Electronic Supplementary Information for Dalton Transactions

Rhodium complexes bearing a tetradentate diamine–bis(phenolate) ligands

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A. General Considerations for X-Ray Crystallography

Diffraction data for the complexes were collected at low temperature (T = 128 K) on a Bruker SMART APEX CCD diffractometer with graphite-monochromated Mo Kα radiation (λ= 0.71073 Å). The cell parameters for the Rh complexes were obtained from the least-squares refinement of the spots (from 60 collected frames) using the SMART program. A hemisphere of the crystal data was collected and the intensity data was processed using the Saint Plus program. All calculations for structure determination were carried out using the SHELXTL package (version 5.1). 2 Initial atomic positions were located by direct methods using XS, and the structure was refined by least-squares methods using SHELX. Absorption corrections were applied by using SADABS.3 Calculated hydrogen positions were input and refined in a riding manner along with the attached carbons.[1]

B. X-Ray Diffraction Data for $Rh(N^{py}N'O_2^{tBu})(Cl)(CH_3OH)$ (**2a**).

Table 1. Crystal data and structure refinement for [Rh C37 H50 Cl N2 O3]*CH3OH.

Empirical formula	C38 H54 Cl N2 O4 Rh	
Formula weight	740.18	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 15.7408(13) Å	$\alpha = 90^0$
	b = 17.9422(10) Å	$\beta = 119.7460(10)^0$
	c = 15.7257(9) Å	$\gamma = 90°$.
Volume	3856.1(4) $Å^3$	
Z	4	
Density (calculated)	1.275 Mg/m^3	
Absorption coefficient	0.551 mm^{-1}	
F(000)	1556	
Crystal size	0.118 x 0.106 x 0.08 mm^3	
Theta range for data collection	1.49 to 26.42°.	
Index ranges	-19<=h<=17, -17<=k<=22, -19<=l<=19	
Reflections collected	22172	
Independent reflections	7877 [R(int) = 0.0366]	
Completeness to theta = 26.42°	99.6 %	
Transmission Factors	min/max ratio: 0.882	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7877 / 0 / 440	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0467, wR2 = 0.1132	
R indices (all data)	R1 = 0.0684, wR2 = 0.1237	
Largest diff. peak and hole	1.367 and -0.559 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Rh C37 H50 Cl N2 O3]*CH3O. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	5667(1)	8338(1)	8407(1)	39(1)
Cl(1)	5797(1)	9644(1)	8253(1)	62(1)
O(1)	4544(2)	8347(1)	6993(2)	45(1)
O(2)	6754(2)	8404(1)	9794(2)	51(1)
O(3)	6588(2)	8177(2)	7817(2)	68(1)
O(4)	5650(3)	8937(2)	6184(3)	105(1)
N(1)	5597(2)	7216(1)	8574(2)	40(1)
N(2)	4774(2)	8393(1)	8951(2)	39(1)
C(1)	4354(3)	9017(2)	9055(3)	54(1)
C(2)	3775(3)	9005(3)	9483(3)	74(1)
C(3)	3601(4)	8331(3)	9794(4)	85(2)
C(4)	4035(3)	7699(3)	9695(3)	70(1)
C(5)	4626(3)	7739(2)	9279(2)	44(1)
C(6)	5194(3)	7087(2)	9238(3)	47(1)
C(7)	3767(3)	7900(2)	6756(2)	42(1)
C(8)	2790(3)	8142(2)	6162(2)	48(1)
C(9)	2537(3)	8936(2)	5728(3)	58(1)
C(10)	3011(4)	9107(3)	5114(4)	94(2)
C(11)	2878(4)	9497(3)	6552(4)	93(2)
C(12)	1432(4)	9037(3)	5053(5)	115(2)
C(13)	2044(3)	7638(2)	5991(3)	51(1)
C(14)	2200(3)	6914(2)	6355(3)	48(1)
C(15)	1363(3)	6387(2)	6197(3)	64(1)
C(16)	1475(4)	6219(3)	7205(4)	98(2)
C(17)	352(3)	6728(3)	5567(4)	83(1)
C(18)	1440(4)	5666(3)	5720(4)	92(2)
C(19)	3163(3)	6686(2)	6893(2)	49(1)
C(20)	3934(3)	7156(2)	7082(2)	43(1)
C(21)	4956(3)	6872(2)	7583(3)	47(1)
C(22)	6591(3)	6869(2)	8985(3)	48(1)
C(23)	7349(2)	7138(2)	9984(2)	44(1)

C(24)	8086(3)	6643(2)	10569(3)	49(1)
C(25)	8842(3)	6826(2)	11488(3)	48(1)
C(26)	9678(3)	6279(2)	12095(3)	56(1)
C(27)	10538(6)	6662(4)	12945(7)	101(3)
C(28)	10084(5)	5996(4)	11431(5)	92(3)
C(29)	9312(6)	5644(5)	12406(8)	100(3)
C(30)	8781(3)	7520(2)	11845(3)	50(1)
C(31)	8059(2)	8040(2)	11316(2)	44(1)
C(32)	8003(3)	8783(2)	11763(3)	56(1)
C(33)	8765(4)	8827(3)	12859(3)	88(2)
C(34)	8185(3)	9435(2)	11240(3)	73(1)
C(35)	6979(3)	8859(2)	11658(3)	71(1)
C(36)	7359(2)	7867(2)	10327(2)	43(1)
C(37)	7601(4)	8416(3)	8360(5)	98(2)
C(38)	6126(7)	9585(4)	6137(5)	145(3)
C(39)	9682(14)	5572(11)	11560(13)	55(6)
C(40)	10680(20)	6625(15)	12510(20)	74(8)
C(41)	9513(15)	5959(12)	12992(16)	59(6)

Table 3. Bond lengths [Å] and angles [°] for [Rh C37 H50 Cl N2 O3]*CH3O.

Rh(1)-N(2)	1.977(3)
Rh(1)-O(2)	1.999(2)
Rh(1)-N(1)	2.040(3)
Rh(1)-O(1)	2.041(2)
Rh(1)-O(3)	2.093(3)
Rh(1)-Cl(1)	2.3757(9)
O(1)-C(7)	1.352(4)
O(2)-C(36)	1.323(4)
O(3)-C(37)	1.451(6)
O(4)-C(38)	1.406(8)
N(1)-C(6)	1.485(4)
N(1)-C(22)	1.499(4)
N(1)-C(21)	1.506(4)
N(2)-C(5)	1.348(4)
N(2)-C(1)	1.351(4)
C(1)-C(2)	1.375(6)
C(2)-C(3)	1.382(6)
C(3)-C(4)	1.371(6)
C(4)-C(5)	1.379(5)
C(5)-C(6)	1.494(5)
C(7)-C(20)	1.406(4)
C(7)-C(8)	1.414(5)
C(8)-C(13)	1.397(5)
C(8)-C(9)	1.545(5)
C(9)-C(11)	1.514(6)
C(9)-C(10)	1.516(6)
C(9)-C(12)	1.534(6)
C(13)-C(14)	1.392(5)
C(14)-C(19)	1.381(5)
C(14)-C(15)	1.539(6)
C(15)-C(17)	1.523(6)
C(15)-C(18)	1.530(6)
C(15)-C(16)	1.536(6)
C(19)-C(20)	1.383(5)

C(20)-C(21)	1.488(5)
C(22)-C(23)	1.505(5)
C(23)-C(24)	1.387(5)
C(23)-C(36)	1.411(4)
C(24)-C(25)	1.380(5)
C(25)-C(30)	1.389(5)
C(25)-C(26)	1.536(5)
C(26)-C(29)	1.465(8)
C(26)-C(40)	1.51(3)
C(26)-C(27)	1.516(8)
C(26)-C(39)	1.524(18)
C(26)-C(28)	1.555(8)
C(26)-C(41)	1.66(2)
C(30)-C(31)	1.385(5)
C(31)-C(36)	1.424(5)
C(31)-C(32)	1.531(5)
C(32)-C(33)	1.536(5)
C(32)-C(34)	1.537(6)
C(32)-C(35)	1.542(6)

N(2)-Rh(1)-O(2)	86.11(11)
N(2)-Rh(1)-N(1)	84.19(11)
O(2)-Rh(1)-N(1)	89.40(10)
N(2)-Rh(1)-O(1)	93.09(10)
O(2)-Rh(1)-O(1)	176.08(9)
N(1)-Rh(1)-O(1)	94.33(10)
N(2)-Rh(1)-O(3)	174.89(11)
O(2)-Rh(1)-O(3)	94.92(12)
N(1)-Rh(1)-O(3)	90.81(11)
O(1)-Rh(1)-O(3)	86.22(11)
N(2)-Rh(1)-Cl(1)	96.35(8)
O(2)-Rh(1)-Cl(1)	88.99(7)
N(1)-Rh(1)-Cl(1)	178.26(8)
O(1)-Rh(1)-Cl(1)	87.29(7)
O(3)-Rh(1)-Cl(1)	88.68(8)
C(7)-O(1)-Rh(1)	118.13(19)

C(36)-O(2)-Rh(1)	127.3(2)
C(37)-O(3)-Rh(1)	120.0(3)
C(6)-N(1)-C(22)	110.5(3)
C(6)-N(1)-C(21)	111.2(3)
C(22)-N(1)-C(21)	107.2(3)
C(6)-N(1)-Rh(1)	108.26(19)
C(22)-N(1)-Rh(1)	110.8(2)
C(21)-N(1)-Rh(1)	108.9(2)
C(5)-N(2)-C(1)	119.1(3)
C(5)-N(2)-Rh(1)	114.7(2)
C(1)-N(2)-Rh(1)	126.1(2)
N(2)-C(1)-C(2)	122.0(4)
C(1)-C(2)-C(3)	118.9(4)
C(4)-C(3)-C(2)	119.1(4)
C(3)-C(4)-C(5)	120.1(4)
N(2)-C(5)-C(4)	120.9(3)
N(2)-C(5)-C(6)	116.3(3)
C(4)-C(5)-C(6)	122.6(3)
N(1)-C(6)-C(5)	112.5(3)
O(1)-C(7)-C(20)	118.9(3)
O(1)-C(7)-C(8)	122.6(3)
C(20)-C(7)-C(8)	118.5(3)
C(13)-C(8)-C(7)	117.6(3)
C(13)-C(8)-C(9)	120.2(3)
C(7)-C(8)-C(9)	122.2(3)
C(11)-C(9)-C(10)	109.5(4)
C(11)-C(9)-C(12)	108.3(4)
C(10)-C(9)-C(12)	106.4(4)
C(11)-C(9)-C(8)	109.3(3)
C(10)-C(9)-C(8)	111.5(3)
C(12)-C(9)-C(8)	111.7(4)
C(14)-C(13)-C(8)	124.3(3)
C(19)-C(14)-C(13)	116.4(3)
C(19)-C(14)-C(15)	120.6(3)
C(13)-C(14)-C(15)	123.0(3)
C(17)-C(15)-C(18)	109.4(4)

