(11)-C(9A)-C(8)	-18(4)
C(10)-C(11)-C(9A)-S(2A)	-8.3(14)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_rs02_0m_a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(14)-H(14)...O(3)#1	0.95	2.64	3.362(4)	133.7
C(26)-H(26)...O(1)	0.95	2.39	3.172(3)	139.4

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1

Optimized Cartesian coordinates (Å)

All compounds were optimized the LC-BLYP [i,ii,iii,iv] functional with the triple-ζ basis set 6-311G(d,p) basis for the lighter atoms (C, H, N, O, S, P), and the LANL2DZ basis set (corresponding to the Los Alamos Effective Core Potential plus DZ) [v] for Rh

1. [Rh((C$_4$H$_3$S)COCHCO(C$_4$H$_3$S))(CO)(PPh$_3$)] (one molecule)

Rh	-0.381458000	-1.055955000	0.051143000
P	1.816926000	-0.463964000	0.010967000
S	-4.854364000	-2.811536000	-0.004960000
S	-0.389575000	3.728620000	-0.149108000
O	-0.812216000	0.951920000	0.108535000
O	-2.416117000	-1.396035000	0.067879000
O	0.123477000	-3.981591000	-0.090546000
C	-2.909210000	3.874908000	0.169806000
H	-3.945967000	3.608907000	0.316921000
C	-5.899309000	-0.494002000	0.048893000
H	-6.027749000	0.578164000	0.078217000
C	3.058853000	-1.733859000	-0.377549000
C	-0.038500000	-2.863530000	-0.033616000
C	3.153966000	-2.837637000	0.457054000
H	2.505730000	-2.919154000	1.322443000
C	-4.690428000	-1.106301000	0.032266000
C	1.563426000	1.065055000	2.291704000
H	0.552329000	1.218482000	1.934821000
C	2.426938000	0.261073000	1.564621000
C	4.068991000	-3.831254000	0.200047000
H	4.133066000	-4.687337000	0.860051000
C	-1.954179000	1.495675000	0.064470000
C	-3.332778000	-0.541239000	0.045205000
C	2.105976000	0.842670000	-1.216748000
C	1.992131000	1.671476000	3.451528000
H	1.309586000	2.298897000	4.011330000
C	-3.174266000	0.846324000	0.026000000
H	-4.062768000	1.452224000	-0.035306000
C	-1.912507000	2.965496000	0.046863000
C	3.890116000	-1.649071000	-1.477604000
H	3.827788000	-0.795005000	-2.139810000
C	3.091475000	1.800165000	-1.055129000
H	3.703923000	1.803411000	-0.161757000
C	3.281932000	1.476991000	3.900722000
H	3.615110000	1.950037000	4.816550000
C	3.720821000	0.072838000	2.018158000
H	4.406298000	-0.555272000	1.463042000

C	4.895781000	-3.740454000	-0.902521000
H	5.612317000	-4.525929000	-1.109238000
C	-2.444104000	5.206986000	0.101824000
H	-3.081155000	6.076435000	0.180663000
C	4.144937000	0.677485000	3.183431000
H	5.158173000	0.519772000	3.532198000
C	4.803291000	-2.651841000	-1.739237000
H	5.446998000	-2.576476000	-2.606954000
C	1.315531000	0.868084000	-2.352358000
H	0.525790000	0.134631000	-2.465552000
C	-6.549049000	-2.690817000	-0.001727000
H	-7.156273000	-3.582900000	-0.021917000
C	-6.975058000	-1.408812000	0.028774000
H	-8.016586000	-1.120713000	0.037689000
C	-1.105371000	5.268524000	-0.070588000
H	-0.495762000	6.154981000	-0.157034000
C	3.288922000	2.763550000	-2.020957000
H	4.059716000	3.512118000	-1.884182000
C	2.503720000	2.777256000	-3.154605000
H	2.656976000	3.537382000	-3.911104000
C	1.517233000	1.828380000	-3.319758000
H	0.890372000	1.842379000	-4.202685000

2. [Rh((C$_4$H$_3$S)COCHCO(C$_4$H$_3$S))(CO)(PPh$_3$)] (two molecules)

Rh	4.180447000	1.611409000	-0.184113000
P	5.522038000	-0.223034000	-0.012629000
S	1.782210000	5.780639000	-0.277711000
S	1.413242000	-2.012921000	-1.717301000
O	2.702913000	0.360218000	-0.875120000
O	2.831722000	3.158923000	-0.351832000
O	6.213534000	3.522057000	0.840185000
C	-0.607323000	-0.497805000	-2.009665000
H	-1.258460000	0.364074000	-2.000863000
C	-0.392533000	4.637645000	-0.936880000
H	-1.125306000	3.886499000	-1.193539000
C	7.152500000	-0.033534000	0.773605000
C	5.462558000	2.770719000	0.450928000
C	8.047543000	0.862729000	0.208628000
H	7.764782000	1.423696000	-0.675306000
C	0.915725000	4.367407000	-0.712396000
C	5.010492000	-0.990396000	-2.619828000
H	4.086182000	-0.444038000	-2.483443000
C	5.927935000	-1.044055000	-1.584046000
C	9.295116000	1.044237000	0.757358000
H	9.984087000	1.747286000	0.306117000
C	1.524266000	0.678292000	-1.215787000
C	1.642549000	3.089144000	-0.749878000
C	4.714043000	-1.517050000	0.976509000
C	5.268242000	-1.637491000	-3.809109000

