

Supporting Information for

Ligand Effects in Rhodium-Catalyzed Hydroformylation with Bisphosphines: Steric or Electronic?

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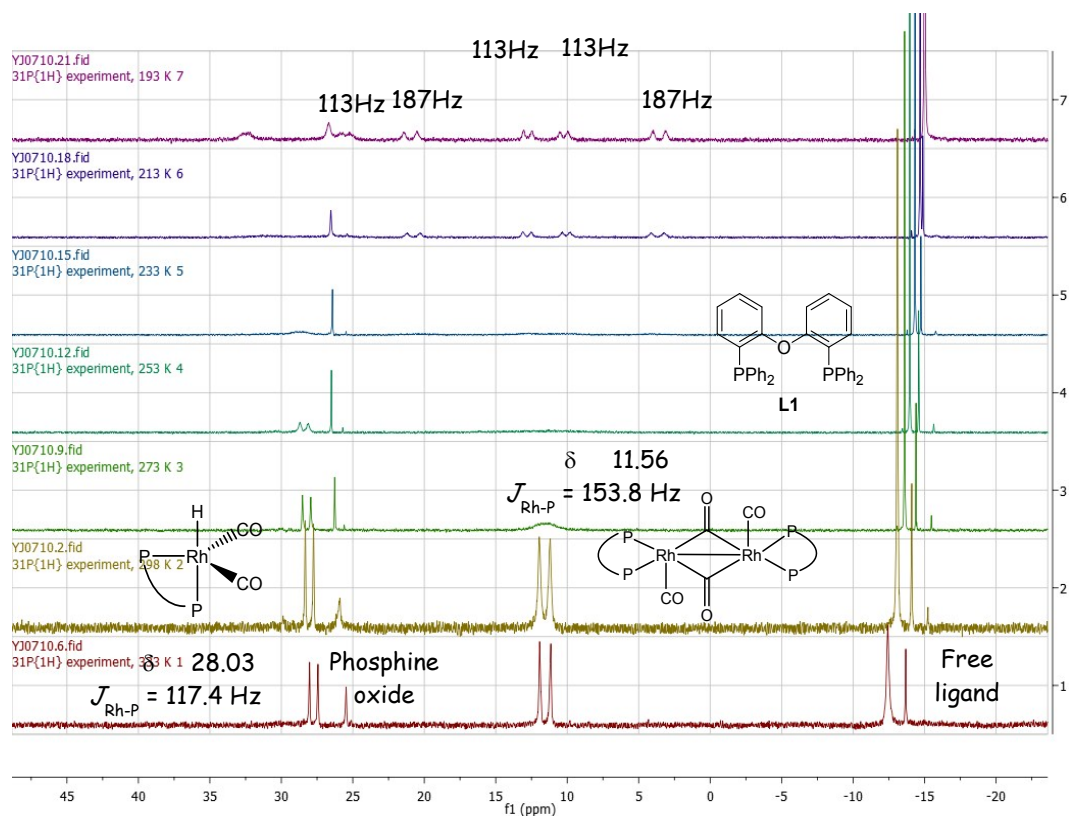
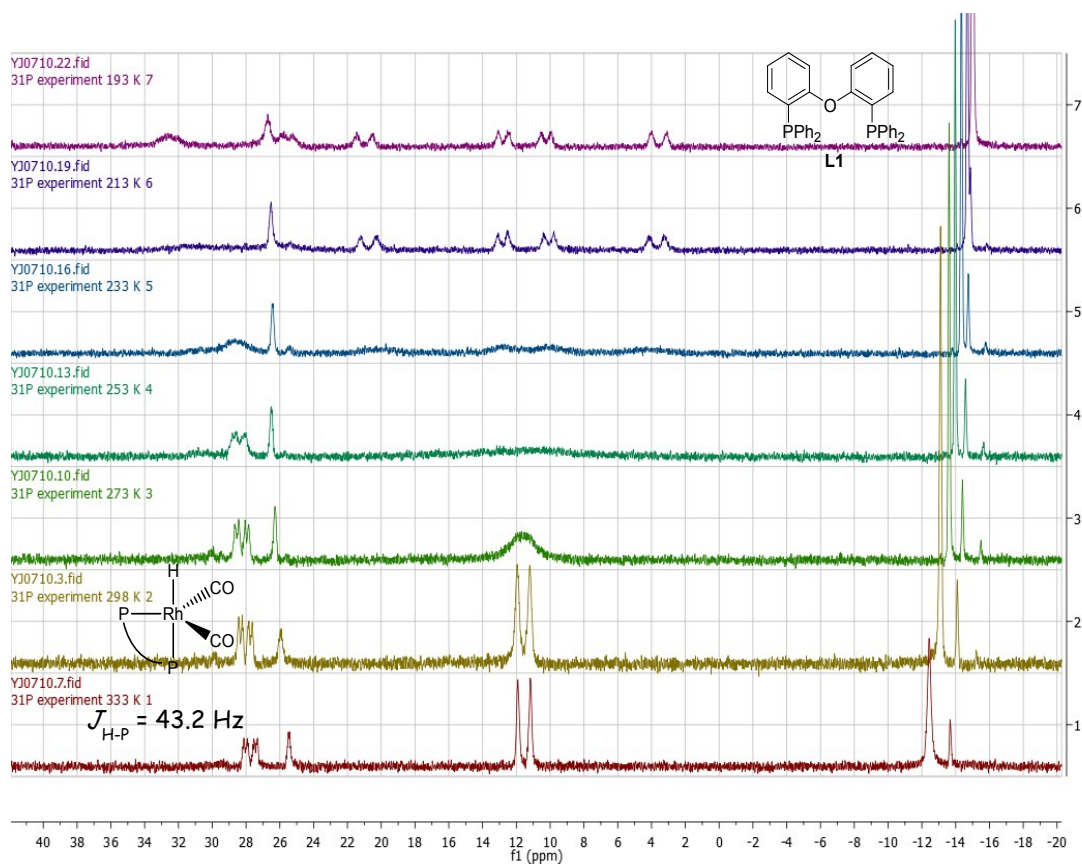


Figure S-1 $^{31}\text{P}\{^1\text{H}\}$ NMR spectra for the reaction of $\text{Rh}(\text{acac})(\text{CO})_2$ with DPEphos in



Toluene- d_8 at 80 °C, 10 bar of CO/H_2 (1:1) after 1 h.

Figure S-2 ^{31}P NMR spectra for the reaction of $\text{Rh}(\text{acac})(\text{CO})_2$ with DPEphos (**L1**) in Toluene- d_8 at 80 °C, 10 bar of CO/H_2 (1:1) after 1 h.

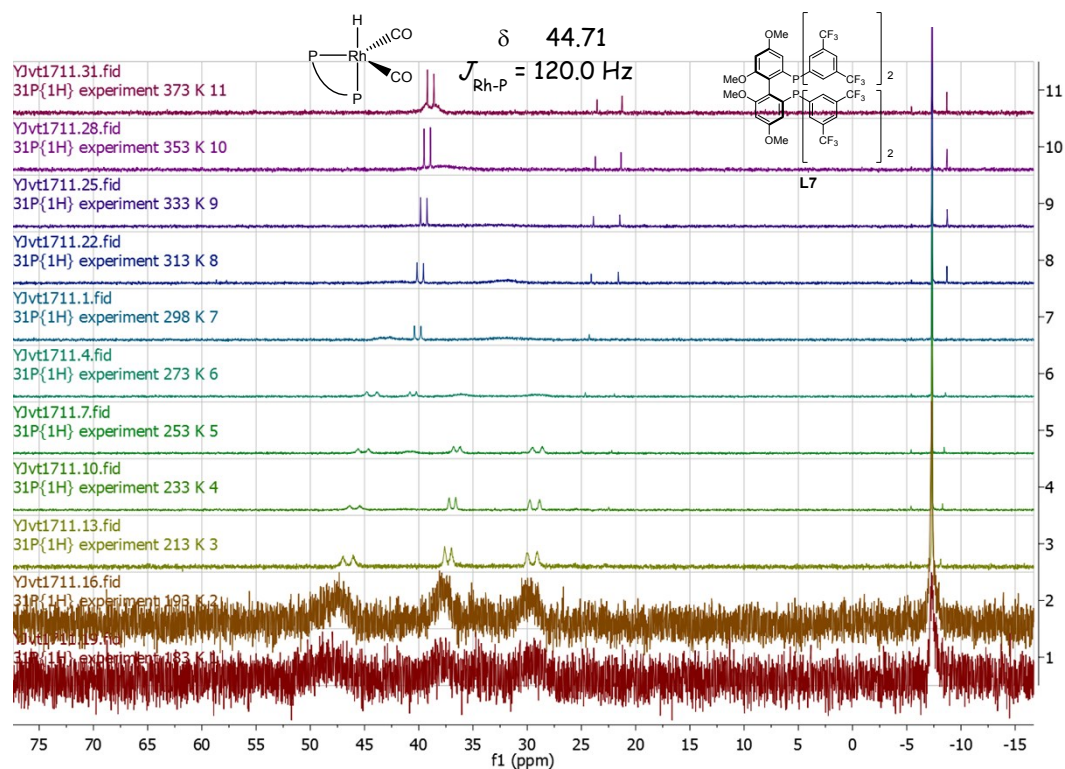


Figure S-3 $^{31}\text{P}\{^1\text{H}\}$ NMR spectra for the reaction of $\text{Rh}(\text{acac})(\text{CO})_2$ with (S)-BTfM-Garphos (**L7**) in Toluene- d_8 at 80 °C, 10 bar of CO/H_2 (1:1) after 1 h.

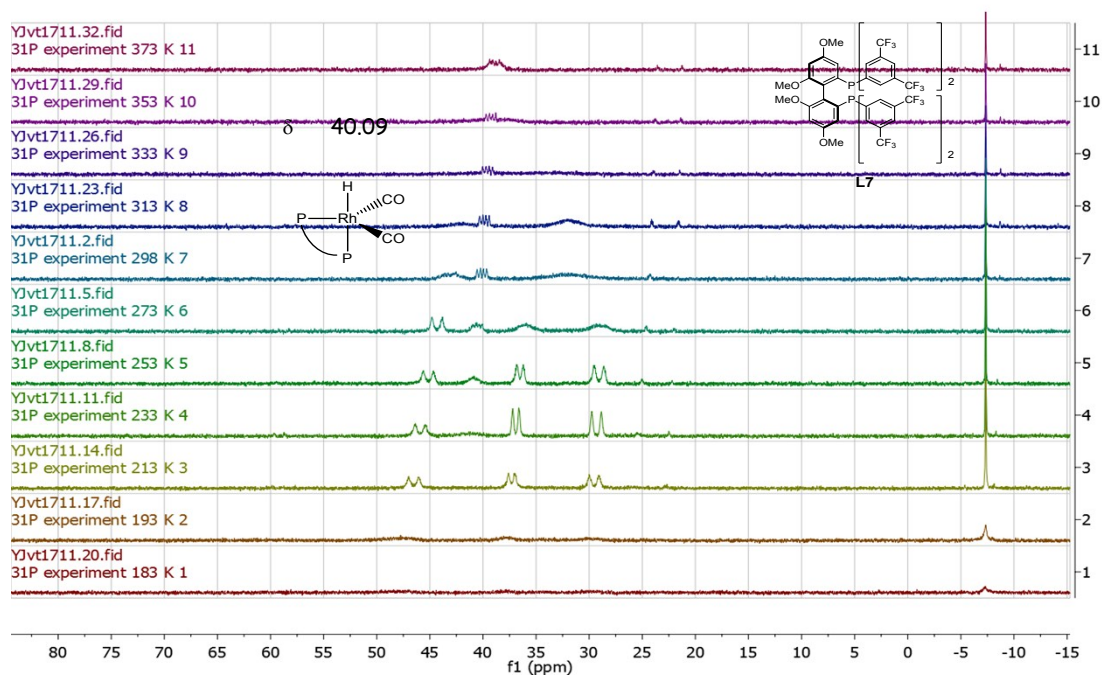


Figure S-4 ^{31}P NMR spectra for the reaction of $\text{Rh}(\text{acac})(\text{CO})_2$ with (S)-BTfM-Garphos (**L7**) in Toluene- d_8 at 80 °C, 10 bar of CO/H_2 (1:1) after 1 h.

Table S-1 Results of hydroformylation of styrene with (S)-(+)-DTBM-SEGPHOS (**L8**).

#	Incubation	Reaction	L/M	Conv. (%)	Aldehyde Sel. (%)	l/b (%)	ee (%)
1	80C/10b/1h	80C/20b/12h	2	12	100	0/100	19
2	60C/10b/0,5h	80C/20b/8h	1.2	96	100	13/87	0
3	60C/10b/0,5h	60C/20b/8h	1.2	51	100	10/90	0
4	80C/10b/1h	80C/30b/8h	2	5	100	0/100	18
5	80C/10b/1h	80C/30b/8h	1.2	96	100	12/88	0
6	80C/6b/1h	80C/10b/8h	2	15	100	0/100	20

Table S-2 Results of the hydroformylation of 1-octene with DPEphos (**L1**) under different incubation conditions. ^a

Incub. Conditions	Conv. (%)	Aldehyde Sel. (%)	l/b ratio
80 °C, 1h	57	100	6.7
RT, 10 min	53	100	6.7
None	57	100	6.7

^a Reaction conditions: P(CO)/P(H₂) = 1, P(CO/H₂) = 20 bar, substrate/L/Rh = 667/3/1, Rh(acac)(CO)₂ = 1 mM. 80 °C, 12 hrs. Each experiment was repeated twice to confirm the reproducibility.

Computational Details

Gaussian 09 reference:

Gaussian 09, Revision E.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Coordinates and energies (a.u.) for stationary points in the two coordination modes (ea and ee) of HRh(CO)₂(bisphosphine) and fragments:

ee-HRh(CO)₂(L1)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2483.47055035, PCM -2483.50334196

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P	5.8549630	8.7255900	-9.7627830
O	5.1706920	7.9245990	-12.6690640
C	6.4366740	7.5267160	-13.0530940
C	4.6254700	7.4539320	-10.3500900
C	7.4124620	7.7300210	-9.6054700
C	4.4466380	7.2107400	-11.7274340
C	8.5032400	11.4028010	-15.1907930

H	7.8566310	10.9345810	-15.9261990
C	5.3553330	8.9394630	-7.9854210
C	8.9752440	6.8544370	-13.9624660
H	9.9690410	6.5986540	-14.3169380
C	7.3041910	8.5582550	-13.4598950
C	9.8159510	6.3100210	-9.2479160
H	10.7440070	5.7618430	-9.1122940
C	5.8913720	8.1738320	-6.9381750
H	6.6361800	7.4133330	-7.1461270
C	8.2147000	11.2765260	-13.8207320
C	10.4485720	12.7509780	-14.6866840
H	11.3086960	13.3239960	-15.0216060
C	4.4032110	9.9251410	-7.6791980
H	4.0065670	10.5478340	-8.4750210
C	3.7838970	6.7577930	-9.4658380
H	3.8857670	6.9246880	-8.3993020
C	2.8120450	5.8675350	-9.9251040
C	9.8302680	7.7023340	-9.3452390
H	10.7700700	8.2440100	-9.2859820
C	9.0575610	11.9076490	-12.8952610
H	8.8282510	11.8365310	-11.8371410
C	8.6024560	5.6257800	-9.3300670
H	8.5809290	4.5418380	-9.2574390
C	6.8190960	6.1865800	-13.0945630
H	6.1238250	5.4175550	-12.7762740
C	3.4668890	6.3358540	-12.1964790
H	3.3538340	6.2115560	-13.2685620
C	8.0955240	5.8547550	-13.5497800
H	8.3963660	4.8116040	-13.5819090
C	8.5781590	8.1922670	-13.9159050
H	9.2714330	8.9648500	-14.2290870
C	3.9832920	10.1269130	-6.3649570
H	3.2446310	10.8934700	-6.1485460
C	8.6393950	8.4059540	-9.5273140
H	8.6572780	9.4873840	-9.6158530
C	9.6115430	12.1335280	-15.6190780
C	2.6484540	5.6581160	-11.2938920
C	7.4095230	6.3294010	-9.5053590
H	6.4737750	5.7829840	-9.5613220
C	4.5230320	9.3595680	-5.3303950
H	4.2059000	9.5252620	-4.3046700
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H	5.9119710	7.7910100	-4.8207780
C	10.1690920	12.6358180	-13.3247930
H	10.8091040	13.1206980	-12.5929950
Rh	5.9007590	10.8448910	-10.9887840
H	7.4413400	10.8805480	-10.5631830
C	4.0090680	10.8150980	-11.4880470
C	5.9443490	12.5701510	-10.1613410
O	6.0244180	13.6101970	-9.6601880
O	2.8907900	10.8010470	-11.7638330
H	1.8852990	4.9782990	-11.6607900
H	2.1788820	5.3486420	-9.2116570
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C	5.5542670	10.5750880	-14.6075910
C	5.3253140	9.6329720	-15.6195550
C	4.8553060	11.7925530	-14.6464750
C	4.4154670	9.9009550	-16.6455250

C	3.9556760	12.0630510	-15.6764480
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H	5.8587800	8.6881460	-15.6101510
H	5.0164460	12.5281510	-13.8630830
H	4.2453630	9.1580300	-17.4200690
H	3.4248680	13.0107230	-15.6920880
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m062_LANL2DZ

E(RM062X): Gas phase -2482.57848008, PCM -2482.61068733

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C	7.3737230	7.7026190	-9.7884690
C	4.3889930	7.3527070	-11.7724970
C	8.5745450	11.3184440	-15.1195360
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C	5.4375500	8.9134020	-8.0387860
C	9.0775560	6.9573850	-13.4555510
H	10.1117140	6.6955990	-13.6530760
C	7.3457510	8.6495540	-13.2938920
C	9.6942650	6.1435220	-9.6997770
H	10.5951080	5.5385800	-9.6670900
C	6.1254240	8.2632030	-7.0113570
H	6.9764620	7.6303640	-7.2395950
C	8.2198330	11.3293360	-13.7645260
C	10.4619010	12.7450910	-14.6494470
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C	4.3528580	9.7386040	-7.7134630
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C	3.7445290	6.8704280	-9.5180220
H	3.8668400	7.0117990	-8.4482420
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C	9.7686540	7.4851640	-10.0565390
H	10.7257310	7.9305870	-10.3095730
C	8.9922220	12.0624650	-12.8616910
H	8.6999000	12.0884780	-11.8155340
C	8.4593310	5.5734710	-9.3916310
H	8.3961430	4.5250550	-9.1168930
C	6.8398750	6.3108890	-12.8214130
H	6.1197480	5.5580560	-12.5176080
C	3.3844990	6.5196910	-12.2503110
H	3.2672510	6.4184340	-13.3241190
C	8.1665500	5.9764520	-13.0781320
H	8.4853720	4.9442620	-12.9752180
C	8.6659310	8.2833640	-13.5647430
H	9.3845490	9.0498030	-13.8385100
C	3.9486380	9.8887580	-6.3927360
H	3.1022910	10.5259010	-6.1568600
C	8.6123240	8.2635750	-10.1017890
H	8.6646330	9.3102660	-10.3899310
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C	2.5578090	5.8511850	-11.3535190
C	7.3054540	6.3469340	-9.4409710
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C	4.6393840	9.2351690	-5.3729720

H	4.3323690	9.3614240	-4.3396220
C	5.7293050	8.4301790	-5.6846060
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C	10.1121840	12.7653270	-13.3032670
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Rh	5.8516710	10.9186350	-10.9575940
H	7.3322830	11.0587920	-10.4419690
C	3.9852800	10.6978150	-11.6176910
C	5.7261250	12.6041480	-10.0739190
O	5.7060150	13.6123140	-9.5261790
O	2.9340400	10.5133680	-12.0184210
H	1.7726800	5.2007090	-11.7244670
H	2.1034900	5.5059850	-9.2780630
H	9.9565750	12.0108710	-16.6109510
C	5.5943650	10.5674050	-14.5485000
C	5.4081180	9.5916350	-15.5302720
C	4.8575200	11.7549470	-14.6178440
C	4.4994580	9.8022340	-16.5654060
C	3.9571510	11.9670040	-15.6559840
C	3.7745020	10.9883410	-16.6309860
H	5.9724970	8.6643600	-15.4855480
H	4.9895980	12.5112610	-13.8467870
H	4.3582590	9.0360050	-17.3213260
H	3.3912640	12.8920980	-15.6988810
H	3.0644120	11.1485260	-17.4360110

ea-HRh(CO)₂(L1)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2483.47146649, PCM -2483.50508153

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C	6.3810210	7.4971410	-13.0301530
C	4.5964300	7.4920580	-10.3072300
C	7.4235350	7.7797090	-9.6891400
C	4.4021000	7.2406430	-11.6798760
C	8.5611450	11.3934810	-15.0790960
H	7.8949950	11.0042560	-15.8424720
C	5.4317980	8.9461120	-7.9505150
C	8.8878330	6.7638750	-13.9722240
H	9.8699120	6.4833620	-14.3405220
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C	10.5723930	12.6046480	-14.4895090
H	11.4629780	13.1510510	-14.7872340
C	4.5112650	9.9422170	-7.5851970
H	4.0880670	10.5853410	-8.3493070
C	3.7588760	6.8160380	-9.4049630
H	3.8742700	6.9921390	-8.3413880
C	2.7714880	5.9339520	-9.8469370
C	9.8521540	7.8007530	-9.5982540
H	10.7838120	8.3589410	-9.6140890
C	9.1294990	11.7294570	-12.7568470
H	8.8897540	11.6115970	-11.7049810

C	8.6659440	5.7026990	-9.4623140
H	8.6709310	4.6200610	-9.3712150
C	6.7151820	6.1462030	-13.1066050
H	5.9969190	5.3930950	-12.8014740
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H	3.2775410	6.2443390	-13.2004840
C	7.9774730	5.7838470	-13.5787680
H	8.2434010	4.7324590	-13.6390510
C	8.5367300	8.1131470	-13.8909160
H	9.2522890	8.8697550	-14.1930840
C	4.1573030	10.1262090	-6.2486420
H	3.4437210	10.9014940	-5.9849440
C	8.6386090	8.4802670	-9.7086690
H	8.6317640	9.5599120	-9.8150180
C	9.7086340	12.0906980	-15.4592590
C	2.5895880	5.7167040	-11.2121700
C	7.4509160	6.3814260	-9.5673690
H	6.5224750	5.8193950	-9.5546760
C	4.7287250	9.3297450	-5.2545850
H	4.4611770	9.4810080	-4.2126440
C	5.6531630	8.3451000	-5.6050270
H	6.1096820	7.7268100	-4.8371660
C	10.2803550	12.4222020	-13.1372770
H	10.9404980	12.8282430	-12.3759590
Rh	5.8466330	10.9126100	-10.9235070
H	5.8279700	12.3496780	-11.5840100
C	7.0147420	11.7841920	-9.6731620
C	3.9216060	11.0107500	-11.1124170
O	2.7806200	11.1738590	-11.2050800
O	7.6638340	12.4011880	-8.9372270
H	1.8129480	5.0443350	-11.5641830
H	2.1394280	5.4290300	-9.1227300
H	9.9250230	12.2359320	-16.5141080
C	5.5867820	10.5579380	-14.5587830
C	5.4310330	9.6575630	-15.6227570
C	4.8301540	11.7405970	-14.5613600
C	4.5396530	9.9324530	-16.6625800
C	3.9482830	12.0188130	-15.6051590
C	3.7975370	11.1136200	-16.6580360
H	6.0063360	8.7377210	-15.6423910
H	4.9275170	12.4410620	-13.7376890
H	4.4281470	9.2210260	-17.4764340
H	3.3716910	12.9393810	-15.5899310
H	3.1039910	11.3264830	-17.4666650

m062_LANL2DZ

E(RM062X): Gas phase -2482.57886652, PCM -2482.61197720

P	6.7835620	10.3544340	-13.0940410
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C	6.4385540	7.6133130	-12.9307830
C	4.5806810	7.5612670	-10.3883820
C	7.3805450	7.6986970	-9.8099590
C	4.3858430	7.3559560	-11.7625890
C	8.5527830	11.3609250	-15.0813950
H	7.8951890	10.8938340	-15.8096750
C	5.4682300	8.9056180	-8.0285430
C	9.0517720	6.9067730	-13.5048460

H	10.0784570	6.6335880	-13.7247990
C	7.3463490	8.6178400	-13.2900570
C	9.7160390	6.1673530	-9.7452390
H	10.6235120	5.5721140	-9.7216850
C	6.1964970	8.2829400	-7.0125100
H	7.0542600	7.6649100	-7.2552170
C	8.2450300	11.2832980	-13.7180670
C	10.5337200	12.6429330	-14.5762030
H	11.4195650	13.1742780	-14.9100570
C	4.3754940	9.7144330	-7.6872080
H	3.8206140	10.2247350	-8.4697200
C	3.7367210	6.8778900	-9.5059760
H	3.8575710	7.0220860	-8.4365270
C	2.7369160	6.0293070	-9.9748190
C	9.7718870	7.5068820	-10.1134590
H	10.7200580	7.9597140	-10.3856210
C	9.0901760	11.8999470	-12.7925250
H	8.8378850	11.8603060	-11.7358690
C	8.4922780	5.5854220	-9.4146400
H	8.4453120	4.5382960	-9.1322000
C	6.8159710	6.2797180	-12.8411200
H	6.0912080	5.5320770	-12.5354120
C	3.3826580	6.5217290	-12.2409900
H	3.2669990	6.4175470	-13.3146620
C	8.1352400	5.9330570	-13.1219090
H	8.4431410	4.8959550	-13.0361880
C	8.6565840	8.2399580	-13.5897260
H	9.3802530	9.0008650	-13.8662990
C	4.0053400	9.8750020	-6.3576730
H	3.1533740	10.4989140	-6.1077060
C	8.6070120	8.2727990	-10.1457980
H	8.6427460	9.3177840	-10.4462610
C	9.6911630	12.0373020	-15.5072010
C	2.5551410	5.8553440	-11.3431050
C	7.3292400	6.3453580	-9.4526080
H	6.3733810	5.8895800	-9.2055180
C	4.7358910	9.2488930	-5.3487380
H	4.4544410	9.3838990	-4.3092460
C	5.8321210	8.4597740	-5.6781250
H	6.4108070	7.9778050	-4.8965260
C	10.2331220	12.5731500	-13.2194540
H	10.8813190	13.0505930	-12.4914540
Rh	5.9266270	10.9597010	-10.8831090
H	5.9518860	12.4097360	-11.4461560
C	7.1047140	11.7210110	-9.5659240
C	3.9856500	11.0869870	-11.1257620
O	2.8604780	11.2449220	-11.2662230
O	7.7859650	12.2452510	-8.8049070
H	1.7707210	5.2038640	-11.7138270
H	2.0954610	5.5133230	-9.2683170
H	9.9194750	12.0957850	-16.5668200
C	5.5906130	10.5658430	-14.4781780
C	5.4427970	9.6339530	-15.5086270
C	4.8018230	11.7210610	-14.4857840
C	4.5215560	9.8546120	-16.5298390
C	3.8882100	11.9440230	-15.5110000
C	3.7439670	11.0091990	-16.5335930
H	6.0486350	8.7321110	-15.5132250

H	4.9029740	12.4436790	-13.6798160
H	4.4110130	9.1211010	-17.3224810
H	3.2815750	12.8439120	-15.5055670
H	3.0238430	11.1780110	-17.3279220

ee-HRh(CO)₂(L2)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2640.72267940, PCM -2640.75573477

P	6.7532840	10.3278390	-13.3846940
P	5.8397750	8.7759560	-9.7137550
O	5.1472410	7.9743230	-12.6518550
C	6.3629140	7.5439180	-13.1478730
C	4.6724430	7.4481330	-10.3302330
C	7.4494080	7.8505220	-9.5075810
C	4.4585990	7.2320770	-11.7071080
C	8.6830610	11.3040780	-15.3632850
C	5.2531990	8.9243150	-7.9357340
C	8.8274300	6.7962520	-14.1981770
H	9.7971010	6.5152160	-14.5972520
C	7.2268340	8.5504350	-13.6224220
C	9.8666290	6.4033110	-9.3350730
H	10.8042150	5.8589460	-9.2656720
C	6.0071740	8.3386100	-6.9039320
H	6.9057210	7.7847560	-7.1468020
C	8.2549150	11.2433710	-14.0089180
C	10.5605030	12.7232010	-14.6789630
H	11.4461770	13.2897470	-14.9530600
C	4.0613860	9.6161760	-7.5933100
C	3.8954780	6.6805690	-9.4433720
H	4.0344470	6.8103350	-8.3762490
C	2.9435010	5.7671410	-9.8960140
C	9.7955270	7.7286000	-8.9124950
H	10.6823340	8.2070080	-8.5034210
C	8.9966580	11.9298620	-13.0342910
H	8.6545680	11.8912480	-12.0064140
C	8.7207410	5.7845570	-9.8261950
H	8.7439960	4.7462370	-10.1441600
C	6.7003060	6.1918900	-13.2265070
H	6.0023480	5.4416400	-12.8725490
C	3.4912120	6.3380300	-12.1699890
H	3.3471220	6.2408510	-13.2411790
C	7.9359690	5.8210600	-13.7555370
H	8.1980090	4.7686240	-13.8142630
C	8.4699810	8.1433790	-14.1300920
H	9.1760210	8.8939110	-14.4661670
C	3.7022600	9.7037460	-6.2408590
H	2.7889210	10.2337790	-5.9830610
C	8.6111620	8.4765570	-8.9846160
C	9.8351200	12.0490590	-15.6597270
C	2.7313880	5.6007420	-11.2643840
C	7.5297740	6.5045830	-9.9009270
H	6.6439130	6.0024840	-10.2682190
C	4.4722460	9.1346960	-5.2284780
H	4.1625130	9.2271170	-4.1913290
C	5.6311580	8.4417070	-5.5647170
H	6.2424490	7.9765680	-4.7966620
C	10.1396260	12.6610970	-13.3538200
H	10.6876610	13.1783280	-12.5716670

Rh	5.9846000	10.8575240	-11.1253740
H	7.5289750	10.7569160	-10.7739400
C	4.1047540	10.9393970	-11.6837450
C	6.1421720	12.5384470	-10.2109180
O	6.2950800	13.5501230	-9.6690150
O	3.0089250	10.9787750	-12.0361650
H	1.9804390	4.9052470	-11.6270980
H	2.3638790	5.1953980	-9.1774890
H	10.1673520	12.0965280	-16.6938450
C	5.4564130	10.6569360	-14.6790060
C	4.8470710	9.5917100	-15.3603400
C	5.0138140	11.9798220	-14.9373540
C	3.8194550	9.8024170	-16.2776370
C	3.9798440	12.1660370	-15.8666900
C	3.3807510	11.0995290	-16.5334780
H	5.1865660	8.5781570	-15.1856430
H	3.3698300	8.9556090	-16.7884330
H	3.6400770	13.1795630	-16.0649280
H	2.5792450	11.2827050	-17.2435160
C	3.1458480	10.2522350	-8.6097740
H	3.6287840	11.1072580	-9.0902640
H	2.8600890	9.5548250	-9.4025510
H	2.2281850	10.6037590	-8.1305820
C	8.6620860	9.8965780	-8.4623590
H	7.6930500	10.2699850	-8.1316760
H	9.3525930	9.9561670	-7.6148200
H	9.0221340	10.5851670	-9.2334370
C	7.9765250	10.6312890	-16.5205870
H	8.6422370	10.5822130	-17.3869780
H	7.6560380	9.6150150	-16.2845990
H	7.0808190	11.1850550	-16.8192170
C	5.6167440	13.2025950	-14.2840650
H	5.7563160	13.0624220	-13.2081120
H	6.6003620	13.4387640	-14.7049870
H	4.9721920	14.0726160	-14.4365900

m062_LANL2DZ

E(RM062X): Gas phase -2639.76678276, PCM -2639.79917228

P	6.7000250	10.4919270	-13.2174360
P	5.8619890	8.7339470	-9.8009260
O	5.0797080	8.1118600	-12.6888980
C	6.3893450	7.7327370	-12.8954980
C	4.5604690	7.5500850	-10.3900770
C	7.3274400	7.5860270	-9.7430460
C	4.3291910	7.4064270	-11.7659290
C	8.7482270	11.3572670	-15.0667830
C	5.4674360	8.8801410	-7.9950420
C	9.0468950	7.0736510	-13.3067680
H	10.0937190	6.8256040	-13.4456660
C	7.2837470	8.7472550	-13.2634230
C	9.4995580	5.8115710	-9.6490070
H	10.3478690	5.1347310	-9.6191620
C	6.4156170	8.4743230	-7.0473160
H	7.3437200	8.0195980	-7.3761280
C	8.1862280	11.4383510	-13.7719460
C	10.4065150	13.0238170	-14.4140070
H	11.2660040	13.6324620	-14.6772120
C	4.2632810	9.4725940	-7.5491760

C	3.7289850	6.8274660	-9.5250300
H	3.8784490	6.9231870	-8.4527680
C	2.7071610	6.0149210	-10.0069670
C	9.7034940	7.1734110	-9.8287960
H	10.7147310	7.5570920	-9.9343790
C	8.7466510	12.3120200	-12.8336670
H	8.2896180	12.3824490	-11.8508600
C	8.2040600	5.3280630	-9.4950750
H	8.0241830	4.2693000	-9.3371700
C	6.7922790	6.4068810	-12.7758260
H	6.0684390	5.6503690	-12.4908880
C	3.3041910	6.6075420	-12.2608700
H	3.1642030	6.5564370	-13.3354330
C	8.1289670	6.0820690	-12.9742210
H	8.4531910	5.0542490	-12.8486510
C	8.6227340	8.3900240	-13.4580990
H	9.3440700	9.1611580	-13.7128010
C	4.0541110	9.5993750	-6.1736600
H	3.1206910	10.0385060	-5.8315610
C	8.6391250	8.0815740	-9.8707550
C	9.8565300	12.1588160	-15.3549150
C	2.4881960	5.9100130	-11.3779710
C	7.1339740	6.2132080	-9.5422190
H	6.1268810	5.8248140	-9.4265810
C	5.0027830	9.1934440	-5.2417130
H	4.8086140	9.3149090	-4.1807610
C	6.1940420	8.6334900	-5.6827460
H	6.9489780	8.3089360	-4.9739200
C	9.8504760	13.1008520	-13.1438570
H	10.2631720	13.7723250	-12.3981710
Rh	5.5951240	11.1259860	-11.0740770
H	6.9825340	11.5910440	-10.5061910
C	3.8096210	10.6144950	-11.8429900
C	5.1333870	12.6893100	-10.1581840
O	4.8974770	13.6794890	-9.6242030
O	2.8100290	10.3018930	-12.2912830
H	1.6860900	5.2873960	-11.7601770
H	2.0779060	5.4713560	-9.3101090
H	10.2949860	12.0985060	-16.3475090
C	5.5447660	10.6589820	-14.6470080
C	5.0886300	9.5402470	-15.3511170
C	5.0757560	11.9415830	-15.0019560
C	4.1775380	9.6676640	-16.3930580
C	4.1610680	12.0452560	-16.0541660
C	3.7091190	10.9281930	-16.7465560
H	5.4640180	8.5543150	-15.0991350
H	3.8414440	8.7846730	-16.9272110
H	3.7999140	13.0320720	-16.3310010
H	2.9958410	11.0434920	-17.5564470
C	3.1958950	10.0005110	-8.4751420
H	3.4944100	10.9721830	-8.8794990
H	3.0014340	9.3417910	-9.3247000
H	2.2578240	10.1320140	-7.9307960
C	8.9464150	9.5484070	-10.0191210
H	8.4459160	10.1477840	-9.2528830
H	10.0225370	9.7200870	-9.9425200
H	8.6073450	9.9310620	-10.9862800
C	8.2137650	10.4708560	-16.1652880