C(17)-C(15)-C(16)	107.3(4)
C(18)-C(15)-C(16)	110.1(4)
C(17)-C(15)-C(14)	113.2(4)
C(18)-C(15)-C(14)	109.2(4)
C(16)-C(15)-C(14)	107.7(3)
C(14)-C(19)-C(20)	122.0(3)
C(19)-C(20)-C(7)	121.0(3)
C(19)-C(20)-C(21)	120.5(3)
C(7)-C(20)-C(21)	118.5(3)
C(20)-C(21)-N(1)	113.6(3)
N(1)-C(22)-C(23)	115.8(3)
C(24)-C(23)-C(36)	119.5(3)
C(24)-C(23)-C(22)	117.1(3)
C(36)-C(23)-C(22)	123.3(3)
C(25)-C(24)-C(23)	123.1(3)
C(24)-C(25)-C(30)	116.1(3)
C(24)-C(25)-C(26)	121.8(3)
C(30)-C(25)-C(26)	122.1(3)
C(29)-C(26)-C(40)	132.3(11)
C(29)-C(26)-C(27)	112.6(6)
C(40)-C(26)-C(27)	31.2(9)
C(29)-C(26)-C(39)	69.4(8)
C(40)-C(26)-C(39)	107.2(12)
C(27)-C(26)-C(39)	128.1(8)
C(29)-C(26)-C(25)	110.3(4)
C(40)-C(26)-C(25)	113.3(11)
C(27)-C(26)-C(25)	111.9(4)
C(39)-C(26)-C(25)	115.2(7)
C(29)-C(26)-C(28)	109.4(5)
C(40)-C(26)-C(28)	74.9(10)
C(27)-C(26)-C(28)	104.7(6)
C(39)-C(26)-C(28)	40.8(7)
C(25)-C(26)-C(28)	107.6(4)
C(29)-C(26)-C(41)	36.3(7)
C(40)-C(26)-C(41)	109.9(12)
C(27)-C(26)-C(41)	81.6(8)

C(39)-C(26)-C(41)	103.1(10)
C(25)-C(26)-C(41)	107.6(8)
C(28)-C(26)-C(41)	138.5(8)
C(31)-C(30)-C(25)	124.2(3)
C(30)-C(31)-C(36)	118.0(3)
C(30)-C(31)-C(32)	121.9(3)
C(36)-C(31)-C(32)	120.2(3)
C(31)-C(32)-C(33)	111.7(3)
C(31)-C(32)-C(34)	110.4(3)
C(33)-C(32)-C(34)	108.2(3)
C(31)-C(32)-C(35)	108.8(3)
C(33)-C(32)-C(35)	108.0(4)
C(34)-C(32)-C(35)	109.8(3)
O(2)-C(36)-C(23)	124.4(3)
O(2)-C(36)-C(31)	117.2(3)
C(23)-C(36)-C(31)	118.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [Rh C37 H50 Cl N2 O3]*CH3O. 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)	44(1)	29(1)	46(1)	1(1)	25(1)	3(1)
Cl(1)	72(1)	34(1)	85(1)	5(1)	42(1)	-2(1)
O(1)	56(2)	42(1)	41(1)	5(1)	26(1)	0(1)
O(2)	50(2)	32(1)	55(1)	-6(1)	13(1)	7(1)
O(3)	75(2)	54(2)	101(2)	-2(2)	64(2)	1(1)
N(1)	41(2)	32(1)	44(2)	0(1)	18(1)	4(1)
N(2)	43(2)	39(2)	34(1)	3(1)	19(1)	7(1)
C(1)	62(3)	48(2)	53(2)	7(2)	28(2)	20(2)
C(2)	86(3)	83(3)	68(3)	21(2)	50(3)	42(3)
C(3)	86(4)	113(4)	83(3)	33(3)	62(3)	38(3)
C(4)	75(3)	76(3)	77(3)	33(2)	51(3)	16(2)
C(5)	46(2)	45(2)	41(2)	7(2)	21(2)	3(2)
C(6)	53(2)	36(2)	49(2)	6(2)	23(2)	3(2)
C(7)	58(2)	35(2)	36(2)	0(1)	26(2)	2(2)
C(8)	59(2)	44(2)	39(2)	3(2)	24(2)	9(2)
C(9)	63(3)	50(2)	56(2)	15(2)	26(2)	14(2)
C(10)	110(4)	93(4)	86(3)	48(3)	55(3)	29(3)
C(11)	135(5)	55(3)	88(3)	10(3)	55(3)	30(3)
C(12)	78(4)	88(4)	135(5)	58(4)	18(4)	27(3)
C(13)	46(2)	55(2)	45(2)	3(2)	18(2)	7(2)
C(14)	50(2)	45(2)	46(2)	-2(2)	20(2)	-1(2)
C(15)	55(3)	59(3)	66(3)	0(2)	20(2)	-9(2)
C(16)	97(4)	95(4)	106(4)	17(3)	54(4)	-20(3)
C(17)	60(3)	81(4)	97(4)	-1(3)	30(3)	-5(2)
C(18)	70(3)	62(3)	122(4)	-22(3)	29(3)	-14(2)
C(19)	57(2)	38(2)	41(2)	2(2)	17(2)	3(2)
C(20)	47(2)	36(2)	39(2)	-2(1)	15(2)	1(2)
C(21)	53(2)	34(2)	47(2)	-7(2)	18(2)	4(2)
C(22)	48(2)	34(2)	56(2)	-4(2)	20(2)	8(2)
C(23)	42(2)	35(2)	50(2)	-2(2)	19(2)	4(1)
C(24)	53(2)	31(2)	60(2)	-2(2)	26(2)	8(2)

C(25)	41(2)	41(2)	60(2)	1(2)	23(2)	4(2)
C(26)	45(2)	46(2)	64(2)	10(2)	18(2)	11(2)
C(27)	76(5)	75(5)	90(6)	10(4)	-6(4)	34(4)
C(28)	73(5)	85(5)	118(6)	25(4)	49(4)	40(4)
C(29)	89(5)	86(6)	140(8)	62(6)	68(5)	47(4)
C(30)	45(2)	43(2)	51(2)	1(2)	16(2)	1(2)
C(31)	41(2)	35(2)	51(2)	-3(2)	20(2)	-1(2)
C(32)	52(2)	46(2)	53(2)	-11(2)	14(2)	2(2)
C(33)	90(4)	63(3)	66(3)	-21(2)	4(3)	15(3)
C(34)	62(3)	36(2)	98(3)	-7(2)	23(2)	-7(2)
C(35)	75(3)	64(3)	80(3)	-19(2)	42(3)	6(2)
C(36)	40(2)	34(2)	51(2)	1(2)	19(2)	6(1)
C(37)	77(4)	99(4)	147(5)	19(4)	78(4)	10(3)
C(38)	208(8)	110(6)	106(5)	15(4)	69(5)	3(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for [Rh C37 H50 Cl N2 O3]*CH3O.

	x	y	z	U(eq)
H(1)	4460	9468	8831	65
H(2)	3505	9443	9561	89
H(3)	3196	8306	10067	102
H(4)	3931	7243	9910	84
H(6A)	5728	6983	9892	57
H(6B)	4772	6652	9016	57
H(10A)	2811	9592	4826	141
H(10B)	2813	8740	4605	141
H(10C)	3710	9095	5521	141
H(11A)	3575	9462	6962	139
H(11B)	2568	9395	6933	139
H(11C)	2708	9991	6284	139
H(12A)	1104	8976	5425	173
H(12B)	1197	8671	4540	173
H(12C)	1304	9527	4770	173
H(13)	1401	7798	5608	61
H(16A)	929	5926	7124	147
H(16B)	1496	6678	7528	147
H(16C)	2070	5946	7594	147
H(17A)	270	6862	4940	125
H(17B)	289	7165	5884	125
H(17C)	-139	6372	5481	125
H(18A)	1379	5778	5095	139
H(18B)	927	5332	5632	139
H(18C)	2063	5437	6134	139
H(19)	3297	6202	7135	58
H(21A)	5242	6968	7171	57
H(21B)	4944	6336	7660	57
H(22A)	6831	6961	8534	58
H(22B)	6522	6334	9017	58

H(24)	8071	6166	10331	59
H(27A)	10361	6804	13425	152
H(27B)	10714	7097	12712	152
H(27C)	11085	6326	13236	152
H(28A)	10612	5654	11793	137
H(28B)	10319	6412	11222	137
H(28C)	9573	5749	10868	137
H(29A)	8756	5432	11846	150
H(29B)	9124	5810	12869	150
H(29C)	9817	5275	12706	150
H(30)	9256	7643	12481	60
H(33A)	8656	8429	13201	132
H(33B)	8704	9297	13117	132
H(33C)	9410	8784	12942	132
H(34A)	8813	9376	11286	110
H(34B)	8171	9896	11542	110
H(34C)	7685	9440	10563	110
H(35A)	6493	8870	10976	107
H(35B)	6947	9312	11965	107
H(35C)	6860	8442	11967	107
H(37A)	7630	8927	8554	147
H(37B)	7894	8368	7954	147
H(37C)	7950	8110	8933	147
H(39A)	10240	5274	11984	82
H(39B)	9713	5702	10984	82
H(39C)	9095	5293	11375	82
H(40A)	11163	6280	12956	111
H(40B)	10704	7072	12860	111
H(40C)	10806	6743	11992	111
H(41A)	8892	5712	12719	88
H(41B)	9528	6367	13394	88
H(41C)	10025	5613	13383	88

C. X-Ray Diffraction Data for Rh($N^{NMe2}N'O_2^{Me}$)(Cl)(CH_3OH) (**2b**).

Table 1. Crystal data and structure refinement for (C23 H33 Cl N2 O3 Rh) * (C H4 O) * 0.5(C6 H6).

Identification code	periana10	
Empirical formula	C27 H40 Cl N2 O4 Rh	
Formula weight	594.97	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 11.740(3) Å	α= 90°.
	b = 19.505(4) Å	β= 90°.
	c = 24.825(5) Å	γ = 90°.
Volume	5685(2) $Å^3$	
Z	8	
Density (calculated)	1.390 Mg/m^3	
Absorption coefficient	0.728 mm^{-1}	
F(000)	2480	
Crystal size	0.12 x 0.12 x 0.03 mm^3	
Theta range for data collection	1.64 to 25.68°.	
Index ranges	-14<=h<=12, -23<=k<=23, -28<=l<=30	
Reflections collected	30572	
Independent reflections	5392 [R(int) = 0.0615]	
Completeness to theta = 25.68°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.645 and 0.580	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5392 / 12 / 325	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0511, wR2 = 0.1307	
R indices (all data)	R1 = 0.0786, wR2 = 0.1504	
Largest diff. peak and hole	1.660 and -0.720 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (C23 H33 Cl N2 O3 Rh) * (C H4 O) * 0.5(C6 H6). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	4676(1)	10224(1)	3501(1)	42(1)
Cl(1)	3295(1)	11009(1)	3206(1)	59(1)
O(1)	5368(3)	11011(2)	3936(1)	53(1)
O(2)	3776(3)	9465(2)	3154(1)	54(1)
O(3)	3662(3)	10071(2)	4201(1)	56(1)
N(1)	5716(3)	10360(2)	2863(2)	43(1)
N(2)	5910(4)	9535(2)	3780(2)	57(1)
C(1)	6377(4)	11299(2)	3823(2)	52(1)
C(2)	7016(5)	11579(2)	4250(2)	57(1)
C(3)	8095(5)	11839(3)	4131(3)	67(2)
C(4)	8564(5)	11838(3)	3621(3)	62(1)
C(5)	7897(4)	11582(2)	3211(2)	54(1)
C(6)	6817(4)	11329(2)	3301(2)	49(1)
C(7)	6551(6)	11586(3)	4813(2)	83(2)
C(8)	9779(5)	12070(4)	3520(3)	86(2)
C(9)	6089(4)	11097(2)	2835(2)	48(1)
C(10)	5110(4)	10207(2)	2338(2)	48(1)
C(11)	4704(4)	9480(2)	2284(2)	48(1)
C(12)	4980(5)	9116(3)	1819(2)	57(1)
C(13)	4577(5)	8460(3)	1724(3)	66(2)
C(14)	3874(5)	8178(3)	2112(2)	64(2)
C(15)	3583(4)	8506(2)	2581(2)	57(1)
C(16)	4034(4)	9176(2)	2679(2)	48(1)
C(17)	4943(7)	8047(3)	1234(3)	96(2)
C(18)	2800(5)	8184(3)	2994(3)	76(2)
C(19)	6730(4)	9893(2)	2908(2)	49(1)
C(20)	6975(7)	9721(4)	3459(3)	105(3)
C(21)	6263(8)	9673(4)	4326(3)	111(3)
C(22)	5607(7)	8830(4)	3746(4)	119(3)
C(23)	2543(5)	9783(3)	4149(3)	76(2)

C(25)	9545(6)	10283(5)	4545(4)	98(2)
C(24)	9491(6)	9604(5)	4626(4)	102(3)
C(26)	9951(7)	9305(4)	5081(4)	101(2)
O(4)	3659(4)	1338(2)	4589(2)	88(1)
C(27)	2802(8)	1811(4)	4482(3)	124(3)

Table 3. Bond lengths [Å] and angles [°] for (C23 H33 Cl N2 O3 Rh) * (C H4 O) * 0.5(C6 H6).