H	4.541414000	-1.591728000	-4.610584000
C	0.978644000	1.949684000	-1.197157000
H	-0.041797000	2.061245000	-1.523321000
C	0.699256000	-0.453613000	-1.656022000
C	7.528644000	-0.739300000	1.899998000
H	6.844233000	-1.444812000	2.353283000
C	4.812889000	-2.862689000	0.675689000
H	5.354564000	-3.183440000	-0.205286000
C	6.444997000	-2.335571000	-3.977764000
H	6.648180000	-2.838822000	-4.915331000
C	7.108296000	-1.747660000	-1.759569000
H	7.839437000	-1.791163000	-0.961799000
C	9.662992000	0.337822000	1.885707000
H	10.643314000	0.484934000	2.322123000
C	-1.040294000	-1.800412000	-2.345357000
H	-2.053970000	-2.050987000	-2.624638000
C	7.365212000	-2.389295000	-2.952230000
H	8.293053000	-2.933009000	-3.081041000
C	8.779467000	-0.550401000	2.454898000
H	9.061714000	-1.106355000	3.340491000
C	3.995792000	-1.125076000	2.093996000
H	3.896160000	-0.067891000	2.314000000
C	0.380299000	6.733308000	-0.413964000
H	0.425086000	7.795005000	-0.224845000
C	-0.702554000	6.006000000	-0.766432000
H	-1.690911000	6.423827000	-0.897563000
C	-0.048489000	-2.709899000	-2.235355000
H	-0.111097000	-3.773678000	-2.407834000
C	4.214503000	-3.802849000	1.489283000
H	4.296091000	-4.854644000	1.243005000
C	3.516356000	-3.406953000	2.610096000
H	3.048449000	-4.146531000	3.248947000
C	3.405870000	-2.064383000	2.911473000
H	2.850522000	-1.746691000	3.785835000
Rh	-4.180400000	-1.611434000	0.184149000
P	-5.521864000	0.223036000	0.011866000
S	-1.782411000	-5.780903000	0.279993000
S	-1.413405000	2.013115000	1.717180000
O	-2.703047000	-0.360190000	0.875450000
O	-2.831862000	-3.159026000	0.352780000
O	-6.213182000	-3.522222000	-0.840489000
C	0.606623000	0.497722000	2.011759000
H	1.257478000	-0.364379000	2.004016000
C	0.392421000	-4.637497000	0.938152000
H	1.125220000	-3.886187000	1.194265000
C	-7.152203000	0.033432000	-0.774607000
C	-5.462327000	-2.770822000	-0.451116000
C	-8.047290000	-0.862829000	-0.209699000
H	-7.764612000	-1.423769000	0.674279000
C	-0.915923000	-4.367448000	0.713941000
C	-5.010901000	0.990868000	2.619073000

H	-4.086627000	0.444355000	2.483071000
C	-5.928033000	1.044442000	1.583016000
C	-9.294809000	-1.044364000	-0.758542000
H	-9.983813000	-1.747414000	-0.307353000
C	-1.524578000	-0.678290000	1.216726000
C	-1.642796000	-3.089207000	0.751129000
C	-4.713656000	1.516786000	-0.977445000
C	-5.268903000	1.638253000	3.808145000
H	-4.542317000	1.592549000	4.609842000
C	-0.979020000	-1.949707000	1.198515000
H	0.041305000	-2.061279000	1.525037000
C	-0.699684000	0.453647000	1.657096000
C	-7.528259000	0.739188000	-1.901037000
H	-6.843827000	1.444720000	-2.354258000
C	-4.811692000	2.862432000	-0.676409000
H	-5.352876000	3.183347000	0.204805000
C	-6.445602000	2.336541000	3.976311000
H	-6.648985000	2.840018000	4.913713000
C	-7.108341000	1.748265000	1.758047000
H	-7.839238000	1.791717000	0.960050000
C	-9.662590000	-0.337972000	-1.886936000
H	-10.642867000	-0.485108000	-2.323444000
C	1.039608000	1.800384000	2.347206000
H	2.053092000	2.050881000	2.627249000
C	-7.365511000	2.390189000	2.950494000
H	-8.293306000	2.934071000	3.078920000
C	-8.779028000	0.550263000	-2.456050000
H	-9.061203000	1.106209000	-3.341672000
C	-3.996027000	1.124601000	-2.095266000
H	-3.896992000	0.067413000	-2.315513000
C	-0.380387000	-6.733412000	0.416215000
H	-0.425144000	-7.795182000	0.227499000
C	0.702510000	-6.005884000	0.768091000
H	1.690950000	-6.423568000	0.899055000
C	0.048069000	2.710025000	2.236038000
H	0.110762000	3.773867000	2.408092000
C	-4.213118000	3.802393000	-1.490103000
H	-4.294069000	4.854194000	-1.243639000
C	-3.515584000	3.406297000	-2.611221000
H	-3.047516000	4.145720000	-3.250135000
C	-3.405909000	2.063708000	-2.912824000
H	-2.851009000	1.745829000	-3.787399000

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