H	8.9765970	10.3313460	-16.9348040
H	7.9150680	9.4874240	-15.7965590
H	7.3323320	10.9178840	-16.6366140
C	5.5447130	13.2026070	-14.3205340
H	5.5336960	13.1000540	-13.2297860
H	6.5713430	13.4497150	-14.6117180
H	4.9031620	14.0424230	-14.5958740

ea-HRh(CO)₂(L2)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2640.71927548, PCM -2640.75205970

P	6.8399420	10.3466160	-13.2341290
P	5.8781940	8.4501580	-9.7161230
O	5.2481470	8.0165480	-12.6322990
C	6.4345930	7.5677580	-13.1686760
C	4.5534470	7.3403940	-10.4303350
C	7.3641260	7.3260210	-9.6888880
C	4.4455930	7.2328080	-11.8290870
C	8.7276320	11.4537260	-15.1993880
C	5.2974900	8.7524250	-7.9722800
C	8.8619690	6.8462630	-14.3012560
H	9.8151730	6.5715490	-14.7425310
C	7.2918340	8.5884750	-13.6236050
C	9.7578150	5.8561380	-9.8899050
H	10.6751280	5.2776990	-9.9561610
C	6.1317360	8.8385780	-6.8294410
C	8.3353740	11.2793410	-13.8448140
C	10.6740940	12.7354890	-14.4429870
H	11.5722990	13.2948520	-14.6897610
C	3.9401880	9.1071100	-7.8459030
H	3.3038110	9.1118050	-8.7240970
C	3.6270990	6.6068140	-9.6684610
H	3.6584920	6.6690800	-8.5877950
C	2.6510750	5.8096650	-10.2661590
C	9.6718930	7.1171390	-10.4719090
H	10.5164190	7.5430950	-11.0046260
C	9.1292700	11.8425800	-12.8321010
H	8.8179170	11.7190000	-11.8006700
C	8.6568850	5.3372890	-9.2093670
H	8.7310660	4.3571220	-8.7447460
C	6.7639490	6.2176260	-13.2765510
H	6.0787870	5.4614260	-12.9103340
C	3.4668680	6.4466930	-12.4397910
H	3.4159070	6.4286830	-13.5234290
C	7.9858890	5.8612900	-13.8479440
H	8.2497750	4.8110540	-13.9307140
C	8.5151270	8.1940020	-14.1844420
H	9.2138800	8.9516780	-14.5204340
C	3.3832360	9.4750740	-6.6249160
H	2.3317590	9.7406360	-6.5696810
C	8.4827350	7.8367320	-10.3665740
H	8.4109560	8.8214750	-10.8155960
C	9.8970020	12.1842420	-15.4608850
C	2.5688240	5.7265320	-11.6564080
C	7.4501390	6.0415360	-9.0916780
C	4.1901770	9.5117300	-5.4896750
H	3.7781820	9.7961970	-4.5257930
C	5.5423840	9.2063200	-5.6078780

H	6.1796570	9.2662720	-4.7294400
C	10.2900010	12.5608950	-13.1165380
H	10.8791800	12.9813520	-12.3068410
Rh	6.1688790	10.7346790	-10.7250270
H	6.2973770	12.2459760	-11.1381680
C	7.5376200	11.2505220	-9.4988900
C	4.2701160	11.1020570	-10.7364960
O	3.1641990	11.4329060	-10.6677160
O	8.3011410	11.6837930	-8.7400720
H	1.8049020	5.1163190	-12.1287000
H	1.9527880	5.2601560	-9.6420790
H	10.2026580	12.3185940	-16.4956380
C	5.4928840	10.7706620	-14.4512210
C	4.8542580	9.7531900	-15.1783680
C	5.0425820	12.1068320	-14.6086300
C	3.7879830	10.0207500	-16.0345770
C	3.9687510	12.3512890	-15.4776250
C	3.3371740	11.3300120	-16.1838740
H	5.2035110	8.7319160	-15.0910430
H	3.3189960	9.2082770	-16.5826430
H	3.6252310	13.3757350	-15.5974850
H	2.5054610	11.5579200	-16.8445040
C	6.3302140	5.3881350	-8.3162600
H	5.5623870	4.9832360	-8.9829520
H	6.7178980	4.5592360	-7.7176760
H	5.8343910	6.0881820	-7.6390430
C	7.6264390	8.5983660	-6.8288690
H	8.0550790	8.9509100	-5.8871160
H	7.8820030	7.5401190	-6.9332230
H	8.1311340	9.1307050	-7.6373200
C	5.6833850	13.2898400	-13.9204370
H	5.8052140	13.1218290	-12.8469020
H	6.6790300	13.5011730	-14.3256050
H	5.0719070	14.1860500	-14.0553090
C	7.9623420	10.9090730	-16.3855660
H	8.5905960	10.9321810	-17.2805670
H	7.6304930	9.8804470	-16.2316380
H	7.0657710	11.5021910	-16.5913560

m062_LANL2DZ

E(RM062X): Gas phase -2639.76154181, PCM -2639.79464576

P	6.7987350	10.3575170	-13.1944390
P	5.8436370	8.5106290	-9.7309960
O	5.1680590	8.0984310	-12.6078790
C	6.3881580	7.6196520	-13.0191050
C	4.5005590	7.4224130	-10.4011420
C	7.3348250	7.4269920	-9.8320060
C	4.3561810	7.3442110	-11.7923140
C	8.7307890	11.3609090	-15.1247680
C	5.3622600	8.7342590	-7.9617330
C	8.8806310	6.8339840	-13.9217040
H	9.8610870	6.5296100	-14.2722980
C	7.2715010	8.6014120	-13.4893150
C	9.7125230	5.9954490	-10.2049950
H	10.6285580	5.4292070	-10.3428970
C	6.2488150	8.7313110	-6.8669740
C	8.2903520	11.2703140	-13.7854320
C	10.5948410	12.7487040	-14.3817120

H	11.4851650	13.3186960	-14.6284650
C	4.0324480	9.1378180	-7.7632160
H	3.3632630	9.2114540	-8.6168480
C	3.5829900	6.7019360	-9.6257930
H	3.6528650	6.7417880	-8.5439030
C	2.5778080	5.9393580	-10.2111760
C	9.6169380	7.3019850	-10.6668720
H	10.4497970	7.7739940	-11.1776060
C	9.0106710	11.9250240	-12.7797500
H	8.6466820	11.8654060	-11.7568250
C	8.6296760	5.4145290	-9.5524980
H	8.7137040	4.3992790	-9.1736170
C	6.7293730	6.2724640	-12.9787610
H	6.0261440	5.5464220	-12.5842000
C	3.3527310	6.5896080	-12.3919910
H	3.2856280	6.5885010	-13.4749590
C	7.9880800	5.8864400	-13.4306440
H	8.2689420	4.8389120	-13.3910950
C	8.5247380	8.1805350	-13.9412940
H	9.2391190	8.9195580	-14.2924770
C	3.5488570	9.4609370	-6.5035200
H	2.5147000	9.7658420	-6.3829630
C	8.4330050	8.0058400	-10.4782130
H	8.3508580	9.0276960	-10.8398590
C	9.8842680	12.1044150	-15.3904880
C	2.4601300	5.8815920	-11.5976940
C	7.4323620	6.1053390	-9.3504580
C	4.4075590	9.4068410	-5.4103340
H	4.0517010	9.6584780	-4.4165000
C	5.7365700	9.0580440	-5.6048210
H	6.4163170	9.0512310	-4.7573250
C	10.1587260	12.6579070	-13.0661110
H	10.6980200	13.1564520	-12.2673930
Rh	6.0108290	10.8210750	-10.6528740
H	6.0667440	12.3367020	-10.9838340
C	7.2057300	11.3544300	-9.2809010
C	4.0776060	11.0287910	-10.9014660
O	2.9529020	11.2390640	-10.9066490
O	7.8237810	11.7325870	-8.3881290
H	1.6722120	5.2953080	-12.0587750
H	1.8837430	5.3936730	-9.5807830
H	10.2310680	12.1760830	-16.4180850
C	5.5258460	10.7075730	-14.4860620
C	4.9245410	9.6730310	-15.2113460
C	5.1176590	12.0372620	-14.7141960
C	3.9315110	9.9319450	-16.1485110
C	4.1180080	12.2756570	-15.6624520
C	3.5236620	11.2418940	-16.3759000
H	5.2504470	8.6492580	-15.0600890
H	3.4826540	9.1121180	-16.7005030
H	3.8060070	13.3015430	-15.8399830
H	2.7485510	11.4582990	-17.1042980
C	6.3272370	5.4160030	-8.5928790
H	5.5529500	5.0400150	-9.2683780
H	6.7276840	4.5671240	-8.0337840
H	5.8441300	6.0936640	-7.8825010
C	7.7263540	8.4355670	-6.9673380
H	8.2196140	8.7226010	-6.0364770

H	7.9262890	7.3747850	-7.1434920
H	8.1998020	8.9913340	-7.7801090
C	5.7533240	13.2143750	-14.0186150
H	5.9322530	13.0131390	-12.9587110
H	6.7214030	13.4599860	-14.4700710
H	5.1108400	14.0943190	-14.0957050
C	8.0178960	10.7071710	-16.2834890
H	8.6779510	10.6654100	-17.1530800
H	7.6951180	9.6904080	-16.0460260
H	7.1202180	11.2687250	-16.5627710

ee-HRh(CO)₂(L3)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2976.67965388, PCM -2976.72219591

P	7.1253320	10.3712440	-13.2369690
P	5.6294550	8.4889380	-9.5419870
C	9.1180480	8.4496610	-12.8209610
C	4.1402510	7.3385980	-9.6037380
C	7.1282230	7.4485300	-9.2334310
C	3.8329650	6.4432650	-10.6651200
C	9.1182510	12.2031600	-14.2339900
H	9.2859640	11.4897140	-15.0328130
C	5.4570170	9.2295860	-7.8304310
C	9.7995280	8.1118210	-15.5013700
H	10.0549110	7.9792470	-16.5494650
C	8.4296980	9.1763380	-13.7983770
C	9.4868000	6.0701710	-8.5778640
H	10.3979520	5.5341280	-8.3270780
C	5.9217020	8.5589240	-6.6864840
H	6.4106730	7.5960160	-6.7815910
C	8.1572150	11.9386070	-13.2404880
C	9.7019160	14.3016020	-13.1786320
H	10.2977250	15.2098580	-13.1546420
C	4.8376530	10.4764010	-7.6647260
H	4.4805240	11.0091180	-8.5377170
C	3.1444600	7.5442940	-8.6326800
H	3.3342930	8.2263030	-7.8147810
C	1.9014990	6.9118590	-8.6824380
C	9.5411380	7.4200990	-8.9313480
H	10.4932660	7.9430670	-8.9529850
C	7.9976220	12.8799540	-12.2138700
H	7.2778640	12.6897680	-11.4283120
C	8.2561930	5.4130750	-8.5477230
H	8.2060960	4.3622520	-8.2766400
C	10.1423420	7.5709020	-13.1762360
H	10.6556200	7.0091220	-12.4010620
C	2.5724840	5.8250340	-10.7078400
H	2.3644710	5.1339360	-11.5183990
C	10.4885820	7.4008340	-14.5166940
H	11.2818900	6.7126400	-14.7946060
C	8.7769920	8.9922760	-15.1457440
H	8.2408040	9.5261800	-15.9253790
C	4.6830150	11.0383480	-6.3961440
H	4.2019760	12.0071650	-6.2942110
C	8.3693520	8.1031400	-9.2590530
H	8.4137460	9.1547960	-9.5290260
C	9.8785320	13.3712710	-14.2058220
C	1.6058000	6.0493030	-9.7305780

C	7.0817740	6.0966890	-8.8687370
H	6.1359120	5.5700370	-8.8548230
C	5.1519060	10.3640240	-5.2682960
H	5.0395260	10.8033470	-4.2809770
C	5.7713720	9.1222500	-5.4185920
H	6.1437750	8.5889830	-4.5482150
C	8.7605580	14.0506020	-12.1822030
H	8.6169740	14.7611150	-11.3728910
Rh	5.5615710	10.2443280	-11.2220980
H	6.8086890	10.7770720	-10.3680700
C	4.0407490	9.4892620	-12.1771150
C	4.8186770	11.9818350	-10.8730200
O	4.3593440	13.0152970	-10.6258160
O	3.1245360	9.0318070	-12.7131100
H	0.6430190	5.5505820	-9.7903970
H	1.1729830	7.1044280	-7.9001230
H	10.6147240	13.5512990	-14.9845580
C	6.0409670	10.6364700	-14.7438290
C	5.2491210	9.6156170	-15.3414280
C	5.8708910	11.9478100	-15.2187340
C	4.3301460	9.9468990	-16.3505630
C	4.9650650	12.2573810	-16.2321870
C	4.1838920	11.2542020	-16.8019470
H	6.4553480	12.7491570	-14.7838130
H	3.6818320	9.1829540	-16.7688950
H	4.8672050	13.2860450	-16.5669450
H	3.4615580	11.4854060	-17.5786890
H	8.8359240	8.5479710	-11.7793040
C	4.8057850	5.9187850	-11.7011320
O	5.8623920	5.3908540	-11.3911830
N	4.3123810	5.9153760	-12.9957030
H	3.6426080	6.6377730	-13.2265910
C	5.3834820	8.2093240	-14.8525350
O	6.0175050	7.9495570	-13.8380300
N	4.7458180	7.2013700	-15.5650500
H	4.4818690	7.4201720	-16.5149760
C	5.0542900	5.8296640	-15.3403290
C	4.9187820	5.2324330	-14.0713850
C	5.4996730	5.0619780	-16.4240930
C	5.3189260	3.8969220	-13.9109750
C	5.8580110	3.7288060	-16.2592070
H	5.5926910	5.5362740	-17.3982100
C	5.7887330	3.1540680	-14.9879360
H	5.2456890	3.4501670	-12.9272810
H	6.2087750	3.1524080	-17.1095460
H	6.0846820	2.1204700	-14.8368840

m062_LANL2DZ

E(RM062X): Gas phase -2975.60398677, PCM -2975.64587530

P	7.0605010	10.4116150	-13.2675900
P	5.6372670	8.5667540	-9.6032120
C	8.3848560	8.0169270	-12.8472540
C	4.1709560	7.4110660	-9.6472560
C	7.1143570	7.5105520	-9.3252660
C	3.8677520	6.5599480	-10.7378440
C	8.6208010	12.4686320	-14.5609740
H	8.3017560	12.0606910	-15.5163620
C	5.4672280	9.2900410	-7.9013460

C	10.1771600	8.2313750	-14.9598790
H	10.8741760	8.3176970	-15.7878200
C	8.3165910	9.1240080	-13.6976550
C	9.4398890	6.0557110	-8.8008670
H	10.3427670	5.4873880	-8.5999220
C	6.0075050	8.6707460	-6.7690260
H	6.5806130	7.7549080	-6.8684770
C	8.1256720	11.9238320	-13.3663590
C	9.8891640	14.1109300	-13.3305900
H	10.5685680	14.9572990	-13.3179630
C	4.7421320	10.4745060	-7.7347990
H	4.3251750	10.9656920	-8.6079590
C	3.2065700	7.5352850	-8.6399370
H	3.3977590	8.1818300	-7.7923590
C	1.9900680	6.8573790	-8.6900890
C	9.5283440	7.3633620	-9.2672400
H	10.4982210	7.8190490	-9.4395400
C	8.5228820	12.5036560	-12.1588210
H	8.1339610	12.1033300	-11.2274330
C	8.1892210	5.4727720	-8.5972760
H	8.1173140	4.4497990	-8.2414160
C	9.3485270	7.0332120	-13.0394670
H	9.3761610	6.1825230	-12.3654740
C	2.6437380	5.8857110	-10.7755240
H	2.4472500	5.2109910	-11.6018690
C	10.2486320	7.1407350	-14.0963500
H	11.0021030	6.3746150	-14.2522380
C	9.2180680	9.2218410	-14.7599080
H	9.1892430	10.0732070	-15.4313920
C	4.5514770	11.0219440	-6.4695050
H	3.9855060	11.9421280	-6.3628470
C	8.3676890	8.0893830	-9.5278040
H	8.4318170	9.1048640	-9.9125610
C	9.4919460	13.5512970	-14.5441870
C	1.7005440	6.0306940	-9.7640340
C	7.0313560	6.1956760	-8.8592690
H	6.0568700	5.7355510	-8.7205040
C	5.0945480	10.3984310	-5.3492940
H	4.9548890	10.8292320	-4.3627070
C	5.8243680	9.2239380	-5.5035620
H	6.2579680	8.7337630	-4.6374500
C	9.4023420	13.5857040	-12.1396060
H	9.6990110	14.0196980	-11.1899520
Rh	5.5484870	10.2936940	-11.2116590
H	6.7554900	10.7760370	-10.3219560
C	4.0178080	9.5161590	-12.2059270
C	4.9433150	12.1004200	-10.8999090
O	4.6183030	13.1626410	-10.6162050
O	3.1535950	9.0006270	-12.7508880
H	0.7597020	5.4928050	-9.8153170
H	1.2758900	6.9827120	-7.8825830
H	9.8608000	13.9603890	-15.4797020
C	5.9136750	10.6601010	-14.7193400
C	5.1565970	9.6323730	-15.3275930
C	5.6044260	11.9781890	-15.0881820
C	4.1774980	9.9343230	-16.2795300
C	4.6361880	12.2696800	-16.0426420
C	3.9211670	11.2452950	-16.6536720

H	6.1219980	12.8011740	-14.6088860
H	3.5660860	9.1390940	-16.6955450
H	4.4318820	13.3053530	-16.2950600
H	3.1529900	11.4642090	-17.3874520
H	7.6503760	7.9056900	-12.0562180
C	4.8603120	6.1857710	-11.8100330
O	6.0323960	5.9837620	-11.5675310
N	4.2985670	5.9299860	-13.0512000
H	3.5169290	6.5134320	-13.3236830
C	5.3216180	8.2323740	-14.8436600
O	5.8455560	8.0025240	-13.7725040
N	4.8175520	7.2040240	-15.6221790
H	4.6775290	7.4142600	-16.6005280
C	5.2086040	5.8684180	-15.3461290
C	5.0331790	5.2977180	-14.0775870
C	5.8052490	5.1212350	-16.3641470
C	5.5446310	4.0191600	-13.8395380
C	6.2753190	3.8393070	-16.1244540
H	5.9306790	5.5764300	-17.3429650
C	6.1678000	3.2965380	-14.8452510
H	5.4269520	3.5998250	-12.8462570
H	6.7453540	3.2782660	-16.9248440
H	6.5521920	2.3039030	-14.6370780

ea-HRh(CO)₂(L3)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2976.67118611, PCM -2976.71507387

P	7.0977050	10.2725480	-13.3098420
P	5.9055380	8.3908390	-9.5980670
C	8.8802130	8.1280100	-12.9259780
C	4.3828010	7.2875340	-9.6097880
C	7.3773490	7.2931910	-9.3335330
C	4.0052420	6.4331890	-10.6844980
C	8.7836900	12.4047770	-14.3450390
H	8.5004440	12.1021230	-15.3473850
C	5.8476410	9.1195520	-7.8731670
C	10.0072590	8.2397660	-15.4723100
H	10.4369650	8.2835450	-16.4696100
C	8.4075750	9.0697300	-13.8451920
C	9.7116250	5.8336810	-8.7633630
H	10.6123570	5.2669670	-8.5445470
C	6.1713810	8.3509360	-6.7401050
H	6.4616280	7.3120430	-6.8546950
C	8.2155440	11.7713540	-13.2250880
C	10.1159220	13.8368490	-12.9192120
H	10.8421250	14.6362860	-12.8029100
C	5.4977080	10.4633480	-7.6837680
H	5.2526170	11.0754260	-8.5424910
C	3.4283970	7.5111180	-8.6034450
H	3.6703570	8.1704610	-7.7800330
C	2.1606090	6.9268010	-8.6258070
C	9.7979040	7.1849310	-9.1039090
H	10.7648980	7.6778840	-9.1504620
C	8.6394800	12.1828840	-11.9527950
H	8.2309180	11.6982070	-11.0721730
C	8.4618880	5.2144530	-8.7062530
H	8.3869380	4.1623980	-8.4455030
C	9.9175660	7.2600820	-13.2694090

H	10.2664010	6.5348590	-12.5400820
C	2.7239650	5.8595040	-10.6950390
H	2.4630380	5.1943330	-11.5117860
C	10.4855750	7.3140610	-14.5422930
H	11.2896840	6.6353240	-14.8125690
C	8.9771600	9.1146820	-15.1259110
H	8.6150080	9.8239980	-15.8638930
C	5.4647530	11.0242970	-6.4042790
H	5.1941350	12.0697360	-6.2852960
C	8.6380670	7.9078190	-9.3870070
H	8.7152940	8.9601850	-9.6492310
C	9.7141190	13.4321410	-14.1942570
C	1.7997500	6.0968730	-9.6796840
C	7.3015490	5.9371140	-8.9876720
H	6.3401310	5.4397900	-8.9575770
C	5.7819420	10.2491870	-5.2900150
H	5.7595780	10.6847250	-4.2949070
C	6.1353360	8.9086740	-5.4628950
H	6.3897570	8.2958140	-4.6024640
C	9.5808560	13.2034330	-11.7992190
H	9.8884870	13.5031880	-10.8014750
Rh	5.3955660	10.2021150	-11.3954000
H	4.1988570	10.3646430	-10.3914320
C	4.0129730	9.3567430	-12.4230410
C	5.6485210	12.0504990	-10.9553590
O	5.5936480	13.1804810	-10.7033080
O	3.0820030	8.9340200	-12.9725000
H	0.8179070	5.6344370	-9.7165660
H	1.4639710	7.1310950	-7.8177560
H	10.1303320	13.9126700	-15.0754410
C	6.0304680	10.5738130	-14.8158150
C	5.3030070	9.5448850	-15.4764080
C	5.7855700	11.8987210	-15.2111890
C	4.4112120	9.8761970	-16.5084260
C	4.9011440	12.2103200	-16.2429150
C	4.2148880	11.1947730	-16.9050520
H	6.2845680	12.7100400	-14.6958740
H	3.8180400	9.1031810	-16.9872440
H	4.7426870	13.2492420	-16.5168770
H	3.5154160	11.4256750	-17.7024320
H	8.4213480	8.0495810	-11.9484170
C	4.9298330	5.9237950	-11.7695940
O	6.0214550	5.4368940	-11.5170450
N	4.3712030	5.8907550	-13.0401470
H	3.6889080	6.6073520	-13.2538190
C	5.4313010	8.1397540	-14.9822460
O	6.0403700	7.8969800	-13.9474410
N	4.8018490	7.1230330	-15.6790630
H	4.5344280	7.3186770	-16.6328630
C	5.0754380	5.7515830	-15.4092130
C	4.9415430	5.1866130	-14.1237560
C	5.4877490	4.9462150	-16.4799300
C	5.3123390	3.8444390	-13.9430360
C	5.8165860	3.6093340	-16.2910530
H	5.5799620	5.3959870	-17.4657210
C	5.7504170	3.0647920	-15.0063960
H	5.2374930	3.4206480	-12.9490240
H	6.1416840	3.0065010	-17.1332080

H	6.0220500	2.0277240	-14.8349710
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m062_LANL2DZ

E(RM062X): Gas phase -2975.60678868, PCM -2975.64876997

P	7.0268630	10.4538890	-13.3519550
P	5.6339660	8.2579900	-9.5949950
C	7.9977610	7.8842990	-12.9803720
C	4.2070830	7.0501490	-9.6172220
C	7.1001050	7.2343210	-9.1690170
C	3.9389310	6.2223760	-10.7324790
C	9.5720690	11.5460280	-14.1115120
H	9.8565150	10.5561100	-14.4504540
C	5.3461210	9.0775100	-7.9580530
C	8.9705150	7.5572380	-15.5692860
H	9.3415140	7.4243220	-16.5814570
C	7.8659990	8.9200230	-13.9042910
C	9.4313640	5.8427370	-8.4963950
H	10.3344180	5.2991870	-8.2369490
C	6.1219030	8.8236280	-6.8241480
H	6.9295820	8.1006460	-6.8668650
C	8.3009730	11.7688630	-13.5748680
C	10.1593400	13.8628060	-13.7534400
H	10.8809620	14.6707490	-13.8215570
C	4.3092820	10.0175000	-7.8616580
H	3.6999650	10.2320480	-8.7351520
C	3.2617500	7.0563570	-8.5853860
H	3.4342770	7.6620510	-7.7042350
C	2.0905470	6.3037010	-8.6511740
C	9.5170530	7.1201940	-9.0403040
H	10.4859590	7.5798560	-9.2079220
C	7.9822060	13.0529470	-13.1070480
H	7.0108970	13.2238780	-12.6474300
C	8.1814300	5.2602570	-8.2873260
H	8.1108630	4.2621720	-7.8658270
C	8.6238070	6.6915580	-13.3412180
H	8.6838770	5.8878210	-12.6149620
C	2.7595380	5.4756130	-10.7940870
H	2.5959410	4.8245040	-11.6466960
C	9.1264770	6.5372190	-14.6277520
H	9.6121230	5.6092960	-14.9139120
C	8.3285350	8.7386880	-15.2155750
H	8.1941990	9.5294300	-15.9510640
C	4.0486310	10.6735080	-6.6649620
H	3.2377910	11.3932150	-6.6111650
C	8.3547300	7.8113110	-9.3777740
H	8.4225980	8.8076050	-9.8114570
C	10.4948240	12.5875890	-14.1951590
C	1.8265830	5.5187850	-9.7638090
C	7.0220660	5.9518220	-8.6198310
H	6.0495160	5.4927240	-8.4646090
C	4.8353280	10.4175630	-5.5424480
H	4.6407850	10.9372350	-4.6095230
C	5.8708420	9.4947490	-5.6270830
H	6.4886820	9.2869430	-4.7589500
C	8.8982330	14.0941590	-13.2082960
H	8.6319640	15.0815550	-12.8449350
Rh	5.8935500	10.7901980	-11.1796460
H	5.1557910	11.4321870	-9.9640820

C	4.1523090	10.9115110	-12.0268230
C	7.3920930	11.5702770	-10.2620070
O	8.2245780	12.1303040	-9.7118400
O	3.1354470	11.0458710	-12.5308440
H	0.9180040	4.9288780	-9.8243750
H	1.3902000	6.3357750	-7.8224740
H	11.4813200	12.3966080	-14.6059660
C	5.8730370	10.7761400	-14.7805350
C	4.9577120	9.7927440	-15.2083450
C	5.8380740	12.0157200	-15.4230720
C	4.0433790	10.0610110	-16.2266900
C	4.9151290	12.2846880	-16.4327300
C	4.0094920	11.3115770	-16.8348040
H	6.5435070	12.7883940	-15.1383310
H	3.3351680	9.2915390	-16.5235760
H	4.9106400	13.2621740	-16.9043610
H	3.2826800	11.5194110	-17.6128500
H	7.5705490	7.9896450	-11.9872450
C	4.9671300	5.9723280	-11.7938350
O	6.1532810	5.9117330	-11.5394620
N	4.4595990	5.6796310	-13.0529110
H	3.6536870	6.2320040	-13.3157980
C	4.9759510	8.4376310	-14.5615190
O	5.0089490	8.3003090	-13.3544670
N	4.9914870	7.3914230	-15.4638730
H	5.0907330	7.7001460	-16.4219630
C	5.5486010	6.1048920	-15.2452350
C	5.3540820	5.3346060	-14.0910990
C	6.3372690	5.5875890	-16.2807110
C	6.0422470	4.1233040	-13.9661930
C	6.9820250	4.3682740	-16.1592070
H	6.4757120	6.1858070	-17.1779850
C	6.8576630	3.6414870	-14.9767480
H	5.8949410	3.5577630	-13.0524390
H	7.5951300	4.0000030	-16.9749830
H	7.3686690	2.6927090	-14.8544770

ee-HRh(CO)₂(L4)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2826.27217123, PCM -2826.31331838

Rh	-1.7703900	14.4349830	5.3443290
P	-1.6451120	15.0118200	7.6676840
P	-0.7838400	16.0656070	3.8865680
C	-3.2761230	15.0875220	8.5465460
C	-4.2226720	14.0936540	8.2512250
H	-3.9893660	13.3356410	7.5088050
C	-5.4578880	14.0739280	8.8974230
H	-6.1772530	13.2958120	8.6587310
C	-5.7730220	15.0567820	9.8382420
H	-6.7398990	15.0486470	10.3333120
C	-4.8409320	16.0506840	10.1363890
H	-5.0780510	16.8199060	10.8660880
C	-3.5960870	16.0633850	9.5029670
H	-2.8746250	16.8328190	9.7560440
C	-1.6692010	16.4536380	2.3039700
C	-2.5123370	15.4817520	1.7496140
C	-3.1459700	15.7077490	0.5258270
H	-3.7969590	14.9453180	0.1076340

C	-2.9505230	16.9118160	-0.1512010
H	-3.4493660	17.0918720	-1.0992860
C	-2.1139340	17.8881640	0.3963580
H	-1.9606340	18.8288000	-0.1254690
C	-1.4723870	17.6596990	1.6134060
H	-0.8280710	18.4204920	2.0420860
C	-3.6293800	15.0033250	5.0542570
C	0.9121590	15.6733820	3.2459900
C	1.3222010	14.3352630	3.1727240
C	1.7790150	16.6742650	2.7764380
C	2.5703040	14.0029330	2.6433990
C	3.0322310	16.3407320	2.2624690
C	3.4301760	15.0044120	2.1915220
H	0.6643490	13.5552190	3.5403570
H	1.4792320	17.7160010	2.8181550
H	2.8717430	12.9604680	2.5935730
H	3.6962100	17.1271490	1.9147350
H	4.4052170	14.7464820	1.7878750
C	-0.6937280	13.8920790	8.7949220
C	-0.0952140	12.7314410	8.2930230
C	-0.6050220	14.1678760	10.1701470
C	0.5872750	11.8609550	9.1476670
C	0.0795000	13.3019560	11.0200570
C	0.6771800	12.1449260	10.5095710
H	-0.1628380	12.5148130	7.2324830
H	1.0488210	10.9639540	8.7447900
H	0.1445880	13.5263440	12.0810580
H	1.2083090	11.4691470	11.1740200
C	-1.9119440	12.5798940	4.8043960
O	-1.9393540	11.4644660	4.4996120
O	-4.7164450	15.3336990	4.8676620
H	-0.2394800	14.0717230	5.6026390
H	-2.6689130	14.5470270	2.2800710
H	-1.0662240	15.0655270	10.5693320
C	0.2220090	17.1386460	7.8593030
C	0.3229830	18.3410790	7.1479160
C	1.6011160	18.9598540	6.9649680
C	2.7775850	18.3176250	7.4747180
C	2.6330020	17.0815310	8.1574620
C	1.4003270	16.5109000	8.3544450
H	0.8715820	20.6880200	5.8811840
C	1.7556530	20.1937230	6.2707910
C	4.0440490	18.9290450	7.2820150
H	3.5221840	16.5899880	8.5439630
H	1.3114930	15.5866960	8.9106180
C	4.1584340	20.1251000	6.6093640
C	3.0001510	20.7592440	6.0992790
H	4.9265140	18.4311490	7.6763580
H	5.1327830	20.5836130	6.4682670
H	3.0942800	21.7033690	5.5699820
C	-0.9204720	18.9091500	6.5337490
C	-1.7639020	19.8148150	7.2548800
C	-1.3012530	18.4638670	5.2630120
C	-1.4106540	20.3236800	8.5375020
C	-3.0203310	20.2142800	6.6901740
C	-2.5596860	18.8537960	4.7236130
C	-2.2473280	21.1851670	9.2125630
H	-0.4629540	20.0269090	8.9748490

C	-3.8577380	21.1043680	7.4128410
C	-3.3905260	19.6945100	5.4221930
H	-2.8465720	18.4971270	3.7417970
C	-3.4829480	21.5835470	8.6479920
H	-1.9551060	21.5661780	10.1871370
H	-4.8057660	21.4000610	6.9702370
H	-4.3476790	19.9839140	4.9961410
H	-4.1311620	22.2648710	9.1912170
N	-0.4145640	17.6775100	4.4972820
N	-1.0519530	16.6020910	8.1493850
H	0.4918040	17.6332070	4.9569000
H	-1.7612990	17.2698630	7.8526610

m062_LANL2DZ

E(RM062X): Gas phase -2825.23977570, PCM -2825.28226475

Rh	-1.6514140	14.7085390	5.4468620
P	-1.6306000	15.1809150	7.7402670
P	-0.6818110	16.2241950	3.9334730
C	-3.2862700	15.2584060	8.5471470
C	-4.2484370	14.3311030	8.1326290
H	-3.9996380	13.6194550	7.3484400
C	-5.5131040	14.3170950	8.7102710
H	-6.2482140	13.5906170	8.3789080
C	-5.8374640	15.2406700	9.7010170
H	-6.8282780	15.2389320	10.1441690
C	-4.8875550	16.1677820	10.1180850
H	-5.1337090	16.8913940	10.8889660
C	-3.6142830	16.1735950	9.5528870
H	-2.8791680	16.8934840	9.8995330
C	-1.5680580	16.5186880	2.3442580
C	-2.4023450	15.5199440	1.8391920
C	-3.0415420	15.6921430	0.6125970
H	-3.6883210	14.9105730	0.2268350
C	-2.8580350	16.8669720	-0.1095190
H	-3.3609980	17.0044900	-1.0615190
C	-2.0305080	17.8702800	0.3929930
H	-1.8888940	18.7897700	-0.1664590
C	-1.3839110	17.6957900	1.6117720
H	-0.7468110	18.4765580	2.0179450
C	-3.5209810	15.3300330	5.1097150
C	1.0027360	15.8168750	3.3122690
C	1.4023260	14.4790050	3.2779560
C	1.8733560	16.8028890	2.8331850
C	2.6523500	14.1301240	2.7743570
C	3.1295550	16.4527940	2.3481250
C	3.5200390	15.1165150	2.3148000
H	0.7322600	13.7134740	3.6577300
H	1.5741440	17.8469380	2.8439170
H	2.9512080	13.0869370	2.7524730
H	3.8028490	17.2262310	1.9924510
H	4.4994020	14.8452400	1.9333690
C	-0.7560440	14.0063120	8.8555470
C	-0.2181490	12.8240700	8.3514990
C	-0.6420420	14.2898570	10.2220430
C	0.4330880	11.9311890	9.2027530
C	0.0115430	13.4027630	11.0677220
C	0.5506930	12.2206190	10.5572410
H	-0.3024590	12.6090940	7.2908420