Rh(1)-O(2)	2.012(3)
Rh(1)-N(1)	2.019(4)
Rh(1)-O(1)	2.046(3)
Rh(1)-N(2)	2.095(4)
Rh(1)-O(3)	2.128(3)
Rh(1)-Cl(1)	2.3475(13)
O(1)-C(1)	1.341(6)
O(2)-C(16)	1.340(6)
O(3)-C(23)	1.435(6)
N(1)-C(19)	1.502(6)
N(1)-C(9)	1.505(5)
N(1)-C(10)	1.514(6)
N(2)-C(22)	1.423(8)
N(2)-C(21)	1.441(8)
N(2)-C(20)	1.527(9)
C(1)-C(6)	1.396(7)
C(1)-C(2)	1.410(7)
C(2)-C(3)	1.397(8)
C(2)-C(7)	1.500(8)
C(3)-C(4)	1.380(8)
C(3)-H(3)	0.9300
C(4)-C(5)	1.378(7)
C(4)-C(8)	1.516(8)
C(5)-C(6)	1.379(7)
C(5)-H(5)	0.9300
C(6)-C(9)	1.507(6)
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700

C(10)-C(11)	1.502(6)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(16)	1.389(7)
C(11)-C(12)	1.395(7)
C(12)-C(13)	1.383(7)
C(12)-H(12)	0.9300
C(13)-C(14)	1.384(8)
C(13)-C(17)	1.520(8)
C(14)-C(15)	1.372(7)
C(14)-H(14)	0.9300
C(15)-C(16)	1.430(6)
C(15)-C(18)	1.514(8)
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-C(20)	1.438(8)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(25)-C(24)	1.341(11)
C(25)-C(26)#1	1.361(11)
C(25)-H(25)	0.9300

C(24)-C(26)	1.381(11)
C(24)-H(24)	0.9300
C(26)-C(25)#1	1.361(11)
C(26)-H(26)	0.9300
O(4)-C(27)	1.391(9)
O(4)-H(4A)	0.8200
C(27)-H(26A)	0.9600
C(27)-H(26B)	0.9600
C(27)-H(26C)	0.9600

O(2)-Rh(1)-N(1)	94.48(14)
O(2)-Rh(1)-O(1)	170.68(13)
N(1)-Rh(1)-O(1)	94.31(14)
O(2)-Rh(1)-N(2)	91.90(16)
N(1)-Rh(1)-N(2)	85.73(16)
O(1)-Rh(1)-N(2)	91.83(16)
O(2)-Rh(1)-O(3)	87.35(14)
N(1)-Rh(1)-O(3)	176.73(14)
O(1)-Rh(1)-O(3)	84.02(13)
N(2)-Rh(1)-O(3)	91.51(15)
O(2)-Rh(1)-Cl(1)	89.07(11)
N(1)-Rh(1)-Cl(1)	94.98(11)
O(1)-Rh(1)-Cl(1)	87.09(10)
N(2)-Rh(1)-Cl(1)	178.75(13)
O(3)-Rh(1)-Cl(1)	87.75(10)
C(1)-O(1)-Rh(1)	123.7(3)
C(16)-O(2)-Rh(1)	124.6(3)
C(23)-O(3)-Rh(1)	119.6(3)
C(19)-N(1)-C(9)	110.6(4)
C(19)-N(1)-C(10)	108.5(3)
C(9)-N(1)-C(10)	106.6(3)
C(19)-N(1)-Rh(1)	109.9(3)
C(9)-N(1)-Rh(1)	109.7(3)
C(10)-N(1)-Rh(1)	111.4(3)
C(22)-N(2)-C(21)	108.0(5)
C(22)-N(2)-C(20)	113.8(6)

C(21)-N(2)-C(20)	102.2(6)
C(22)-N(2)-Rh(1)	115.3(4)
C(21)-N(2)-Rh(1)	112.9(4)
C(20)-N(2)-Rh(1)	104.0(3)
O(1)-C(1)-C(6)	122.6(4)
O(1)-C(1)-C(2)	118.4(5)
C(6)-C(1)-C(2)	119.0(5)
C(3)-C(2)-C(1)	117.7(5)
C(3)-C(2)-C(7)	121.6(5)
C(1)-C(2)-C(7)	120.7(5)
C(4)-C(3)-C(2)	123.8(5)
C(4)-C(3)-H(3)	118.1
C(2)-C(3)-H(3)	118.1
C(5)-C(4)-C(3)	116.8(5)
C(5)-C(4)-C(8)	121.3(6)
C(3)-C(4)-C(8)	121.7(5)
C(4)-C(5)-C(6)	122.2(5)
C(4)-C(5)-H(5)	118.9
C(6)-C(5)-H(5)	118.9
C(5)-C(6)-C(1)	120.4(5)
C(5)-C(6)-C(9)	120.3(5)
C(1)-C(6)-C(9)	119.3(4)
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(4)-C(8)-H(8A)	109.5
C(4)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(4)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
N(1)-C(9)-C(6)	114.6(4)
N(1)-C(9)-H(9A)	108.6

C(6)-C(9)-H(9A)	108.6
N(1)-C(9)-H(9B)	108.6
C(6)-C(9)-H(9B)	108.6
H(9A)-C(9)-H(9B)	107.6
C(11)-C(10)-N(1)	114.3(4)
C(11)-C(10)-H(10A)	108.7
N(1)-C(10)-H(10A)	108.7
C(11)-C(10)-H(10B)	108.7
N(1)-C(10)-H(10B)	108.7
H(10A)-C(10)-H(10B)	107.6
C(16)-C(11)-C(12)	119.9(5)
C(16)-C(11)-C(10)	121.3(4)
C(12)-C(11)-C(10)	118.7(4)
C(13)-C(12)-C(11)	122.2(5)
C(13)-C(12)-H(12)	118.9
C(11)-C(12)-H(12)	118.9
C(12)-C(13)-C(14)	116.9(5)
C(12)-C(13)-C(17)	122.0(6)
C(14)-C(13)-C(17)	121.0(5)
C(15)-C(14)-C(13)	123.7(5)
C(15)-C(14)-H(14)	118.2
C(13)-C(14)-H(14)	118.2
C(14)-C(15)-C(16)	118.6(5)
C(14)-C(15)-C(18)	122.2(5)
C(16)-C(15)-C(18)	119.2(5)
O(2)-C(16)-C(11)	124.6(4)
O(2)-C(16)-C(15)	116.8(4)
C(11)-C(16)-C(15)	118.6(5)
C(13)-C(17)-H(17A)	109.5
C(13)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(13)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5

H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(20)-C(19)-N(1)	111.8(5)
C(20)-C(19)-H(19A)	109.3
N(1)-C(19)-H(19A)	109.3
C(20)-C(19)-H(19B)	109.3
N(1)-C(19)-H(19B)	109.3
H(19A)-C(19)-H(19B)	107.9
C(19)-C(20)-N(2)	112.9(6)
C(19)-C(20)-H(20A)	109.0
N(2)-C(20)-H(20A)	109.0
C(19)-C(20)-H(20B)	109.0
N(2)-C(20)-H(20B)	109.0
H(20A)-C(20)-H(20B)	107.8
N(2)-C(21)-H(21A)	109.5
N(2)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
N(2)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(2)-C(22)-H(22A)	109.5
N(2)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(2)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(3)-C(23)-H(23A)	109.5
O(3)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
O(3)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(24)-C(25)-C(26)#1	120.1(8)
C(24)-C(25)-H(25)	120.0

C(26)#1-C(25)-H(25)	120.0
C(25)-C(24)-C(26)	121.4(8)
C(25)-C(24)-H(24)	119.3
C(26)-C(24)-H(24)	119.3
C(25)#1-C(26)-C(24)	118.5(8)
C(25)#1-C(26)-H(26)	120.7
C(24)-C(26)-H(26)	120.7
C(27)-O(4)-H(4A)	109.5
O(4)-C(27)-H(26A)	109.5
O(4)-C(27)-H(26B)	109.5
H(26A)-C(27)-H(26B)	109.5
O(4)-C(27)-H(26C)	109.5
H(26A)-C(27)-H(26C)	109.5
H(26B)-C(27)-H(26C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (C23 H33 Cl N2 O3 Rh) * (C H4 O) * 0.5(C6 H6). 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)	35(1)	44(1)	47(1)	0(1)	0(1)	2(1)
Cl(1)	50(1)	66(1)	61(1)	1(1)	-1(1)	18(1)
O(1)	48(2)	60(2)	51(2)	-8(2)	1(2)	-6(2)
O(2)	43(2)	54(2)	64(2)	-9(2)	6(2)	-8(2)
O(3)	46(2)	69(2)	53(2)	5(2)	7(2)	-3(2)
N(1)	38(2)	42(2)	48(2)	-3(2)	-1(2)	-1(2)
N(2)	50(3)	57(2)	63(3)	15(2)	0(2)	7(2)
C(1)	51(3)	47(3)	58(3)	-5(2)	-5(2)	-2(2)
C(2)	56(3)	51(3)	65(3)	-5(2)	-7(3)	-5(3)
C(3)	64(4)	52(3)	85(4)	-9(3)	-21(3)	-7(3)
C(4)	53(3)	46(3)	88(4)	-7(3)	-5(3)	-6(3)
C(5)	53(3)	40(2)	69(3)	-6(2)	5(3)	-2(2)
C(6)	49(3)	42(3)	57(3)	-5(2)	-4(2)	-1(2)
C(7)	99(5)	90(4)	59(4)	-10(3)	-12(3)	-26(4)
C(8)	62(4)	72(4)	123(6)	-10(4)	-2(4)	-17(3)
C(9)	50(3)	43(2)	50(3)	-3(2)	4(2)	-3(2)
C(10)	46(3)	51(3)	46(3)	-3(2)	0(2)	2(2)
C(11)	39(3)	43(2)	60(3)	-5(2)	-4(2)	4(2)
C(12)	53(3)	60(3)	58(3)	-14(3)	1(2)	1(3)
C(13)	63(4)	59(3)	75(4)	-23(3)	-6(3)	0(3)
C(14)	53(3)	45(3)	94(4)	-23(3)	-5(3)	-4(3)
C(15)	44(3)	45(3)	83(4)	1(3)	-4(3)	0(2)
C(16)	35(3)	48(3)	62(3)	-5(2)	-4(2)	5(2)
C(17)	112(6)	77(4)	99(5)	-38(4)	6(5)	-7(4)
C(18)	66(4)	57(3)	106(5)	-1(3)	9(4)	-8(3)
C(19)	38(3)	47(3)	61(3)	0(2)	4(2)	3(2)
C(20)	81(5)	126(5)	107(5)	23(4)	17(4)	31(4)
C(21)	122(7)	104(5)	107(6)	10(4)	-65(5)	17(5)
C(22)	120(5)	67(4)	169(6)	9(4)	-57(5)	4(4)
C(23)	52(3)	96(5)	78(4)	7(3)	10(3)	-11(3)
C(25)	77(5)	122(7)	94(6)	19(5)	-7(4)	17(5)