H	0.8519350	11.0135160	8.8024760
H	0.1023910	13.6297050	12.1253390
H	1.0619670	11.5285720	11.2191990
C	-1.7214810	12.8263240	4.9148310
O	-1.6238280	11.7159620	4.6469880
O	-4.5742200	15.7188960	4.9112800
H	-0.1485620	14.3867810	5.7596350
H	-2.5478240	14.6058700	2.4102370
H	-1.0512190	15.2196250	10.6081230
C	0.2378800	17.1899660	7.9347650
C	0.3276910	18.3224000	7.1361080
C	1.6100750	18.8423860	6.7788510
C	2.7863780	18.1621620	7.2015720
C	2.6517120	16.9945420	7.9968300
C	1.4206240	16.5263710	8.3641570
H	0.8556640	20.5237180	5.6419820
C	1.7510720	20.0005590	5.9649060
C	4.0552750	18.6587860	6.8100090
H	3.5500510	16.4771190	8.3219090
H	1.3282070	15.6510910	8.9974310
C	4.1614710	19.7766010	6.0226860
C	2.9937590	20.4519460	5.5964260
H	4.9441390	18.1289150	7.1418540
H	5.1370940	20.1454950	5.7237870
H	3.0821970	21.3385350	4.9763870
C	-0.9276670	18.8835490	6.5566890
C	-1.8491210	19.6284630	7.3554370
C	-1.2618580	18.5458620	5.2530850
C	-1.5472160	20.0057360	8.6938960
C	-3.1281150	19.9618700	6.8277040
C	-2.5411520	18.8847420	4.7337200
C	-2.4668770	20.6816150	9.4560620
H	-0.5727280	19.7521030	9.1010040
C	-4.0524380	20.6679460	7.6388870
C	-3.4470650	19.5611170	5.5039440
H	-2.7815800	18.6034590	3.7135080
C	-3.7337420	21.0203410	8.9253160
H	-2.2187330	20.9648090	10.4741070
H	-5.0236240	20.9181080	7.2202330
H	-4.4266670	19.8073770	5.1037490
H	-4.4493920	21.5576930	9.5388000
N	-0.3431080	17.8693880	4.4237440
N	-1.0185540	16.7022560	8.3587590
H	0.5850720	17.8814670	4.8402370
H	-1.7350080	17.3983480	8.1615970

ea-HRh(CO)₂(L4)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2826.27100821, PCM -2826.31228661

Rh	-2.4927910	14.6161820	5.3710060
P	-1.6740860	15.0755350	7.6386410
P	-0.9386900	15.9641560	4.0405120
C	-2.9671860	14.7950680	8.9249910
C	-3.8778050	13.7409650	8.7529270
H	-3.8320770	13.1337790	7.8543550
C	-4.8507650	13.4858320	9.7193710
H	-5.5503850	12.6676850	9.5747830
C	-4.9342820	14.2876220	10.8596960

H	-5.6993710	14.0945290	11.6063660
C	-4.0387710	15.3445040	11.0323430
H	-4.1049990	15.9768550	11.9132860
C	-3.0577910	15.5978900	10.0717940
H	-2.3664590	16.4244570	10.1980190
C	-1.4104100	16.4281210	2.3034080
C	-2.2991160	15.6192220	1.5842070
C	-2.6144160	15.9193300	0.2569220
H	-3.3055070	15.2826560	-0.2880880
C	-2.0533480	17.0366310	-0.3615260
H	-2.3045060	17.2743760	-1.3913680
C	-1.1714040	17.8532610	0.3512710
H	-0.7353290	18.7284470	-0.1225190
C	-0.8480410	17.5495280	1.6728520
H	-0.1710050	18.1897010	2.2290770
C	-4.1701200	15.5701350	5.6156310
C	0.7620760	15.2808840	3.7217600
C	0.9173780	13.8884510	3.6564740
C	1.8829150	16.0964750	3.4926560
C	2.1615830	13.3227440	3.3703000
C	3.1290710	15.5291420	3.2241930
C	3.2718220	14.1416860	3.1590150
H	0.0621370	13.2460930	3.8419450
H	1.7849490	17.1767720	3.5203900
H	2.2611050	12.2421690	3.3195250
H	3.9877560	16.1740730	3.0598690
H	4.2420210	13.7026380	2.9445100
C	-0.2580280	14.0598310	8.2338620
C	0.7740720	13.7592240	7.3325190
C	-0.1852480	13.5600060	9.5441870
C	1.8684920	12.9951350	7.7369990
C	0.9073540	12.7891340	9.9437860
C	1.9374300	12.5086460	9.0433990
H	0.7209670	14.1152550	6.3097090
H	2.6593870	12.7756610	7.0258720
H	0.9502680	12.4039180	10.9585640
H	2.7850570	11.9059860	9.3571060
C	-2.1164560	12.7321500	5.4505260
O	-1.9467650	11.5867710	5.4309720
O	-5.2137100	16.0592510	5.6862330
H	-3.1471800	14.2152540	3.9875050
H	-2.7507370	14.7580550	2.0667380
H	-0.9801710	13.7703290	10.2513510
C	0.0091420	17.3895010	7.9965260
C	0.1517500	18.5730760	7.2572530
C	1.3946270	19.2853810	7.2837620
C	2.4858130	18.7796210	8.0639490
C	2.2898420	17.5888090	8.8110990
C	1.0935180	16.9175860	8.7904140
H	0.7823890	20.8750830	5.9457750
C	1.5999470	20.4827890	6.5411290
C	3.7199200	19.4810150	8.0767390
H	3.1055440	17.2150560	9.4248040
H	0.9581480	16.0323510	9.3973850
C	3.8850710	20.6366500	7.3467930
C	2.8118730	21.1371640	6.5713680
H	4.5358900	19.0852120	8.6765690
H	4.8336210	21.1652720	7.3636340

H	2.9453240	22.0487580	5.9956090
C	-1.0166140	19.0720490	6.4608330
C	-1.8707470	20.1034970	6.9735230
C	-1.3108210	18.4736320	5.2304140
C	-1.6234530	20.7520060	8.2170370
C	-3.0343780	20.4929020	6.2309390
C	-2.4768340	18.8623280	4.5110620
C	-2.4701930	21.7317810	8.6873040
H	-0.7513330	20.4655620	8.7947210
C	-3.8843140	21.5077790	6.7435160
C	-3.3078590	19.8371320	5.0025880
H	-2.6946650	18.3934770	3.5594980
C	-3.6118050	22.1194580	7.9461580
H	-2.2588190	22.2133130	9.6380280
H	-4.7609880	21.7907090	6.1661410
H	-4.1942940	20.1220200	4.4419680
H	-4.2690970	22.8944120	8.3292680
N	-0.4313850	17.5175710	4.6896050
N	-1.2415730	16.7375840	8.0170900
H	0.3805340	17.3995450	5.2901250
H	-1.9311630	17.3262450	7.5533400

m062_LANL2DZ

E(RM062X): Gas phase -2825.24166695, PCM -2825.28196428

Rh	-2.8485200	14.7991240	5.3753460
P	-1.7837140	15.1316390	7.5326380
P	-1.1126890	15.9131910	4.1120890
C	-2.7621520	14.6752730	9.0092410
C	-3.6506470	13.6000810	8.9285560
H	-3.7820360	13.0814250	7.9824870
C	-4.3742890	13.2065220	10.0518790
H	-5.0625900	12.3703100	9.9846180
C	-4.2267700	13.8970880	11.2515640
H	-4.7992570	13.5978440	12.1238030
C	-3.3561460	14.9826750	11.3301170
H	-3.2527650	15.5299120	12.2616860
C	-2.6242780	15.3719530	10.2129510
H	-1.9619660	16.2317820	10.2619310
C	-1.4090700	16.3420800	2.3426600
C	-2.1919860	15.4843970	1.5679770
C	-2.3748120	15.7380400	0.2106600
H	-2.9837180	15.0662670	-0.3858500
C	-1.7889550	16.8561840	-0.3757590
H	-1.9409050	17.0588410	-1.4311890
C	-1.0132050	17.7191460	0.3958110
H	-0.5602810	18.5955980	-0.0569570
C	-0.8178890	17.4611300	1.7488600
H	-0.2214490	18.1340030	2.3591810
C	-4.3653830	15.9954040	5.7258620
C	0.5015030	15.0426150	3.9078030
C	0.5347760	13.6536280	4.0404320
C	1.6816910	15.7295750	3.5994500
C	1.7304260	12.9586180	3.8762650
C	2.8796310	15.0361140	3.4572790
C	2.9053200	13.6486850	3.5944090
H	-0.3763510	13.1198790	4.2954860
H	1.6628990	16.8076370	3.4652130
H	1.7443620	11.8793490	3.9886040

H	3.7916830	15.5780850	3.2276600
H	3.8403350	13.1094440	3.4786900
C	-0.1971400	14.2655950	7.8202750
C	0.9429980	14.6643770	7.1154970
C	-0.1208260	13.1497430	8.6591490
C	2.1376280	13.9669280	7.2427220
C	1.0750980	12.4451990	8.7799480
C	2.2038100	12.8507340	8.0738070
H	0.9058630	15.5344600	6.4689230
H	3.0075630	14.2923770	6.6811840
H	1.1216160	11.5788360	9.4318530
H	3.1338490	12.2997490	8.1711550
C	-2.7980130	12.8749850	5.4078760
O	-2.8035340	11.7272350	5.3920730
O	-5.3081490	16.6317810	5.8461660
H	-3.5783620	14.5780730	4.0179280
H	-2.6609520	14.6203280	2.0308330
H	-0.9923200	12.8304850	9.2221170
C	-0.2488610	17.4807540	8.0222740
C	0.0382910	18.6328000	7.2909680
C	1.2613170	19.3306180	7.5266340
C	2.1699140	18.8506130	8.5111780
C	1.8225330	17.6940700	9.2563790
C	0.6496720	17.0300200	9.0284940
H	0.9191380	20.8742600	6.0475660
C	1.6099900	20.5005700	6.7970780
C	3.3861540	19.5441990	8.7354740
H	2.5044850	17.3412420	10.0249990
H	0.3909540	16.1516940	9.6106360
C	3.6968720	20.6690030	8.0157810
C	2.7955970	21.1484460	7.0355970
H	4.0677680	19.1647510	9.4920760
H	4.6295910	21.1935430	8.1947120
H	3.0460630	22.0390020	6.4680030
C	-1.0033480	19.1510020	6.3518950
C	-1.8084060	20.2707620	6.7400230
C	-1.2965040	18.4675140	5.1755850
C	-1.5535320	21.0134240	7.9266080
C	-2.9215650	20.6503190	5.9388670
C	-2.4359050	18.8349110	4.4031430
C	-2.3448630	22.0795120	8.2728740
H	-0.7196820	20.7315940	8.5599680
C	-3.7203140	21.7570190	6.3235100
C	-3.2199860	19.8886420	4.7806760
H	-2.6720780	18.2767700	3.5043410
C	-3.4393550	22.4636350	7.4639330
H	-2.1285060	22.6343900	9.1802820
H	-4.5641210	22.0298950	5.6956040
H	-4.0878190	20.1576860	4.1852730
H	-4.0539830	23.3102580	7.7511650
N	-0.4771490	17.4206250	4.7298300
N	-1.4513830	16.8029630	7.7805550
H	0.3584800	17.3132590	5.2975970
H	-2.0578860	17.3443440	7.1713500

ee-HRh(CO)₂(L5)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2866.34400862, PCM -2866.37655708

P	5.3923410	8.6347620	-12.7812500
P	4.6917790	8.3465840	-9.2098500
C	3.5294300	8.0199020	-7.7943670
C	3.9451310	7.4249370	-6.5902400
C	6.3057450	9.5321900	-15.3488370
H	6.7439920	8.5473410	-15.4696640
C	6.0341160	9.2606740	-8.3221810
C	6.9978990	8.6101310	-7.5357200
H	7.0494320	7.5266840	-7.5265000
C	5.6068930	9.8533170	-14.1726250
C	5.8756690	11.7388650	-16.2447960
H	5.9766120	12.4649700	-17.0467270
C	6.0184210	10.6620090	-8.3514500
H	5.2851710	11.1721940	-8.9682240
C	2.1957940	8.4320920	-7.9118360
H	1.8722430	8.9085100	-8.8319880
C	1.2949230	8.2483220	-6.8592570
C	5.0408690	11.1305230	-14.0569100
H	4.4847690	11.3810770	-13.1605090
C	3.0463030	7.2370330	-5.5421330
H	3.3841020	6.7716840	-4.6202410
C	6.9377710	11.3990600	-7.6026360
H	6.9108830	12.4845820	-7.6362370
C	6.4385600	10.4672080	-16.3750730
C	1.7170400	7.6488490	-5.6740140
C	7.8872910	10.7446690	-6.8172380
H	8.6014840	11.3178120	-6.2323130
C	7.9169680	9.3484320	-6.7889850
H	8.6537480	8.8315130	-6.1794480
C	5.1776890	12.0679350	-15.0830080
H	4.7305360	13.0519870	-14.9735760
Rh	3.6424800	9.2539490	-11.2030960
H	4.6245200	10.5033080	-10.9981570
C	2.4157860	7.7530220	-11.4520600
C	2.3512790	10.6569010	-11.3611010
O	1.6137480	11.5467960	-11.4407400
O	1.6678820	6.8865580	-11.5916600
H	1.0183480	7.5047300	-4.8545750
H	0.2653010	8.5765690	-6.9700340
H	6.9796210	10.1999760	-17.2786720
C	5.3028990	7.0562650	-13.7471990
C	6.4355410	6.3008060	-14.0861720
C	4.0513170	6.6491070	-14.2341410
C	6.3143080	5.1642020	-14.8893710
C	3.9320050	5.5153110	-15.0378360
C	5.0641940	4.7679020	-15.3671490
H	7.4108980	6.5895460	-13.7117910
H	3.1655010	7.2260590	-13.9896850
H	7.2021730	4.5931450	-15.1483070
H	2.9539820	5.2169970	-15.4045620
H	4.9726440	3.8844230	-15.9929170
H	4.9739050	7.1038130	-6.4682470
C	7.3907860	7.6847430	-10.9384590
C	8.6650120	7.8011230	-10.3371990
C	9.5812230	8.7915510	-10.7060470
C	9.2303600	9.6908820	-11.7132750
C	7.9892450	9.5890190	-12.3442050
C	7.0729250	8.5983850	-11.9758280

C	6.5207690	6.5486550	-10.4770260
C	6.9025300	5.2401270	-10.8496820
C	6.1855660	4.1073150	-10.4473710
C	5.0672630	4.2724550	-9.6290150
C	4.6841510	5.5490630	-9.2127850
C	5.4009980	6.6801260	-9.6177660
H	10.5393940	8.8606380	-10.2127020
H	7.7638790	10.3046090	-13.1231830
H	6.4932920	3.1232750	-10.7686280
H	3.8137420	5.6292770	-8.5749840
O	10.0378340	10.6984230	-12.1561460
O	8.9455230	6.8833630	-9.3637930
O	4.2921380	3.2451580	-9.1752900
O	8.0211800	5.1481350	-11.6298410
C	11.3004860	10.8741720	-11.5375940
H	11.2011470	11.0856120	-10.4648430
H	11.9459400	9.9956670	-11.6712750
H	11.7610290	11.7322630	-12.0298630
C	10.2122960	6.9181600	-8.7320600
H	10.2153730	6.0894920	-8.0214990
H	11.0297290	6.7764680	-9.4511290
H	10.3689360	7.8582450	-8.1875570
C	8.4844900	3.8671980	-12.0177650
H	8.7288580	3.2428800	-11.1485170
H	7.7526330	3.3427710	-12.6454400
H	9.3926470	4.0405680	-12.5981120
C	4.6026320	1.9271700	-9.5935900
H	3.8523540	1.2807160	-9.1355360
H	4.5477620	1.8244060	-10.6851970
H	5.5995040	1.6157110	-9.2537160

m062_LANL2DZ

E(RM062X): Gas phase -2865.30442455, PCM -2865.33525671

P	5.3950430	8.7646700	-12.6879490
P	4.7935800	8.4434670	-9.2771080
C	3.6199170	8.0824790	-7.8985250
C	3.9382370	8.2491970	-6.5475960
C	6.8455190	9.6308150	-15.0108510
H	7.7080360	9.0910050	-14.6314540
C	6.2681380	9.0893780	-8.3887530
C	7.0591880	8.2613740	-7.5815600
H	6.8258160	7.2024550	-7.5038300
C	5.6626170	9.6821220	-14.2618010
C	5.8568000	11.0334540	-16.7077080
H	5.9346880	11.5586450	-17.6545380
C	6.5939830	10.4417200	-8.5083580
H	5.9864890	11.0791880	-9.1439570
C	2.3185480	7.6840960	-8.2334530
H	2.0415410	7.5737420	-9.2777170
C	1.3737570	7.4226390	-7.2479340
C	4.5874380	10.4299740	-14.7480420
H	3.6806970	10.4952950	-14.1517070
C	2.9843230	8.0076400	-5.5604860
H	3.2474710	8.1509890	-4.5171260
C	7.6980030	10.9626750	-7.8345010
H	7.9457990	12.0142410	-7.9412500
C	6.9415600	10.3049730	-16.2232750
C	1.7044430	7.5875410	-5.9049170

C	8.4769280	10.1364180	-7.0302850
H	9.3330490	10.5428520	-6.4994040
C	8.1517390	8.7856870	-6.8995870
H	8.7524240	8.1396740	-6.2655890
C	4.6804930	11.0957310	-15.9682790
H	3.8356500	11.6714520	-16.3326420
Rh	3.7893080	9.7823780	-11.1951450
H	5.0395890	10.7415470	-11.0865730
C	2.1406200	8.7580840	-11.5546690
C	2.9402100	11.4640780	-11.0390450
O	2.4825590	12.5135910	-10.9607790
O	1.1540720	8.2339490	-11.8013070
H	0.9644140	7.3997830	-5.1335600
H	0.3753420	7.1055800	-7.5314570
H	7.8672520	10.2660600	-16.7888410
C	5.2414990	7.0256660	-13.3019940
C	6.2183530	6.4360200	-14.1121710
C	4.1110230	6.2815090	-12.9596160
C	6.0545060	5.1377850	-14.5823760
C	3.9478110	4.9781590	-13.4245190
C	4.9175740	4.4051260	-14.2402690
H	7.1161390	6.9873540	-14.3710980
H	3.3615540	6.7146200	-12.3058480
H	6.8148730	4.6970730	-15.2208570
H	3.0646850	4.4136700	-13.1405240
H	4.7902730	3.3930180	-14.6133510
H	4.9292660	8.5790090	-6.2567970
C	7.4021550	7.7873730	-10.9496200
C	8.6431150	7.8954900	-10.2954350
C	9.4663320	9.0057970	-10.4659690
C	9.0422470	10.0319590	-11.3129400
C	7.8520750	9.9179180	-12.0238220
C	7.0451360	8.7902360	-11.8627070
C	6.5219110	6.6353580	-10.6016150
C	6.8701970	5.3636230	-11.0840480
C	6.0691140	4.2467100	-10.8511450
C	4.9031790	4.4064970	-10.1038820
C	4.5649970	5.6456280	-9.5638050
C	5.3652260	6.7606030	-9.8103630
H	10.3972550	9.0861830	-9.9242160
H	7.5672320	10.7338550	-12.6788190
H	6.3343650	3.2861280	-11.2675980
H	3.6681770	5.7028750	-8.9588930
O	9.7454260	11.1784500	-11.5077860
O	8.9588200	6.8696110	-9.4639830
O	4.0329960	3.3934850	-9.8489330
O	8.0094000	5.3093450	-11.8188890
C	10.8791990	11.3936860	-10.6991890
H	10.6191570	11.3562740	-9.6336970
H	11.6668180	10.6574050	-10.9028830
H	11.2476280	12.3884370	-10.9490970
C	10.2229240	6.8908530	-8.8444810
H	10.2857380	5.9775370	-8.2524290
H	11.0296230	6.9002100	-9.5879380
H	10.3291590	7.7598630	-8.1832190
C	8.4161760	4.0557800	-12.3138060
H	8.6058720	3.3462630	-11.4987430
H	7.6659730	3.6361460	-12.9949970

H	9.3423490	4.2326540	-12.8610610
C	4.3002330	2.1408300	-10.4361770
H	3.4703950	1.4909880	-10.1596270
H	4.3553340	2.2182660	-11.5296300
H	5.2367930	1.7110920	-10.0598050

ea-HRh(CO)₂(L5)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2866.34663072, PCM -2866.37983398

P	5.4673770	8.8185650	-12.7096650
P	4.8280700	8.4474980	-9.2238150
C	3.5024220	8.0097800	-7.9931340
C	3.7721240	7.7487940	-6.6402200
C	6.6377850	9.5259200	-15.2423010
H	7.3998860	8.7787090	-15.0503310
C	6.1472020	9.1231740	-8.1112490
C	7.0448370	8.3016210	-7.4110300
H	7.0289300	7.2282740	-7.5660960
C	5.6375070	9.7808510	-14.2874220
C	5.7151870	11.2184550	-16.7049140
H	5.7482350	11.7745380	-17.6376320
C	6.2037560	10.5100790	-7.9100100
H	5.5237450	11.1561880	-8.4552050
C	2.1727730	7.9363790	-8.4361840
H	1.9465720	8.1562000	-9.4733840
C	1.1432990	7.5974800	-7.5571000
C	4.6793580	10.7654160	-14.5662780
H	3.9071290	10.9739630	-13.8329770
C	2.7409700	7.4197710	-5.7590060
H	2.9693160	7.2274840	-4.7142350
C	7.1290300	11.0643880	-7.0245030
H	7.1579080	12.1409030	-6.8816760
C	6.6785440	10.2419320	-16.4370900
C	1.4240880	7.3404820	-6.2145360
C	8.0154290	10.2396320	-6.3299010
H	8.7358460	10.6704260	-5.6398580
C	7.9718780	8.8578250	-6.5269030
H	8.6558800	8.2083720	-5.9867210
C	4.7158260	11.4765440	-15.7685590
H	3.9636260	12.2349450	-15.9657890
Rh	4.0012260	9.8683970	-11.0564210
H	3.1343680	10.5710420	-9.9317950
C	2.2816120	9.4515500	-11.8009970
C	4.9039860	11.5803450	-11.1174570
O	5.3306340	12.6555490	-11.1183610
O	1.2047310	9.2981690	-12.2044890
H	0.6222640	7.0861210	-5.5269280
H	0.1214290	7.5455160	-7.9222010
H	7.4638650	10.0377480	-17.1595600
C	5.1270670	7.1214770	-13.3693140
C	6.1012800	6.3812410	-14.0590270
C	3.8320440	6.5988940	-13.2626470
C	5.7779970	5.1576230	-14.6433880
C	3.5097240	5.3712090	-13.8461100
C	4.4792880	4.6509280	-14.5423780
H	7.1211770	6.7446770	-14.1172620
H	3.0756530	7.1522660	-12.7175290
H	6.5402440	4.6006840	-15.1819890

H	2.4995640	4.9825370	-13.7546010
H	4.2277120	3.6995260	-15.0030110
H	4.7880520	7.8086140	-6.2666250
C	7.5052890	7.8101120	-10.9885760
C	8.7800590	7.9216440	-10.3887820
C	9.6775300	8.9395820	-10.7296620
C	9.3071460	9.8709900	-11.7019260
C	8.0637550	9.7743830	-12.3300060
C	7.1727280	8.7508210	-11.9908890
C	6.6300520	6.6660350	-10.5676270
C	7.0070570	5.3710200	-10.9859190
C	6.2870900	4.2288540	-10.6201220
C	5.1620500	4.3751960	-9.8069150
C	4.7720380	5.6410980	-9.3645310
C	5.4925590	6.7824840	-9.7320550
H	10.6387380	9.0052950	-10.2417260
H	7.8150190	10.5205500	-13.0734050
H	6.5929150	3.2540140	-10.9700830
H	3.8968990	5.7044720	-8.7317090
O	10.0963820	10.9061200	-12.1100580
O	9.0787260	6.9715870	-9.4548140
O	4.3826880	3.3364210	-9.3861270
O	8.1140870	5.3093530	-11.7842650
C	11.3475520	11.0967010	-11.4717230
H	11.2306820	11.2659580	-10.3934480
H	12.0204440	10.2433090	-11.6302800
H	11.7863460	11.9854610	-11.9278930
C	10.3401120	7.0138760	-8.8116590
H	10.3578940	6.1600440	-8.1318710
H	11.1656070	6.9172620	-9.5289640
H	10.4688240	7.9366420	-8.2319210
C	8.5750710	4.0432130	-12.2199230
H	8.8372410	3.3926500	-11.3753390
H	7.8331440	3.5357890	-12.8498000
H	9.4717670	4.2380400	-12.8111530
C	4.7103580	2.0270070	-9.8174900
H	3.9603900	1.3676930	-9.3774900
H	4.6704430	1.9376920	-10.9110570
H	5.7057440	1.7201620	-9.4693560

m062_LANL2DZ

E(RM062X): Gas phase -2865.31109721, PCM -2865.34358859

P	5.4286840	8.7832090	-12.6473920
P	4.8285060	8.4848960	-9.2716520
C	3.6329030	8.1093590	-7.9175640
C	3.9867890	8.0099280	-6.5689770
C	6.8395680	9.6515490	-14.9882560
H	7.7069350	9.1092400	-14.6234260
C	6.3065000	9.1143480	-8.3696830
C	7.1075200	8.2805200	-7.5787220
H	6.8839010	7.2183990	-7.5168870
C	5.6679220	9.7021220	-14.2215890
C	5.8217740	11.0538860	-16.6682100
H	5.8845810	11.5803100	-17.6154100
C	6.6365970	10.4660720	-8.4849730
H	6.0295610	11.1083930	-9.1161960
C	2.2925890	7.9198160	-8.2766240
H	2.0015830	8.0226190	-9.3179700

C	1.3355270	7.6093230	-7.3160580
C	4.5812040	10.4445090	-14.6922140
H	3.6790450	10.5026900	-14.0888500
C	3.0247130	7.7149680	-5.6059080
H	3.3148420	7.6507360	-4.5618270
C	7.7444810	10.9833170	-7.8154920
H	7.9930010	12.0349880	-7.9194040
C	6.9152580	10.3265760	-16.2014010
C	1.6996950	7.5079670	-5.9760710
C	8.5271030	10.1520300	-7.0196540
H	9.3862280	10.5548640	-6.4909190
C	8.2036980	8.8003380	-6.8983910
H	8.8097520	8.1491230	-6.2748660
C	4.6554640	11.1116810	-15.9128810
H	3.8032060	11.6836480	-16.2653220
Rh	3.8416910	9.7815780	-11.1035630
H	2.9219570	10.4466840	-10.0368380
C	2.1704550	9.1184650	-11.7848710
C	4.5769360	11.5726920	-11.3021870
O	4.9244540	12.6597580	-11.4077710
O	1.1287940	8.7946110	-12.1454230
H	0.9520730	7.2792300	-5.2230510
H	0.3028790	7.4605390	-7.6151630
H	7.8316290	10.2892160	-16.7819170
C	5.2165700	7.0529710	-13.2464240
C	6.1758360	6.4397660	-14.0599580
C	4.0631470	6.3465920	-12.9002900
C	5.9750380	5.1468130	-14.5288020
C	3.8663040	5.0469810	-13.3642650
C	4.8190890	4.4469100	-14.1807260
H	7.0871210	6.9687470	-14.3202140
H	3.3258680	6.8091260	-12.2505770
H	6.7198050	4.6850780	-15.1706780
H	2.9685260	4.5063960	-13.0798400
H	4.6629320	3.4380480	-14.5518290
H	5.0121080	8.1775510	-6.2585910
C	7.4431770	7.7988330	-10.9326970
C	8.6856700	7.9056140	-10.2835510
C	9.5071440	9.0185130	-10.4544660
C	9.0806070	10.0472370	-11.2960920
C	7.8879990	9.9342230	-12.0054450
C	7.0847010	8.8046110	-11.8423070
C	6.5517990	6.6554680	-10.5833310
C	6.8772660	5.3797480	-11.0689990
C	6.0552210	4.2771400	-10.8391340
C	4.8891300	4.4563440	-10.0961490
C	4.5701650	5.7010670	-9.5570810
C	5.3917600	6.8003360	-9.8011710
H	10.4402980	9.0977870	-9.9164090
H	7.6049400	10.7492010	-12.6627700
H	6.3043860	3.3123540	-11.2558490
H	3.6647070	5.7817400	-8.9667150
O	9.7818320	11.1938370	-11.4902300
O	9.0062180	6.8779300	-9.4575360
O	3.9990570	3.4593570	-9.8492330
O	8.0151620	5.3073820	-11.8049010
C	10.9165100	11.4099310	-10.6824160
H	10.6575090	11.3682550	-9.6169310

H	11.7056370	10.6764440	-10.8900190
H	11.2812910	12.4065320	-10.9298770
C	10.2724710	6.8990570	-8.8415110
H	10.3376010	5.9845260	-8.2517060
H	11.0768220	6.9104260	-9.5873910
H	10.3795980	7.7667780	-8.1788860
C	8.3996300	4.0476480	-12.3022130
H	8.5745010	3.3327270	-11.4886390
H	7.6427710	3.6432130	-12.9851780
H	9.3299600	4.2083580	-12.8473460
C	4.2346190	2.2092360	-10.4552970
H	3.3889260	1.5763960	-10.1877210
H	4.2912730	2.3024390	-11.5474660
H	5.1601770	1.7503650	-10.0859440

ee-HRh(CO)₂(L6)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2564.24893269, PCM -2564.28224419

P	10.2233510	0.6940600	-6.2374930
P	10.0157490	-2.8145220	-8.1223490
C	8.4713620	-3.6803690	-8.6884920
C	7.2224850	-3.2105790	-8.2537750
C	11.7271540	2.9147020	-5.2603820
H	10.8285820	3.5023750	-5.4172600
C	11.2509400	-4.1973920	-8.2383820
C	12.0045920	-4.4538880	-9.3943540
H	11.9014700	-3.8113090	-10.2625400
C	11.7310100	1.5422690	-5.5661620
C	14.0348790	2.7895160	-4.5416680
H	14.9239310	3.2717270	-4.1451060
C	11.4121520	-5.0391270	-7.1274700
H	10.8512300	-4.8358000	-6.2205460
C	8.5063630	-4.8129330	-9.5196440
H	9.4581810	-5.2091460	-9.8558310
C	7.3252610	-5.4380830	-9.9206370
C	12.8980640	0.8029710	-5.3268410
H	12.8982140	-0.2648050	-5.5195090
C	6.0403000	-3.8330570	-8.6582050
H	5.0851720	-3.4514620	-8.3088790
C	12.2974200	-6.1159130	-7.1727840
H	12.4103440	-6.7554990	-6.3019330
C	12.8706070	3.5323360	-4.7555860
C	6.0885580	-4.9483190	-9.4954090
C	13.0447680	-6.3620930	-8.3265140
H	13.7417900	-7.1947800	-8.3587970
C	12.8970220	-5.5278250	-9.4351670
H	13.4778890	-5.7086270	-10.3355040
C	14.0446760	1.4239530	-4.8252460
H	14.9397600	0.8349590	-4.6462490
Rh	10.0772220	-1.7439090	-5.8720080
H	11.6342230	-1.7407660	-6.2335800
C	8.2015550	-1.7774670	-5.3311850
C	10.7567850	-2.6479810	-4.3284540
O	11.2138310	-3.1756340	-3.4054430
O	7.1128980	-1.8086610	-4.9506420
H	5.1704890	-5.4391040	-9.8056390
H	7.3730760	-6.3123530	-10.5638930
H	12.8512580	4.5938960	-4.5250910

C	8.8966200	1.6544330	-5.3576200
C	8.1683460	2.6980460	-5.9472620
C	8.6375980	1.3250720	-4.0165760
C	7.2020280	3.3913860	-5.2133500
C	7.6794490	2.0238900	-3.2838560
C	6.9553770	3.0581590	-3.8817210
H	8.3505280	2.9699550	-6.9811190
H	9.1880590	0.5132280	-3.5494260
H	6.6433790	4.1938330	-5.6873590
H	7.4928530	1.7542360	-2.2482090
H	6.2023020	3.5970480	-3.3138020
H	7.1706120	-2.3550870	-7.5910070
C	12.2924130	2.2637050	-8.7180170
C	13.1863620	1.0391210	-9.2544970
H	12.5545240	3.1476980	-9.3077950
H	12.5942570	2.4711250	-7.6936240
H	13.9395790	1.4474570	-9.9366900
H	13.7228810	0.6187270	-8.3982000
C	12.3741530	-0.0450210	-9.9269730
C	11.7815460	-1.0354740	-9.1436670
C	11.9537690	0.0348680	-11.2594510
C	10.6045130	-1.7102670	-9.5137930
H	12.1669160	-1.1892980	-8.1407020
C	10.7982290	-0.6320690	-11.6536170
H	12.4414250	0.7183390	-11.9507170
C	10.0074940	-1.3758640	-10.7555750
H	10.4057790	-0.4511130	-12.6518560
C	10.7938670	2.0406550	-8.8553460
C	10.2256390	2.4273380	-10.0851030
C	9.9747310	1.2615490	-7.9999510
C	9.0823620	1.8286730	-10.6040910
H	10.7877780	3.1114450	-10.7167760
C	8.8209210	0.6701630	-8.5462080
C	8.4476220	0.8103360	-9.8831440
H	8.7729890	2.0559200	-11.6215830
H	8.2714320	-0.0397510	-7.9340200
C	7.6358860	-0.2758900	-10.5531480
C	8.5330920	-1.4904300	-11.1071570
H	7.0629090	0.1301500	-11.3933810
H	6.9129400	-0.6918600	-9.8445840
H	8.4456570	-1.4950070	-12.1981430
H	8.0913510	-2.4189840	-10.7527490

m062_LANL2DZ

E(RM062X): Gas phase -2563.32365404, PCM -2563.35728306

P	10.2404320	0.6408320	-6.2288750
P	10.0185650	-2.8002850	-8.0637480
C	8.4942920	-3.6307940	-8.6837170
C	7.2516170	-3.1184920	-8.3007540
C	11.6930260	2.8893670	-5.2933550
H	10.7546240	3.4331490	-5.3526990
C	11.2352580	-4.1809010	-8.1877240
C	11.9940520	-4.4290240	-9.3361880
H	11.9093630	-3.7688660	-10.1948340
C	11.7327520	1.5287590	-5.6243600
C	14.0630230	2.8614320	-4.8382950
H	14.9677460	3.3809760	-4.5386090
C	11.3641460	-5.0359570	-7.0890910

H	10.7931390	-4.8312030	-6.1872530
C	8.5331630	-4.7418080	-9.5354100
H	9.4884830	-5.1673870	-9.8266420
C	7.3540150	-5.2964760	-10.0226280
C	12.9413950	0.8367590	-5.5186290
H	12.9646400	-0.2292000	-5.7292500
C	6.0707370	-3.6684440	-8.7942910
H	5.1147880	-3.2523970	-8.4923380
C	12.2256520	-6.1271890	-7.1401610
H	12.3158930	-6.7823430	-6.2795240
C	12.8524720	3.5506820	-4.9048310
C	6.1213110	-4.7546650	-9.6625990
C	12.9776880	-6.3693230	-8.2871470
H	13.6561110	-7.2157930	-8.3248560
C	12.8618930	-5.5181180	-9.3823970
H	13.4488080	-5.6996030	-10.2774810
C	14.1052030	1.5034570	-5.1385280
H	15.0406870	0.9575400	-5.0683040
Rh	10.0769030	-1.7854400	-5.7849320
H	11.6195700	-1.8474990	-6.0775950
C	8.1504520	-1.7174340	-5.3019140
C	10.6949880	-2.7174970	-4.2505010
O	11.1299380	-3.2782860	-3.3483620
O	7.0565550	-1.6641710	-4.9794280
H	5.2031000	-5.1875890	-10.0466570
H	7.3970830	-6.1545850	-10.6859170
H	12.8134000	4.6061850	-4.6546100
C	8.9188530	1.5877930	-5.3526680
C	8.1841920	2.6206290	-5.9417130
C	8.6769240	1.2599990	-4.0128700
C	7.2231340	3.3093400	-5.2035380
C	7.7230900	1.9541660	-3.2763330
C	6.9910270	2.9790540	-3.8721770
H	8.3618520	2.8893530	-6.9784660
H	9.2405670	0.4514130	-3.5518780
H	6.6568020	4.1071040	-5.6739570
H	7.5455740	1.6891780	-2.2388710
H	6.2400020	3.5153440	-3.3009010
H	7.2032170	-2.2770280	-7.6161640
C	12.2308730	2.2940270	-8.6851530
C	13.1518630	1.0636100	-9.0971630
H	12.4617590	3.1245310	-9.3586040
H	12.5226450	2.6121500	-7.6851550
H	13.9632020	1.4439530	-9.7254020
H	13.6059890	0.6589410	-8.1876970
C	12.3774460	-0.0256010	-9.7953030
C	11.7818670	-1.0223350	-9.0307640
C	11.9782110	0.0689810	-11.1283010
C	10.6248940	-1.7054950	-9.4329100
H	12.1435920	-1.1719060	-8.0155040
C	10.8459240	-0.6126720	-11.5518560
H	12.4594680	0.7794450	-11.7965840
C	10.0568590	-1.3854740	-10.6837570
H	10.4660840	-0.4219070	-12.5531390
C	10.7436840	2.0097410	-8.8217370
C	10.1701370	2.3618340	-10.0546440
C	9.9573440	1.2039770	-7.9718230
C	9.0457580	1.7296960	-10.5668470

H	10.7182420	3.0490810	-10.6950410
C	8.8182980	0.5828600	-8.5041900
C	8.4345770	0.7113960	-9.8343180
H	8.7366770	1.9286130	-11.5904060
H	8.2942380	-0.1478000	-7.8880440
C	7.6548970	-0.4018390	-10.4875860
C	8.5993470	-1.5365610	-11.0857550
H	7.0261130	-0.0204710	-11.2978440
H	6.9903390	-0.8643980	-9.7522140
H	8.5549340	-1.4649620	-12.1762650
H	8.1773200	-2.5043360	-10.8185410

ea-HRh(CO)₂(L6)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2564.25148088, PCM -2564.28661732

P	10.0240790	0.6986500	-6.2962030
P	9.8911240	-2.7162620	-8.0999060
C	8.6909570	-3.9415550	-8.8212720
C	7.4880210	-4.2082650	-8.1547890
C	12.0889660	2.3069050	-5.1396250
H	11.3455520	3.0924710	-5.0576270
C	11.3953280	-3.8137450	-7.9745930
C	12.2757850	-4.0552690	-9.0423120
H	12.1409890	-3.5393910	-9.9868840
C	11.7392020	1.0653180	-5.6964240
C	14.3586570	1.5416890	-4.7870030
H	15.3692240	1.7259020	-4.4338170
C	11.6148380	-4.4855800	-6.7625800
H	10.9518490	-4.3007240	-5.9243050
C	8.9716320	-4.6351740	-10.0105860
H	9.9009650	-4.4518670	-10.5398320
C	8.0654900	-5.5617380	-10.5228900
C	12.7165070	0.0597180	-5.7655690
H	12.4519990	-0.9208990	-6.1476710
C	6.5810580	-5.1406020	-8.6666310
H	5.6532410	-5.3340350	-8.1357180
C	12.6775940	-5.3792600	-6.6215730
H	12.8277860	-5.8884370	-5.6737290
C	13.3888320	2.5420200	-4.6910200
C	6.8663720	-5.8174660	-9.8514110
C	13.5474970	-5.6087590	-7.6882250
H	14.3799660	-6.2979230	-7.5774190
C	13.3441760	-4.9417150	-8.8974400
H	14.0181810	-5.1097380	-9.7331050
C	14.0185220	0.2988640	-5.3228750
H	14.7602460	-0.4922570	-5.3837870
Rh	9.2506420	-1.6443620	-5.9231430
H	8.7481560	-3.1057490	-5.5934610
C	7.3684710	-1.2076420	-5.7943040
C	10.4370170	-1.9856200	-4.4513370
O	11.0484140	-2.2549970	-3.5053300
O	6.2382110	-1.0431140	-5.6084050
H	6.1621920	-6.5420960	-10.2505450
H	8.2969260	-6.0882320	-11.4447730
H	13.6420570	3.5072770	-4.2616460
C	9.0237340	1.9169660	-5.3211590
C	8.6607390	3.1773110	-5.8193810
C	8.6327400	1.5631840	-4.0195530

C	7.9253170	4.0645400	-5.0299120
C	7.9048740	2.4542230	-3.2315120
C	7.5473630	3.7066290	-3.7353330
H	8.9460380	3.4659650	-6.8255840
H	8.8875680	0.5813330	-3.6327680
H	7.6460670	5.0347460	-5.4313720
H	7.6083610	2.1644100	-2.2275230
H	6.9721330	4.3967140	-3.1245930
H	7.2629270	-3.6820060	-7.2337120
C	12.1385810	2.2662430	-8.7405750
C	12.9227540	1.1864700	-9.6392680
H	12.4550710	3.2605290	-9.0734670
H	12.4741240	2.1567650	-7.7134730
H	13.3844900	1.7108010	-10.4821100
H	13.7368050	0.7832530	-9.0276190
C	12.0340840	0.0780500	-10.1593100
C	11.5769490	-0.9275070	-9.3068680
C	11.4258710	0.1544230	-11.4197390
C	10.3679040	-1.6142570	-9.5216980
H	12.1155530	-1.0955300	-8.3785170
C	10.2286230	-0.5148640	-11.6530020
H	11.8086740	0.8441930	-12.1680540
C	9.5842940	-1.2546130	-10.6464830
H	9.6924950	-0.3229170	-12.5801260
C	10.6275310	2.1558350	-8.8512030
C	10.0439330	2.6696190	-10.0223120
C	9.7982910	1.3429760	-8.0336350
C	8.8631990	2.1513610	-10.5505790
H	10.6202190	3.3731910	-10.6193820
C	8.6028180	0.8482800	-8.5799320
C	8.2082830	1.1051460	-9.8934630
H	8.5409190	2.4609540	-11.5421380
H	8.0476340	0.1101580	-8.0098680
C	7.3622650	0.0890510	-10.6350110
C	8.0639930	-1.3405340	-10.7112740
H	7.1760600	0.4551810	-11.6501630
H	6.3814980	-0.0531630	-10.1660440
H	7.7316180	-1.8265570	-11.6361590
H	7.6843140	-1.9499150	-9.8929860

m062_LANL2DZ

E(RM062X): Gas phase -2563.32580897, PCM -2563.36069316

P	10.1314330	0.6750530	-6.2338250
P	9.9801370	-2.7324490	-8.0956000
C	8.5704530	-3.7115390	-8.7607560
C	7.2782860	-3.3743450	-8.3501540
C	11.8951400	2.6405630	-5.1807840
H	11.0270040	3.2888430	-5.1091860
C	11.3225840	-4.0027240	-8.1263130
C	12.1779780	-4.1967490	-9.2168800
H	12.0944870	-3.5591560	-10.0923480
C	11.7547970	1.3394160	-5.6802470
C	14.2643220	2.2877720	-4.8781420
H	15.2364160	2.6566400	-4.5669310
C	11.4548190	-4.8324520	-7.0074150
H	10.8027460	-4.6821860	-6.1514710
C	8.7431430	-4.7456470	-9.6883380
H	9.7440860	-5.0311620	-9.9983530

C	7.6385370	-5.3990950	-10.2238450
C	12.8796230	0.5109980	-5.7380200
H	12.7769030	-0.5154100	-6.0798930
C	6.1710660	-4.0233910	-8.8930050
H	5.1719480	-3.7463070	-8.5721550
C	12.4142490	-5.8396530	-6.9811520
H	12.5028670	-6.4740130	-6.1048910
C	13.1430450	3.1109170	-4.7864060
C	6.3503610	-5.0312990	-9.8356610
C	13.2621750	-6.0253640	-8.0698430
H	14.0160120	-6.8061490	-8.0469680
C	13.1419970	-5.2019860	-9.1855980
H	13.8014870	-5.3394010	-10.0369940
C	14.1305060	0.9852040	-5.3485230
H	14.9946660	0.3308570	-5.4009850
Rh	9.6546140	-1.7323140	-5.7872120
H	9.2656160	-3.1864280	-5.4056140
C	7.8150060	-1.3972940	-5.2969520
C	11.1880610	-2.0955110	-4.6699910
O	12.0245680	-2.3661540	-3.9336860
O	6.7440910	-1.2649170	-4.9086360
H	5.4897430	-5.5396280	-10.2589790
H	7.7813760	-6.1949950	-10.9479030
H	13.2405030	4.1214850	-4.4027870
C	8.9773200	1.7649680	-5.3004400
C	8.3776970	2.8967010	-5.8586430
C	8.7303410	1.4487270	-3.9592200
C	7.5414250	3.6995110	-5.0847060
C	7.9010550	2.2559330	-3.1883340
C	7.3033050	3.3818940	-3.7510290
H	8.5632780	3.1505190	-6.8980810
H	9.1839790	0.5598550	-3.5269440
H	7.0757620	4.5739190	-5.5281990
H	7.7135620	2.0002790	-2.1504120
H	6.6496860	4.0069750	-3.1509430
H	7.1428470	-2.5998590	-7.5997200
C	12.0448820	2.3738170	-8.7095360
C	13.0025900	1.2021940	-9.2106980
H	12.2380790	3.2528850	-9.3309870
H	12.3357130	2.6367970	-7.6938740
H	13.7430050	1.6342800	-9.8904450
H	13.5435120	0.8130070	-8.3434950
C	12.2440940	0.0838290	-9.8790770
C	11.6791200	-0.9162620	-9.0964870
C	11.8305920	0.1467880	-11.2104420
C	10.5433380	-1.6419080	-9.4824740
H	12.0473140	-1.0432600	-8.0787950
C	10.7113630	-0.5678680	-11.6140980
H	12.2894130	0.8580040	-11.8933580
C	9.9515610	-1.3501010	-10.7284820
H	10.3180630	-0.4001940	-12.6141950
C	10.5688690	2.0427870	-8.8370390
C	9.9740670	2.3708510	-10.0657260
C	9.8164320	1.2197820	-7.9742330
C	8.8616400	1.7036440	-10.5602790
H	10.4986180	3.0658700	-10.7174790
C	8.6786200	0.5760170	-8.4814670
C	8.2808570	0.6812340	-9.8099390

H	8.5397600	1.8821810	-11.5837440
H	8.1760540	-0.1589590	-7.8552130
C	7.5239600	-0.4628740	-10.4372620
C	8.4905420	-1.5375630	-11.1021510
H	6.8288010	-0.1105060	-11.2054540
H	6.9308810	-0.9673840	-9.6683760
H	8.4186860	-1.4245890	-12.1878140
H	8.1058970	-2.5289790	-10.8648870

ee-HRh(CO)₂(L7)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -5562.57546170, PCM(n-hexane) -5562.60146742,

PCM(toluene) -5562.60521990, PCM(THF) -5562.61769892

Rh	-1.0817180	14.5713860	18.3637510
P	-2.8634970	13.9578030	16.8232140
P	0.7224650	13.6873070	17.0541950
C	-0.2043300	13.9784170	12.4964500
H	-0.3975150	14.1062770	11.4395570
C	1.0867810	14.6139410	14.4400370
H	1.8632440	15.2168710	14.8841660
C	0.3649300	13.6987300	15.2310030
C	-0.6842470	12.9346500	14.6757460
C	-3.1829750	14.9126480	15.2659540
C	-3.9741600	14.3816930	14.2340420
H	-4.3779680	13.3792080	14.3159520
C	-4.2339590	15.1388250	13.0918420
C	-3.6964750	16.4216290	12.9443010
H	-3.8936010	17.0031050	12.0505670
C	-2.9012070	16.9389700	13.9635020
C	-2.6507100	16.1961790	15.1224640
H	-2.0333460	16.6112090	15.9117820
C	2.3015720	14.6758210	17.2037860
C	2.2761320	15.9057840	17.8697970
C	3.4482610	16.6507620	18.0275330
C	4.6644500	16.1859530	17.5272670
H	5.5725380	16.7629050	17.6559920
C	4.6906430	14.9592310	16.8622480
C	3.5240500	14.2066240	16.7035590
H	3.5775710	13.2562260	16.1837010
C	-1.2936290	13.0887470	19.6214470
C	1.4369270	12.0135050	17.4274760
C	1.6802540	11.7110180	18.7739100
C	1.8137450	11.0895310	16.4446750
C	2.2952750	10.5100810	19.1321060
C	2.4364620	9.8932900	16.8158900
C	2.6829880	9.5926630	18.1564010
H	1.3949770	12.4147440	19.5489740
H	1.6185850	11.2895380	15.3978620
H	3.1658440	8.6632660	18.4349980
C	-2.6393180	12.2189710	16.2122580
C	-1.5377370	11.9161010	15.3817510
C	-3.4916690	11.2077030	16.6865410
C	-2.1825060	9.5464120	15.5097040
H	-4.3398470	11.4593280	17.3048680
H	-2.0304460	8.5056720	15.2553500
C	-4.5492670	13.9887390	17.6188700
C	-5.6390150	14.6838530	17.0801470
C	-4.7154290	13.3774360	18.8729330

C	-6.8567630	14.7504720	17.7664370
C	-5.9400420	13.4274750	19.5386450
C	-7.0251690	14.1190980	18.9957600
H	-5.5566090	15.1846160	16.1241720
H	-7.9707780	14.1686120	19.5213720
C	-1.2228470	15.9777980	19.6712760
O	-1.3128460	16.8545220	20.4144000
O	-1.3987310	12.2309570	20.3824270
H	-0.8071480	15.8256080	17.4031690
H	1.3385350	16.2678970	18.2767390
H	-3.8863480	12.8614050	19.3419910
O	-0.3102500	10.2948370	14.1866360
O	-1.9338890	12.3235130	12.7704610
C	-0.2973480	9.0532720	13.4816010
H	-0.1003200	8.2089620	14.1489810
H	-1.2459190	8.8966140	12.9558190
H	0.5181470	9.1308720	12.7619310
C	-2.0827250	12.2418370	11.3553320
H	-2.3862100	13.2000680	10.9200990
H	-1.1537460	11.9052470	10.8805190
H	-2.8718270	11.5092820	11.1829400
O	-4.0203820	8.8278700	16.7483310
O	1.4341450	15.6133350	12.2434850
C	-5.1205080	9.0772730	17.6172440
H	-5.5653810	8.1029890	17.8210870
H	-4.7938990	9.5298260	18.5611070
H	-5.8692270	9.7233420	17.1428210
C	2.4486510	16.4635750	12.7696510
H	3.2827020	15.8831870	13.1827470
H	2.8056640	17.0553940	11.9265240
H	2.0475810	17.1345620	13.5380930
C	5.9903070	14.4065680	16.3368510
C	3.3859520	17.9986670	18.7003510
C	-6.0942390	12.6801820	20.8379850
C	-7.9813930	15.5537970	17.1643890
C	2.8231620	8.8816180	15.7699830
C	2.5887680	10.2347690	20.5850680
F	-7.7879430	16.8932530	17.3237580
F	-9.1832620	15.2612930	17.7205800
F	-8.0954010	15.3406090	15.8248000
F	2.9538040	9.4292970	14.5349290
F	3.9980640	8.2654400	16.0617560
F	1.8910390	7.8859990	15.6562960
F	5.8399210	13.8528110	15.1008360
F	6.9538090	15.3558080	16.2344280
F	6.4879810	13.4234420	17.1379430
F	4.5549330	18.3203160	19.3134030
F	2.4071310	18.0620950	19.6354410
F	3.1333560	18.9956790	17.8018180
F	2.7251300	8.9080100	20.8393240
F	1.6107810	10.7046380	21.4004690
F	3.7481760	10.8304640	20.9873720
F	-7.1472590	13.1200140	21.5689990
F	-6.3003990	11.3438710	20.6211670
F	-4.9891170	12.7720660	21.6197330
C	-2.2389850	18.2814340	13.7921060
C	-5.1188850	14.6009600	11.9980360
F	-2.9111030	19.0838600	12.9281230

F	-2.1266500	18.9531450	14.9656370
F	-0.9713420	18.1527810	13.2974540
F	-5.3899740	13.2800300	12.1469400
F	-6.3146070	15.2474640	11.9436890
F	-4.5482910	14.7513900	10.7664160
C	-1.3513800	10.5522150	15.0282930
C	-0.9295280	13.0887280	13.2792520
C	0.7998010	14.7566420	13.0818270
C	-3.2582070	9.8739610	16.3412910

m062_LANL2DZ

E(RM062X): Gas phase -5560.69756390, PCM(n-hexane) -5560.71971103,
PCM(toluene) -5560.72338087, PCM(THF) -5560.73638198

Rh	-0.9383360	14.9997410	18.4465910
P	-2.7140030	14.1231670	16.9834360
P	0.7257750	13.8562270	17.1170990
C	-0.4002180	14.3811320	12.6427070
H	-0.6439840	14.5509580	11.6016380
C	0.9047970	15.0522780	14.5705740
H	1.6549160	15.6930110	15.0114350
C	0.3149180	14.0252800	15.3199240
C	-0.6646830	13.1947960	14.7623640
C	-3.0719100	14.8794380	15.3418940
C	-3.9097580	14.2388900	14.4246380
H	-4.3629010	13.2801930	14.6671730
C	-4.1470350	14.8159100	13.1803420
C	-3.5274050	16.0049330	12.8095570
H	-3.6909370	16.4336990	11.8261190
C	-2.6741150	16.6191140	13.7191740
C	-2.4584980	16.0795860	14.9836190
H	-1.7832450	16.5703780	15.6782140
C	2.3924100	14.6436850	17.2644260
C	2.4433300	16.0417650	17.3125830
C	3.6631020	16.7014080	17.4133610
C	4.8584110	15.9986370	17.5211390
H	5.8060240	16.5180790	17.6110920
C	4.7988700	14.6113000	17.5214690
C	3.5879400	13.9339490	17.3893720
H	3.5984390	12.8496760	17.3924930
C	-1.1790560	13.7700490	19.9848370
C	1.1288660	12.0584140	17.1859210
C	0.5462900	11.2601850	18.1707790
C	1.9286790	11.4601870	16.2098640
C	0.7607600	9.8865100	18.1711190
C	2.1687770	10.0896990	16.2500670
C	1.5847580	9.2870870	17.2233970
H	-0.1170640	11.6970300	18.9093410
H	2.3429860	12.0531220	15.3975500
H	1.7457550	8.2135790	17.2287700
C	-2.3561160	12.3725930	16.4945090
C	-1.3877240	12.1244570	15.5132350
C	-2.9461220	11.3192990	17.2070180
C	-1.6809810	9.7268430	15.8906190
H	-3.6991460	11.5133770	17.9564170
H	-1.4532770	8.6887770	15.6839110
C	-4.3998110	14.0384480	17.7408330
C	-5.5513590	14.5533240	17.1409100
C	-4.5138620	13.5029480	19.0292160

C	-6.7789070	14.4892080	17.7974740
C	-5.7500590	13.4211310	19.6592460
C	-6.9019360	13.9128490	19.0549530
H	-5.5121400	15.0131460	16.1596330
H	-7.8637050	13.8543770	19.5526440
C	-0.8348090	16.6005270	19.4861080
O	-0.7512310	17.5896950	20.0528720
O	-1.3077020	13.0882880	20.8908070
H	-0.6887400	16.0640990	17.3108690
H	1.5217510	16.6186410	17.2770510
H	-3.6349510	13.1392260	19.5547150
O	-0.1922520	10.5917780	14.2057840
O	-1.9087950	12.5201030	12.8967950
C	-0.0157740	9.2761090	13.7161720
H	0.3926730	8.6123870	14.4881330
H	-0.9651750	8.8650920	13.3555480
H	0.6971230	9.3519720	12.8966930
C	-2.1176740	12.5249090	11.4975970
H	-2.5351180	13.4809450	11.1579890
H	-1.1797940	12.3330000	10.9644820
H	-2.8338130	11.7301330	11.2958210
O	-3.0690870	8.9287870	17.5763200
O	1.0131020	16.2135880	12.4462300
C	-3.9643940	9.1529680	18.6516300
H	-4.1860020	8.1707480	19.0656020
H	-3.5048490	9.7780210	19.4248010
H	-4.8923700	9.6203650	18.3021170
C	1.9863640	17.0921790	12.9848940
H	2.8889710	16.5443360	13.2797250
H	2.2291180	17.7924970	12.1875100
H	1.5905130	17.6425050	13.8440970
C	6.0550530	13.8061240	17.7066450
C	3.6616950	18.2037300	17.3689210
C	-5.8202160	12.7404980	20.9969720
C	-7.9821230	15.0966280	17.1298130
C	3.0915300	9.4860940	15.2291600
C	0.0823780	9.0210160	19.1952240
F	-8.0266730	16.4324410	17.3064120
F	-9.1334700	14.5980020	17.6136680
F	-7.9748490	14.8831130	15.8005110
F	2.9652900	10.0792210	14.0257700
F	4.3831810	9.6103930	15.5882280
F	2.8599650	8.1698520	15.0511770
F	6.0472450	12.6904960	16.9519870
F	7.1573460	14.5053440	17.3833850
F	6.2054460	13.4049230	18.9854850
F	4.8506410	18.7267800	17.7096450
F	2.7347120	18.7300220	18.1883300
F	3.3740750	18.6536910	16.1256940
F	-0.3234660	7.8523450	18.6672000
F	-1.0001820	9.6225500	19.7257860
F	0.9017840	8.7166980	20.2225770
F	-6.9733790	12.9875060	21.6380650
F	-5.7209150	11.3972910	20.8648740
F	-4.8137790	13.1174330	21.8055690
C	-1.9823680	17.8957920	13.3328320
C	-5.1279160	14.1607480	12.2503740
F	-1.7212170	17.9467200	12.0145680

F	-2.7291290	18.9812000	13.6232210
F	-0.8120350	18.0486250	13.9836010
F	-5.0785030	12.8166380	12.3275940
F	-6.3956160	14.5172540	12.5342730
F	-4.9084920	14.4949940	10.9628140
C	-1.0967780	10.7748480	15.1950800
C	-0.9824530	13.3718670	13.3933920
C	0.5292600	15.2378340	13.2430910
C	-2.5868530	10.0049060	16.9201040

ea-HRh(CO)₂(L7)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -5562.57945524, PCM(n-hexane) -5562.60673225,
PCM(toluene) -5562.61082669, PCM(THF) -5562.62430854

Rh	-0.8950070	15.3153820	17.9054890
P	-2.6557740	14.1654380	16.6685440
P	0.8176880	13.9530050	16.8648320
C	0.0453910	14.1973580	12.2989100
H	-0.1219270	14.3142030	11.2362930
C	1.2780490	14.8748160	14.2697930
H	2.0243170	15.5010140	14.7365540
C	0.5550750	13.9425340	15.0372500
C	-0.4660300	13.1600350	14.4663110
C	-3.3267260	14.9892720	15.1442610
C	-3.8934020	14.2769550	14.0762950
H	-3.8890810	13.1935860	14.0769910
C	-4.4521510	14.9641570	12.9971800
C	-4.4476890	16.3613630	12.9528150
H	-4.8793730	16.8885530	12.1096000
C	-3.8683700	17.0645350	14.0060300
C	-3.3128150	16.3866930	15.0958940
H	-2.8583500	16.9479420	15.9054340
C	2.5568980	14.5713840	17.1099640
C	2.7926500	15.4513300	18.1743460
C	4.0882570	15.8924900	18.4557940
C	5.1688450	15.4851240	17.6731670
H	6.1715640	15.8335700	17.8897140
C	4.9327410	14.6195930	16.6053050
C	3.6430610	14.1587250	16.3272790
H	3.4954010	13.4961250	15.4821500
C	-0.6356050	14.8958520	19.7741350
C	1.0438240	12.1759750	17.3612490
C	0.4547590	11.7288490	18.5452630
C	1.8411590	11.2883350	16.6219160
C	0.6640700	10.4184390	18.9912210
C	2.0547130	9.9904360	17.0813830
C	1.4690540	9.5423850	18.2705840
H	-0.1743760	12.3977720	19.1212650
H	2.2713230	11.5893360	15.6751650
H	1.6343140	8.5296090	18.6203740
C	-2.3108930	12.4209670	16.1201880
C	-1.2748740	12.1356750	15.2059040
C	-3.0321990	11.3809770	16.7359270
C	-1.7428660	9.7411240	15.5046840
H	-3.8133630	11.6097460	17.4446110
H	-1.5487500	8.6986370	15.2892300
C	-4.2303880	13.9937560	17.6591670
C	-5.5011890	13.9339440	17.0746880

C	-4.1338790	13.9355020	19.0564190
C	-6.6452540	13.8162000	17.8704280
C	-5.2796830	13.8123370	19.8438130
C	-6.5465320	13.7561810	19.2595140
H	-5.6175500	13.9780320	15.9988500
H	-7.4357650	13.6705220	19.8737360
C	-0.3066160	16.9598510	17.0519120
O	0.0191180	17.9827890	16.6294670
O	-0.4980530	14.7552120	20.9127230
H	-2.0507390	16.2333760	18.4790470
H	1.9588690	15.7919670	18.7794220
H	-3.1605840	14.0021050	19.5270210
O	-0.0056940	10.5387500	14.0308450
O	-1.6564500	12.5032540	12.5416490
C	0.1488470	9.2281460	13.4907810
H	0.4459270	8.5031350	14.2561950
H	-0.7756010	8.8903680	13.0082300
H	0.9444020	9.3060690	12.7491280
C	-1.7335570	12.3678000	11.1235800
H	-2.0413640	13.3013410	10.6412760
H	-0.7729040	12.0401820	10.7098450
H	-2.4938310	11.6082000	10.9402420
O	-3.3840870	8.9804100	16.9715260
O	1.6587750	15.8620830	12.0737850
C	-4.3978910	9.2079660	17.9469470
H	-4.7578600	8.2201350	18.2354050
H	-3.9944460	9.7177420	18.8290930
H	-5.2301790	9.7882270	17.5305260
C	2.6418790	16.7368310	12.6187160
H	3.4855970	16.1780560	13.0419000
H	2.9955330	17.3424650	11.7839660
H	2.2129960	17.3924960	13.3860520
C	6.0627520	14.1530690	15.7245080
C	4.3118340	16.8712580	19.5816710
C	-5.1615650	13.6945950	21.3424700
C	-8.0019650	13.8026360	17.2140950
C	2.9278950	9.0368750	16.3091670
C	-0.0518240	9.9510710	20.2317090
F	-8.4840140	15.0610490	17.0125450
F	-8.9269600	13.1459360	17.9605610
F	-7.9707540	13.2019400	15.9940650
F	3.2979380	9.5292290	15.1003450
F	4.0699600	8.7306130	16.9814740
F	2.2944210	7.8495440	16.0740630
F	5.8176090	14.4289190	14.4097450
F	7.2456390	14.7323520	16.0379120
F	6.2427280	12.8056790	15.8015050
F	3.4199740	16.7050040	20.5885760
F	4.1893400	18.1614850	19.1576480
F	5.5553220	16.7563400	20.1174110
F	0.5030630	8.8334760	20.7631920
F	-1.3599330	9.6506710	19.9679010
F	-0.0663220	10.8990810	21.2017860
F	-6.1262250	14.4038680	21.9866890
F	-5.3010910	12.3986130	21.7521870
F	-3.9647360	14.1249650	21.8043220
C	-3.8622510	18.5721900	14.0038530
C	-5.0721800	14.2191280	11.8448290

F	-4.0980840	19.0878660	12.7700950
F	-4.8175510	19.0824660	14.8317800
F	-2.6743120	19.0745110	14.4300420
F	-5.0801300	12.8757660	12.0298230
F	-6.3590590	14.6006510	11.6251730
F	-4.4048030	14.4504990	10.6735360
C	-1.0200590	10.7680060	14.9085350
C	-0.6849170	13.2977460	13.0670740
C	1.0200930	15.0006040	12.9034430
C	-2.7466440	10.0480090	16.4306670

m062_LANL2DZ

E(RM062X): Gas phase -5560.69950846, PCM(n-hexane) -5560.72202818,
PCM(toluene) -5560.72581087, PCM(THF) -5560.73919005

Rh	-0.9927810	15.0303870	18.3600990
P	-2.6707030	14.1002880	16.9350930
P	0.7286250	13.9331560	17.0218130
C	-0.3981000	14.4598430	12.5523160
H	-0.6567480	14.6442050	11.5173940
C	0.9463250	15.0923540	14.4650480
H	1.7189130	15.7138820	14.8916350
C	0.3485580	14.0716580	15.2170220
C	-0.6408360	13.2509900	14.6635970
C	-3.0984530	14.8894770	15.3235360
C	-3.9588650	14.2812820	14.4068730
H	-4.4178250	13.3213370	14.6333440
C	-4.2055420	14.8905770	13.1789800
C	-3.5676990	16.0741630	12.8217720
H	-3.7363400	16.5238850	11.8485740
C	-2.6845870	16.6517290	13.7280200
C	-2.4637990	16.0817720	14.9769350
H	-1.7583450	16.5349370	15.6669530
C	2.4242040	14.6477210	17.2042280
C	2.5704900	16.0354130	17.1004770
C	3.8198080	16.6304280	17.2358900
C	4.9506000	15.8754630	17.5259020
H	5.9221370	16.3437760	17.6375330
C	4.7947370	14.5039180	17.6761550
C	3.5541250	13.8890270	17.5174550
H	3.4882410	12.8143030	17.6461260
C	-0.7324580	14.1470400	20.0726500
C	1.0398380	12.1285230	17.1973760
C	0.3700390	11.4054040	18.1843150
C	1.8893680	11.4583280	16.3138480
C	0.5530870	10.0298630	18.2815370
C	2.0938590	10.0890060	16.4544050
C	1.4256040	9.3586200	17.4322910
H	-0.3292360	11.9070830	18.8464770
H	2.3773180	11.9949680	15.5034700
H	1.5651820	8.2854730	17.5151710
C	-2.3234280	12.3707400	16.3788370
C	-1.3472080	12.1589050	15.3990110
C	-2.9280430	11.2930270	17.0410830
C	-1.6115330	9.7505920	15.7145920
H	-3.6830360	11.4639050	17.7946750
H	-1.3667960	8.7207950	15.4871670
C	-4.3020110	13.9588700	17.7849770
C	-5.5188980	14.3709970	17.2440360