C(24)	56(4)	138(8)	112(7)	-20(6)	-15(4)	16(5)
C(26)	76(5)	95(5)	131(7)	14(6)	1(5)	6(5)
O(4)	89(3)	96(3)	79(3)	-18(2)	25(2)	-11(3)
C(27)	134(7)	94(5)	144(7)	-11(5)	52(6)	26(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (C23 H33 Cl N2 O3 Rh) * (C H4 O) * 0.5(C6 H6).

	x	y	z	U(eq)
H(3)	8523	12023	4411	80
H(5)	8186	11579	2862	65
H(7A)	7145	11709	5060	124
H(7B)	6265	11139	4901	124
H(7C)	5944	11914	4837	124
H(8A)	10255	11676	3465	128
H(8B)	10048	12324	3826	128
H(8C)	9801	12356	3206	128
H(9A)	5416	11385	2819	57
H(9B)	6511	11166	2504	57
H(10A)	4460	10511	2306	57
H(10B)	5622	10307	2042	57
H(12)	5451	9320	1564	68
H(14)	3583	7741	2052	77
H(17A)	4293	7958	1011	144
H(17B)	5269	7620	1350	144
H(17C)	5499	8301	1033	144
H(18A)	2083	8420	2994	115
H(18B)	3141	8218	3345	115
H(18C)	2681	7710	2906	115
H(19A)	6585	9477	2706	58
H(19B)	7389	10116	2750	58
H(20A)	7349	10107	3630	126
H(20B)	7499	9336	3466	126
H(21A)	5610	9663	4559	167
H(21B)	6613	10118	4343	167
H(21C)	6800	9331	4439	167
H(22A)	6205	8555	3898	178
H(22B)	5499	8706	3375	178
H(22C)	4914	8752	3942	178

H(23A)	2159	9991	3850	113
H(23B)	2119	9867	4473	113
H(23C)	2602	9297	4091	113
H(25)	9238	10473	4234	117
H(24)	9135	9329	4371	122
H(26)	9918	8833	5132	121
H(4A)	4238	1446	4425	132
H(26A)	2225	1781	4755	186
H(26B)	2472	1715	4136	186
H(26C)	3119	2265	4480	186

D. X-Ray Diffraction Data for Rh($N^{py}N'O_2^{Me}$)(Cl)(CH_3OH) (**2c**).

Table 1. Crystal data and structure refinement for C24 H27 Cl N2 O4 Rh.

Identification code	rhnnoom	
Empirical formula	C24 H27 Cl N2 O4 Rh	
Formula weight	545.84	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.2566(18) Å	α= 76.053(3)°.
	b = 9.2615(18) Å	β= 77.247(3)°.
	c = 13.978(3) Å	γ = 81.376(3)°.
Volume	1128.4(4) $Å^3$	
Z	2	
Density (calculated)	1.607 Mg/m^3	
Absorption coefficient	0.909 mm^{-1}	
F(000)	558	
Crystal size	0.13 x 0.10 x 0.02 mm^3	
Theta range for data collection	1.53 to 27.54°.	
Index ranges	-11<=h<=10, -11<=k<=11, -17<=l<=18	
Reflections collected	6872	
Independent reflections	4846 [R(int) = 0.0315]	
Completeness to theta = 27.54°	93.0 %	
Transmission factors	min/max ratio: 0.574	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4846 / 0 / 289	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0684, wR2 = 0.1880	
R indices (all data)	R1 = 0.0970, wR2 = 0.2514	
Largest diff. peak and hole	1.573 and -2.497 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C24 H27 Cl N2 O4 Rh. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	7855(1)	5957(1)	6193(1)	23(1)
Cl(1)	7139(2)	5617(2)	4732(1)	29(1)
O(1)	8632(7)	6328(7)	7323(4)	36(1)
O(2)	9878(6)	6637(8)	5340(4)	39(2)
O(3)	8829(6)	3893(6)	6392(4)	28(1)
O(4)	766(14)	8368(17)	6719(11)	134(5)
N(1)	5852(7)	5455(7)	7060(5)	25(1)
N(2)	6822(7)	7981(7)	6062(4)	25(1)
C(1)	4742(8)	6588(9)	6618(6)	28(2)
C(2)	5314(10)	8070(10)	6341(6)	33(2)
C(3)	4442(11)	9403(10)	6378(6)	39(2)
C(4)	5133(14)	10751(10)	6063(6)	48(3)
C(5)	6659(14)	10655(11)	5754(7)	50(3)
C(6)	7480(12)	9296(11)	5756(7)	43(2)
C(7)	8423(9)	5257(10)	8182(6)	32(2)
C(8)	9641(10)	4577(13)	8644(7)	49(3)
C(9)	9373(11)	3465(15)	9516(7)	59(3)
C(10)	7961(10)	3018(11)	9936(7)	41(2)
C(11)	6809(9)	3723(9)	9490(6)	28(2)
C(12)	7015(9)	4823(8)	8630(5)	24(2)
C(13)	11183(12)	5060(19)	8183(8)	83(5)
C(14)	7776(12)	1732(13)	10841(7)	53(3)
C(15)	5732(9)	5615(9)	8130(6)	27(2)
C(16)	5569(8)	3913(9)	7041(6)	26(2)
C(17)	6665(8)	2662(8)	7437(5)	21(1)
C(18)	6129(9)	1413(9)	8140(6)	29(2)
C(19)	7047(10)	216(9)	8492(6)	33(2)
C(20)	8559(12)	268(12)	8168(8)	59(3)
C(21)	9172(10)	1477(11)	7473(7)	48(3)
C(22)	8221(9)	2708(9)	7093(6)	29(2)
C(23)	6464(11)	-1118(10)	9250(7)	43(2)

C(24)	10833(16)	1576(17)	7144(11)	81(4)

Table 3. Bond lengths [Å] and angles [°] for C24 H27 Cl N2 O4 Rh.

Rh(1)-N(2)	1.958(6)
Rh(1)-O(3)	1.971(5)
Rh(1)-O(1)	1.992(6)
Rh(1)-N(1)	2.029(6)
Rh(1)-O(2)	2.081(5)
Rh(1)-Cl(1)	2.3821(19)
O(1)-C(7)	1.358(10)
O(3)-C(22)	1.380(10)
N(1)-C(1)	1.478(10)
N(1)-C(16)	1.498(10)
N(1)-C(15)	1.516(9)
N(2)-C(2)	1.360(11)
N(2)-C(6)	1.376(11)
C(1)-C(2)	1.478(12)
C(2)-C(3)	1.375(11)
C(3)-C(4)	1.418(14)
C(4)-C(5)	1.379(15)
C(5)-C(6)	1.369(14)
C(7)-C(12)	1.389(11)
C(7)-C(8)	1.413(12)
C(8)-C(9)	1.395(14)
C(8)-C(13)	1.517(14)
C(9)-C(10)	1.390(13)
C(10)-C(11)	1.357(12)
C(10)-C(14)	1.512(13)
C(11)-C(12)	1.374(11)
C(12)-C(15)	1.514(10)
C(16)-C(17)	1.505(10)
C(17)-C(18)	1.399(11)
C(17)-C(22)	1.418(10)
C(18)-C(19)	1.353(11)
C(19)-C(20)	1.377(14)
C(19)-C(23)	1.503(12)
C(20)-C(21)	1.393(14)

C(21)-C(22)	1.404(11)
C(21)-C(24)	1.515(17)

N(2)-Rh(1)-O(3)	177.1(2)
N(2)-Rh(1)-O(1)	87.7(3)
O(3)-Rh(1)-O(1)	91.1(2)
N(2)-Rh(1)-N(1)	81.2(3)
O(3)-Rh(1)-N(1)	96.3(2)
O(1)-Rh(1)-N(1)	93.6(2)
N(2)-Rh(1)-O(2)	94.9(3)
O(3)-Rh(1)-O(2)	87.6(2)
O(1)-Rh(1)-O(2)	83.8(2)
N(1)-Rh(1)-O(2)	175.4(2)
N(2)-Rh(1)-Cl(1)	92.18(18)
O(3)-Rh(1)-Cl(1)	89.32(17)
O(1)-Rh(1)-Cl(1)	174.26(17)
N(1)-Rh(1)-Cl(1)	92.05(18)
O(2)-Rh(1)-Cl(1)	90.53(17)
C(7)-O(1)-Rh(1)	115.1(5)
C(22)-O(3)-Rh(1)	123.8(4)
C(1)-N(1)-C(16)	110.8(6)
C(1)-N(1)-C(15)	107.2(6)
C(16)-N(1)-C(15)	110.8(6)
C(1)-N(1)-Rh(1)	105.5(5)
C(16)-N(1)-Rh(1)	110.4(4)
C(15)-N(1)-Rh(1)	112.0(5)
C(2)-N(2)-C(6)	117.8(7)
C(2)-N(2)-Rh(1)	115.9(6)
C(6)-N(2)-Rh(1)	126.3(6)
N(1)-C(1)-C(2)	109.3(7)
N(2)-C(2)-C(3)	122.8(8)
N(2)-C(2)-C(1)	112.5(7)
C(3)-C(2)-C(1)	124.7(8)
C(2)-C(3)-C(4)	118.8(9)
C(5)-C(4)-C(3)	118.1(8)
C(6)-C(5)-C(4)	120.8(9)

C(5)-C(6)-N(2)	121.7(10)
O(1)-C(7)-C(12)	120.9(7)
O(1)-C(7)-C(8)	120.3(8)
C(12)-C(7)-C(8)	118.7(8)
C(9)-C(8)-C(7)	118.1(9)
C(9)-C(8)-C(13)	122.2(9)
C(7)-C(8)-C(13)	119.7(9)
C(10)-C(9)-C(8)	122.1(9)
C(11)-C(10)-C(9)	118.3(9)
C(11)-C(10)-C(14)	122.6(9)
C(9)-C(10)-C(14)	119.1(8)
C(10)-C(11)-C(12)	121.8(8)
C(11)-C(12)-C(7)	120.9(7)
C(11)-C(12)-C(15)	122.0(7)
C(7)-C(12)-C(15)	117.1(7)
C(12)-C(15)-N(1)	115.2(6)
N(1)-C(16)-C(17)	115.8(6)
C(18)-C(17)-C(22)	119.6(7)
C(18)-C(17)-C(16)	119.0(7)
C(22)-C(17)-C(16)	121.3(7)
C(19)-C(18)-C(17)	122.2(8)
C(18)-C(19)-C(20)	118.2(8)
C(18)-C(19)-C(23)	121.9(8)
C(20)-C(19)-C(23)	119.8(8)
C(19)-C(20)-C(21)	122.7(9)
C(20)-C(21)-C(22)	119.2(9)
C(20)-C(21)-C(24)	123.2(9)
C(22)-C(21)-C(24)	117.5(9)
O(3)-C(22)-C(21)	119.1(7)
O(3)-C(22)-C(17)	122.8(7)
C(21)-C(22)-C(17)	118.1(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C24 H27 Cl N2 O4 Rh. 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)	15(1)	32(1)	21(1)	-5(1)	0(1)	-6(1)
Cl(1)	21(1)	41(1)	24(1)	-11(1)	-3(1)	-3(1)
O(1)	36(3)	49(4)	24(3)	5(3)	-7(2)	-24(3)
O(2)	21(3)	66(4)	28(3)	-16(3)	11(2)	-18(3)
O(3)	14(3)	32(3)	30(3)	5(2)	-4(2)	10(2)
O(4)	106(10)	158(13)	146(12)	-35(10)	-19(9)	-44(9)
N(1)	19(3)	33(3)	24(3)	-13(3)	0(2)	-3(3)
N(2)	30(4)	25(3)	18(3)	5(2)	-17(3)	6(3)
C(1)	20(4)	36(4)	26(4)	-7(3)	-1(3)	0(3)
C(2)	38(5)	41(5)	24(4)	-17(4)	0(3)	-5(4)
C(3)	49(6)	38(5)	29(4)	-14(4)	-9(4)	12(4)
C(4)	88(9)	37(5)	25(4)	-9(4)	-32(5)	12(5)
C(5)	77(8)	39(5)	42(5)	-12(4)	-21(5)	-18(5)
C(6)	61(7)	44(5)	28(4)	-7(4)	-9(4)	-24(5)
C(7)	29(4)	46(5)	20(4)	-5(3)	-3(3)	-12(4)
C(8)	26(5)	88(8)	30(5)	4(5)	-9(4)	-16(5)
C(9)	23(5)	116(10)	30(5)	6(5)	-9(4)	-11(5)
C(10)	30(5)	60(6)	28(4)	1(4)	-9(4)	1(4)
C(11)	24(4)	37(4)	23(4)	-9(3)	-3(3)	-6(3)
C(12)	26(4)	28(4)	20(4)	-4(3)	-7(3)	-2(3)
C(13)	32(6)	171(15)	39(6)	14(7)	-14(5)	-38(8)
C(14)	45(6)	70(7)	36(5)	4(5)	-4(4)	-7(5)
C(15)	26(4)	32(4)	23(4)	-9(3)	-1(3)	0(3)
C(16)	19(4)	32(4)	29(4)	-9(3)	0(3)	-8(3)
C(17)	16(4)	25(4)	19(3)	-3(3)	-2(3)	-2(3)
C(18)	24(4)	31(4)	32(4)	-10(3)	0(3)	-8(3)
C(19)	35(5)	28(4)	26(4)	6(3)	-4(3)	3(3)
C(20)	44(6)	58(7)	52(6)	5(5)	16(5)	6(5)
C(21)	23(5)	49(6)	47(6)	22(4)	2(4)	13(4)
C(22)	23(4)	38(4)	21(4)	-5(3)	4(3)	0(3)
C(23)	48(6)	33(5)	39(5)	-3(4)	3(4)	5(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C24 H27 Cl N2 O4 Rh.