C	-4.2894570	13.4500840	19.0897360
C	-6.6949400	14.2434370	17.9835770
C	-5.4731450	13.3045710	19.8018870
C	-6.6933340	13.6999140	19.2604250
H	-5.5738250	14.8018480	16.2500040
H	-7.6143950	13.5972520	19.8242510
C	-0.5357740	16.8966290	17.9869130
O	-0.3648370	18.0186620	17.8416600
O	-0.6512720	13.6833430	21.1153160
H	-2.1562220	15.7157190	19.1205470
H	1.7094190	16.6683060	16.9054000
H	-3.3460830	13.1717880	19.5542310
O	-0.0797010	10.6778650	14.1016960
O	-1.9196580	12.6101290	12.8105390
C	0.1556880	9.3726710	13.6087110
H	0.5599460	8.7176820	14.3903250
H	-0.7672680	8.9339350	13.2137340
H	0.8927610	9.4773010	12.8145210
C	-2.1893600	12.6673260	11.4227100
H	-2.6023000	13.6424930	11.1350350
H	-1.2804450	12.4767680	10.8411490
H	-2.9290700	11.8930140	11.2267040
O	-3.0600120	8.8888300	17.3127380
O	1.0494460	16.2647710	12.3480040
C	-4.0732730	9.0596140	18.2896830
H	-4.3429590	8.0568180	18.6166770
H	-3.7066460	9.6344040	19.1458550
H	-4.9523200	9.5534390	17.8593780
C	2.0328550	17.1332240	12.8851700
H	2.9336590	16.5781380	13.1715800
H	2.2761770	17.8356440	12.0898730
H	1.6465340	17.6829170	13.7495130
C	5.9759670	13.6503460	18.0491680
C	3.9234430	18.1139420	17.0163610
C	-5.4284710	12.6610880	21.1592200
C	-7.9778300	14.7516900	17.3860140
C	3.0856140	9.4070210	15.5552500
C	-0.1993740	9.2567660	19.3282310
F	-8.1092840	16.0835670	17.5476600
F	-9.0583150	14.1804430	17.9469850
F	-8.0373760	14.5166620	16.0612420
F	3.0810560	9.9301380	14.3134720
F	4.3440900	9.5251240	16.0199370
F	2.8359360	8.0880700	15.4338820
F	5.9531890	12.4652380	17.4109040
F	7.1429320	14.2481230	17.7524820
F	5.9969840	13.3779320	19.3693270
F	2.9798980	18.7894520	17.6929640
F	3.7544420	18.4236440	15.7095690
F	5.1188580	18.6019440	17.3840370
F	-0.4780060	8.0056360	18.9240840
F	-1.3683210	9.8511620	19.6418590
F	0.5003990	9.1490610	20.4753580
F	-6.4618230	13.0340910	21.9330770
F	-5.4814970	11.3124900	21.0620530
F	-4.2960090	12.9539250	21.8198300
C	-1.9557730	17.9104910	13.3508820
C	-5.2093870	14.2706230	12.2492550

F	-1.7040830	17.9675120	12.0306720
F	-2.6616890	19.0170590	13.6597650
F	-0.7742140	18.0141440	13.9923610
F	-5.1743150	12.9241340	12.2929530
F	-6.4678850	14.6341430	12.5631960
F	-5.0068320	14.6332300	10.9668340
C	-1.0214130	10.8227350	15.0626160
C	-0.9789110	13.4482220	13.3018630
C	0.5571540	15.2932380	13.1435470
C	-2.5585650	9.9907050	16.7164370

ee-HRh(CO)₂(L8)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -4501.41378015, PCM -4501.45454961

Rh	-1.2463210	14.0152250	18.3632810
P	-3.0485940	13.8686800	16.7427540
P	0.5720580	13.1908460	16.9643490
C	-0.1568140	13.3890970	12.3786090
C	1.0420550	14.0288730	14.3099480
H	1.8693850	14.5661560	14.7552080
C	0.2099320	13.2627860	15.1390920
C	-0.9008830	12.5567460	14.5685900
C	-3.1576390	14.9827530	15.2721450
C	-3.8517240	14.6274250	14.1060550
H	-4.2050900	13.6096830	14.0053970
C	-4.0954150	15.5482570	13.0817550
C	-3.6044290	16.8704010	13.2669740
C	-2.7353670	17.2076840	14.3272350
C	-2.5807700	16.2467930	15.3413540
H	-1.9784830	16.4808590	16.2111700
C	2.1332700	14.1942630	17.1578150
C	2.0710040	15.4801390	17.7072470
C	3.2170630	16.2366160	17.9771000
C	4.4713660	15.6353140	17.6953480
C	4.5762790	14.4173670	16.9845330
C	3.3845370	13.7037610	16.7792170
H	3.4401300	12.7299960	16.3097970
C	-1.7790170	12.3729820	19.2684700
C	1.2721100	11.4836820	17.1769440
C	1.3551510	10.9440430	18.4596600
C	1.8217440	10.7555280	16.1131770
C	2.0488290	9.7530920	18.7394970
C	2.5649570	9.5867460	16.3181940
C	2.7503170	9.1637400	17.6619890
H	0.8714620	11.4748780	19.2723050
H	1.6854950	11.1295140	15.1081480
C	-3.0236510	12.1482140	16.0552650
C	-1.9237140	11.6941250	15.2522880
C	-3.9913650	11.2370950	16.4967880
C	-2.9060880	9.4496390	15.3985980
H	-4.8036420	11.5945800	17.1173350
C	-4.7443330	14.0582320	17.4777670
C	-5.9129200	14.0572690	16.7142740
C	-4.8598890	14.1936230	18.8643820
C	-7.1852550	14.2441480	17.2764010
C	-6.0898890	14.4071440	19.4968090
C	-7.2305020	14.5302730	18.6627230
H	-5.8357320	13.9071070	15.6453840

C	-1.0363130	15.1087380	19.9189000
O	-0.8965780	15.8241990	20.8204920
O	-2.1524400	11.4320800	19.8228710
H	-0.9074260	15.3993650	17.6379860
H	1.0962980	15.8766220	17.9513020
H	-3.9498650	14.1541850	19.4471480
C	-1.9292380	10.3389120	14.9526130
C	-1.0075470	12.6388440	13.1862190
C	0.8757360	14.1217340	12.9175170
C	-3.9587940	9.8688300	16.1779780
C	-6.1771490	14.4218360	21.0451530
C	-7.1769220	13.3321450	21.5070500
C	-4.8115890	14.0915730	21.6883520
C	-6.6170590	15.7946740	21.6065720
H	-8.1774820	13.5137260	21.1117910
H	-6.8474560	12.3404780	21.1787180
H	-7.2350610	13.3195680	22.6016650
H	-4.0556330	14.8556680	21.4805610
H	-4.9348580	14.0422350	22.7749580
H	-4.4217570	13.1238510	21.3577150
H	-6.5063820	15.7973920	22.6968190
H	-5.9945240	16.6037780	21.2092850
H	-7.6615800	16.0121600	21.3849620
C	-8.4073700	14.0779590	16.3274070
C	-8.2148390	12.7776940	15.4988740
C	-9.7750130	13.9143230	17.0301170
C	-8.4800710	15.2742610	15.3485300
H	-7.3259660	12.7990940	14.8644400
H	-8.1368440	11.9049710	16.1553130
H	-9.0784430	12.6296670	14.8418540
H	-10.1358750	14.8286380	17.4987710
H	-10.5164260	13.6211650	16.2783250
H	-9.7449220	13.1348970	17.7954970
H	-9.3004990	15.1343960	14.6350410
H	-8.6534630	16.2182250	15.8751030
H	-7.5510240	15.3806320	14.7796890
C	-1.8848360	18.5031600	14.4575930
C	-0.4131590	18.0773660	14.7152400
C	-1.8385010	19.4066380	13.2043040
C	-2.3771110	19.3415010	15.6612500
H	-0.2938330	17.4886980	15.6270860
H	-0.0309800	17.4789530	13.8820110
H	0.2167030	18.9684720	14.8121680
H	-2.7732500	19.9327560	13.0126470
H	-1.0681460	20.1701780	13.3613310
H	-1.5770460	18.8436540	12.3055490
H	-1.7494300	20.2313980	15.7842020
H	-3.4099090	19.6779380	15.5217890
H	-2.3375400	18.7717180	16.5946020
C	3.0887520	17.6919760	18.4978790
C	3.8035610	18.6487730	17.5111280
C	1.6116260	18.1350640	18.5798670
C	3.6866170	17.8749520	19.9136680
H	4.8642940	18.4097340	17.4205080
H	3.3479930	18.5916470	16.5165130
H	3.7121870	19.6834970	17.8616430
H	1.0424010	17.5587780	19.3157150
H	1.5743680	19.1850810	18.8872330

H	1.1035240	18.0588640	17.6137450
H	3.4203090	18.8661020	20.2978450
H	3.2867220	17.1319930	20.6121460
H	4.7740150	17.8081050	19.9107550
C	5.8727500	13.8115500	16.3733020
C	6.2779220	12.5379130	17.1524570
C	5.5790030	13.4147870	14.8999090
C	7.0849370	14.7689940	16.3032020
H	6.5240830	12.7636950	18.1949360
H	5.4694590	11.8001920	17.1573230
H	7.1591430	12.0739610	16.6938890
H	5.2799650	14.2901840	14.3140700
H	6.4829910	12.9971310	14.4438770
H	4.7908320	12.6645860	14.8063980
H	7.8593710	14.3006970	15.6852000
H	6.8199520	15.7245970	15.8446590
H	7.5315270	14.9768100	17.2746670
C	3.1075860	8.7805650	15.1075320
C	2.5861310	7.3242140	15.1791780
C	2.6249380	9.3811820	13.7685300
C	4.6540570	8.7560700	15.0546670
H	2.9150690	6.8275130	16.0926350
H	1.4916420	7.3005300	15.1505270
H	2.9551550	6.7512560	14.3205380
H	3.0410400	10.3785390	13.5894730
H	2.9624130	8.7386070	12.9487240
H	1.5352290	9.4532360	13.7138400
H	4.9812650	8.3133570	14.1069230
H	5.0709970	9.7675060	15.1084300
H	5.0801590	8.1572530	15.8585050
C	1.9431440	9.1948080	20.1882790
C	0.4455690	9.1797710	20.5969660
C	2.4319740	7.7399320	20.3788750
C	2.7091460	10.1179890	21.1661300
H	-0.0132870	10.1689490	20.5972370
H	-0.1363490	8.5434110	19.9225740
H	0.3480960	8.7754050	21.6101670
H	3.5139530	7.6298080	20.3200040
H	2.1292640	7.4048340	21.3772000
H	1.9841150	7.0630890	19.6474590
H	2.6019480	9.7529950	22.1939080
H	3.7788130	10.1561250	20.9351760
H	2.3275570	11.1431940	21.1334120
O	3.6303900	8.1148340	17.8880270
C	4.9003720	8.5193620	18.4019920
H	4.8116070	8.9965490	19.3830680
H	5.4986140	7.6101240	18.4994980
H	5.4051460	9.2140130	17.7213830
O	5.6143030	16.2960640	18.1213770
C	6.1899610	15.7513850	19.3101850
H	7.0161950	16.4115720	19.5851040
H	5.4627650	15.7196240	20.1285470
H	6.5789940	14.7401600	19.1496730
O	-8.4220020	14.9207590	19.2557390
C	-8.7439330	16.2983930	19.0580130
H	-9.6519290	16.4904260	19.6347970
H	-7.9412100	16.9520970	19.4158490
H	-8.9350120	16.5251740	18.0037510

O	-3.9766620	17.8324150	12.3390010
C	-4.9994890	18.7148230	12.8040170
H	-5.9205940	18.1697620	13.0393900
H	-4.6860940	19.2690370	13.6947130
H	-5.1937510	19.4199860	11.9922300
C	-4.7864400	15.1010680	11.7661630
C	-3.8148410	15.3492810	10.5849960
C	-5.1286580	13.5953440	11.7890750
C	-6.1124970	15.8515520	11.4954230
H	-3.5858470	16.4111990	10.4809830
H	-2.8718860	14.8123880	10.7309390
H	-4.2662020	15.0028800	9.6474940
H	-5.8776390	13.3560510	12.5523120
H	-5.5544810	13.3124570	10.8207640
H	-4.2508700	12.9691470	11.9676410
H	-6.6266850	15.3904390	10.6443910
H	-6.7870940	15.7949200	12.3569000
H	-5.9448630	16.8984200	11.2480170
H	1.5371950	14.7210340	12.3023720
H	-4.7252020	9.1835460	16.5211900
O	-1.9631020	12.0397410	12.3911240
O	-0.5478520	13.2824210	11.0648390
C	-1.4796690	12.1958860	11.0555770
H	-2.3120300	12.4361110	10.3922530
H	-0.9652640	11.2748950	10.7418130
O	-1.0414830	9.6610750	14.1462340
O	-2.6629060	8.1951890	14.8998380
C	-1.3876560	8.2765010	14.2600570
H	-1.4498800	7.8339120	13.2613480
H	-0.6373260	7.7590490	14.8731520

ea-HRh(CO)₂(L8)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -4501.41516778, PCM -4501.45481795

Rh	-1.2136520	14.3234910	18.3177780
P	-2.9669980	13.7594240	16.6935090
P	0.6068820	13.4231960	16.9400260
C	-0.0298250	13.4179090	12.3391120
C	1.0843910	14.2010070	14.2698950
H	1.8599490	14.8123230	14.7136300
C	0.2980040	13.3950220	15.1056660
C	-0.7362530	12.5829080	14.5386070
C	-3.1689540	14.7665970	15.1595910
C	-3.9128650	14.2998820	14.0648150
H	-4.2627940	13.2760450	14.0768840
C	-4.2181300	15.1225600	12.9764210
C	-3.7691300	16.4720510	13.0373750
C	-2.8630830	16.9194130	14.0222570
C	-2.6202670	16.0429180	15.0953790
H	-1.9779690	16.3630780	15.9053880
C	2.1689850	14.4238710	17.1029040
C	2.0788070	15.7766090	17.4549920
C	3.2110440	16.5716850	17.6656470
C	4.4768840	15.9381340	17.5500430
C	4.6172570	14.6286550	17.0370930
C	3.4354120	13.8889010	16.8679410
H	3.5122420	12.8583110	16.5483950

C	-1.7113270	13.1236730	19.7474600
C	1.2455750	11.7100660	17.2578050
C	1.1209560	11.1628840	18.5326490
C	1.9152700	10.9649980	16.2762380
C	1.7211550	9.9436250	18.8964670
C	2.5749160	9.7681320	16.5743380
C	2.5499110	9.3349440	17.9275980
H	0.5317010	11.7025270	19.2642690
H	1.9287630	11.3421650	15.2628700
C	-2.7928720	12.0212370	16.0686730
C	-1.6829430	11.6524660	15.2380230
C	-3.7056680	11.0465140	16.4887410
C	-2.5210190	9.3471610	15.3535330
H	-4.5542640	11.3446540	17.0902470
C	-4.6508360	13.8736000	17.4684060
C	-5.6492430	14.6839040	16.9333770
C	-4.9170740	13.2114760	18.6776560
C	-6.8684250	14.9267460	17.5925320
C	-6.1068710	13.3966570	19.3854720
C	-7.0211190	14.3590120	18.8741240
H	-5.4756780	15.1586900	15.9778650
C	-1.6021490	16.1951990	18.4349810
O	-1.8342210	17.3131600	18.6463210
O	-1.9125620	12.5604830	20.7418420
H	-0.0468570	14.6809710	19.3268860
H	1.0920760	16.1969170	17.5914570
H	-4.1687150	12.5437210	19.0799480
C	-1.6077230	10.3042210	14.9155260
C	-0.8298100	12.6203960	13.1528430
C	0.9355180	14.2411450	12.8730000
C	-3.5922940	9.6883420	16.1459740
C	-6.4288450	12.5247210	20.6273400
C	-7.7818170	11.8043420	20.4001330
C	-5.3607680	11.4307310	20.8428060
C	-6.4988590	13.3508190	21.9336040
H	-8.5974650	12.5156100	20.2637430
H	-7.7331130	11.1575830	19.5171800
H	-8.0159470	11.1722260	21.2645090
H	-4.3806720	11.8442600	21.0957720
H	-5.6708460	10.7925660	21.6765030
H	-5.2483870	10.7869220	19.9641270
H	-6.5749520	12.6740630	22.7922170
H	-5.5964470	13.9567410	22.0683930
H	-7.3697660	14.0051620	21.9554640
C	-7.9267460	15.7608170	16.8163750
C	-8.0767450	15.1491530	15.3961850
C	-9.3519120	15.7608220	17.4156430
C	-7.4427170	17.2239960	16.6760660
H	-7.1445780	15.1603840	14.8274680
H	-8.4224890	14.1118300	15.4542870
H	-8.8177340	15.7201940	14.8259800
H	-9.4350980	16.3377310	18.3360220
H	-10.0301210	16.2182080	16.6863500
H	-9.7081430	14.7485320	17.6193830
H	-8.1672510	17.8100010	16.0986420
H	-7.3265870	17.7046450	17.6526940
H	-6.4772450	17.2818890	16.1639600
C	-2.0689160	18.2557760	14.0170840

C	-0.5674350	17.9157530	14.2241960
C	-2.1275890	19.0685650	12.7033230
C	-2.5405030	19.1545290	15.1853210
H	-0.3736370	17.3995480	15.1663140
H	-0.1979590	17.2783040	13.4148080
H	0.0203110	18.8400830	14.2269680
H	-3.0947080	19.5383380	12.5251790
H	-1.3869460	19.8733500	12.7673400
H	-1.8846750	18.4550800	11.8327490
H	-1.9552480	20.0808510	15.2080940
H	-3.5953300	19.4299120	15.0796010
H	-2.4207810	18.6609310	16.1541050
C	3.0651320	18.0918390	17.9385970
C	3.8468720	18.8766510	16.8552460
C	1.5911410	18.5417730	17.8559070
C	3.5796880	18.5001190	19.3398650
H	4.9092840	18.6291430	16.8700800
H	3.4520540	18.6564060	15.8573870
H	3.7412790	19.9543490	17.0258830
H	0.9689870	18.0904960	18.6341520
H	1.5422210	19.6273870	17.9890980
H	1.1450890	18.3115830	16.8838860
H	3.3077120	19.5425690	19.5400030
H	3.1260530	17.8839350	20.1237840
H	4.6639360	18.4259670	19.4152340
C	5.9445580	13.9417010	16.6054640
C	6.3019460	12.8102110	17.5988400
C	5.7364210	13.3112060	15.2007120
C	7.1606000	14.8847890	16.4526600
H	6.4858020	13.1987380	18.6055310
H	5.4948730	12.0742110	17.6711210
H	7.2090210	12.2888990	17.2712700
H	5.4621670	14.0755940	14.4663070
H	6.6681600	12.8418920	14.8672110
H	4.9621030	12.5409070	15.1880600
H	7.9697860	14.3277130	15.9668970
H	6.9250640	15.7502360	15.8283930
H	7.5482510	15.2533720	17.4012890
C	3.2239300	8.9242330	15.4460640
C	2.5890950	7.5111780	15.4492670
C	2.9642560	9.5443440	14.0554630
C	4.7575650	8.7929360	15.6013050
H	2.7805980	6.9895690	16.3879860
H	1.5048650	7.5790190	15.3122730
H	2.9998460	6.9104500	14.6292390
H	3.4554820	10.5163150	13.9364950
H	3.3757410	8.8799860	13.2883650
H	1.8973150	9.6724740	13.8545150
H	5.1775410	8.3150510	14.7087620
H	5.2321330	9.7749080	15.7041870
H	5.0296940	8.1801110	16.4595910
C	1.3646680	9.3704680	20.2982200
C	-0.1829140	9.3715100	20.4339660
C	1.7970500	7.9087090	20.5573680
C	1.9598000	10.2719320	21.4061200
H	-0.6175690	10.3699350	20.3824480
H	-0.6406210	8.7600820	19.6493760
H	-0.4655570	8.9451560	21.4025820

H	2.8727920	7.7851650	20.6796280
H	1.3281450	7.5759950	21.4900390
H	1.4693310	7.2393570	19.7586510
H	1.6699530	9.8973380	22.3944030
H	3.0541490	10.2934980	21.3651230
H	1.6037810	11.3032230	21.3229670
O	3.3489110	8.2531550	18.2699760
C	4.5459720	8.6183790	18.9585970
H	4.3336160	9.1210560	19.9078330
H	5.0857880	7.6893310	19.1574310
H	5.1724650	9.2781160	18.3474000
O	5.5966650	16.6603370	17.9363840
C	6.0955450	16.3069070	19.2276960
H	6.9046180	17.0069760	19.4499830
H	5.3179050	16.3946860	19.9939290
H	6.4909630	15.2857760	19.2468480
O	-8.0965480	14.7141550	19.6740060
C	-7.9155040	15.9559360	20.3593660
H	-8.7921080	16.0876640	20.9981800
H	-7.0120340	15.9422830	20.9783380
H	-7.8484930	16.7989500	19.6632620
O	-4.2283920	17.3458620	12.0635330
C	-5.2775870	18.2055370	12.5131780
H	-6.1450860	17.6303770	12.8563720
H	-4.9482900	18.8591520	13.3277770
H	-5.5655710	18.8182310	11.6556150
C	-4.9293230	14.5445160	11.7240980
C	-4.0303380	14.7862780	10.4850000
C	-5.1454790	13.0208440	11.8561020
C	-6.3182720	15.1763500	11.4693110
H	-3.9121610	15.8520050	10.2839570
H	-3.0334100	14.3596380	10.6341460
H	-4.4770650	14.3169790	9.6003990
H	-5.8426100	12.7715610	12.6633900
H	-5.5807750	12.6421310	10.9254800
H	-4.2089140	12.4849160	12.0343480
H	-6.8221630	14.6372380	10.6588950
H	-6.9575570	15.1092640	12.3560700
H	-6.2423760	16.2205330	11.1686840
H	1.5618430	14.8698540	12.2504200
H	-4.3180360	8.9540880	16.4760490
O	-1.7165260	11.9212670	12.3587540
O	-0.3887550	13.2463080	11.0222740
C	-1.2207450	12.0830810	11.0277230
H	-2.0573290	12.2295430	10.3428960
H	-0.6209510	11.2023480	10.7510430
O	-0.6627040	9.6889600	14.1232580
O	-2.1765530	8.1125830	14.8632030
C	-1.1639340	8.3702410	13.8873190
H	-1.6041960	8.3215430	12.8799400
H	-0.3538060	7.6468010	14.0003700

m062_LANL2DZ

E(RM062X): Gas phase -4499.67523704, PCM -4499.71217554

Rh	-0.9260840	14.4813690	18.5155630
P	-2.7190710	13.8394910	16.9821330
P	0.7440770	13.5964470	17.0509790
C	-0.1948800	13.4258000	12.5354760

C	0.9425090	14.4389230	14.3399010
H	1.6857170	15.1435420	14.6962920
C	0.3129000	13.5946960	15.2531940
C	-0.6518080	12.6490080	14.8045900
C	-2.9782960	14.6935760	15.3870880
C	-3.6809620	14.0981500	14.3328510
H	-3.8867900	13.0339510	14.3835350
C	-4.1421350	14.8518710	13.2555660
C	-3.8806560	16.2460500	13.2778380
C	-3.0384780	16.8415810	14.2295880
C	-2.6317100	16.0300280	15.2986750
H	-2.0406570	16.4642300	16.0968470
C	2.3037740	14.5617300	17.1461880
C	2.2469590	15.9537470	17.0058840
C	3.3697770	16.7562200	17.1855070
C	4.5703930	16.1163970	17.5814610
C	4.6993160	14.7202520	17.6120770
C	3.5276980	13.9727960	17.4234980
H	3.5811600	12.8953010	17.5141910
C	-1.4212550	13.2893580	19.9671940
C	1.3321960	11.8554640	17.1415080
C	0.8622170	10.9979940	18.1220080
C	2.1663850	11.3541290	16.1423900
C	1.1924110	9.6339360	18.1458780
C	2.5729780	10.0247180	16.1198090
C	2.0920370	9.1810770	17.1538970
H	0.1782280	11.4035130	18.8584390
H	2.4896620	12.0323760	15.3614630
C	-2.5269730	12.0718300	16.5029140
C	-1.4607090	11.7018200	15.6308650
C	-3.3347950	11.0977840	17.0858400
C	-2.0911270	9.3822850	16.0481220
H	-4.1564660	11.4013190	17.7241800
C	-4.4034560	13.9938010	17.7105430
C	-5.4125610	14.6792360	17.0507650
C	-4.6701070	13.4838410	18.9859600
C	-6.6658640	14.9209940	17.6281980
C	-5.8952710	13.6810790	19.6170440
C	-6.8500130	14.4870050	18.9485690
H	-5.2267470	15.0627390	16.0561140
C	-1.0498200	16.3999260	18.3802320
O	-1.0215060	17.5489460	18.3204940
O	-1.6114860	12.6278180	20.8876490
H	0.2545730	14.8195060	19.4723840
H	1.2916440	16.4091560	16.7631810
H	-3.8952240	12.9256450	19.4969250
C	-1.2838690	10.3441620	15.4449920
C	-0.8412140	12.5908020	13.4396640
C	0.6903080	14.3866340	12.9582120
C	-3.1397520	9.7252920	16.8643890
C	-6.2190660	12.9716320	20.9433080
C	-7.4495720	12.0717080	20.7265720
C	-5.0566210	12.0740830	21.3917590
C	-6.5063560	13.9527090	22.0929970
H	-8.3188840	12.6586430	20.4247570
H	-7.2463570	11.3218350	19.9553290
H	-7.6911790	11.5455560	21.6566090
H	-4.1552690	12.6490670	21.6245810

H	-5.3533760	11.5379920	22.2978340
H	-4.8009980	11.3253180	20.6344330
H	-6.5432060	13.4009110	23.0381330
H	-5.7162170	14.7060460	22.1768960
H	-7.4673570	14.4503820	21.9637230
C	-7.7066270	15.6069540	16.7171820
C	-7.7565020	14.8260260	15.3846330
C	-9.1496140	15.6203250	17.2469580
C	-7.2578940	17.0475020	16.4129220
H	-6.7912740	14.8083070	14.8710210
H	-8.0682480	13.7907260	15.5547240
H	-8.4826180	15.2965230	14.7122970
H	-9.2976050	16.3060360	18.0812020
H	-9.8072320	15.9499600	16.4357700
H	-9.4680010	14.6254570	17.5652140
H	-7.9626860	17.5205880	15.7194120
H	-7.2143550	17.6579060	17.3201490
H	-6.2634520	17.0630170	15.9522330
C	-2.4936110	18.2833740	14.2045360
C	-0.9710610	18.2125760	14.4547450
C	-2.6759480	19.0270730	12.8719130
C	-3.1240860	19.1030200	15.3438930
H	-0.7313220	17.8308050	15.4506410
H	-0.4828730	17.5690210	13.7151010
H	-0.5394730	19.2162950	14.3822270
H	-3.7097650	19.3090840	12.6726930
H	-2.0877510	19.9495660	12.9129970
H	-2.3205960	18.4298580	12.0287980
H	-2.7003060	20.1129580	15.3540120
H	-4.2086860	19.1933940	15.2279820
H	-2.9251780	18.6444790	16.3175670
C	3.3221710	18.2648720	16.8843110
C	4.3705900	18.5887150	15.8037190
C	1.9510800	18.6700600	16.3277580
C	3.5858300	19.1287870	18.1292770
H	5.3786880	18.3454750	16.1422080
H	4.1613480	18.0262340	14.8880180
H	4.3331080	19.6565310	15.5615910
H	1.1472700	18.5266270	17.0577140
H	1.9733370	19.7312790	16.0619300
H	1.7038450	18.1069160	15.4218350
H	3.3532760	20.1741250	17.9002250
H	2.9498340	18.8197890	18.9653040
H	4.6307390	19.0836450	18.4360500
C	6.0084180	13.9211080	17.7843800
C	6.0110950	13.1953360	19.1402910
C	6.0647880	12.8548050	16.6666360
C	7.3003070	14.7422070	17.6396740
H	5.9822860	13.8996570	19.9765110
H	5.1469400	12.5305800	19.2348320
H	6.9191550	12.5905170	19.2389440
H	6.0356450	13.3286840	15.6800830
H	6.9981050	12.2881140	16.7472550
H	5.2397090	12.1392740	16.7237320
H	8.1429770	14.0454090	17.5819920
H	7.2896520	15.3452980	16.7289800
H	7.4865170	15.4080400	18.4818290
C	3.4716770	9.5211330	14.9731240

C	2.7626480	8.4208430	14.1642030
C	3.7992130	10.6519120	13.9848380
C	4.8115720	8.9894280	15.5091890
H	2.5069690	7.5620200	14.7868430
H	1.8532430	8.8236940	13.7063940
H	3.4210610	8.0785550	13.3581040
H	4.3656640	11.4613830	14.4574520
H	4.4138860	10.2448380	13.1766660
H	2.8946250	11.0754370	13.5362630
H	5.4901810	8.7935170	14.6722340
H	5.2904900	9.7224620	16.1668950
H	4.6872770	8.0564360	16.0558220
C	0.5339340	8.7471330	19.2247690
C	-0.7535870	9.4047640	19.7626450
C	0.0976760	7.3781700	18.6706650
C	1.4697000	8.6009500	20.4402230
H	-0.5512520	10.2875010	20.3737400
H	-1.4304480	9.6920050	18.9522570
H	-1.2725400	8.6853320	20.4031900
H	0.9157100	6.7715890	18.2884930
H	-0.4027640	6.8164050	19.4659180
H	-0.6236100	7.5148350	17.8562340
H	0.9797070	7.9995210	21.2137690
H	2.4234050	8.1318270	20.2027560
H	1.6823130	9.5874950	20.8639280
O	2.4655850	7.8528340	17.0669010
C	3.4041390	7.3484510	18.0034470
H	2.9006280	6.7910320	18.7984790
H	4.0658400	6.6619400	17.4689180
H	4.0006130	8.1555680	18.4418520
O	5.6288450	16.9214350	17.9519270
C	5.7613000	17.0165720	19.3629220
H	6.5720060	17.7221110	19.5565530
H	4.8362000	17.3831340	19.8206430
H	6.0090130	16.0464680	19.8067250
O	-7.9847800	14.8518840	19.6437310
C	-7.8996230	16.1785200	20.1457610
H	-8.8449210	16.3853070	20.6517240
H	-7.0711850	16.2792490	20.8549420
H	-7.7524930	16.9012130	19.3361530
O	-4.4856780	17.0199180	12.3100210
C	-5.6379260	17.6829730	12.8089140
H	-6.3635720	16.9625010	13.2062770
H	-5.3756520	18.3893220	13.6044200
H	-6.0802690	18.2257330	11.9708460
C	-4.8011750	14.1782810	12.0371650
C	-3.8857350	14.4221890	10.8232910
C	-4.9338240	12.6640000	12.2508880
C	-6.2100120	14.7066490	11.7108470
H	-3.8367550	15.4870640	10.5849080
H	-2.8683530	14.0731100	11.0261000
H	-4.2740380	13.8891610	9.9474620
H	-5.6144100	12.4344280	13.0783650
H	-5.3508570	12.2140340	11.3447260
H	-3.9701790	12.1910430	12.4570460
H	-6.6600660	14.0641510	10.9466570
H	-6.8629750	14.6804690	12.5891690
H	-6.1826780	15.7207150	11.3144980

H	1.1896690	15.0481580	12.2605710
H	-3.7809900	8.9749990	17.3112050
O	-1.6942120	11.7650800	12.7562250
O	-0.6210230	13.1324320	11.2666240
C	-1.3010780	11.8892260	11.3956620
H	-2.1887780	11.8921290	10.7610010
H	-0.6148570	11.0695950	11.1408180
O	-0.3740940	9.7208140	14.6379870
O	-1.7028830	8.1393560	15.6399030
C	-0.4610600	8.3360730	14.9710770
H	-0.4439050	7.7425210	14.0554840
H	0.3621970	8.0658390	15.6454850

ee-HRh(CO)₂(BDPP)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2142.72594257, PCM -2142.75298371

Rh	5.5291130	8.4957250	26.7377280
P	6.8613520	10.4946100	27.0875330
P	4.7433630	8.3435310	29.0212510
C	6.1039310	11.6594200	28.3751930
C	4.5171810	10.0404240	29.8132580
C	7.0122280	11.5358830	25.5677700
C	7.9008290	11.1216600	24.5587440
C	7.9724110	11.8021000	23.3452630
C	7.1467840	12.9037710	23.1052040
C	6.2506730	13.3160000	24.0900780
C	6.1834190	12.6391550	25.3107550
C	8.6141910	10.3337330	27.6680730
C	8.9798000	9.2225420	28.4434830
C	10.2757410	9.0985690	28.9487200
C	11.2325880	10.0756200	28.6746580
C	10.8855470	11.1813690	27.8955410
C	9.5878580	11.3125460	27.4006450
C	5.8487730	7.4436650	30.2114910
C	6.1838060	7.9022400	31.4948030
C	7.0026630	7.1427650	32.3356250
C	7.4914810	5.9076700	31.9126120
C	7.1631320	5.4374160	30.6386630
C	6.3585810	6.2013900	29.7950010
C	3.1119410	7.5319200	29.3740530
C	2.3330330	7.0742870	28.3038110
C	1.0917520	6.4747850	28.5328700
C	0.6178000	6.3240280	29.8357290
C	1.3910510	6.7687570	30.9121090
C	2.6302290	7.3651830	30.6834770
H	5.1562760	11.9689320	27.9203270
H	4.3498180	9.8688710	30.8841460
H	8.6697750	11.4666780	22.5827930
H	7.1989940	13.4307000	22.1569530
H	5.5994010	14.1675660	23.9141630
H	5.4730810	12.9821240	26.0558130
H	8.2520310	8.4424000	28.6387700
H	10.5356690	8.2299240	29.5468850
H	12.2438810	9.9741850	29.0583830
H	11.6255480	11.9445000	27.6707150
H	9.3368140	12.1749420	26.7924720
H	7.2558100	7.5215410	33.3220280
H	8.1262140	5.3174160	32.5673540

H	7.5407520	4.4779140	30.2967590
H	6.1294430	5.8410660	28.7966280
H	2.7131120	7.1823760	27.2920630
H	0.4996970	6.1242300	27.6922230
H	-0.3463430	5.8566860	30.0153340
H	1.0305770	6.6453960	31.9296740
H	3.2290370	7.6889110	31.5303130
H	5.8168400	8.8570120	31.8561070
H	8.5381860	10.2578740	24.7236630
C	3.2543660	10.7388720	29.2830000
H	3.2478920	10.8244130	28.1930440
H	2.3534900	10.1932950	29.5730160
H	3.1826380	11.7509770	29.6985850
C	6.9343530	12.9206220	28.6680570
H	6.3581680	13.6106620	29.2959190
H	7.8546090	12.6713040	29.2042920
H	7.2127720	13.4534140	27.7554720
C	4.0144310	9.4334130	25.9307540
O	3.1409340	9.9778950	25.4084080
C	5.7236570	7.1689320	25.3732560
O	5.8921900	6.3487840	24.5741320
H	6.7856070	7.6934920	27.3007240
C	5.7877880	10.9288440	29.7088630
H	5.6611730	11.7183300	30.4626730
H	6.6718980	10.3646460	30.0302670

m062_LANL2DZ

E(RM062X): Gas phase -2141.93745723, PCM -2141.96384787

Rh	5.3925280	8.5270370	26.6388100
P	6.7670360	10.4523980	27.0699790
P	4.7157420	8.3639550	28.9536890
C	5.9813600	11.6428740	28.2879870
C	4.4762460	10.0226020	29.7760870
C	7.0671430	11.4751380	25.5757790
C	8.0667910	11.0675180	24.6829100
C	8.2562250	11.7343800	23.4789760
C	7.4399510	12.8120340	23.1389450
C	6.4329730	13.2137530	24.0100510
C	6.2454070	12.5491640	25.2208730
C	8.4522450	10.2591990	27.7825380
C	8.7287560	9.1397340	28.5736470
C	9.9640350	9.0044590	29.2046130
C	10.9448420	9.9760990	29.0337240
C	10.6867360	11.0871200	28.2328540
C	9.4486050	11.2312040	27.6155350
C	5.9163120	7.5062910	30.0578630
C	6.3946700	8.0150100	31.2687080
C	7.3500710	7.3141950	32.0049520
C	7.8271000	6.0905170	31.5478950
C	7.3433530	5.5651040	30.3500750
C	6.4031180	6.2707680	29.6093810
C	3.1422850	7.5271940	29.4183150
C	2.2406580	7.1810080	28.4111410
C	1.0182020	6.5929640	28.7320510
C	0.6936260	6.3446040	30.0617200
C	1.5929770	6.6804380	31.0734220
C	2.8117600	7.2678340	30.7535580
H	5.0224370	11.9137660	27.8269370