	x	y	z	U(eq)
H(2)	10009	6426	4773	58
H(1A)	3793	6614	7110	34
H(1B)	4551	6326	6015	34
H(3)	3396	9421	6609	47
H(4)	4561	11693	6064	58
H(5)	7147	11543	5538	59
H(6)	8530	9260	5540	51
H(9)	10183	2998	9834	71
H(11)	5833	3449	9781	33
H(13A)	11891	4503	8602	125
H(13B)	11167	6133	8143	125
H(13C)	11488	4857	7507	125
H(14A)	6738	1784	11199	80
H(14B)	8430	1795	11290	80
H(14C)	8039	783	10620	80
H(15A)	5654	6692	8131	33
H(15B)	4799	5224	8539	33
H(16A)	5564	3881	6338	31
H(16B)	4562	3725	7438	31
H(18)	5085	1404	8377	34
H(20)	9211	-553	8429	71
H(23A)	5374	-1006	9368	65
H(23B)	6793	-1192	9882	65
H(23C)	6846	-2027	8995	65
H(24A)	11146	1472	6445	122
H(24B)	11363	773	7574	122
H(24C)	11066	2547	7200	122

E. X-Ray Diffraction Data for Rh($N^{py}N'O_2^{Me}$)(Ph)(CH_3OH) (**3**).

Table 1. Crystal data and structure refinement for C31 H34 N2 O5 Rh.

Identification code	rhn2o2m	
Empirical formula	C31 H34 N2 O5 Rh	
Formula weight	617.51	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.3395(14) Å	α= 90°.
	b = 14.753(2) Å	β= 90°.
	c = 23.961(3) Å	γ = 90°.
Volume	3654.9(8) $Å^3$	
Z	4	
Density (calculated)	1.122 Mg/m^3	
Absorption coefficient	0.500 mm^{-1}	
F(000)	1276	
Crystal size	0.42 x 0.18 x 0.03 mm^3	
Theta range for data collection	1.62 to 25.68°.	
Index ranges	-12<=h<=12, -16<=k<=17, -19<=l<=29	
Reflections collected	20150	
Independent reflections	6911 [R(int) = 0.0598]	
Completeness to theta = 25.68°	99.9 %	
Transmission factors	min/max ratio: 0.252	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6911 / 0 / 352	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0690, wR2 = 0.2131	
R indices (all data)	R1 = 0.1005, wR2 = 0.2348	
Absolute structure parameter	0.47(8)	
Largest diff. peak and hole	1.445 and -0.657 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C31 H34 N2 O5 Rh. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	2532(1)	2081(1)	1423(1)	37(1)
O(1)	1034(6)	2729(4)	1063(2)	39(2)
O(2)	2657(6)	3178(4)	2018(2)	49(1)
O(3)	1178(6)	1480(5)	1962(3)	51(2)
O(4)	9609(8)	116(6)	1663(4)	84(2)
O(5)	1041(10)	4432(7)	2319(4)	98(3)
N(1)	3899(7)	2686(5)	931(3)	38(2)
N(2)	4109(8)	1521(6)	1786(3)	45(2)
C(1)	3405(8)	2809(6)	358(3)	41(2)
C(2)	2287(9)	3418(5)	322(3)	42(2)
C(3)	2329(10)	4102(6)	-83(3)	47(2)
C(4)	1312(11)	4715(7)	-167(4)	54(2)
C(5)	187(10)	4605(7)	153(4)	51(2)
C(6)	113(9)	3902(6)	556(3)	44(2)
C(7)	1183(8)	3327(6)	654(3)	39(2)
C(8)	1403(12)	5462(7)	-578(5)	70(3)
C(9)	-1079(9)	3781(8)	890(4)	60(3)
C(10)	4291(9)	3593(7)	1146(4)	50(2)
C(11)	4781(9)	3590(6)	1745(4)	45(2)
C(12)	6049(9)	3761(7)	1872(4)	54(2)
C(13)	6451(10)	3747(7)	2445(4)	57(3)
C(14)	5538(10)	3569(7)	2844(4)	56(3)
C(15)	4269(9)	3386(7)	2723(4)	50(2)
C(16)	3866(8)	3396(6)	2167(4)	43(2)
C(17)	7839(9)	3953(9)	2599(5)	75(3)
C(18)	3278(11)	3149(8)	3168(4)	66(3)
C(19)	5036(8)	2065(7)	933(4)	44(2)
C(20)	5202(9)	1619(7)	1507(4)	47(2)
C(21)	6359(10)	1289(7)	1702(4)	57(3)
C(22)	6384(11)	857(8)	2181(6)	73(3)
C(23)	5245(12)	752(7)	2511(5)	69(3)

C(24)	4135(11)	1091(7)	2285(5)	58(3)
C(25)	2247(7)	985(6)	920(3)	40(2)
C(26)	2870(9)	149(6)	1040(4)	49(2)
C(27)	2563(14)	-630(6)	738(4)	67(3)
C(28)	1668(10)	-599(7)	307(4)	60(3)
C(29)	1082(12)	229(8)	191(5)	74(3)
C(30)	1368(11)	971(7)	492(4)	56(3)
C(31)	114(14)	2055(11)	2182(6)	94(4)

Table 3. Bond lengths [Å] and angles [°] for C31 H34 N2 O5 Rh.

Rh(1)-O(1)	2.013(6)
Rh(1)-N(2)	2.025(8)
Rh(1)-C(25)	2.037(9)
Rh(1)-N(1)	2.045(8)
Rh(1)-O(3)	2.101(6)
Rh(1)-O(2)	2.161(6)
O(1)-C(7)	1.329(10)
O(2)-C(16)	1.339(11)
O(3)-C(31)	1.486(16)
N(1)-C(1)	1.476(10)
N(1)-C(19)	1.490(11)
N(1)-C(10)	1.490(12)
N(2)-C(20)	1.319(12)
N(2)-C(24)	1.355(12)
C(1)-C(2)	1.467(12)
C(2)-C(7)	1.397(12)
C(2)-C(3)	1.401(11)
C(3)-C(4)	1.401(14)
C(4)-C(5)	1.403(14)
C(4)-C(8)	1.481(14)
C(5)-C(6)	1.418(13)
C(6)-C(7)	1.414(12)
C(6)-C(9)	1.481(12)
C(10)-C(11)	1.522(12)
C(11)-C(12)	1.369(13)
C(11)-C(16)	1.415(13)
C(12)-C(13)	1.436(13)
C(13)-C(14)	1.367(14)
C(13)-C(17)	1.513(14)
C(14)-C(15)	1.370(13)
C(15)-C(16)	1.395(12)
C(15)-C(18)	1.520(13)
C(19)-C(20)	1.534(12)
C(20)-C(21)	1.374(13)

C(21)-C(22)	1.312(16)
C(22)-C(23)	1.426(17)
C(23)-C(24)	1.364(15)
C(25)-C(30)	1.371(12)
C(25)-C(26)	1.420(12)
C(26)-C(27)	1.394(12)
C(27)-C(28)	1.389(14)
C(28)-C(29)	1.391(16)
C(29)-C(30)	1.343(14)

O(1)-Rh(1)-N(2)	175.6(3)
O(1)-Rh(1)-C(25)	90.7(3)
N(2)-Rh(1)-C(25)	92.7(3)
O(1)-Rh(1)-N(1)	94.5(2)
N(2)-Rh(1)-N(1)	82.4(3)
C(25)-Rh(1)-N(1)	96.1(3)
O(1)-Rh(1)-O(3)	87.2(3)
N(2)-Rh(1)-O(3)	95.8(3)
C(25)-Rh(1)-O(3)	86.1(3)
N(1)-Rh(1)-O(3)	177.2(3)
O(1)-Rh(1)-O(2)	88.5(2)
N(2)-Rh(1)-O(2)	88.5(3)
C(25)-Rh(1)-O(2)	173.2(3)
N(1)-Rh(1)-O(2)	90.7(3)
O(3)-Rh(1)-O(2)	87.1(3)
C(7)-O(1)-Rh(1)	122.9(5)
C(16)-O(2)-Rh(1)	114.3(5)
C(31)-O(3)-Rh(1)	118.1(7)
C(1)-N(1)-C(19)	110.6(7)
C(1)-N(1)-C(10)	107.8(7)
C(19)-N(1)-C(10)	109.6(7)
C(1)-N(1)-Rh(1)	110.5(5)
C(19)-N(1)-Rh(1)	106.0(5)
C(10)-N(1)-Rh(1)	112.4(5)
C(20)-N(2)-C(24)	118.7(9)
C(20)-N(2)-Rh(1)	115.4(6)

C(24)-N(2)-Rh(1)	125.9(7)
C(2)-C(1)-N(1)	113.7(7)
C(7)-C(2)-C(3)	119.2(9)
C(7)-C(2)-C(1)	123.5(7)
C(3)-C(2)-C(1)	117.2(8)
C(2)-C(3)-C(4)	122.8(9)
C(3)-C(4)-C(5)	118.0(8)
C(3)-C(4)-C(8)	121.9(9)
C(5)-C(4)-C(8)	120.2(10)
C(4)-C(5)-C(6)	120.1(9)
C(7)-C(6)-C(5)	120.6(8)
C(7)-C(6)-C(9)	119.3(8)
C(5)-C(6)-C(9)	120.1(9)
O(1)-C(7)-C(2)	125.3(8)
O(1)-C(7)-C(6)	115.5(7)
C(2)-C(7)-C(6)	119.2(8)
N(1)-C(10)-C(11)	114.5(8)
C(12)-C(11)-C(16)	121.2(8)
C(12)-C(11)-C(10)	121.9(8)
C(16)-C(11)-C(10)	116.9(8)
C(11)-C(12)-C(13)	119.2(9)
C(14)-C(13)-C(12)	118.1(9)
C(14)-C(13)-C(17)	121.6(9)
C(12)-C(13)-C(17)	120.3(10)
C(13)-C(14)-C(15)	123.4(9)
C(14)-C(15)-C(16)	119.1(9)
C(14)-C(15)-C(18)	122.8(9)
C(16)-C(15)-C(18)	118.1(8)
O(2)-C(16)-C(15)	122.1(8)
O(2)-C(16)-C(11)	118.8(8)
C(15)-C(16)-C(11)	119.0(8)
N(1)-C(19)-C(20)	110.8(7)
N(2)-C(20)-C(21)	122.3(9)
N(2)-C(20)-C(19)	113.8(8)
C(21)-C(20)-C(19)	123.7(9)
C(22)-C(21)-C(20)	119.1(10)

C(21)-C(22)-C(23)	121.4(10)
C(24)-C(23)-C(22)	115.8(10)
N(2)-C(24)-C(23)	122.6(11)
C(30)-C(25)-C(26)	116.0(8)
C(30)-C(25)-Rh(1)	123.4(7)
C(26)-C(25)-Rh(1)	120.3(6)
C(27)-C(26)-C(25)	120.5(8)
C(28)-C(27)-C(26)	120.7(9)
C(27)-C(28)-C(29)	117.8(9)
C(30)-C(29)-C(28)	120.9(10)
C(29)-C(30)-C(25)	124.0(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C31 H34 N2 O5 Rh. 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)	37(1)	42(1)	33(1)	2(1)	1(1)	0(1)
O(1)	35(3)	44(4)	38(3)	11(3)	-5(3)	2(3)
O(2)	45(4)	53(3)	48(3)	-10(2)	16(3)	8(3)
O(3)	48(4)	63(5)	41(4)	17(3)	9(3)	-4(3)
O(4)	59(5)	96(6)	98(6)	22(5)	-3(4)	-18(4)
N(1)	44(4)	44(5)	26(4)	-1(3)	-2(3)	5(3)
N(2)	58(5)	50(5)	28(4)	6(3)	-3(3)	-6(4)
C(1)	38(4)	50(5)	37(4)	-5(4)	5(4)	-3(4)
C(2)	54(6)	37(4)	35(4)	-1(3)	-6(4)	-12(4)
C(3)	53(6)	52(5)	35(4)	-1(3)	-9(4)	-5(5)
C(4)	78(7)	50(6)	33(5)	1(4)	-4(5)	-8(5)
C(5)	61(6)	56(6)	36(5)	0(4)	-10(4)	5(5)
C(6)	44(5)	49(5)	39(5)	-4(4)	-2(4)	2(4)
C(7)	39(5)	49(5)	28(4)	-10(4)	0(4)	5(4)
C(8)	92(9)	54(6)	65(7)	18(5)	-18(6)	1(6)
C(9)	42(5)	91(8)	46(6)	7(5)	9(4)	24(5)
C(10)	48(5)	57(6)	46(5)	6(4)	4(4)	-7(5)
C(11)	44(5)	46(5)	46(5)	-14(4)	1(4)	-1(4)
C(12)	41(5)	67(7)	54(6)	-10(5)	3(4)	-7(5)
C(13)	52(6)	55(6)	64(7)	-10(5)	-20(5)	-6(5)
C(14)	70(7)	52(6)	45(6)	-18(5)	4(5)	-8(5)
C(15)	57(6)	56(6)	36(5)	-11(4)	3(4)	-5(5)
C(16)	38(5)	42(5)	48(5)	-8(4)	1(4)	-2(4)
C(17)	48(7)	91(9)	85(8)	-25(7)	-13(5)	8(5)
C(18)	77(7)	76(8)	45(6)	-8(5)	4(5)	-15(6)
C(19)	38(5)	52(5)	43(5)	1(4)	5(4)	3(4)
C(20)	41(5)	53(5)	46(5)	-12(4)	-10(4)	-3(4)
C(21)	61(6)	63(6)	46(6)	-5(5)	-16(5)	7(5)
C(22)	43(6)	81(8)	94(9)	-11(7)	-21(6)	17(6)
C(23)	89(9)	45(6)	72(8)	8(5)	-38(7)	-1(6)
C(24)	62(6)	53(6)	60(6)	-13(5)	-24(5)	-1(5)

C(25)	34(6)	47(5)	37(4)	13(3)	0(3)	-7(4)
C(26)	50(6)	46(5)	51(5)	2(4)	-13(4)	-3(4)
C(27)	81(7)	44(5)	75(6)	3(4)	-28(8)	-3(7)
C(28)	63(6)	53(6)	65(7)	-17(5)	-11(5)	-7(5)
C(29)	77(8)	75(8)	71(7)	10(6)	-34(6)	-16(6)
C(30)	73(7)	44(6)	50(6)	-6(5)	-13(5)	-3(5)
C(31)	93(10)	115(11)	74(9)	24(8)	6(7)	-22(9)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C31 H34 N2 O5 Rh.

	x	y	z	U(eq)
H(1A)	4109	3053	121	50
H(1B)	3159	2209	205	50
H(3)	3078	4153	-310	56
H(5)	-526	5002	100	61
H(8A)	1664	6021	-388	106
H(8B)	559	5552	-756	106
H(8C)	2046	5307	-863	106
H(9A)	-1512	3219	778	90
H(9B)	-1660	4296	827	90
H(9C)	-854	3749	1287	90
H(10A)	3539	4007	1121	60
H(10B)	4979	3839	901	60
H(12)	6655	3887	1584	65
H(14)	5796	3573	3224	67
H(17A)	7859	4339	2931	112
H(17B)	8262	4267	2288	112
H(17C)	8298	3385	2676	112
H(18A)	3694	3153	3535	99
H(18B)	2923	2545	3093	99
H(18C)	2578	3597	3162	99
H(19A)	5826	2411	839	53
H(19B)	4916	1590	646	53
H(21)	7131	1372	1494	68
H(22)	7177	609	2311	88
H(23)	5260	465	2866	82
H(24)	3348	1022	2486	70
H(26)	3500	121	1328	59
H(27)	2971	-1188	829	80
H(28)	1462	-1126	97	72
H(29)	471	270	-104	89

H(30)	935	1519	402	67
H(31A)	407	2369	2519	141
H(31B)	-633	1674	2272	141
H(31C)	-134	2503	1899	141

1. (a) G.M. Sheldrick, *SHELXTL*, version 6.14; Bruker Analytical X-ray System, Inc.: Madison, WI, 1997 (b) R. H. Blessing, Acta Crystallogr. A51, 1995, **33**. (c) Internal Tables for Crystallographers, Vol. A, Space-Group Symmetry. D. Reidel Publishing Company, 1983, ISBN 90-277-1445-2.

Theory: All theoretical calculations were performed with the B3LYP[1,2] density functional, in combination with the Jaguar 6.5[3] computational package. Rhodium was described with the effective core potential of Hay and Wadt[4], while all other atoms used the 6-31G** all electron basis set. [5]

The following includes the Cartesian coordinates (in Angstroms) and gas-phase electronic energies (in Hartrees) for *cis*-O,O and *trans*-O,O isomers of species **2a**, **2b** and **2c**.

Compound 2a – trans-O,O R=t-Bu S=CH_3OH, N=C_6H_4N

Electronic Energy: -2347.50313294350

H	1.3882676385	-1.1450654190	-0.1925091806
C	1.9601820507	-1.8680241226	0.3771649273
C	3.4253624592	-3.6992899083	1.8164713244
C	1.2929742616	-2.5938710515	1.3660641263
C	3.3290294121	-1.9958251591	0.0756010642
C	4.0413030042	-2.9316074755	0.8200006743
C	2.0516542731	-3.5427127430	2.1282311962
H	5.1010033079	-3.0899402186	0.6387522649
O	1.4640098086	-4.2767369583	3.0705722035
C	4.2537471741	-4.6845240873	2.5883080142
H	3.8788537465	-5.7089571554	2.5036611630
H	5.2871704635	-4.6707186804	2.2154410403
Rh	2.3671729761	-4.8190465104	4.8481732539
N	2.4948134485	-2.9223569833	5.5365170826
C	2.9177776345	-0.3777210373	6.5352993879
C	1.5490401015	-2.3323947384	6.2955054645
C	3.6461600626	-2.2778221249	5.2524762573
C	3.8844328701	-0.9968977775	5.7496431531
C	1.7292690880	-1.0551015758	6.8075168871
H	0.6606163752	-2.9275083147	6.4726492272
H	4.8199444359	-0.4995775739	5.5143522232
H	0.9480508476	-0.6102345455	7.4138711082
H	3.0894297393	0.6194271673	6.9297568692
C	4.6310042424	-2.9604597425	4.3390442603
H	5.6340380392	-2.8914852679	4.7687139632
H	4.6316781499	-2.4246736617	3.3853193446
O	3.1697120519	-5.6750295348	6.5679107701
N	4.2881855037	-4.3965709655	4.0712036938
C	5.2792919579	-5.3188735533	4.7345056346
H	4.9117588231	-6.3311274719	4.5401270433
H	6.2430733585	-5.2010915085	4.2203090977
C	5.4460566282	-5.0540361896	6.2014428833
C	5.7962158953	-4.6543080331	8.8975471977
C	4.3456971879	-5.2764726797	7.0629730543
C	6.6782208491	-4.6023627671	6.6873672357
C	6.8815323727	-4.3761366751	8.0464401819
C	4.5428998021	-5.1007945251	8.4698345155

H	7.4825963835	-4.4448024031	5.9745580897
H	5.9443558284	-4.5051999342	9.9605713469
C	3.4205406200	-5.4205332143	9.4805047185
C	8.2075230355	-3.8524720849	8.6296508188
C	-0.2147163927	-2.3878463150	1.6302439505
C	3.9681911861	-1.1150712114	-1.0142657252
Cl	0.1763779072	-5.2700884217	5.7667679112
O	2.4487309180	-6.8895591599	4.2552097860
C	1.3421232069	-7.4688437900	3.5193004061
H	1.6087293866	-8.4917077137	3.2365395410
H	0.4315978883	-7.4407979177	4.1188590027
H	1.2111674907	-6.8436462192	2.6374712999
H	2.4940467842	-7.2531533950	5.1585092799
C	-0.4412003469	-1.9346327297	3.0931703055
H	-0.1030585135	-2.6996785038	3.7918483495
H	0.0945535259	-0.9992710900	3.2971164103
H	-1.5085505794	-1.7539699682	3.2692386679
C	-0.9742978180	-3.7131745647	1.3790048517
H	-2.0458435927	-3.5759211625	1.5677797332
H	-0.8542129041	-4.0350191104	0.3381697816
H	-0.6061905531	-4.5013759494	2.0371461787
C	-0.8283668824	-1.3143116641	0.7082645735
H	-0.3668761162	-0.3306720773	0.8531320189
H	-0.7435647535	-1.5804162976	-0.3512958865
H	-1.8950763070	-1.2118491945	0.9351087819
C	3.8024744139	0.3774854935	-0.6389143600
H	4.2451635252	1.0220670835	-1.4079398141
H	2.7490219288	0.6548263274	-0.5385660264
H	4.2967705352	0.5981376478	0.3138249050
C	3.2757805364	-1.3777851990	-2.3726285338
H	2.2046974616	-1.1577845319	-2.3312063168
H	3.7145685294	-0.7510868788	-3.1584079515
H	3.3888848383	-2.4253883132	-2.6703197486
C	5.4733573366	-1.3984074293	-1.1825757069
H	6.0304965406	-1.2004036550	-0.2599796402
H	5.6620186973	-2.4357786380	-1.4794311726
H	5.8890720108	-0.7513332249	-1.9626122140
C	2.1839343792	-4.5307357479	9.2118991741
H	2.4464350184	-3.4691419249	9.2981990356
H	1.7728026142	-4.7181203833	8.2197294682
H	1.4029901389	-4.7421013579	9.9524779279
C	3.0220786783	-6.9111622724	9.3465060592
H	3.8768043125	-7.5628595801	9.5627544954
H	2.2233986492	-7.1549615403	10.0571758192
H	2.6633663224	-7.1261935334	8.3387610618
C	3.8610720387	-5.1830328377	10.9394400902
H	3.0333251349	-5.4356011611	11.6107743620