H	4.3365760	9.8293690	30.8483220
H	9.0385880	11.4079390	22.8011900
H	7.5854410	13.3301220	22.1966790
H	5.7889750	14.0479700	23.7504130
H	5.4505730	12.8763940	25.8857080
H	7.9788700	8.3633410	28.6907150
H	10.1547620	8.1308530	29.8200940
H	11.9114480	9.8664910	29.5154870
H	11.4508420	11.8444600	28.0888460
H	9.2571720	12.0995550	26.9914470
H	7.7217080	7.7303680	32.9360530
H	8.5730730	5.5477390	32.1197160
H	7.7089100	4.6101740	29.9863160
H	6.0533460	5.8783590	28.6578110
H	2.5110370	7.3678270	27.3743920
H	0.3237540	6.3256360	27.9419400
H	-0.2562390	5.8827390	30.3122160
H	1.3452690	6.4780410	32.1107810
H	3.5183550	7.5127540	31.5436400
H	6.0401670	8.9688470	31.6472170
H	8.6975940	10.2190880	24.9359740
C	3.1885700	10.6808690	29.2730450
H	3.1605500	10.7536920	28.1818070
H	2.3106320	10.1115140	29.5867890
H	3.1028070	11.6949970	29.6784180
C	6.7947570	12.9154090	28.5396400
H	6.2009970	13.6295100	29.1199590
H	7.6968750	12.6831690	29.1138650
H	7.1018140	13.4032530	27.6109730
C	3.9125250	9.6270430	25.9110330
O	3.1078890	10.2947560	25.4487120
C	5.4447110	7.2176240	25.2557900
O	5.5358070	6.4083470	24.4473180
H	6.6274890	7.6674620	27.0845640
C	5.7032930	10.9506350	29.6422680
H	5.5542540	11.7568050	30.3738260
H	6.6154490	10.4283930	29.9621900

ea-HRh(CO)₂(BDPP)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2142.72984361, PCM -2142.75738761

Rh	5.4978380	8.5558480	26.6626540
P	6.8229200	10.5378150	27.1618590
P	4.7713660	8.3345050	28.9806350
C	6.0009450	11.6943840	28.4168300
C	4.4354880	10.0046320	29.7753720
C	7.0559660	11.6102010	25.6753890
C	8.1231490	11.3605320	24.7957720
C	8.2511640	12.0760980	23.6056430
C	7.3125080	13.0520680	23.2654230
C	6.2412080	13.3010100	24.1234510
C	6.1115830	12.5846800	25.3146320
C	8.5448680	10.3439430	27.8231390
C	8.8846640	9.1285070	28.4352880
C	10.1500760	8.9369340	28.9949240
C	11.1019880	9.9541880	28.9358800
C	10.7837560	11.1644250	28.3140870
C	9.5167220	11.3598240	27.7647220

C	5.9116940	7.4854870	30.1769110
C	6.2711950	8.0000130	31.4322700
C	7.1162770	7.2839140	32.2845220
C	7.6097150	6.0375200	31.9019740
C	7.2526000	5.5089060	30.6594420
C	6.4166400	6.2271430	29.8060010
C	3.1976010	7.4114210	29.3107760
C	2.4833300	6.8521900	28.2438440
C	1.2901430	6.1618420	28.4739560
C	0.7999880	6.0228970	29.7717730
C	1.5105080	6.5687920	30.8448630
C	2.7030810	7.2529880	30.6169050
H	5.0623190	11.9744320	27.9270670
H	4.2384550	9.7993320	30.8352260
H	9.0855030	11.8667300	22.9420550
H	7.4116840	13.6080630	22.3377180
H	5.4996110	14.0524430	23.8672150
H	5.2589870	12.7887460	25.9544060
H	8.1556900	8.3252750	28.4588980
H	10.3894040	7.9882030	29.4664890
H	12.0900660	9.8041760	29.3619770
H	11.5241020	11.9574430	28.2539460
H	9.2915900	12.2996430	27.2718000
H	7.3859510	7.7055670	33.2487920
H	8.2662230	5.4818920	32.5653380
H	7.6272660	4.5374940	30.3500030
H	6.1568720	5.8041780	28.8416960
H	2.8706310	6.9546650	27.2351730
H	0.7474800	5.7333880	27.6362230
H	-0.1279020	5.4869980	29.9505840
H	1.1385680	6.4554970	31.8593640
H	3.2562860	7.6522230	31.4625550
H	5.9014190	8.9637960	31.7633630
H	8.8585990	10.6003970	25.0401210
C	3.1576300	10.6445890	29.2067380
H	3.2001700	10.7671780	28.1214080
H	2.2784830	10.0374900	29.4348520
H	3.0067550	11.6343410	29.6536740
C	6.7817780	12.9815660	28.7263870
H	6.1676680	13.6527300	29.3387550
H	7.6974770	12.7668110	29.2849610
H	7.0574070	13.5200130	27.8160810
C	3.8167720	9.1259850	25.8939620
O	2.8612100	9.4515360	25.3270660
C	6.3967570	6.8679380	26.4421130
O	6.9270700	5.8689890	26.1896850
H	6.0109470	8.7645080	25.1814110
C	5.6554400	10.9644050	29.7388970
H	5.4377170	11.7498460	30.4761960
H	6.5520620	10.4563800	30.1133810

m062_LANL2DZ

E(RM062X): Gas phase -2141.94097900, PCM -2141.96795653

Rh	5.3955200	8.5806170	26.6080820
P	6.7252170	10.5073030	27.1426790
P	4.7480670	8.3501660	28.9333480
C	5.8863770	11.6824360	28.3392770
C	4.4093320	9.9865840	29.7532620

C	7.0909800	11.5582560	25.6840940
C	8.2058260	11.2576400	24.8928240
C	8.4514670	11.9608770	23.7187900
C	7.5836060	12.9718160	23.3129710
C	6.4644830	13.2686530	24.0850740
C	6.2166700	12.5637530	25.2607640
C	8.3887030	10.2990320	27.9085730
C	8.6749480	9.0871490	28.5428270
C	9.8853310	8.8988910	29.2087500
C	10.8340850	9.9151400	29.2243120
C	10.5727830	11.1187590	28.5697290
C	9.3591730	11.3115160	27.9188270
C	5.9577470	7.5250630	30.0511900
C	6.4564030	8.0777190	31.2339080
C	7.4236160	7.4026430	31.9783500
C	7.8938080	6.1633430	31.5577240
C	7.3831310	5.5906870	30.3935520
C	6.4254360	6.2672440	29.6481650
C	3.2174520	7.4170990	29.3469560
C	2.3762250	6.9788080	28.3238010
C	1.1920970	6.3079360	28.6273930
C	0.8461820	6.0693060	29.9529190
C	1.6875780	6.4955130	30.9805350
C	2.8685280	7.1633700	30.6792150
H	4.9350770	11.9254380	27.8503030
H	4.2397110	9.7669680	30.8161200
H	9.3218220	11.7155680	23.1184980
H	7.7753610	13.5203390	22.3965130
H	5.7785940	14.0496430	23.7723320
H	5.3316970	12.8019110	25.8448910
H	7.9488950	8.2804570	28.5019200
H	10.0799540	7.9523930	29.7034730
H	11.7821530	9.7696330	29.7327050
H	11.3176080	11.9086010	28.5649320
H	9.1703410	12.2472070	27.3998750
H	7.8100410	7.8515770	32.8878370
H	8.6511170	5.6423380	32.1347600
H	7.7355690	4.6197020	30.0611320
H	6.0411140	5.8182310	28.7366440
H	2.6579810	7.1569920	27.2898600
H	0.5443220	5.9698930	27.8249890
H	-0.0741480	5.5445230	30.1888300
H	1.4254630	6.2999060	32.0155430
H	3.5324660	7.4761570	31.4821990
H	6.1055180	9.0425340	31.5857330
H	8.8848520	10.4663380	25.1990850
C	3.1126630	10.5876710	29.2008760
H	3.1373500	10.6788270	28.1108760
H	2.2505430	9.9703580	29.4632950
H	2.9582940	11.5875140	29.6208100
C	6.6507950	12.9789530	28.6163490
H	6.0160960	13.6712640	29.1797630
H	7.5423650	12.7780410	29.2180530
H	6.9643290	13.4775820	27.6955580
C	3.6937370	9.1622150	25.8850710
O	2.7238150	9.5119860	25.3811560
C	6.3424970	6.9070950	26.3779700
O	6.9184320	5.9414610	26.1484990

H	5.8661270	8.7928740	25.1408530
C	5.5897140	10.9786510	29.6797360
H	5.3636480	11.7717010	30.4060850
H	6.5164420	10.5077350	30.0334980

ee-HRh(CO)₂(CHIRAPHOS)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2103.40946072, PCM -2103.43583245

Rh	6.5220260	7.9838080	26.8654810
P	7.1669390	10.2914290	27.1952550
P	5.1004420	8.2619990	28.8173270
C	6.4756750	10.7632980	28.9090560
C	5.0651160	10.1371900	29.1374780
C	6.5675120	11.5944370	26.0176170
C	6.5882360	11.2689270	24.6511050
C	6.1983460	12.1975690	23.6862430
C	5.7695130	13.4693610	24.0697700
C	5.7417080	13.8072580	25.4230730
C	6.1414060	12.8800110	26.3877660
C	8.9651750	10.7280110	27.3113420
C	9.9218250	9.7052650	27.2639700
C	11.2841380	10.0018680	27.3522240
C	11.7067720	11.3241830	27.4854910
C	10.7617290	12.3528410	27.5254850
C	9.4019820	12.0578700	27.4353200
C	5.6606850	7.5002570	30.4144780
C	5.2975650	7.9859010	31.6811920
C	5.7104780	7.3317490	32.8422870
C	6.4870820	6.1743880	32.7572780
C	6.8507330	5.6787960	31.5050280
C	6.4444240	6.3390110	30.3438740
C	3.3166610	7.7533280	28.7930620
C	2.8917730	6.8828630	27.7804950
C	1.5699950	6.4319160	27.7334000
C	0.6538920	6.8494200	28.6975950
C	1.0651600	7.7149500	29.7150550
C	2.3856980	8.1584890	29.7652370
H	6.3411690	11.8511020	28.9424400
H	4.8136970	10.3174250	30.1899540
H	6.2225150	11.9229520	22.6356390
H	5.4567160	14.1906620	23.3203170
H	5.4090410	14.7942770	25.7323530
H	6.1127930	13.1735110	27.4320170
H	9.5904310	8.6780750	27.1509100
H	12.0126920	9.1970900	27.3112870
H	12.7662320	11.5555170	27.5508010
H	11.0838970	13.3861020	27.6210320
H	8.6811300	12.8696130	27.4491420
H	5.4251230	7.7270720	33.8132840
H	6.8080330	5.6655750	33.6617870
H	7.4571420	4.7808070	31.4277680
H	6.7426440	5.9625360	29.3703930
H	3.6060800	6.5540370	27.0321030
H	1.2603130	5.7564750	26.9411060
H	-0.3749200	6.5026970	28.6608520
H	0.3573350	8.0418820	30.4717230
H	2.6866350	8.8228880	30.5695660
H	4.6936340	8.8828900	31.7771140

H	6.9104560	10.2777900	24.3454480
C	3.9864620	10.8097750	28.2701230
H	4.1220910	10.5968690	27.2059350
H	2.9840760	10.4793480	28.5481370
H	4.0297590	11.8969860	28.3942140
C	7.4755840	10.3913630	30.0185540
H	7.0211570	10.5573280	31.0012230
H	7.7784830	9.3423810	29.9691930
H	8.3776130	11.0030820	29.9547140
C	5.2080970	8.2111420	25.4430730
O	4.4499950	8.3303300	24.5817610
C	7.4023170	6.4592500	26.1173300
O	7.9676840	5.5378600	25.7022990
H	7.6470920	7.7752520	27.9897760

m062_LANL2DZ

E(RM062X): Gas phase -2102.64037793, PCM -2102.66670610

Rh	6.5364260	7.9555640	26.8415850
P	7.1659730	10.2530940	27.1870800
P	5.1235550	8.2480290	28.7822630
C	6.4995140	10.7008570	28.8928910
C	5.0832160	10.1046420	29.0870120
C	6.5502990	11.5627510	26.0430350
C	6.5065810	11.2322790	24.6837860
C	6.0840280	12.1600440	23.7363740
C	5.6877190	13.4330160	24.1360420
C	5.7255560	13.7751210	25.4849690
C	6.1565230	12.8486660	26.4304950
C	8.9433860	10.7106670	27.3258520
C	9.9087630	9.7040650	27.2717040
C	11.2604150	10.0168720	27.4074310
C	11.6558600	11.3365570	27.5968550
C	10.6979320	12.3486410	27.6455950
C	9.3501130	12.0378150	27.5072310
C	5.6787480	7.5169370	30.3818700
C	5.2755890	7.9991630	31.6323790
C	5.7090350	7.3844650	32.8024230
C	6.5463000	6.2725880	32.7384130
C	6.9471670	5.7804850	31.5006770
C	6.5192030	6.4017420	30.3294860
C	3.3427490	7.7777570	28.7733560
C	2.9074170	6.8677090	27.8085650
C	1.5760440	6.4542170	27.7731700
C	0.6674520	6.9531240	28.6997480
C	1.0914120	7.8631610	29.6677290
C	2.4200050	8.2681420	29.7065180
H	6.4030360	11.7912350	28.9685970
H	4.7916900	10.3035920	30.1266380
H	6.0576610	11.8840230	22.6871540
H	5.3472690	14.1551030	23.4008120
H	5.4172730	14.7656060	25.8045200
H	6.1756070	13.1409630	27.4762900
H	9.5914820	8.6765730	27.1169970
H	12.0027880	9.2264700	27.3595910
H	12.7085620	11.5800050	27.7010040
H	11.0027680	13.3808450	27.7867950
H	8.6111090	12.8342530	27.5322030
H	5.3924900	7.7736210	33.7650520

H	6.8849560	5.7941250	33.6519460
H	7.5994870	4.9149520	31.4435080
H	6.8441100	6.0324720	29.3606490
H	3.6222150	6.4780620	27.0880990
H	1.2513250	5.7453110	27.0183090
H	-0.3703020	6.6364560	28.6705350
H	0.3850480	8.2559700	30.3922380
H	2.7363620	8.9800820	30.4646440
H	4.6238330	8.8649560	31.7058610
H	6.8092220	10.2359520	24.3707040
C	4.0563880	10.7565340	28.1539270
H	4.2235760	10.4735050	27.1084920
H	3.0366280	10.4689100	28.4145750
H	4.1318610	11.8468440	28.2129700
C	7.4867960	10.2373110	29.9714370
H	7.0245260	10.3143110	30.9609010
H	7.7879280	9.1942810	29.8286160
H	8.3904770	10.8499190	29.9605030
C	5.1595420	8.2364500	25.4490620
O	4.3621150	8.4169650	24.6517180
C	7.4197430	6.4414640	26.0811590
O	7.9909840	5.5345300	25.6700670
H	7.6503510	7.7385150	27.9362430

ea-HRh(CO)₂(CHIRAPHOS)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2103.41292882, PCM -2103.43931104

Rh	6.6035980	8.1058330	27.0032180
P	7.2040760	10.4615180	27.2733760
P	5.3624900	8.4027400	29.0394010
C	6.5524860	10.9879330	28.9858870
C	5.2150600	10.2775770	29.3316230
C	6.4781870	11.6333820	26.0334130
C	6.6374090	11.2958330	24.6784290
C	6.1651240	12.1351590	23.6708920
C	5.5165280	13.3279710	23.9975530
C	5.3533570	13.6773680	25.3374950
C	5.8351340	12.8400640	26.3472930
C	8.9633100	11.0554340	27.3036150
C	9.9999260	10.1512130	27.5732820
C	11.3257540	10.5837780	27.6372360
C	11.6355240	11.9280360	27.4299510
C	10.6120950	12.8382870	27.1579800
C	9.2871540	12.4067110	27.0935960
C	6.0606320	7.7097670	30.6143310
C	5.8723500	8.2773060	31.8857630
C	6.4153470	7.6796700	33.0249110
C	7.1496910	6.4981520	32.9148490
C	7.3399430	5.9199040	31.6588560
C	6.8055140	6.5234480	30.5199170
C	3.6066180	7.8032550	29.1131470
C	2.9557010	7.4890990	27.9107880
C	1.6284400	7.0564130	27.9093190
C	0.9327410	6.9242560	29.1112820
C	1.5720700	7.2255060	30.3156990
C	2.8980130	7.6594340	30.3176310
H	6.3531930	12.0657950	28.9557870
H	5.0331600	10.4497110	30.3991620

H	6.2976120	11.8520430	22.6307920
H	5.1400900	13.9785070	23.2134660
H	4.8507690	14.6031510	25.6032590
H	5.7001550	13.1430640	27.3795970
H	9.7727170	9.1041230	27.7307780
H	12.1144150	9.8658860	27.8431760
H	12.6674720	12.2644680	27.4740680
H	10.8441940	13.8862800	26.9898960
H	8.5058100	13.1252530	26.8687780
H	6.2637970	8.1397550	33.9974940
H	7.5736090	6.0344760	33.8009720
H	7.9127340	5.0021020	31.5613300
H	6.9741510	6.0799250	29.5435410
H	3.4979640	7.5778360	26.9759390
H	1.1435970	6.8154790	26.9675370
H	-0.0981530	6.5814950	29.1117660
H	1.0409620	7.1167690	31.2573310
H	3.3824760	7.8690710	31.2652820
H	5.3032150	9.1943520	32.0023400
H	7.1312430	10.3660700	24.4130360
C	4.0137290	10.8528140	28.5628510
H	4.0697380	10.6480380	27.4899970
H	3.0747840	10.4360810	28.9328030
H	3.9731130	11.9396440	28.6937610
C	7.6329750	10.7541180	30.0582210
H	7.2209730	10.9677860	31.0500490
H	7.9917040	9.7211610	30.0671200
H	8.4935370	11.4070810	29.9020640
C	5.5851180	8.2359540	25.3609530
O	4.9782280	8.1846850	24.3768120
C	8.3105190	7.2019390	27.0860770
O	9.2611960	6.5401980	27.0807950
H	6.0513950	6.6239950	27.0214280

m062_LANL2DZ

E(RM062X): Gas phase -2102.64284594, PCM -2102.66922461

Rh	6.5857590	8.1023100	26.9922610
P	7.1833970	10.4424080	27.2734520
P	5.3820640	8.3955540	29.0053790
C	6.5429720	10.9539910	28.9711990
C	5.2049960	10.2503290	29.2801740
C	6.4629410	11.6113190	26.0477350
C	6.6098630	11.2635430	24.6993830
C	6.1356050	12.0981070	23.6934090
C	5.4992150	13.2929080	24.0206500
C	5.3507460	13.6515300	25.3565850
C	5.8343640	12.8192300	26.3639460
C	8.9244400	11.0422400	27.3301620
C	9.9449420	10.1379050	27.6332470
C	11.2626790	10.5708410	27.7526500
C	11.5742290	11.9141670	27.5659250
C	10.5639910	12.8228660	27.2588310
C	9.2465130	12.3911390	27.1407910
C	6.0928470	7.7310020	30.5722550
C	5.9125070	8.3080640	31.8353110
C	6.4859150	7.7356590	32.9674050
C	7.2418980	6.5719290	32.8551300
C	7.4235260	5.9850780	31.6060780

C	6.8588940	6.5648140	30.4731960
C	3.6362880	7.8126380	29.1051540
C	2.9675870	7.5135450	27.9145530
C	1.6315760	7.1210230	27.9322800
C	0.9510530	7.0156120	29.1414100
C	1.6113390	7.3026870	30.3340010
C	2.9454350	7.6976480	30.3166100
H	6.3666420	12.0368370	28.9723560
H	4.9681440	10.4396800	30.3346400
H	6.2570520	11.8102730	22.6542520
H	5.1198420	13.9415540	23.2376950
H	4.8569690	14.5816870	25.6194940
H	5.7155070	13.1260990	27.3978770
H	9.7079820	9.0895390	27.7792110
H	12.0445970	9.8552250	27.9854990
H	12.6016270	12.2530220	27.6533930
H	10.8018820	13.8708880	27.1062110
H	8.4674020	13.1061970	26.8924330
H	6.3425580	8.2010300	33.9375810
H	7.6904890	6.1273460	33.7377580
H	8.0134600	5.0791480	31.5099080
H	7.0178320	6.1182620	29.4951410
H	3.5030730	7.5854200	26.9729290
H	1.1266080	6.8907900	26.9995980
H	-0.0886390	6.7040040	29.1565610
H	1.0890550	7.2132940	31.2814060
H	3.4522830	7.8998120	31.2550170
H	5.3260490	9.2155430	31.9481540
H	7.0995460	10.3280290	24.4400190
C	4.0481120	10.7867880	28.4315950
H	4.1650260	10.5271440	27.3733960
H	3.0927040	10.3824900	28.7720760
H	4.0034580	11.8779260	28.5066310
C	7.6148110	10.6516030	30.0265250
H	7.1950620	10.7832210	31.0285420
H	7.9783210	9.6205000	29.9550870
H	8.4721180	11.3186580	29.9193270
C	5.5189100	8.2969860	25.3720160
O	4.8529080	8.3229510	24.4391750
C	8.2926750	7.1761520	27.0905450
O	9.2312690	6.5184730	27.1448700
H	6.0335470	6.6474920	26.9929140

ee-HRh(CO)₂(SPANphos)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2988.75493343, PCM -2988.79310445

Rh	1.6010140	13.8591090	6.0230080
P	0.1976080	12.9088500	7.7935070
O	0.9279830	14.9235070	9.9154230
C	1.5868550	16.1805500	10.1359340
P	1.9364430	16.2670320	5.9062980
C	0.6363060	17.2168790	10.7723920
H	1.2028550	17.8508020	11.4586870
H	0.2748520	17.8568320	9.9620920
O	1.9220950	16.7015690	8.8443370
C	2.8410610	15.8367120	10.9480790
H	3.1322520	14.8225050	10.6564560
H	2.5745380	15.8022120	12.0085120

C	4.0623960	16.7673430	10.7351690
C	4.3128680	16.8437800	9.2313600
C	5.5776770	17.0204220	8.6591900
H	6.4465670	17.0945110	9.3066430
C	5.7611100	17.1098520	7.2768730
C	4.6389180	16.9739590	6.4503240
H	4.7729690	16.9999440	5.3736640
C	3.3583170	16.7733250	6.9746870
C	3.2105040	16.7497810	8.3742300
C	3.8411920	18.1970640	11.2874130
H	3.5554880	18.1724840	12.3461090
H	3.0720280	18.7403590	10.7329880
C	5.2470120	16.1330310	11.4913890
H	5.4995680	15.1492290	11.0842400
H	4.9922880	16.0088310	12.5497210
H	6.1412070	16.7614940	11.4458080
C	7.1301270	17.3519140	6.6835740
H	7.2690800	16.7885070	5.7554660
H	7.9238130	17.0579440	7.3769750
C	1.1168190	11.9610110	9.0995450
C	0.5445920	11.6932620	10.3537880
H	-0.4469140	12.0684470	10.5861250
C	1.2383690	10.9504140	11.3093580
H	0.7814500	10.7570740	12.2761700
C	2.5135150	10.4568250	11.0248320
H	3.0541220	9.8789330	11.7693690
C	3.0880750	10.7104890	9.7790550
H	4.0791630	10.3309010	9.5466550
C	2.3958840	11.4596050	8.8247480
H	2.8527500	11.6629090	7.8633640
C	2.4855040	16.8316010	4.2157450
C	3.1279820	15.9136940	3.3701080
C	3.5712410	16.2953140	2.1025140
H	4.0668600	15.5678340	1.4657190
C	3.3676200	17.6001330	1.6523920
H	3.7027120	17.8961670	0.6622220
C	2.7238330	18.5211420	2.4805460
H	2.5549460	19.5381490	2.1372040
C	2.2893010	18.1425410	3.7515890
H	1.7864260	18.8718400	4.3767600
C	0.3830570	13.7849070	4.4853840
C	0.5994240	17.4956630	6.2749870
C	-0.7264760	17.1381450	5.9979820
C	0.8591270	18.7721140	6.7978270
C	-1.7696070	18.0384120	6.2228830
C	-0.1837810	19.6697770	7.0308780
C	-1.5013100	19.3058290	6.7413470
H	-0.9440380	16.1455690	5.6148730
H	1.8799040	19.0609330	7.0300080
H	-2.7916860	17.7445700	6.0010760
H	0.0330150	20.6539980	7.4375810
H	-2.3127970	20.0051030	6.9226330
C	-0.9576950	13.9385460	8.8282320
C	-0.4379390	14.8888220	9.7244560
C	-2.3540000	13.8353460	8.7317410
C	-1.2739020	15.6973330	10.5095980
C	-3.2154490	14.6514820	9.4699000
C	-2.6551660	15.5765240	10.3573560

H	-2.7864710	13.0967060	8.0668380
H	-3.3155260	16.2023340	10.9503940
C	-0.5920150	16.6286040	11.5041240
C	-0.1887610	15.8250900	12.7647530
H	0.4200910	14.9528170	12.5147440
H	-1.0840800	15.4670900	13.2831380
H	0.3751590	16.4548010	13.4636030
H	7.2819790	18.4120210	6.4433990
C	-1.4888800	17.8030660	11.9337030
H	-1.8528880	18.3671170	11.0690520
H	-2.3547640	17.4611710	12.5090430
H	-0.9248680	18.4898460	12.5742260
C	-4.7143980	14.5436500	9.3074070
H	-5.0017400	13.5738220	8.8910080
H	-5.2324560	14.6661730	10.2643590
H	-5.1004060	15.3167470	8.6307980
C	-0.9462600	11.6017760	7.1194790
C	-0.9352220	10.2764800	7.5796340
C	-1.8196370	11.9305280	6.0676060
C	-1.7698520	9.3133140	7.0063150
C	-2.6638000	10.9735500	5.5064200
C	-2.6388660	9.6569110	5.9720120
H	-0.2720020	9.9872480	8.3863190
H	-1.7374700	8.2916620	7.3748180
H	-3.3319390	11.2554030	4.6974830
H	-3.2871910	8.9069600	5.5279120
H	4.7682550	18.7731580	11.2032570
C	2.9802070	12.6955810	5.3607680
O	3.8367030	12.0050600	4.9999100
O	-0.2906680	13.7826640	3.5484360
H	2.5969580	14.0058190	7.2513690
H	3.2736350	14.8940570	3.7109370
H	-1.8438650	12.9439180	5.6814790

m062_LANL2DZ

E(RM062X): Gas phase -2987.65097024, PCM -2987.68695897

Rh	1.9034400	13.7337080	6.2051360
P	0.2993600	12.9078250	7.7886200
O	0.9759880	14.8399650	9.9683060
C	1.6981540	16.0578210	10.1017900
P	1.9112180	16.1544580	5.9539840
C	0.8386490	17.1661970	10.7505560
H	1.4140770	17.6697010	11.5317630
H	0.6150910	17.8987270	9.9670500
O	1.9782070	16.4706580	8.7759120
C	2.9715720	15.6909220	10.8524600
H	3.2616060	14.6951950	10.4956490
H	2.7333460	15.6045050	11.9187390
C	4.1620670	16.6493200	10.6423770
C	4.3462690	16.8377530	9.1452080
C	5.5658750	17.1650840	8.5466000
H	6.4469650	17.2860990	9.1721800
C	5.6933100	17.3413630	7.1708310
C	4.5682090	17.1348500	6.3649730
H	4.6646610	17.2189480	5.2851730
C	3.3398480	16.7931170	6.9192560
C	3.2385140	16.6960960	8.3150230
C	3.9585750	18.0291460	11.2934080

H	3.6999520	17.9310220	12.3545340
H	3.1787470	18.6073460	10.7919350
C	5.3863930	15.9834390	11.2840350
H	5.6269690	15.0413220	10.7835630
H	5.1835330	15.7739330	12.3394390
H	6.2657530	16.6314470	11.2417970
C	7.0105070	17.7429870	6.5571970
H	7.1530820	17.2681210	5.5831250
H	7.8488160	17.4594200	7.1981790
C	1.0128500	11.9635210	9.2018090
C	0.3026000	11.7665620	10.3913470
H	-0.6871310	12.2008470	10.5074640
C	0.8565240	11.0209220	11.4268900
H	0.2984710	10.8779370	12.3471030
C	2.1249080	10.4600270	11.2844670
H	2.5573220	9.8799870	12.0938750
C	2.8345760	10.6484120	10.1032720
H	3.8230870	10.2158580	9.9850900
C	2.2822310	11.3996920	9.0676340
H	2.8402620	11.5598020	8.1505220
C	2.2898790	16.7740040	4.2595490
C	3.0760270	15.9650640	3.4298030
C	3.4353200	16.3941430	2.1554270
H	4.0506480	15.7587380	1.5263120
C	2.9963570	17.6297740	1.6869360
H	3.2678170	17.9616640	0.6897850
C	2.2023050	18.4348290	2.4995260
H	1.8513470	19.3957470	2.1364870
C	1.8540820	18.0131270	3.7800730
H	1.2346000	18.6484660	4.4050810
C	0.9783050	13.3180600	4.4805470
C	0.5168620	17.2284350	6.4928830
C	-0.7665400	16.6818860	6.5028530
C	0.7080650	18.5296020	6.9706310
C	-1.8475280	17.4233730	6.9758240
C	-0.3689190	19.2681480	7.4508260
C	-1.6490740	18.7136360	7.4569880
H	-0.9139620	15.6579820	6.1660330
H	1.7108150	18.9510730	6.9897550
H	-2.8389430	16.9815780	6.9854520
H	-0.2100350	20.2744340	7.8269570
H	-2.4885200	19.2878770	7.8375680
C	-0.8632620	14.0378410	8.6746850
C	-0.3508100	14.9317620	9.6179140
C	-2.2405330	14.0764650	8.4253180
C	-1.1697340	15.8353820	10.3003630
C	-3.0787460	14.9876100	9.0638790
C	-2.5256080	15.8658990	9.9994390
H	-2.6754360	13.3748150	7.7204690
H	-3.1759040	16.5714650	10.5102710
C	-0.4884620	16.6795110	11.3573140
C	-0.2313220	15.8160430	12.6058750
H	0.3517990	14.9240750	12.3610440
H	-1.1811660	15.4917660	13.0415130
H	0.3120850	16.3949350	13.3618120
H	7.0620030	18.8263130	6.4042860
C	-1.3138680	17.9055930	11.7476560
H	-1.5791860	18.4947770	10.8638730

H	-2.2342330	17.6188940	12.2652940
H	-0.7374800	18.5416390	12.4269900
C	-4.5541700	15.0329670	8.7555160
H	-4.8573270	14.1771970	8.1484760
H	-5.1509730	15.0276920	9.6721130
H	-4.8165460	15.9430710	8.2045430
C	-0.8727350	11.6768140	7.0653030
C	-1.0425030	10.3893460	7.5813000
C	-1.5887370	12.0369660	5.9152570
C	-1.9069100	9.4876410	6.9622670
C	-2.4633900	11.1436800	5.3076570
C	-2.6212340	9.8608010	5.8293130
H	-0.4952970	10.0815940	8.4659100
H	-2.0203930	8.4891120	7.3726480
H	-3.0120460	11.4448270	4.4208950
H	-3.2943000	9.1563720	5.3511050
H	4.8868690	18.6039140	11.2204330
C	3.5528930	12.8194410	5.8835490
O	4.5612740	12.2810410	5.7768900
O	0.4897140	13.1022380	3.4719660
H	2.6381030	14.0626320	7.5450380
H	3.4092020	14.9968580	3.7958550
H	-1.4641040	13.0321410	5.4942480

ea-HRh(CO)₂(SPANphos)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2988.75595103, PCM -2988.79517611

Rh	1.7691940	13.7667470	5.9349540
P	0.2625050	12.9460650	7.8311230
O	0.9206650	14.9333700	10.0307490
C	1.5704860	16.1963700	10.2158750
P	1.9244700	16.2462440	5.9551520
C	0.6196090	17.2394650	10.8479770
H	1.1727770	17.8458340	11.5689660
H	0.2933050	17.9043870	10.0431700
O	1.8796040	16.6778440	8.9007110
C	2.8377270	15.8792980	11.0140840
H	3.1483480	14.8732400	10.7135430
H	2.5797560	15.8321490	12.0764550
C	4.0346790	16.8391590	10.7962260
C	4.2613970	16.9504050	9.2901980
C	5.5096560	17.2098160	8.7146010
H	6.3750690	17.3282390	9.3601570
C	5.6836510	17.3242230	7.3330490
C	4.5703490	17.1239210	6.5089390
H	4.7013910	17.1656880	5.4327340
C	3.3042210	16.8430950	7.0345800
C	3.1615950	16.8024550	8.4352290
C	3.7987740	18.2528890	11.3822550
H	3.5343490	18.2013170	12.4454550
H	3.0101750	18.7952780	10.8549310
C	5.2449310	16.2113740	11.5184000
H	5.5097910	15.2428690	11.0837010
H	5.0095230	16.0576470	12.5773280
H	6.1257500	16.8583030	11.4740310
C	7.0333640	17.6558240	6.7395420
H	7.1900840	17.1367870	5.7888890
H	7.8466810	17.3728440	7.4144660

C	1.1349480	11.9623770	9.1460120
C	0.6406520	11.8288110	10.4531910
H	-0.2782680	12.3303870	10.7378870
C	1.3170500	11.0532740	11.3963480
H	0.9193870	10.9656470	12.4039600
C	2.4957070	10.3912890	11.0479760
H	3.0221350	9.7884960	11.7827800
C	2.9914990	10.5087240	9.7489100
H	3.9068230	9.9973060	9.4644650
C	2.3183580	11.2896320	8.8077860
H	2.7155680	11.3776200	7.8028730
C	2.4331940	16.8757210	4.2798730
C	3.1992820	16.0441250	3.4463250
C	3.6237950	16.4876300	2.1926830
H	4.2149220	15.8288860	1.5628230
C	3.2787570	17.7637240	1.7460060
H	3.6000070	18.1056570	0.7661120
C	2.5111150	18.5957360	2.5624210
H	2.2315670	19.5884120	2.2203820
C	2.0943180	18.1580880	3.8203810
H	1.4941630	18.8173200	4.4374330
C	3.6148400	13.5704840	6.4457920
C	0.4672720	17.3114690	6.3419800
C	-0.8102870	16.8032800	6.0749180
C	0.5881310	18.6104180	6.8599810
C	-1.9467000	17.5804500	6.3078400
C	-0.5479060	19.3850610	7.0969050
C	-1.8180450	18.8719240	6.8194490
H	-0.9117020	15.7919890	5.6934700
H	1.5716740	19.0125840	7.0841070
H	-2.9306680	17.1724090	6.0957980
H	-0.4415910	20.3897790	7.4971190
H	-2.7015860	19.4764340	7.0045550
C	-0.9148850	13.9910600	8.8204770
C	-0.4335840	14.9195160	9.7559220
C	-2.3048950	13.9338870	8.6254350
C	-1.2939700	15.7433680	10.4964760
C	-3.1893320	14.7651380	9.3170900
C	-2.6648350	15.6626360	10.2551710
H	-2.7100670	13.2202350	7.9168720
H	-3.3459940	16.2996810	10.8116850
C	-0.6410000	16.6540320	11.5285880
C	-0.2824500	15.8325480	12.7913640
H	0.3391030	14.9666830	12.5507260
H	-1.1944500	15.4650720	13.2726600
H	0.2540460	16.4541720	13.5184140
H	7.1317310	18.7308710	6.5415730
C	-1.5430300	17.8290020	11.9432920
H	-1.8717150	18.4088360	11.0749270
H	-2.4316690	17.4842210	12.4810950
H	-0.9980510	18.5015020	12.6146550
C	-4.6770390	14.7033160	9.0561530
H	-4.9583060	13.7640220	8.5717180
H	-5.2515250	14.7887460	9.9846390
H	-5.0027010	15.5205780	8.4001040
C	-0.9088570	11.6623870	7.1511790
C	-1.1931880	10.4624860	7.8209080
C	-1.5435080	11.9033010	5.9219790

C	-2.0805720	9.5322710	7.2752390
C	-2.4404290	10.9806460	5.3824370
C	-2.7088320	9.7878620	6.0562410
H	-0.7186400	10.2462670	8.7712670
H	-2.2786110	8.6056610	7.8071720
H	-2.9182080	11.1907950	4.4295940
H	-3.3972530	9.0623820	5.6319350
H	4.7140700	18.8466420	11.2927200
C	0.8634800	13.7014670	4.2420570
O	0.3998330	13.5920310	3.1863590
O	4.7334210	13.3761960	6.6698900
H	1.8458260	12.1990010	5.7291640
H	-1.3288140	12.8163530	5.3779440
H	3.4489200	15.0423410	3.7810840

m062_LANL2DZ

E(RM062X): Gas phase -2987.65462853, PCM -2987.69084207

Rh	2.2641290	13.5503210	6.5181460
P	0.3854260	12.8195830	7.9739320
O	0.9995590	14.7792710	10.2234630
C	1.7445880	15.9910560	10.2284380
P	1.8527190	16.0352590	6.0749420
C	0.9237530	17.1679700	10.8064340
H	1.4805330	17.6440500	11.6175740
H	0.7931070	17.9043220	10.0063780
O	1.9832140	16.2229750	8.8525680
C	3.0413190	15.6983290	10.9651300
H	3.3597340	14.7032180	10.6411890
H	2.8302330	15.6468800	12.0392880
C	4.1950690	16.6933970	10.6982820
C	4.2586890	16.9917040	9.2068060
C	5.3898970	17.5372860	8.5874900
H	6.2557830	17.7860650	9.1967030
C	5.4543350	17.7620940	7.2158090
C	4.3580580	17.3927110	6.4246740
H	4.4135940	17.5086130	5.3447560
C	3.2109700	16.8596300	6.9981320
C	3.1660210	16.7105730	8.3948070
C	4.0554920	18.0167400	11.4718700
H	3.8843900	17.8306750	12.5385320
H	3.2445920	18.6388480	11.0866540
C	5.4800080	15.9911090	11.1656990
H	5.6632640	15.0895780	10.5751990
H	5.3846270	15.7054270	12.2189020
H	6.3503150	16.6469760	11.0799500
C	6.6749180	18.3797340	6.5818380
H	6.9441460	17.8605720	5.6581080
H	7.5342150	18.3401290	7.2553640
C	0.9392160	11.7266620	9.3441650
C	0.3539220	11.7332340	10.6127950
H	-0.4522870	12.4266170	10.8350700
C	0.8006000	10.8534750	11.5958010
H	0.3439700	10.8713280	12.5805220
C	1.8283010	9.9562260	11.3182980
H	2.1762480	9.2725930	12.0863220
C	2.4111780	9.9402090	10.0538240
H	3.2141230	9.2446280	9.8316520
C	1.9730120	10.8240840	9.0725100

H	2.4373080	10.8240880	8.0890350
C	2.1369270	16.6535380	4.3625630
C	2.5922720	15.7594830	3.3909140
C	2.8429920	16.1952090	2.0908040
H	3.1969410	15.4899160	1.3455940
C	2.6366730	17.5279220	1.7510170
H	2.8283560	17.8680600	0.7380470
C	2.1778400	18.4269590	2.7132880
H	2.0104880	19.4670150	2.4509810
C	1.9291520	17.9931050	4.0104880
H	1.5641360	18.6958810	4.7547280
C	3.5384490	13.5681230	7.9703690
C	0.3622810	16.9997500	6.5671010
C	-0.8852670	16.4286400	6.3106020
C	0.4188570	18.2490170	7.1934050
C	-2.0571130	17.0999620	6.6496370
C	-0.7517350	18.9145910	7.5476550
C	-1.9932390	18.3421190	7.2735890
H	-0.9393930	15.4414470	5.8555310
H	1.3865350	18.6949690	7.4129270
H	-3.0193110	16.6399160	6.4442920
H	-0.6940330	19.8838320	8.0350940
H	-2.9057750	18.8616900	7.5505180
C	-0.7685710	13.9927680	8.8025590
C	-0.2922610	14.8948520	9.7556790
C	-2.1244700	14.0688820	8.4558810
C	-1.1137460	15.8756810	10.3180830
C	-2.9696330	15.0294950	9.0030450
C	-2.4431200	15.9397330	9.9223830
H	-2.5297650	13.3714800	7.7291790
H	-3.0925230	16.7075630	10.3351180
C	-0.4644290	16.7748370	11.3493630
C	-0.3205360	16.0021470	12.6735260
H	0.2548450	15.0827680	12.5357150
H	-1.3077940	15.7342130	13.0617420
H	0.1850050	16.6234650	13.4216240
H	6.4990980	19.4302680	6.3274800
C	-1.2636560	18.0552120	11.5921330
H	-1.4578380	18.5776410	10.6492850
H	-2.2211960	17.8426870	12.0772340
H	-0.7016670	18.7253930	12.2505350
C	-4.4221300	15.1060600	8.6082400
H	-4.6279770	14.4894500	7.7301150
H	-5.0729350	14.7608030	9.4181350
H	-4.7093170	16.1368450	8.3768500
C	-0.8179690	11.7391080	7.0892320
C	-1.4333560	10.6416060	7.6980580
C	-1.1748150	12.0788170	5.7798140
C	-2.3860900	9.8978210	7.0065680
C	-2.1360560	11.3423130	5.0938360
C	-2.7416500	10.2483310	5.7066250
H	-1.1678360	10.3682800	8.7148600
H	-2.8530360	9.0434780	7.4863200
H	-2.4030540	11.6173510	4.0785020
H	-3.4855550	9.6676990	5.1703550
H	4.9796990	18.5945930	11.3729630
C	1.9192380	12.3043340	5.0902780
O	1.8452050	11.5301240	4.2463390

O	4.3693340	13.5108120	8.7594610
H	3.5372350	13.8478020	5.6765570
H	-0.6918040	12.9245920	5.2963950
H	2.7493380	14.7184920	3.6583210

ee-HRh(CO)₂(PPh₃)₂

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2409.46548158, PCM -2409.49846370

P	7.2911540	10.3963030	-13.0422870
P	5.5120290	8.8410850	-9.6361780
C	8.8498220	8.1060360	-12.6175780
C	3.7627800	8.4997850	-10.1489770
C	6.3131640	7.1724090	-9.7612750
C	3.4446900	8.5998780	-11.5129190
C	7.6537560	12.1327730	-15.2963610
H	7.2628040	11.3246680	-15.9060040
C	5.3572820	9.0336880	-7.7952210
C	10.8431500	8.7424830	-14.4564270
H	11.6228100	9.0025130	-15.1670800
C	8.7564370	9.3037940	-13.3440260
C	7.6385690	4.6945620	-9.9325180
H	8.1492010	3.7378700	-9.9968230
C	5.3404680	7.9359380	-6.9192690
H	5.4498840	6.9294190	-7.3096600
C	7.7592510	11.9742850	-13.9037970
C	8.5448570	14.3775030	-15.1381410
H	8.8433730	15.3071570	-15.6144650
C	5.2172450	10.3228710	-7.2606940
H	5.2503490	11.1798420	-7.9260930
C	2.7487070	8.1474730	-9.2445490
H	2.9671380	8.0704450	-8.1851620
C	1.4508690	7.9005120	-9.6963060
C	8.2924490	5.8056710	-9.3909670
H	9.3135960	5.7166440	-9.0307240
C	8.2618590	13.0391570	-13.1426220
H	8.3313500	12.9326480	-12.0650850
C	6.3273750	4.8230720	-10.3888890
H	5.8103820	3.9661700	-10.8118460
C	9.9162280	7.2303690	-12.8210640
H	9.9648640	6.3081300	-12.2493030
C	2.1503410	8.3395560	-11.9640160
H	1.9291770	8.4200530	-13.0242270
C	10.9188950	7.5480060	-13.7395480
H	11.7566610	6.8729140	-13.8903600
C	9.7675060	9.6129290	-14.2660640
H	9.7247790	10.5358450	-14.8334860
C	5.0560740	10.5119490	-5.8877020
H	4.9505240	11.5181770	-5.4921480
C	7.6394960	7.0349300	-9.3146210
H	8.1625010	7.8961580	-8.9089810
C	8.0418600	13.3260500	-15.9072010
C	1.1485320	7.9924900	-11.0558220
C	5.6656230	6.0514300	-10.2993580
H	4.6421380	6.1319450	-10.6490170
C	5.0442920	9.4141810	-5.0255290
H	4.9294080	9.5613830	-3.9553310
C	5.1886100	8.1263770	-5.5444500
H	5.1846480	7.2666950	-4.8799920

C	8.6563220	14.2299780	-13.7550300
H	9.0422770	15.0440260	-13.1480130
Rh	6.6472490	10.7060020	-10.7046860
H	7.9421610	9.8268490	-10.4037170
C	5.0488160	11.7779250	-11.0794460
C	7.6127880	11.9600370	-9.6087110
O	8.2362200	12.6669410	-8.9381280
O	4.1159270	12.4192470	-11.2985050
H	0.1374570	7.8006880	-11.4040870
H	0.6757360	7.6368850	-8.9820130
H	7.9489370	13.4336930	-16.9843810
C	6.0243670	9.7123600	-14.2191210
C	6.1531880	8.4590820	-14.8350650
C	4.8535600	10.4569040	-14.4531550
C	5.1408890	7.9639380	-15.6620590
C	3.8498170	9.9662530	-15.2870340
C	3.9886120	8.7141120	-15.8935010
H	7.0464520	7.8650980	-14.6752920
H	4.7253520	11.4295620	-13.9873060
H	5.2613090	6.9908660	-16.1302250
H	2.9589350	10.5629360	-15.4623710
H	3.2058860	8.3305970	-16.5417680
H	8.0912760	7.8625240	-11.8817660
H	4.2114850	8.8874340	-12.2246810

m062_LANL2DZ

E(RM062X): Gas phase -2408.57906490, PCM -2408.61189040

P	6.8222770	10.5512280	-13.0466120
P	5.5514530	8.8924070	-9.7293000
C	7.2438550	7.7832020	-13.0765360
C	3.9817390	8.0062650	-10.1189250
C	6.8028230	7.5497720	-9.8773450
C	3.5359410	8.0001330	-11.4461050
C	8.3311620	11.9004810	-15.0312490
H	7.8938340	11.1972150	-15.7348840
C	5.4358980	9.0750850	-7.8975350
C	10.0010770	7.9212950	-13.3779820
H	11.0795570	7.9822450	-13.4870630
C	7.8599490	9.0372390	-13.1871280
C	8.7921330	5.5818170	-9.9821420
H	9.5634730	4.8189130	-10.0270140
C	5.9610660	8.1377430	-7.0022640
H	6.4882520	7.2648600	-7.3756670
C	7.9747220	11.8441760	-13.6782480
C	9.8085540	13.7539170	-14.5807390
H	10.5180190	14.4962120	-14.9329000
C	4.7646970	10.1940030	-7.3933400
H	4.3762990	10.9366310	-8.0858430
C	3.2296180	7.3320940	-9.1510200
H	3.5562110	7.3328440	-8.1151860
C	2.0614770	6.6618980	-9.5060770
C	9.1437240	6.9289390	-9.9198380
H	10.1891560	7.2208370	-9.9244500
C	8.5426740	12.7549240	-12.7859060
H	8.2585600	12.7180810	-11.7385710
C	7.4492200	5.2190170	-9.9995370
H	7.1677860	4.1715550	-10.0521640
C	7.9921380	6.6152150	-13.1469040

H	7.4981910	5.6531810	-13.0551150
C	2.3730190	7.3231360	-11.8013510
H	2.0407560	7.3311290	-12.8345270
C	9.3765700	6.6824600	-13.2968270
H	9.9639180	5.7701780	-13.3344660
C	9.2477260	9.0942670	-13.3319690
H	9.7469260	10.0548470	-13.4132160
C	4.6077130	10.3666020	-6.0222480
H	4.0839100	11.2393850	-5.6453750
C	8.1565300	7.9063970	-9.8728730
H	8.4327480	8.9569190	-9.8436140
C	9.2412790	12.8510810	-15.4793460
C	1.6325100	6.6534050	-10.8306780
C	6.4573570	6.1972340	-9.9483040
H	5.4123430	5.9019060	-9.9577280
C	5.1357530	9.4296610	-5.1363250
H	5.0240420	9.5694940	-4.0656790
C	5.8138680	8.3187740	-5.6284310
H	6.2319750	7.5886920	-4.9424590
C	9.4596510	13.7040050	-13.2351980
H	9.8937150	14.4073640	-12.5317450
Rh	5.8837720	10.9635740	-10.8890100
H	7.3890530	10.7683690	-10.4707580
C	3.9812250	11.2031410	-11.3986670
C	6.1474490	12.6108220	-9.9240330
O	6.3926220	13.5639170	-9.3358050
O	2.8830380	11.3362100	-11.6797820
H	0.7203430	6.1326630	-11.1041080
H	1.4849840	6.1476530	-8.7435060
H	9.5083420	12.8886140	-16.5308270
C	5.6717380	10.3865230	-14.4830210
C	5.7809830	9.3909970	-15.4586990
C	4.6521520	11.3391750	-14.6032550
C	4.8795260	9.3401720	-16.5202550
C	3.7586460	11.2928770	-15.6678590
C	3.8660750	10.2869750	-16.6262850
H	6.5733330	8.6525510	-15.3942440
H	4.5653900	12.1283510	-13.8603900
H	4.9760860	8.5589600	-17.2677860
H	2.9756340	12.0402310	-15.7466480
H	3.1642920	10.2447500	-17.4531010
H	6.1672540	7.7182820	-12.9310110
H	4.0941940	8.5449970	-12.2052290

ea-HRh(CO)₂(PPh₃)₂

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2409.46398406, PCM -2409.49820931

P	6.5925290	10.1899330	-13.2446320
P	5.6447620	8.8813080	-9.6745260
C	5.9778170	7.4787490	-13.6182410
C	4.4525590	7.4880770	-9.9520760
C	7.3041130	8.0670280	-9.6611220
C	3.5000640	7.5870600	-10.9741560
C	8.5378820	11.7562150	-14.6682190
H	7.8289060	11.8026850	-15.4873770
C	5.3620980	9.2656500	-7.8814930
C	8.5717670	6.6262320	-14.1569390
H	9.5871930	6.3018290	-14.3676550

C	7.0211320	8.4205770	-13.6188430
C	9.8981000	6.9761630	-9.7229150
H	10.8983590	6.5531090	-9.7439040
C	5.9633570	8.5370500	-6.8423320
H	6.6731710	7.7483330	-7.0695320
C	8.2146160	11.0537610	-13.4985210
C	10.6986870	12.3521740	-13.7511590
H	11.6553620	12.8578570	-13.8470940
C	4.4736040	10.3008650	-7.5538620
H	4.0255980	10.8896150	-8.3476080
C	4.4437490	6.3473590	-9.1309390
H	5.1619200	6.2523140	-8.3231520
C	3.5130470	5.3307930	-9.3378440
C	9.6706680	8.2117710	-9.1105670
H	10.4923440	8.7533820	-8.6503880
C	9.1541000	11.0161700	-12.4539780
H	8.9156680	10.4893590	-11.5348850
C	8.8341640	6.2940700	-10.3106510
H	9.0001680	5.3389920	-10.8001320
C	6.2253380	6.1345710	-13.8909120
H	5.4020560	5.4256290	-13.8898840
C	2.5628140	6.5707840	-11.1785480
H	1.8279270	6.6691710	-11.9723880
C	7.5270930	5.7022930	-14.1602930
H	7.7227580	4.6548340	-14.3721320
C	8.3224370	7.9757500	-13.8911280
H	9.1461220	8.6809680	-13.9000450
C	4.1818110	10.5910900	-6.2202850
H	3.4923250	11.3967950	-5.9850860
C	8.3877160	8.7560180	-9.0852250
H	8.2291700	9.7177120	-8.6067950
C	9.7691670	12.4055600	-14.7893950
C	2.5692640	5.4401880	-10.3630320
C	7.5451800	6.8332930	-10.2804100
H	6.7329310	6.2906640	-10.7500870
C	4.7825710	9.8595130	-5.1950690
H	4.5621340	10.0913870	-4.1569210
C	5.6764360	8.8342630	-5.5093990
H	6.1556300	8.2660730	-4.7169610
C	10.3891600	11.6500100	-12.5837660
H	11.1042850	11.6060180	-11.7671290
Rh	5.5115130	10.8960280	-11.0889320
H	5.4648730	12.2779830	-11.8575260
C	6.7665020	11.8532460	-9.9838620
C	3.5939710	11.0446290	-11.1861850
O	2.4571810	11.2634650	-11.2299880
O	7.4594590	12.5131760	-9.3333200
H	1.8407240	4.6496030	-10.5189450
H	3.5201710	4.4555770	-8.6943250
H	9.9986590	12.9531230	-15.6993730
C	5.6404160	10.6419520	-14.7764060
C	5.8411800	9.9800110	-16.0002270
C	4.7041380	11.6854290	-14.7257720
C	5.1235160	10.3519490	-17.1376410
C	3.9900070	12.0600690	-15.8654240
C	4.1951890	11.3929960	-17.0735830
H	6.5590740	9.1691790	-16.0659940
H	4.5315710	12.2012770	-13.7876120

H	5.2902430	9.8259610	-18.0736880
H	3.2680160	12.8693990	-15.8037930
H	3.6342610	11.6795420	-17.9587590
H	4.9627120	7.7999510	-13.4085330
H	3.4881270	8.4682660	-11.6061140

m062_LANL2DZ

E(RM062X): Gas phase -2408.58352065, PCM -2408.61567078

P	6.4099930	10.2355860	-13.2395860
P	5.6152100	8.9290210	-9.7530230
C	5.4311450	7.6479710	-13.2482870
C	4.7200370	7.3432900	-10.0282470
C	7.3891900	8.4575510	-9.7214170
C	3.4330870	7.4064540	-10.5706830
C	8.6956170	11.3046240	-14.5882850
H	8.0619230	11.4413310	-15.4595100
C	5.2608260	9.2391670	-7.9717870
C	7.7878640	6.3984100	-14.0225330
H	8.7093490	5.9121350	-14.3291040
C	6.5619030	8.4235020	-13.5239550
C	10.1584580	8.0822450	-9.9293270
H	11.2313870	7.9408890	-10.0142170
C	5.6774330	8.3415880	-6.9806640
H	6.2459970	7.4569080	-7.2553850
C	8.1595060	10.7799160	-13.4092820
C	10.8688460	11.4708670	-13.5463950
H	11.9187730	11.7413390	-13.6003000
C	4.5405990	10.3770630	-7.6046190
H	4.2237430	11.0772640	-8.3727230
C	5.2459610	6.0959700	-9.6772180
H	6.2452350	6.0244210	-9.2584350
C	4.5061040	4.9353460	-9.8843390
C	9.6427690	8.9855030	-9.0009880
H	10.3106530	9.5493320	-8.3573730
C	8.9927610	10.6138260	-12.2958680
H	8.5859620	10.2193570	-11.3673540
C	9.2913130	7.3640110	-10.7473120
H	9.6801760	6.6619030	-11.4784090
C	5.4794430	6.2602450	-13.3342700
H	4.6005840	5.6756920	-13.0774600
C	2.6885030	6.2468700	-10.7681950
H	1.6909340	6.3141120	-11.1903000
C	6.6646690	5.6323120	-13.7150170
H	6.7131280	4.5493830	-13.7722150
C	7.7407890	7.7882310	-13.9256530
H	8.6285230	8.3762050	-14.1410070
C	4.2394350	10.6146540	-6.2635410
H	3.6791870	11.5023010	-5.9881420
C	8.2673800	9.1740670	-8.8977750
H	7.8745150	9.8873730	-8.1782240
C	10.0434750	11.6542220	-14.6517550
C	3.2271340	5.0075370	-10.4310110
C	7.9144690	7.5475950	-10.6461750
H	7.2535780	6.9828670	-11.2977390
C	4.6589780	9.7212500	-5.2851720
H	4.4283520	9.9092000	-4.2412540
C	5.3805390	8.5823990	-5.6452020
H	5.7125130	7.8839650	-4.8835650

C	10.3409650	10.9455660	-12.3683960
H	10.9732810	10.7992720	-11.4977050
Rh	5.2575640	10.9431330	-11.1443260
H	5.0744170	12.3165340	-11.8441810
C	6.5305150	11.9371980	-10.0624750
C	3.3377680	10.9136400	-11.2766380
O	2.1936720	10.9804570	-11.3486880
O	7.2449780	12.5690220	-9.4281850
H	2.6520780	4.1010750	-10.5920530
H	4.9303320	3.9728180	-9.6162980
H	10.4476430	12.0681750	-15.5703040
C	5.6622900	10.7981980	-14.8259230
C	5.7298100	10.0347020	-15.9970790
C	5.0343280	12.0469940	-14.8656410
C	5.1813090	10.5144990	-17.1832960
C	4.4934440	12.5285700	-16.0546060
C	4.5643050	11.7623080	-17.2149140
H	6.2119060	9.0613940	-15.9821930
H	4.9653030	12.6381310	-13.9571000
H	5.2349880	9.9109110	-18.0839580
H	4.0089140	13.4996850	-16.0710580
H	4.1363550	12.1345310	-18.1404280
H	4.5159540	8.1408130	-12.9296080
H	3.0132710	8.3689820	-10.8502850

ee-HRh(CO)₂(PEtPh₂)₂

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2104.62629043, PCM -2104.65245722

P	6.7185080	10.4846090	-13.3788800
P	5.6801710	8.6609960	-9.6793190
C	7.1842810	7.6176180	-9.3945290
C	8.5672800	11.8829890	-15.0373270
H	7.9591660	11.5441600	-15.8708130
C	5.1972250	9.1592480	-7.9645150
C	9.4683250	5.9997220	-9.0915380
H	10.3503480	5.3767700	-8.9724580
C	6.1741770	9.5856390	-7.0494120
H	7.2248820	9.5389770	-7.3192210
C	8.1969140	11.5609990	-13.7203920
C	10.4869770	13.1143140	-14.2304920
H	11.3689640	13.7174070	-14.4273040
C	3.8472470	9.2503570	-7.5887200
H	3.0638500	8.9507570	-8.2782340
C	9.3659540	6.8716440	-10.1753450
H	10.1701680	6.9348320	-10.9030980
C	8.9877810	12.0362000	-12.6659330
H	8.7014320	11.8092660	-11.6444500
C	8.4363430	5.9400520	-8.1519760
H	8.5140950	5.2719680	-7.2987320
C	3.4860210	9.7354100	-6.3306120
H	2.4354850	9.7926880	-6.0595560
C	8.2340900	7.6765580	-10.3212070
H	8.1622060	8.3757810	-11.1471520
C	9.7022460	12.6528480	-15.2899820
C	7.3040940	6.7414350	-8.3006910
H	6.5203020	6.6979100	-7.5519850
C	4.4668140	10.1452580	-5.4268910
H	4.1856920	10.5237980	-4.4484790

C	5.8121720	10.0708880	-5.7930470
H	6.5842590	10.3936930	-5.1001770
C	10.1269790	12.8040510	-12.9193090
H	10.7263510	13.1654650	-12.0883190
Rh	5.8121710	10.5803690	-11.1387950
H	7.3481300	10.5470730	-10.6964290
C	3.9380980	10.4841070	-11.6821830
C	5.8174290	12.2971320	-10.2284860
O	5.8576510	13.3061210	-9.6679740
O	2.8263700	10.3978500	-11.9789820
H	9.9705670	12.8967250	-16.3142750
C	5.5427640	11.0602530	-14.6932460
C	5.3325870	10.3886730	-15.9071240
C	4.8286100	12.2474120	-14.4559830
C	4.4316930	10.8861070	-16.8531650
C	3.9401820	12.7503500	-15.4045160
C	3.7349100	12.0680700	-16.6062270
H	5.8677710	9.4719270	-16.1298870
H	4.9701240	12.7747220	-13.5167960
H	4.2786110	10.3461770	-17.7835650
H	3.4019540	13.6718570	-15.2014850
H	3.0351050	12.4540220	-17.3418780
C	7.3738010	8.8650470	-14.0559340
H	7.6995490	9.0087390	-15.0927820
H	8.2843530	8.6707170	-13.4782760
C	6.4111800	7.6805330	-13.9302240
H	5.4819500	7.8464860	-14.4834410
H	6.1459220	7.5123410	-12.8832020
H	6.8735040	6.7654030	-14.3153650
C	4.3727600	7.4001520	-10.1539640
H	3.4515430	7.9762830	-10.2948710
H	4.6634430	7.0711840	-11.1572720
C	4.1223920	6.1905190	-9.2487720
H	3.8481150	6.4914070	-8.2335850
H	5.0046580	5.5485530	-9.1848360
H	3.3011810	5.5867840	-9.6509770

m062_LANL2DZ

E(RM062X): Gas phase -2103.83759054, PCM -2103.86409558

P	6.8540500	10.5359290	-13.2793080
P	5.7402300	8.7393390	-9.7525940
C	7.1247740	7.5720960	-9.4186290
C	8.5062070	11.8849180	-15.1396200
H	7.9116860	11.3893390	-15.9037570
C	5.1734160	9.1413130	-8.0497510
C	9.2223820	5.7600280	-9.0087000
H	10.0348180	5.0583150	-8.8484290
C	6.1188120	9.5292300	-7.0921130
H	7.1770010	9.5035050	-7.3410850
C	8.2051530	11.6879970	-13.7863410
C	10.2945380	13.3889100	-14.5433160
H	11.1026470	14.0513040	-14.8374110
C	3.8172560	9.2007240	-7.7166340
H	3.0600720	8.9207150	-8.4438950
C	9.2768110	6.6619910	-10.0663800
H	10.1347520	6.6713560	-10.7311230
C	8.9572600	12.3569390	-12.8197460
H	8.7157640	12.2178570	-11.7703500

C	8.1282390	5.7688690	-8.1454030
H	8.0877030	5.0771140	-7.3099940
C	3.4152710	9.6223630	-6.4505390
H	2.3578480	9.6585910	-6.2079110
C	8.2365090	7.5679740	-10.2647690
H	8.2880500	8.2966140	-11.0693720
C	9.5442930	12.7294360	-15.5159550
C	7.0872400	6.6682910	-8.3481680
H	6.2453140	6.6811680	-7.6617160
C	4.3629440	9.9934260	-5.5029290
H	4.0492860	10.3216130	-4.5173460
C	5.7174050	9.9471850	-5.8287440
H	6.4635690	10.2425880	-5.0977350
C	9.9995260	13.2022870	-13.1970660
H	10.5746420	13.7192520	-12.4353890
Rh	6.1146640	10.7067810	-11.0451930
H	7.6403140	10.4628560	-10.7411190
C	4.1909620	10.9032450	-11.4754100
C	6.4370150	12.3301660	-10.0105940
O	6.7195540	13.2532750	-9.3951260
O	3.0777220	10.9685630	-11.7227430
H	9.7646050	12.8795210	-16.5682490
C	5.5819890	10.9480060	-14.5488490
C	5.2860110	10.1593550	-15.6639550
C	4.8797090	12.1468390	-14.3681550
C	4.3028120	10.5566650	-16.5705090
C	3.9103570	12.5491400	-15.2775660
C	3.6147400	11.7498510	-16.3807940
H	5.8162280	9.2279460	-15.8383020
H	5.1023770	12.7654070	-13.5009640
H	4.0778770	9.9295740	-17.4276560
H	3.3809780	13.4838280	-15.1228170
H	2.8505200	12.0570590	-17.0875470
C	7.5714470	8.9446830	-13.9042070
H	7.7962770	9.0445980	-14.9724950
H	8.5380260	8.8468750	-13.3964750
C	6.6958790	7.7260580	-13.6197230
H	5.6827370	7.8524600	-14.0143210
H	6.6126940	7.5621730	-12.5422680
H	7.1251610	6.8249360	-14.0663030
C	4.3957380	7.6162680	-10.3808740
H	3.5112380	8.2547840	-10.4920620
H	4.6972630	7.3627930	-11.4023690
C	4.0694230	6.3551160	-9.5855500
H	3.8162670	6.5876160	-8.5470300
H	4.9171540	5.6662150	-9.5805650
H	3.2166740	5.8361800	-10.0325820

ea-HRh(CO)₂(PEtPh₂)₂

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2104.62435121, PCM -2104.65207070

P	6.9830120	10.2587000	-13.3249730
P	5.9106220	8.4884700	-9.8940510
C	7.3489940	7.3494630	-9.6584930
C	8.3761460	11.8315090	-15.2692710
H	7.6526830	11.4622420	-15.9896710
C	5.2668350	8.7055600	-8.1752810
C	9.5786990	5.6529900	-9.3936040

H	10.4385330	4.9971310	-9.2908950
C	6.1523980	8.8064410	-7.0902700
H	7.2186800	8.6761380	-7.2454810
C	8.2720660	11.4626600	-13.9183780
C	10.3291810	13.1759690	-14.7848640
H	11.1207210	13.8409160	-15.1189850
C	3.8955190	8.8949410	-7.9401770
H	3.1847730	8.8490020	-8.7591900
C	9.6561330	6.7900870	-10.1971470
H	10.5786140	7.0285130	-10.7188590
C	9.2113020	11.9702600	-13.0097190
H	9.1307560	11.7117560	-11.9594050
C	8.3949990	5.3682030	-8.7079510
H	8.3331450	4.4928720	-8.0675320
C	3.4225010	9.1601390	-6.6542920
H	2.3573740	9.3003450	-6.4936500
C	8.5498830	7.6334900	-10.3249680
H	8.6148300	8.5307730	-10.9325370
C	9.3949260	12.6830700	-15.6980620
C	7.2907180	6.2104420	-8.8347250
H	6.3894520	5.9922180	-8.2722690
C	4.3115600	9.2498000	-5.5825570
H	3.9430520	9.4590340	-4.5825410
C	5.6781430	9.0751660	-5.8060970
H	6.3803070	9.1499530	-4.9805960
C	10.2355410	12.8160620	-13.4400790
H	10.9529370	13.2002030	-12.7202520
Rh	6.2850210	10.6708030	-10.9499180
H	6.4319100	12.1627220	-11.4648710
C	4.4093900	11.0999010	-10.8517290
C	7.7029780	11.1722880	-9.7478700
O	8.5016610	11.5608880	-9.0045820
O	3.3071460	11.4383330	-10.7466300
H	9.4559710	12.9638650	-16.7460090
C	5.6172560	10.5478600	-14.5492400
C	5.3948000	9.7496490	-15.6826590
C	4.7580390	11.6385110	-14.3279280
C	4.3426780	10.0274860	-16.5605100
C	3.7181260	11.9241080	-15.2104510
C	3.5021430	11.1149790	-16.3286670
H	6.0389340	8.9047710	-15.8995250
H	4.9065830	12.2657790	-13.4549120
H	4.1860230	9.3910970	-17.4272310
H	3.0711680	12.7756100	-15.0194220
H	2.6851430	11.3307170	-17.0112480
C	7.8057110	8.6965950	-13.9708330
H	8.0216550	8.8393130	-15.0359830
H	8.7799430	8.6702640	-13.4701400
C	7.0626400	7.3784760	-13.7322740
H	6.0420740	7.4025220	-14.1258140
H	7.0112280	7.1430070	-12.6672240
H	7.5881530	6.5521260	-14.2234750
C	4.5938310	7.4573560	-10.7362170
H	3.7366370	8.1320270	-10.8374880
H	4.9627400	7.3058710	-11.7547710
C	4.1652530	6.1243500	-10.1154790
H	3.8260570	6.2466720	-9.0826980
H	4.9809180	5.3967290	-10.1226070

H	3.3362700	5.6967070	-10.6899640
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m062_LANL2DZ