H	4.7150766416	-5.8085128750	11.2224376325
H	4.1252438667	-4.1359106375	11.1271584174
C	8.7916009711	-4.8891151844	9.6189865804
H	9.7324296878	-4.5252528253	10.0494535320
H	8.1043138079	-5.0924972432	10.4457550486
H	8.9944483016	-5.8393599572	9.1134161105
C	9.2602574430	-3.5900740761	7.5353862031
H	9.5150179411	-4.5031918587	6.9865271278
H	8.9171867230	-2.8416335621	6.8122161368
H	10.1823970119	-3.2106609390	7.9889277824
C	7.9548704562	-2.5205301754	9.3774332690
H	7.5557949542	-1.7602399682	8.6966453237
H	7.2380451210	-2.6424796177	10.1950487017
H	8.8874224502	-2.1345735216	9.8066873364

Compound 2a′ – cis-O,O R=t-Bu S=CH_3OH, N=C_6H_4N

Electronic Energy: -2347.49778372243

H	2.8091897068	-1.2107471942	0.5650202719
C	2.1892182646	-0.9612251739	1.4176666623
C	0.5688425516	-0.2658012850	3.5288556883
C	1.1664880542	-1.8478954613	1.7639670774
C	2.4707375720	0.2369999586	2.0965799996
C	1.6132435434	0.5779488677	3.1394665149
C	0.3792360261	-1.5239073780	2.9116200186
H	1.7346021732	1.5175802011	3.6694597749
O	-0.5810370519	-2.3442605972	3.3582377576
C	-0.4989389892	0.2643248097	4.4474333430
H	-0.2564627484	1.2927538955	4.7431359079
H	-1.4443276692	0.2911944721	3.8935783460
Rh	-0.9671799828	-2.5043561354	5.3697865054
N	-2.9323610801	-1.9960893389	4.9321664691
C	-5.4054443753	-0.9318010975	4.3130574988
C	-3.8088984933	-2.7186360076	4.2219051369
C	-3.2477990732	-0.7521101453	5.3502313444
C	-4.4830756711	-0.1861454533	5.0465932410
C	-5.0661628881	-2.2188268388	3.8972150653
H	-3.4733507843	-3.7063342217	3.9269130464
H	-4.7126692538	0.8211698169	5.3789239024
H	-5.7566094272	-2.8263862337	3.3223212294
H	-6.3745967236	-0.5097084695	4.0644088266
O	0.9700062400	-2.9225388199	5.8085577476
N	-0.8209469328	-0.4893764522	5.7222754735
C	0.1754143679	-0.2400696287	6.8169179491
H	0.1749376190	0.8397992591	7.0202346681
H	-0.2308140359	-0.7564220041	7.6915314089
C	1.5862826676	-0.6963897065	6.5509594028
C	4.2306386531	-1.4781194437	6.5437074380
C	1.8918357598	-2.0316596232	6.1762633142
C	2.6038424522	0.2178066032	6.8574906320
C	3.9476717474	-0.1367167670	6.8517199543
C	3.2705822957	-2.4353005527	6.2202352713
H	2.3078981859	1.2275291751	7.1284035636
H	5.2676124902	-1.7905687661	6.5677052292
C	3.6814045010	-3.9052758107	5.9770960639
C	5.0906678267	0.8309240349	7.2109500284
C	0.8471526763	-3.0765916287	0.8794100244
C	3.6679997822	1.1019186746	1.6588914473
C	-2.1884981823	-0.0773552556	6.1841878701
H	-2.2862521586	1.0150179435	6.1550755067
H	-2.2935612604	-0.4213734695	7.2176009831
O	-1.2383909456	-4.5593240136	4.7380768468
C	-0.7037661844	-5.6487880594	5.5256217692

H	-1.1888880311	-5.5821893816	6.4980618087
H	-0.9512292395	-6.5948291652	5.0337708000
H	0.3745741400	-5.5405441001	5.6473664088
Cl	-1.6426196831	-2.9965206492	7.6553806133
H	-0.7609549656	-4.4798726890	3.8932200207
C	-0.6301505411	-3.0067514655	0.4183433366
H	-1.3113262917	-2.9922375021	1.2711666034
H	-0.8039520194	-2.1007276543	-0.1724979468
H	-0.8730890673	-3.8713143918	-0.2117928750
C	1.0938987414	-4.3973751439	1.6399965388
H	2.1533906825	-4.5211281225	1.8788517507
H	0.5460465130	-4.4182619899	2.5830238071
H	0.7761573521	-5.2553683036	1.0352199936
C	1.7193839646	-3.1265162675	-0.3931225299
H	1.4281678050	-3.9926367759	-0.9976807650
H	1.5923301113	-2.2329608223	-1.0130711728
H	2.7843511882	-3.2352145928	-0.1613676222
C	3.8031678807	2.3773140971	2.5113553216
H	4.6756006790	2.9534539815	2.1841909334
H	2.9255158637	3.0264099075	2.4153655115
H	3.9391908914	2.1414330265	3.5719484729
C	3.5044496492	1.5301635177	0.1807274810
H	4.3610954276	2.1349465056	-0.1409705711
H	3.4389235819	0.6676612512	-0.4898436828
H	2.5966165261	2.1280436090	0.0438731581
C	4.9716503832	0.2808606496	1.8101190199
H	4.9550115059	-0.6208511867	1.1896853049
H	5.8425217612	0.8761622290	1.5092653217
H	5.1141704133	-0.0336793035	2.8491812251
C	3.2702025700	-4.3537724684	4.5568071564
H	2.1985019873	-4.2344630345	4.4089475923
H	3.7849273920	-3.7526209082	3.7988078859
H	3.5390993706	-5.4055974633	4.3946039627
C	3.0001241791	-4.8016121059	7.0408901192
H	3.2079897230	-5.8605543785	6.8402843319
H	3.3836891235	-4.5684139140	8.0405218410
H	1.9205480465	-4.6474668372	7.0522986091
C	5.2031223703	-4.1274959778	6.1032388040
H	5.5752527412	-3.8743100036	7.1016225469
H	5.4269024850	-5.1862963965	5.9302056712
H	5.7700036640	-3.5481389617	5.3659587991
C	5.7924975970	0.3398177148	8.5010733638
H	6.6161031908	1.0102415630	8.7765494396
H	5.0873873010	0.3041427052	9.3384648204
H	6.2083118976	-0.6648100401	8.3754098693
C	4.5837240238	2.2645301525	7.4590962669
H	3.8928109706	2.3096399948	8.3077516843

H	5.4275395526	2.9249067415	7.6877628916
H	4.0722436527	2.6721746293	6.5799816574
C	6.1272448683	0.8819982788	6.0639109609
H	6.5492767977	-0.1055473065	5.8554756432
H	5.6723219501	1.2506773840	5.1383972163
H	6.9579596156	1.5499662084	6.3228165481

Compound 2b – trans-O,O R=Me S=CH_3OH, N=$CH_2N(CH_3)_2$

Electronic Energy: -1801.92856443459

H	0.9386203159	-1.8188115608	-0.6645450435
C	1.6353441341	-2.2648329705	0.0443304654
C	3.3956142238	-3.4435774250	1.8577834051
C	1.1150757549	-2.9417524312	1.1426290096
C	3.0146759389	-2.1317654120	-0.1796191506
C	3.8676032671	-2.7317443828	0.7428971961
C	1.9991447846	-3.5403739715	2.0863055954
H	4.9438808557	-2.6694321424	0.5858801514
O	1.4569518794	-4.1413603890	3.1391156694
C	4.3998911741	-4.2073160873	2.6837186340
H	4.2819231250	-5.2837059571	2.5360581146
H	5.4127721098	-3.9243631730	2.3674617555
Rh	2.4728125557	-4.6387060480	4.8422568095
N	2.2798589370	-2.6188753421	5.6352741294
C	3.6994047218	-2.1761783986	5.7721569759
C	4.5062528074	-2.5599059282	4.5364840744
H	5.5682523770	-2.3530440497	4.7105468631
H	4.1871967589	-1.9786587676	3.6687553968
O	3.1502462735	-5.2332059191	6.6928984077
N	4.3309630483	-4.0112383766	4.1822731291
C	5.3951662910	-4.8846240724	4.8006206360
H	5.1590925468	-5.8965293214	4.4599160791
H	6.3539033389	-4.5855657157	4.3561617387
C	5.5118342236	-4.8478092984	6.3007922470
C	5.9070887356	-5.0918269517	9.0448405055
C	4.3985042631	-5.1225440485	7.1335952511
C	6.7818582200	-4.6662082137	6.8672910191
C	7.0108038407	-4.7787604937	8.2365195057
C	4.6238607065	-5.2626577945	8.5339392180
H	7.6199623440	-4.4499789098	6.2054263458
H	6.0531215452	-5.2024048273	10.1188648427
C	3.4634167354	-5.6108324131	9.4321441044
H	2.6937945106	-4.8284512230	9.4323588807
H	2.9682805901	-6.5301648781	9.0989979820
H	3.7962110053	-5.7543748288	10.4644756836
C	8.3885834295	-4.5974214624	8.8310454275
H	8.3784640280	-3.8950901253	9.6733676086
H	8.7962081509	-5.5434440584	9.2101510125
H	9.0947924004	-4.2126765801	8.0885397341
C	-0.3722084543	-3.0761218041	1.3523420199
H	-0.6747191970	-4.1297681519	1.3819539477
H	-0.6878255698	-2.6379478006	2.3072183454
H	-0.9290387837	-2.5828014066	0.5501687847
C	3.5416498941	-1.3690107948	-1.3736520358
H	3.1127449403	-1.7406132822	-2.3121068131

H	3.3002977558	-0.2997046975	-1.3149982360
H	4.6298790997	-1.4554128634	-1.4522931465
O	0.4450296007	-5.1659307203	5.3864909625
C	0.2232438317	-6.3604840472	6.1744809550
H	-0.8360399143	-6.4121850251	6.4450575758
H	0.5384084273	-7.2457791977	5.6203128877
H	0.8454372232	-6.2525932949	7.0614330654
H	0.1114618267	-5.2878178920	4.4802403463
Cl	2.7363230210	-6.8641738841	3.9773732541
H	4.1136637314	-2.6579615750	6.6569462765
H	3.7414897143	-1.0872601485	5.9221885416
C	1.5196469750	-1.7053403495	4.7472515641
H	1.4380202872	-0.7176455917	5.2211621070
H	2.0092427165	-1.6062516331	3.7802619499
H	0.5256572040	-2.1186490647	4.5807532399
C	1.6180511425	-2.6458344283	6.9628260182
H	0.5754370379	-2.9347096718	6.8228575359
H	2.1109753601	-3.3905217231	7.5845938108
H	1.6633087132	-1.6535634688	7.4316545881