E(RM062X): Gas phase -2103.83720229, PCM -2103.86490464

P	6.9642140	10.2397800	-13.2428980
P	5.8558120	8.5915690	-9.9012050
C	7.2940420	7.4547010	-9.7812240
C	8.4549860	11.6670190	-15.1991860
H	7.7831440	11.2263360	-15.9312930
C	5.3132380	8.7282120	-8.1514190
C	9.5319630	5.7724300	-9.7060600
H	10.3965520	5.1167930	-9.6808230
C	6.2352070	8.6530570	-7.1030110
H	7.2777420	8.4325530	-7.3132170
C	8.2652330	11.4098610	-13.8369120
C	10.3467530	13.0759620	-14.6922850
H	11.1509560	13.7251910	-15.0239670
C	3.9790280	9.0329140	-7.8574700
H	3.2483920	9.1301340	-8.6562280
C	9.5906760	6.9775120	-10.3983630
H	10.5021960	7.2712130	-10.9093440
C	9.1279780	11.9996010	-12.9101570
H	8.9744290	11.8190650	-11.8502960
C	8.3669160	5.4163170	-9.0277810
H	8.3260090	4.4877690	-8.4673920
C	3.5726280	9.2321160	-6.5420530
H	2.5334900	9.4626800	-6.3300270
C	8.4786410	7.8166530	-10.4283450
H	8.5218580	8.7695810	-10.9506380
C	9.4874480	12.4968910	-15.6238410
C	7.2568270	6.2536310	-9.0589760
H	6.3652780	5.9867240	-8.4995200
C	4.4959420	9.1442710	-5.5030460
H	4.1789250	9.3035910	-4.4774970
C	5.8279550	8.8600690	-5.7877120
H	6.5562280	8.7985510	-4.9852740
C	10.1669460	12.8243590	-13.3357130
H	10.8296800	13.2759460	-12.6042320
Rh	6.1672390	10.7572040	-10.9423360
H	6.2918250	12.2151180	-11.4916210
C	4.2622820	11.1000290	-10.9557730
C	7.5128170	11.3377760	-9.6830900
O	8.2611870	11.7507910	-8.9183670
O	3.1449860	11.3573390	-10.9140290
H	9.6195550	12.6948110	-16.6830180
C	5.6628630	10.4718850	-14.5332030
C	5.5413430	9.6624150	-15.6677270
C	4.7621560	11.5324790	-14.3719160
C	4.5439310	9.9013470	-16.6114610
C	3.7742460	11.7788250	-15.3195380
C	3.6585370	10.9596200	-16.4405670
H	6.2244550	8.8357310	-15.8337660
H	4.8413540	12.1685230	-13.4944490
H	4.4642370	9.2574320	-17.4818240
H	3.0886470	12.6081260	-15.1774530
H	2.8818870	11.1451660	-17.1756290
C	7.7820290	8.6622910	-13.8015720
H	8.0650680	8.7721750	-14.8546130

H	8.7225700	8.6060220	-13.2425390
C	6.9532380	7.4011010	-13.5680700
H	5.9468550	7.4941530	-13.9878860
H	6.8578890	7.1920880	-12.4998100
H	7.4322470	6.5329820	-14.0295790
C	4.4891390	7.6083060	-10.6822370
H	3.6300540	8.2887580	-10.6747500
H	4.7659420	7.5077810	-11.7360480
C	4.1197340	6.2595780	-10.0743740
H	3.9247230	6.3482440	-9.0010120
H	4.9170260	5.5273360	-10.2211620
H	3.2157390	5.8674180	-10.5483770

ee-HRh(CO)₂(pySPAN)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2900.45423780, PCM -2900.49080203

Rh	1.4626280	13.8307680	6.0214800
P	0.3691590	12.8372340	7.9167040
O	0.9706180	14.8568130	10.1284120
C	1.5673390	16.1521330	10.2819070
P	1.8067440	16.1892970	6.0167330
C	0.5781040	17.1664290	10.9019470
H	1.1055840	17.7912550	11.6268950
H	0.2376590	17.8186000	10.0922250
O	1.8366810	16.6211890	8.9529710
C	2.8571840	15.8997630	11.0693760
H	3.1883960	14.8888290	10.8102850
H	2.6198270	15.8963330	12.1376970
C	4.0229520	16.8808430	10.7851190
C	4.2253980	16.9192320	9.2722220
C	5.4579980	17.1488120	8.6532550
H	6.3408190	17.2849410	9.2711890
C	5.5996270	17.2145830	7.2623560
C	4.4641480	17.0065420	6.4724780
H	4.5573120	17.0205180	5.3909240
C	3.2132220	16.7600540	7.0495000
C	3.1040660	16.7424520	8.4513360
C	3.7398670	18.3155720	11.2943550
H	3.4992680	18.3124730	12.3642140
H	2.9164350	18.7913070	10.7557410
C	5.2609290	16.3352500	11.5245270
H	5.5542640	15.3530170	11.1417940
H	5.0428270	16.2327380	12.5930840
H	6.1180670	17.0087720	11.4332430
C	6.9385200	17.5154520	6.6291910
H	7.0264310	17.0512820	5.6425790
H	7.7645170	17.1518010	7.2480610
C	2.6853660	12.6760330	5.0532830
C	-0.8193190	13.8200230	8.9226130
C	-0.3749210	14.7799520	9.8446880
C	-2.1997710	13.7391890	8.6686120
C	-1.2758250	15.5928350	10.5491520
C	-3.1186160	14.5593980	9.3251790
C	-2.6363480	15.4734230	10.2721460
H	-2.5632830	13.0161170	7.9465900
H	-3.3465900	16.1017940	10.8012180
C	-0.6674640	16.5397710	11.5764990
C	-0.2874920	15.7452710	12.8506140

H	0.3740750	14.9050430	12.6259420
H	-1.1873300	15.3440790	13.3277780
H	0.2143740	16.3971440	13.5754820
H	7.0832460	18.5948170	6.4938600
C	-1.6190090	17.6821600	11.9697430
H	-1.9589960	18.2419500	11.0927190
H	-2.4994240	17.3075700	12.5012740
H	-1.1082680	18.3807420	12.6410840
C	-4.5957230	14.4734480	9.0175930
H	-4.8457680	13.5324440	8.5200290
H	-5.1990310	14.5443190	9.9286940
H	-4.9125690	15.2891890	8.3560760
H	4.6259490	18.9422000	11.1513660
C	-0.0520580	13.8461640	4.7521510
O	-0.9186840	13.8889310	3.9975940
O	3.4576100	11.9972170	4.5306200
H	2.6812170	13.9060250	7.0324280
C	-1.9030680	9.6111270	7.6663130
C	-1.4096290	10.6824590	8.3636750
N	-0.6304700	11.4566800	7.5024080
C	-0.6288040	10.8278010	6.2570490
C	-1.4081930	9.7035930	6.3289420
H	-2.5482170	8.8419640	8.0689180
H	-1.5437350	10.9659540	9.3946320
H	-0.0504450	11.2347540	5.4446840
H	-1.6010600	9.0185210	5.5150630
C	3.1806830	11.1207350	10.0462300
C	2.7099720	11.7225800	8.9075110
N	1.4067290	12.1540830	9.1393980
C	1.0649400	11.8012610	10.4419750
C	2.1365060	11.1719140	11.0206460
H	4.1655280	10.6917670	10.1698900
H	3.1748830	11.8856850	7.9492480
H	0.1005820	12.0609330	10.8483120
H	2.1744900	10.7976730	12.0347250
C	3.1608930	16.8473440	2.3788280
C	2.7922250	16.0227040	3.4110800
N	2.2553620	16.8026150	4.4338760
C	2.3014070	18.1344540	4.0247590
C	2.8456440	18.1853790	2.7668120
H	3.5950620	16.5264450	1.4419330
H	2.8571850	14.9533110	3.5248620
H	1.9107840	18.9182220	4.6532120
H	2.9851120	19.0824860	2.1787580
C	-0.5451920	19.1834520	7.0618270
C	0.7009920	18.6290370	6.9088240
N	0.5513700	17.3309200	6.4288820
C	-0.8090230	17.0799810	6.2870320
C	-1.5034630	18.2004200	6.6648800
H	-0.7500080	20.1829030	7.4212800
H	1.6821380	19.0257640	7.1180650
H	-1.1587770	16.1225740	5.9348930
H	-2.5795510	18.3049470	6.6636820

m062_LANL2DZ

E(RM062X): Gas phase -2899.42509444, PCM -2899.45947733

Rh	2.0083470	13.7114070	6.4338600
P	0.4664380	12.8225580	7.9203090

O	1.1035930	14.8395710	10.1179320
C	1.6970470	16.1330840	10.2078960
P	1.8831650	16.0463490	6.0505330
C	0.7413080	17.1622660	10.8480790
H	1.2844090	17.7575430	11.5862090
H	0.4065980	17.8305170	10.0465030
O	1.9037660	16.5398360	8.8633830
C	3.0190830	15.9290160	10.9366500
H	3.4104020	14.9605970	10.6033210
H	2.8146710	15.8522920	12.0102700
C	4.0946560	17.0051480	10.6708040
C	4.2346150	17.1495170	9.1646760
C	5.3988390	17.5737170	8.5207120
H	6.2743840	17.8140340	9.1188650
C	5.4853170	17.7013810	7.1337740
C	4.3779270	17.3377280	6.3621810
H	4.4386790	17.3737360	5.2757750
C	3.2042480	16.9020850	6.9708780
C	3.1295990	16.8602010	8.3680520
C	3.7484740	18.3810200	11.2671150
H	3.5141450	18.3007850	12.3351220
H	2.9056770	18.8503630	10.7541590
C	5.3936510	16.5053180	11.3155560
H	5.7301840	15.5732820	10.8529200
H	5.2315390	16.3229090	12.3828050
H	6.1949260	17.2437290	11.2277600
C	6.7433700	18.2140410	6.4806330
H	6.8733350	17.7834060	5.4849930
H	7.6263830	17.9681080	7.0755910
C	3.8141460	12.9833660	6.3652400
C	-0.6974220	13.8519970	8.8920420
C	-0.2367090	14.7948830	9.8108480
C	-2.0769790	13.7617750	8.6632590
C	-1.1220590	15.6232170	10.5067250
C	-2.9769010	14.6028890	9.3104920
C	-2.4802810	15.5287810	10.2325530
H	-2.4605170	13.0234520	7.9644770
H	-3.1791500	16.1788920	10.7526220
C	-0.4966220	16.5519800	11.5255710
C	-0.1014800	15.7461120	12.7764740
H	0.5504870	14.9054000	12.5240460
H	-0.9965740	15.3474380	13.2631570
H	0.4188270	16.3907490	13.4943100
H	6.7129130	19.3027780	6.3669460
C	-1.4306650	17.6919160	11.9308270
H	-1.7764650	18.2464750	11.0525400
H	-2.3038930	17.3183480	12.4739320
H	-0.9040670	18.3872250	12.5921760
C	-4.4543230	14.5249260	9.0220740
H	-4.7027560	13.6056670	8.4876310
H	-5.0401600	14.5531460	9.9449240
H	-4.7777440	15.3685860	8.4030750
H	4.6079060	19.0494980	11.1570950
C	1.3598400	13.0390310	4.6527930
O	1.0328630	12.6676870	3.6276930
O	4.8746300	12.5625580	6.4352200
H	2.5048260	14.2044150	7.8293680
C	-2.2473310	10.0980660	7.1551790

C	-1.2316350	10.5947190	7.9288830
N	-0.6546250	11.6588530	7.2601020
C	-1.3316250	11.8423460	6.0671980
C	-2.3167920	10.8948300	5.9754860
H	-2.8589040	9.2408940	7.3965360
H	-0.8430390	10.2724930	8.8838170
H	-1.0701990	12.6524260	5.4034730
H	-3.0011190	10.7757200	5.1483320
C	2.4485810	10.3256730	10.1515750
C	2.2582290	11.0506480	9.0086330
N	1.1567030	11.8709540	9.1857730
C	0.6510870	11.6509930	10.4587740
C	1.4289120	10.7092100	11.0736150
H	3.2364720	9.6056450	10.3164810
H	2.7995780	11.0661070	8.0751960
H	-0.2140920	12.1945350	10.8064840
H	1.2931110	10.3419790	12.0804980
C	3.2484720	16.7094720	2.4659800
C	2.9732580	15.8983530	3.5336040
N	2.1946620	16.6066490	4.4347730
C	1.9950330	17.8793520	3.9298400
C	2.6219280	17.9661020	2.7160320
H	3.8218130	16.4307320	1.5940940
H	3.2714740	14.8841490	3.7544670
H	1.3929730	18.5943490	4.4692800
H	2.6159290	18.8288680	2.0658650
C	-0.8082740	18.5653170	7.3658450
C	0.4557840	18.2940370	6.9168230
N	0.4887700	16.9848890	6.4658470
C	-0.7634010	16.4281620	6.6600280
C	-1.5842860	17.3769970	7.2024250
H	-1.1452610	19.5112650	7.7656650
H	1.3514570	18.8980910	6.9020760
H	-0.9450670	15.3960470	6.3975970
H	-2.6242370	17.2363170	7.4582350

ea-HRh(CO)₂(pySPAN)

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -2900.45163344, PCM -2900.48812486

Rh	2.3072920	13.5949870	6.6242270
P	0.4873270	12.8231370	8.0402020
O	1.1733720	14.8886640	10.2161410
C	1.7375010	16.2126380	10.3108100
P	1.9029630	15.9980960	6.1058080
C	0.7500330	17.2036040	10.9721390
H	1.2953080	17.8533130	11.6596520
H	0.3419640	17.8325240	10.1754800
O	1.9117070	16.6358550	8.9541670
C	3.0788830	16.0479280	11.0266570
H	3.4814640	15.0776800	10.7234060
H	2.8958860	15.9997790	12.1042380
C	4.1501400	17.1315310	10.7183100
C	4.2474940	17.2726110	9.2000300
C	5.4010040	17.6995580	8.5313890
H	6.2792420	17.9634680	9.1136790
C	5.4732640	17.7892350	7.1372050
C	4.3616720	17.3816280	6.3894080
H	4.4189450	17.3799050	5.3055120

C	3.1874450	16.9495740	7.0143550
C	3.1316510	16.9510490	8.4211370
C	3.8277930	18.5113480	11.3415810
H	3.6530220	18.4272480	12.4209650
H	2.9543500	18.9817310	10.8836200
C	5.4738910	16.6193290	11.3255640
H	5.7898910	15.6850050	10.8527090
H	5.3476030	16.4354460	12.3982080
H	6.2801590	17.3501810	11.2158040
C	6.7198350	18.3013940	6.4535630
H	6.8475430	17.8486360	5.4658800
H	7.6164780	18.0847870	7.0422930
C	3.6073770	13.6071500	8.0523810
C	-0.6579590	13.8607920	9.0440930
C	-0.1825780	14.7979980	9.9730910
C	-2.0483000	13.7458440	8.8658230
C	-1.0667330	15.5840080	10.7301050
C	-2.9487220	14.5298850	9.5867120
C	-2.4359940	15.4412310	10.5191780
H	-2.4366640	13.0300720	8.1509940
H	-3.1296950	16.0493620	11.0920640
C	-0.4326190	16.5466740	11.7244980
C	0.0434440	15.7711710	12.9773400
H	0.7160970	14.9504450	12.7184080
H	-0.8155720	15.3466230	13.5067460
H	0.5654200	16.4423710	13.6696000
H	6.6793030	19.3885870	6.3094830
C	-1.3923050	17.6629880	12.1699210
H	-1.8001730	18.2103320	11.3141740
H	-2.2282820	17.2651790	12.7538970
H	-0.8629170	18.3782430	12.8083590
C	-4.4381640	14.4120480	9.3618560
H	-4.6838740	13.5180560	8.7828160
H	-4.9835700	14.3611110	10.3104260
H	-4.8262620	15.2785710	8.8127120
H	4.6735090	19.1901740	11.1920750
C	2.0149930	12.3051850	5.2092380
O	2.0006050	11.5245610	4.3595930
O	4.4621630	13.5713970	8.8275240
H	3.5936950	13.9034290	5.7571740
C	-2.2912770	10.3839710	6.6679990
C	-1.3668540	10.7361850	7.6202170
N	-0.6481350	11.8317030	7.1485230
C	-1.1486090	12.1699740	5.8931900
C	-2.1574210	11.2948230	5.5763800
H	-2.9742470	9.5481110	6.7350000
H	-1.1372680	10.3002660	8.5799950
H	-0.7208080	12.9885880	5.3357550
H	-2.7217450	11.2923570	4.6540980
C	2.1144160	9.9182250	10.0951480
C	2.0582530	10.7680660	9.0221540
N	1.0253920	11.6813280	9.2346260
C	0.4286000	11.3792920	10.4605540
C	1.0848310	10.3073400	11.0073460
H	2.8219160	9.1103870	10.2209300
H	2.6487560	10.8177860	8.1206930
H	-0.3958550	11.9669060	10.8302050
H	0.8615120	9.8564790	11.9647340

C	2.8324560	16.3044690	2.2911960
C	2.6528500	15.5872540	3.4456430
N	2.2258710	16.4571600	4.4475200
C	2.1361930	17.7345990	3.8955750
C	2.5021640	17.6654170	2.5758900
H	3.1550410	15.8983020	1.3425000
H	2.7878370	14.5394050	3.6559970
H	1.7913180	18.5674490	4.4873730
H	2.5195430	18.4966430	1.8839850
C	-0.9953510	18.5862720	6.8224770
C	0.3379610	18.2645870	6.7599540
N	0.4512990	16.9240990	6.4071740
C	-0.8300210	16.4101990	6.2487700
C	-1.7368110	17.4098210	6.4950850
H	-1.3977730	19.5571780	7.0783860
H	1.2193470	18.8550540	6.9567200
H	-0.9771200	15.3755210	5.9796810
H	-2.8125690	17.3101170	6.4536830

m062_LANL2DZ

E(RM062X): Gas phase -2899.42724580, PCM -2899.46166603

Rh	2.3018360	13.5592870	6.5846100
P	0.5344100	12.7928150	8.0398040
O	1.1172930	14.7644620	10.2749570
C	1.7502480	16.0417100	10.2657140
P	1.8371960	15.9575510	6.1051570
C	0.8318650	17.1463610	10.8347610
H	1.3800330	17.7320000	11.5770490
H	0.5631120	17.8079080	10.0035270
O	1.9512390	16.2903600	8.8840360
C	3.0733190	15.8679050	10.9957280
H	3.4579720	14.8842380	10.7108410
H	2.8740040	15.8467470	12.0729260
C	4.1558780	16.9258010	10.6787440
C	4.2125900	17.1316000	9.1724480
C	5.3249620	17.6614320	8.5099990
H	6.1931180	17.9546610	9.0954840
C	5.3750170	17.8141700	7.1256920
C	4.2792900	17.3851910	6.3674530
H	4.3154670	17.4407580	5.2810600
C	3.1489430	16.8699950	6.9906380
C	3.1170990	16.7818130	8.3903880
C	3.9039680	18.2837490	11.3584580
H	3.7304620	18.1584850	12.4335650
H	3.0535000	18.8117440	10.9215170
C	5.4814370	16.3537800	11.2043650
H	5.7433400	15.4342680	10.6737660
H	5.3901230	16.1269790	12.2717940
H	6.3008490	17.0680210	11.0891640
C	6.5797760	18.4183300	6.4506460
H	6.8205810	17.8870370	5.5263520
H	7.4569450	18.3842840	7.1008910
C	3.6026660	13.6688600	8.0182010
C	-0.6526840	13.8319370	8.9607090
C	-0.2055220	14.7651930	9.8929490
C	-2.0228980	13.7779910	8.6685350
C	-1.0855520	15.6590200	10.5088440
C	-2.9218730	14.6528070	9.2693780

C	-2.4329710	15.5955120	10.1798910
H	-2.3950480	13.0500250	7.9525740
H	-3.1304810	16.2913270	10.6394680
C	-0.4631880	16.6288730	11.4908850
C	-0.1508730	15.8980040	12.8093230
H	0.4956280	15.0320650	12.6443950
H	-1.0771400	15.5474810	13.2741680
H	0.3465150	16.5786120	13.5096600
H	6.3994550	19.4660880	6.1887920
C	-1.3671040	17.8282930	11.7744970
H	-1.6665530	18.3201870	10.8433600
H	-2.2683350	17.5284390	12.3177340
H	-0.8355770	18.5567050	12.3950190
C	-4.3897680	14.6090130	8.9301290
H	-4.6323610	13.7193570	8.3455120
H	-5.0048410	14.6017410	9.8343530
H	-4.6830220	15.4857190	8.3428700
H	4.7822130	18.9237420	11.2286090
C	2.0026010	12.2471370	5.1753340
O	1.9579740	11.4566720	4.3507430
O	4.4374940	13.7037910	8.7999370
H	3.5586780	13.8847390	5.7202670
C	-2.2693050	10.3219830	6.9037550
C	-1.2985790	10.6988450	7.7933730
N	-0.5623030	11.7223730	7.2235010
C	-1.0945120	12.0045090	5.9753030
C	-2.1449790	11.1548280	5.7524740
H	-2.9787050	9.5203880	7.0490270
H	-1.0426690	10.3234090	8.7737580
H	-0.6670880	12.7852000	5.3621850
H	-2.7439990	11.1171290	4.8545300
C	2.2624350	10.0935440	10.2341560
C	2.1610960	10.8678420	9.1132060
N	1.1120480	11.7586210	9.2898910
C	0.5487300	11.5278450	10.5372140
C	1.2412830	10.5146370	11.1387190
H	2.9940900	9.3160180	10.3968810
H	2.7297050	10.8762940	8.1948230
H	-0.2869220	12.1193300	10.8787770
H	1.0494510	10.1231780	12.1271890
C	2.8016120	16.5373860	2.3716080
C	2.5946690	15.7401290	3.4634090
N	2.0805940	16.5220980	4.4853080
C	1.9691960	17.8235420	4.0253760
C	2.4009320	17.8604470	2.7278910
H	3.1839210	16.2090920	1.4163950
H	2.7627010	14.6855680	3.6212080
H	1.5679730	18.5960870	4.6638630
H	2.4138810	18.7352670	2.0940560
C	-0.9189680	18.4108040	7.4472150
C	0.3712970	18.1542790	7.0651230
N	0.4313820	16.8653770	6.5671660
C	-0.8293340	16.3063640	6.6554390
C	-1.6838620	17.2348910	7.1836990
H	-1.2798520	19.3414450	7.8620930
H	1.2647500	18.7592560	7.1219930
H	-1.0003240	15.2909870	6.3261140
H	-2.7386070	17.0889220	7.3651960

HRh(CO)₂ fragment

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -336.79519502, PCM(n-hexane) -336.79583322,
PCM(toluene) , PCM(THF)

Rh	-0.5425400	1.0800940	-2.3384450
C	0.0708060	2.3559470	-1.0259670
C	-0.4543120	-0.1861180	-3.7929760
O	-0.2623550	-0.9320150	-4.6441100
O	0.5641280	3.0780970	-0.2826220
H	0.4669830	0.1496230	-1.6761160

m062_LANL2DZ

E(RM062X): Gas phase -336.56465748, PCM(n-hexane) -336.56452430,
PCM(toluene) -336.56559278, PCM(THF) -336.57148120

Rh	-0.3608800	1.2119130	-2.4986610
C	0.0598510	2.3840530	-0.9908050
C	-0.4633790	-0.2359300	-3.8071110
O	-0.4480300	-1.1319740	-4.5065170
O	0.3710410	2.9924260	-0.0824400
H	0.6841080	0.3251400	-1.8747030

L7

b3lyp_LANL2DZ

E(RB3LYP): Gas phase -5225.73536263, PCM(n-hexane) -5225.76377085,
PCM(toluene) -5225.76711226, PCM(THF) -5225.77719805

P	-1.8075470	-0.6695430	0.0407890
P	1.7565480	0.5578200	0.1704870
C	1.0435800	-2.9614800	3.1256650
H	0.8996090	-3.7947900	3.8009180
C	2.3571650	-1.9726290	1.3411070
H	3.1886170	-2.0137230	0.6508770
C	1.4991100	-0.8579510	1.3392730
C	0.4035560	-0.7823280	2.2145710
C	-3.0593520	-1.8425000	0.7484470
C	-3.7393400	-1.6203150	1.9520140
H	-3.5701420	-0.7057270	2.5080350
C	-4.6411490	-2.5715740	2.4388560
C	-4.8789140	-3.7578300	1.7446880
H	-5.5857400	-4.4874800	2.1219900
C	-4.1957750	-3.9831250	0.5478800
C	-3.2852140	-3.0438060	0.0589680
H	-2.7516890	-3.2492810	-0.8642540
C	2.7348170	-0.2530930	-1.1847470
C	2.0011190	-1.0137670	-2.1100780
C	2.6349900	-1.6221850	-3.1931940
C	4.0105450	-1.4782830	-3.3914560
H	4.4983110	-1.9398840	-4.2412160
C	4.7375640	-0.7129860	-2.4816950
C	4.1121560	-0.1089940	-1.3843200
H	4.7081970	0.4760420	-0.6927400
C	3.0500990	1.5683080	1.0365720
C	3.3480070	2.8319420	0.5033820
C	3.6832580	1.1733440	2.2219330
C	4.2792100	3.6656380	1.1267860
C	4.6092870	2.0180290	2.8416550
C	4.9193380	3.2661370	2.3013520
H	2.8444710	3.1745040	-0.3958710

H	3.4558590	0.2099390	2.6633860
H	5.6377190	3.9159940	2.7865480
C	-1.5954900	0.5769130	1.3977000
C	-0.5158310	0.3971320	2.2776310
C	-2.4603970	1.6792350	1.5228860
C	-1.1794800	2.4484960	3.4347280
H	-3.2812800	1.8034390	0.8304440
H	-1.0488310	3.1947000	4.2073070
C	-2.8190440	0.2881390	-1.1880350
C	-4.1725430	0.0654670	-1.4619870
C	-2.1333410	1.2554830	-1.9423060
C	-4.8226920	0.7921530	-2.4666750
C	-2.7930590	1.9850190	-2.9303410
C	-4.1452150	1.7603950	-3.2045570
H	-4.7310030	-0.6754750	-0.9016670
H	-4.6517120	2.3178520	-3.9834640
H	0.9282550	-1.1295130	-1.9838790
H	-1.0792080	1.4385220	-1.7557530
O	0.7342770	1.1341820	4.1283590
O	-0.8739910	-1.7291310	3.9475380
C	0.9408930	2.0173720	5.2264260
H	1.1396600	3.0410390	4.8867210
H	0.0769380	2.0209010	5.9016310
H	1.8170010	1.6391310	5.7525540
C	-1.0878700	-2.7272260	4.9408360
H	-1.2894650	-3.7064840	4.4902590
H	-0.2260950	-2.8079900	5.6138980
H	-1.9644760	-2.4060050	5.5028080
O	-3.0192920	3.7081130	2.7580870
O	2.8871070	-4.1413270	2.3264680
C	-4.1209890	3.9480420	1.8902920
H	-4.5839400	4.8697530	2.2439960
H	-3.7929690	4.0830880	0.8523580
H	-4.8546800	3.1338930	1.9372220
C	3.9992380	-4.2817030	1.4503980
H	4.7370690	-3.4849530	1.6056910
H	4.4519880	-5.2430570	1.6949330
H	3.6847160	-4.2867600	0.3996460
C	6.2295670	-0.5714080	-2.6353950
C	1.8229910	-2.4768480	-4.1312910
C	-2.0538100	3.0659710	-3.6751570
C	-6.2936270	0.5647230	-2.6996690
C	5.2395820	1.5886500	4.1401050
C	4.6214730	4.9941730	0.5029380
F	-6.6457380	-0.7367680	-2.5290420
F	-6.6852200	0.9287900	-3.9462080
F	-7.0575910	1.2860430	-1.8251450
F	5.4622450	0.2489500	4.1862730
F	6.4276130	2.2021510	4.3699430
F	4.4403970	1.8800430	5.2125690
F	6.9033200	-1.4117230	-1.7932790
F	6.6543470	-0.8579740	-3.8907610
F	6.6570150	0.6846410	-2.3404720
F	2.4232910	-2.6412690	-5.3364320
F	0.5892220	-1.9539470	-4.3630910
F	1.6184130	-3.7279340	-3.6226890
F	5.0828950	5.8877300	1.4160710
F	3.5497530	5.5626620	-0.1095740

F	5.5909540	4.8734470	-0.4480960
F	-2.5412180	3.2579130	-4.9270760
F	-2.1467930	4.2693570	-3.0346980
F	-0.7274770	2.7970160	-3.7950960
C	-4.3919780	-5.2849180	-0.1854560
C	-5.3289320	-2.3254560	3.7557660
F	-5.6352750	-5.7983850	0.0008310
F	-4.2053150	-5.1547820	-1.5238290
F	-3.5116250	-6.2387950	0.2377510
F	-5.5999800	-1.0093430	3.9573010
F	-6.5014620	-2.9993380	3.8643430
F	-4.5558730	-2.7225880	4.8130100
C	-0.3267640	1.3564720	3.3059870
C	0.1963070	-1.8578130	3.1173020
C	2.1253810	-3.0203980	2.2350710
C	-2.2487310	2.6103740	2.5422360

m062_LANL2DZ

E(RM062X): Gas phase -5224.07303602, PCM(n-hexane) -5224.09865276,
PCM(toluene) -5224.10201618, PCM(THF) -5224.11260342

P	-1.6560780	0.0780790	-0.4518760
P	1.7355770	0.7916180	0.0960860
C	0.3485900	-2.5993610	2.9454090
H	0.0789490	-3.3934820	3.6304450
C	1.7506840	-1.8802410	1.1023910
H	2.5404060	-2.0830610	0.3930800
C	1.1363260	-0.6197760	1.1390220
C	0.0976100	-0.3517940	2.0320720
C	-2.1457170	-1.4984960	0.3666120
C	-3.0768250	-1.5587090	1.4056070
H	-3.5698210	-0.6538410	1.7538560
C	-3.3463610	-2.7752820	2.0259960
C	-2.6788080	-3.9374510	1.6509820
H	-2.8703840	-4.8765160	2.1606790
C	-1.7390170	-3.8645110	0.6278350
C	-1.4793290	-2.6624270	-0.0230080
H	-0.7258890	-2.6204120	-0.8050160
C	2.6295850	-0.1477860	-1.2216760
C	1.9079300	-0.4173550	-2.3877120
C	2.4670700	-1.1916690	-3.4012170
C	3.7533310	-1.7071240	-3.2888040
H	4.1833760	-2.3118260	-4.0793020
C	4.4722400	-1.4254870	-2.1323960
C	3.9270740	-0.6536890	-1.1091280
H	4.5150790	-0.4648090	-0.2139560
C	3.1467760	1.3590730	1.1470180
C	4.1484880	2.1461380	0.5753240
C	3.1760560	1.1334430	2.5280580
C	5.1757980	2.6647130	1.3619260
C	4.1986340	1.6747730	3.2978280
C	5.2156040	2.4392300	2.7308730
H	4.1424490	2.3555290	-0.4927630
H	2.3983600	0.5496430	3.0103920
H	6.0163640	2.8453020	3.3400690
C	-1.5937830	1.2201200	1.0097410
C	-0.6763200	0.9214360	2.0237110
C	-2.3519470	2.3957070	1.0529990
C	-1.2789150	2.9973640	3.1453210

H	-3.0740100	2.6134240	0.2793510
H	-1.1854410	3.7155010	3.9491240
C	-3.2243450	0.5934620	-1.2790410
C	-4.4150490	-0.1353210	-1.2557930
C	-3.1828760	1.7719040	-2.0336340
C	-5.5356730	0.3245390	-1.9442240
C	-4.3189550	2.2317750	-2.6918450
C	-5.5104290	1.5150110	-2.6597390
H	-4.4854580	-1.0660160	-0.7018780
H	-6.3914990	1.8734720	-3.1801090
H	0.8979190	-0.0284350	-2.4992570
H	-2.2608170	2.3469350	-2.0977130
O	0.3612080	1.4678050	4.0467260
O	-1.2631920	-1.0325800	3.8159280
C	0.4909490	2.3038230	5.1821500
H	0.8676440	3.2945510	4.9031180
H	-0.4683930	2.4093930	5.7005610
H	1.2110940	1.8145640	5.8357660
C	-1.5161090	-1.9208410	4.8883830
H	-1.8861620	-2.8888520	4.5286600
H	-0.6084230	-2.0819440	5.4807490
H	-2.2835370	-1.4482260	5.4990720
O	-2.8683610	4.4375360	2.2530710
O	1.8436270	-4.1207040	2.0233720
C	-3.7788550	4.7909440	1.2300070
H	-4.2016960	5.7512280	1.5217310
H	-3.2722750	4.8933150	0.2635230
H	-4.5838760	4.0520110	1.1405760
C	2.8909550	-4.4360310	1.1226210
H	3.7718530	-3.8115050	1.3114850
H	3.1370260	-5.4806160	1.3057800
H	2.5683010	-4.3155860	0.0831000
C	5.8532860	-1.9836240	-1.9327330
C	1.6395570	-1.4573630	-4.6272990
C	-4.2399490	3.5498320	-3.4083540
C	-6.7830290	-0.5151820	-1.9242480
C	4.2032720	1.4725170	4.7856470
C	6.2392560	3.4832960	0.6858530
F	-6.6923750	-1.5613450	-2.7700770
F	-7.8728560	0.1867300	-2.2824180
F	-7.0173960	-1.0289660	-0.7016720
F	3.3490130	0.5098460	5.1785630
F	5.4237830	1.1393710	5.2467710
F	3.8441640	2.5995780	5.4430290
F	5.8979390	-2.7969830	-0.8526750
F	6.2752910	-2.7020820	-2.9856370
F	6.7607460	-1.0139610	-1.7148330
F	2.2664300	-2.2569830	-5.5055470
F	1.3287880	-0.3169300	-5.2751620
F	0.4671880	-2.0478810	-4.3137760
F	7.1767420	3.9176430	1.5447070
F	5.7185020	4.5704660	0.0804140
F	6.8716850	2.7793580	-0.2747850
F	-5.3390240	3.8063870	-4.1352660
F	-4.0976000	4.5719170	-2.5321950
F	-3.1808800	3.6119370	-4.2360860
C	-0.9967080	-5.1080010	0.2279680
C	-4.3976580	-2.8275820	3.0979640

F	-0.7389670	-5.9001480	1.2834460
F	-1.6981340	-5.8523830	-0.6523130
F	0.1812800	-4.8228420	-0.3618780
F	-4.4221620	-1.6984120	3.8326840
F	-5.6334650	-2.9799640	2.5830610
F	-4.2026560	-3.8536710	3.9511310
C	-0.5389710	1.8247120	3.0987910
C	-0.2678250	-1.3582940	2.9608480
C	1.3408300	-2.8678780	1.9927340
C	-2.1865290	3.2779660	2.1190410