Compound 2b′ – cis-O,O R=Me S=CH_3OH, N=$CH_2N(CH_3)_2$

Electronic Energy: -1801.92416317448

H	3.1005709538	-1.2846638064	0.8657245647
C	2.4162721575	-0.9527691439	1.6458074090
C	0.6538653114	-0.1069345165	3.6086814684
C	1.3140059295	-1.7534489909	1.9422265963
C	2.6858496418	0.2492666177	2.3179139370
C	1.7826979590	0.6561955806	3.2987950153
C	0.4125808048	-1.3301481851	2.9510885001
H	1.9575772514	1.5863171358	3.8364227373
O	-0.6817941715	-2.0543426648	3.2302292846
C	-0.4036291001	0.4350706639	4.5271871281
H	-0.0689692807	1.3766862301	4.9782993812
H	-1.2916255817	0.6569562302	3.9300087060
Rh	-1.0339365469	-2.4668211319	5.1974390879
N	-3.1839641596	-2.0503857383	4.8363442186
C	-3.2752418947	-0.5690683948	5.0064063264
O	0.9248329503	-2.8457761696	5.4820629618
N	-0.8754700142	-0.4536866268	5.6640002211
C	0.0386101053	-0.3245045148	6.8534980085
H	0.0169658850	0.7265670130	7.1737131450
H	-0.4107878603	-0.9355365056	7.6402243172
C	1.4647518260	-0.7400896731	6.5975120712
C	4.1465175013	-1.4437485026	6.3427455905
C	1.7973807892	-1.9708033961	5.9803141106
C	2.4837407395	0.1054043814	7.0603760457
C	3.8324555040	-0.2217879404	6.9557801645
C	3.1749524013	-2.3088875941	5.8534709798
H	2.2029962428	1.0501469605	7.5255037296
H	5.1926303947	-1.7266889382	6.2311714311
C	3.5482984442	-3.6008712645	5.1736205827
H	3.1232162325	-4.4658407111	5.6967553479
H	3.1608933551	-3.6295979471	4.1483100438
H	4.6349149266	-3.7250992765	5.1351894064
C	4.9169063452	0.6843575000	7.4910991482
H	5.3025049223	0.3345054739	8.4581953420
H	5.7717539608	0.7344506863	6.8072125539
H	4.5496778957	1.7052165825	7.6388776293
C	1.0653821640	-3.0418374803	1.1987630178
H	0.0325323147	-3.1070850847	0.8411069872
H	1.7346697650	-3.1326154136	0.3379948332
H	1.2337063548	-3.9104772231	1.8459659609
C	3.9158430265	1.0622973642	1.9861405115
H	4.8363339523	0.5125713841	2.2186007044
H	3.9563788525	1.3179228022	0.9203217556
H	3.9407319690	1.9977466403	2.5532024020
C	-2.2738237916	-0.0686666715	6.0458553534

H	-2.3446259598	1.0232954131	6.1477587518
H	-2.4765481654	-0.5183494159	7.0202896921
O	-1.2984984454	-4.6019805775	4.8428514777
C	-0.2539467347	-5.2978040408	4.1264742384
H	0.7251859211	-4.9907055642	4.4984928961
H	-0.4033359661	-6.3764908092	4.2375379259
H	-0.3584935374	-5.0124388533	3.0812195207
Cl	-1.4454498846	-3.2773670161	7.5015979177
H	-1.2577658747	-4.8384041205	5.7918774374
H	-3.0802806329	-0.1124335485	4.0343892698
H	-4.2929593061	-0.2793029056	5.3018473870
C	-4.0964515586	-2.7314084821	5.7876857482
H	-5.1392393176	-2.4888835374	5.5379884925
H	-3.9456247507	-3.8087144334	5.7166520086
H	-3.8740384521	-2.4312783131	6.8094131521
C	-3.5659239215	-2.4384427285	3.4555630180
H	-4.5831687260	-2.0923032657	3.2253921483
H	-2.8422450468	-2.0210398131	2.7565690642
H	-3.5317797655	-3.5270038652	3.3829262974

Compound 2c – cis-O,O R=Me S=CH_3OH, N=C_6H_4N

Electronic Energy: -1875.73808553718

H	3.2860966340	-1.6854986324	1.0798840404
C	2.5380092764	-1.2897579222	1.7656348864
C	0.6242686318	-0.2908007099	3.5137494396
C	1.4652145494	-2.1060116923	2.1185008261
C	2.6991167656	0.0091576994	2.2706684025
C	1.7258879678	0.4881473749	3.1468133713
C	0.4889069889	-1.6026137993	3.0115096778
H	1.8240968921	1.4912678096	3.5582121141
O	-0.5669638410	-2.3598458056	3.3389816364
C	-0.4928219148	0.3011445414	4.3279944505
H	-0.2564309537	1.3389580015	4.5947988934
H	-1.4061246122	0.3094695529	3.7222822851
Rh	-1.0927750945	-2.4362139101	5.3123251769
N	-3.0200100276	-1.8704891280	4.7862474942
C	-5.4410212895	-0.7509655210	4.0650916739
C	-3.8985500889	-2.5868139097	4.0722579796
C	-3.3080983534	-0.6050353712	5.1580524244
C	-4.5161180032	-0.0112341399	4.8015617032
C	-5.1304445837	-2.0598506514	3.6972614021
H	-3.5855098432	-3.5927458095	3.8156074001
H	-4.7242524425	1.0115948390	5.0986261685
H	-5.8237272508	-2.6641223446	3.1225554102
H	-6.3899550842	-0.3080447463	3.7781440069
O	0.8098362603	-2.9039564308	5.7910379568
N	-0.8878032589	-0.4061785119	5.6140392512
C	0.0758773573	-0.1604239178	6.7440542199
H	0.1063776663	0.9232622631	6.9237030774
H	-0.3806157242	-0.6450807949	7.6122867766
C	1.4747586499	-0.6733293736	6.5232382600
C	4.1144771853	-1.5458833358	6.3715902328
C	1.7365177102	-2.0043284298	6.1144173807
C	2.5403984594	0.1824727235	6.8379553848
C	3.8693544140	-0.2249179132	6.7775266578
C	3.0941688363	-2.4281724276	6.0358544139
H	2.3135096472	1.2013647172	7.1505764252
H	5.1434939210	-1.8978106197	6.3061266104
C	3.3889371413	-3.8355114762	5.5847272804
C	5.0067762564	0.7112946217	7.1154996804
C	1.3190443961	-3.5025414982	1.5687267045
C	3.8810633336	0.8575501147	1.8617892719
C	-2.2571083110	0.0612795062	6.0102320000
H	-2.3207735763	1.1548432312	5.9482115436
H	-2.4114315382	-0.2506375017	7.0476487480
O	-1.3107750429	-4.4942084478	4.6891944939
C	-0.7106258153	-5.5156560507	5.5229399088

H	-1.3244522547	-5.5713206753	6.4203392398
H	-0.7304630420	-6.4678457869	4.9839424330
H	0.3059803155	-5.2256397388	5.7925735599
Cl	-1.8770205769	-2.8351345640	7.5837270693
H	-0.7694592252	-4.3444300294	3.8886030787
H	2.1364987673	-3.7435078662	0.8829508469
H	0.3732297867	-3.6273123619	1.0281268154
H	1.3259140386	-4.2484662878	2.3741415485
H	4.0048682385	1.7166336295	2.5280078498
H	4.8138646642	0.2830354555	1.8839531892
H	3.7687610926	1.2466920670	0.8413928421
H	5.6064651767	0.9610634712	6.2305883552
H	5.6920294418	0.2686548169	7.8486970351
H	4.6375017504	1.6520497212	7.5362446751
H	2.9549350054	-4.0278141439	4.5964067575
H	4.4672232472	-4.0136249365	5.5294349152
H	2.9545815919	-4.5757527602	6.2678500896

Compound 2c′ – trans-O,O R=Me S=CH_3OH, N=C_6H_4N

Electronic Energy: -1875.73568430996

H	1.2787389916	-1.0863905510	-0.2372112570
C	1.8985305321	-1.7750306164	0.3362593629
C	3.4645014748	-3.5302898118	1.8177849137
C	1.3128826431	-2.4643133566	1.3928682196
C	3.2535158662	-1.9176207890	-0.0096077935
C	4.0144438056	-2.7991315903	0.7526648099
C	2.1001415223	-3.3689114905	2.1653700771
H	5.0694475870	-2.9353069368	0.5154242133
O	1.4970138752	-4.0248477410	3.1482310352
C	4.3384372578	-4.4869734405	2.5787681164
H	4.0176784266	-5.5275131950	2.4675810884
H	5.3706781981	-4.4135988771	2.2088966508
Rh	2.4320730671	-4.7297713783	4.8387516886
N	2.5972610374	-2.9120860472	5.7127601735
C	3.1223492729	-0.5293253349	7.0172678779
C	1.7052779323	-2.4190594520	6.5949305981
C	3.7432853394	-2.2461955686	5.4525697467
C	4.0335214633	-1.0475850950	6.1022512739
C	1.9372519799	-1.2230044258	7.2612367843
H	0.8186872212	-3.0260436682	6.7414467376
H	4.9648011826	-0.5348199703	5.8848552723
H	1.1994389184	-0.8546596925	7.9654680438
H	3.3348011011	0.4022357475	7.5333610892
C	4.6367993430	-2.8034484271	4.3772515039
H	5.6874764483	-2.6732139422	4.6545433679
H	4.4546007630	-2.2294142403	3.4625681235
O	3.2445359358	-5.7200978337	6.4659646175
N	4.3537276457	-4.2414058747	4.0684347796
C	5.3835762152	-5.1414167079	4.7040433330
H	5.0763454684	-6.1607668361	4.4485961997
H	6.3485033859	-4.9426178713	4.2175266772
C	5.5033630776	-4.9619563416	6.1879819601
C	5.7190426012	-4.7196482253	8.9418926255
C	4.3899721326	-5.2896559022	6.9950477054
C	6.6940011499	-4.5076873653	6.7674304418
C	6.8275396362	-4.3775863845	8.1495728254
C	4.5128534048	-5.1670228509	8.4051337916
H	7.5382053984	-4.2649449919	6.1226488909
H	5.7980951651	-4.6224982348	10.0242217281
C	3.3369656856	-5.5238301386	9.2768676258
C	8.1156037532	-3.8979233503	8.7795839888
C	-0.1395353238	-2.2852306577	1.7520422804
C	3.8538927877	-1.1285539779	-1.1506280823
Cl	0.2581394690	-5.2361127245	5.7653237632
O	2.4981865011	-6.7353744222	4.0708485990

C	1.3588640621	-7.2484366399	3.3347484878
H	1.6194147754	-8.2315968850	2.9312692274
H	0.4813831871	-7.2959164482	3.9804383066
H	1.1747658229	-6.5343220642	2.5337444040
H	2.5778766977	-7.1725585903	4.9389796945
H	4.9028504798	-1.3965492863	-1.3121107247
H	3.8155709764	-0.0475717240	-0.9634936119
H	3.3198796801	-1.3062050548	-2.0918961559
H	-0.6110686803	-1.5235351050	1.1235343640
H	-0.6963612668	-3.2224280012	1.6388681522
H	-0.2514963881	-1.9962128827	2.8028993071
H	8.6316742295	-4.7047786713	9.3153934344
H	8.8091614275	-3.5114710618	8.0260665457
H	7.9363839475	-3.0974691838	9.5072843978
H	3.5125620858	-5.2319954342	10.3167202332
H	3.1383084184	-6.6021054792	9.2545077148
H	2.4224607891	-5.0417027343	8.9175140286

[1] A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648.
[2] C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B.* 1988, **37**, 785.
[3] Jaguar 6.0. Schrodinger, LLC: Portland, Oregon, 2005.
[4] P. J. Hay, W. R. Wadt, *J. Chem. Phys.* 1985, **82**, 299.
[5] P. C. Harihara, J. A. Pople, *Theo. Chim. Acta.* 1973, **28**, 213.