Supporting Information for

Experimental and Theoretical Study of Si−Cl and Ge−Cl σ-Bond Activation Reactions by Iridium-Hydride

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This PDF file includes:

X-ray Crystal Structure Details for 5.

1) Labeling Scheme

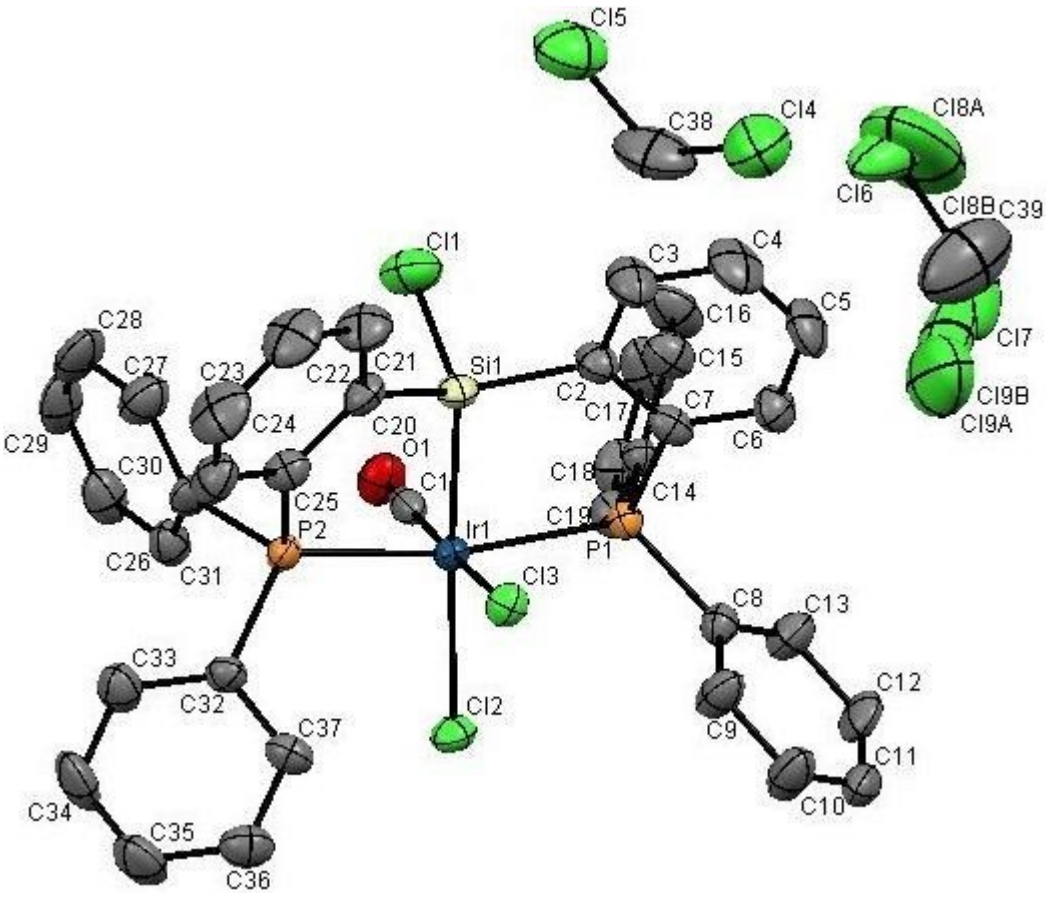


Fig S1 Molecular structure of **5** (Hydrogen atoms are omitted for clarity).

Table S1. Crystal data and structure refinement for 5.

Identification code	crystalclear	
Empirical formula	$C_{37}H_{28}Cl_3IrOP_2Si$, $2(CH_2Cl_2)$	
Formula weight	1047.03	
Temperature	200(2) K	
Wavelength	0.71070 Å	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.2652(2) Å	α= 90°.
	b = 15.8355(3) Å	β= 90°.
	c = 25.8307(7) Å	γ = 90°.
Volume	4198.90(16) $Å^3$	
Z	4	
Density (calculated)	1.656 Mg/m^3	
Absorption coefficient	3.761 mm^{-1}	
F(000)	2056	
Crystal size	0.20 x 0.19 x 0.08 mm^3	
Theta range for data collection	2.13 to 27.49°.	
Index ranges	-13<=h<=13, -18<=k<=20, -20<=l<=33	
Reflections collected	31365	
Independent reflections	8965 [R(int) = 0.0352]	
Completeness to theta = 27.48°	97 %	
Max. and min. transmission	0.5201 and 0.7529	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9362/ 0 / 487	
Goodness-of-fit on F^2	1.094	
Final R indices [I>2sigma(I)]	R1 = 0.0307, wR2 = 0.0642	
R indices (all data)	R1 = 0.0329, wR2 = 0.0661	
Largest diff. peak and hole	1.617 and -0.886 $e.Å^{-3}$	

X-ray Crystal Structure Details for 7.

1) Labeling Scheme

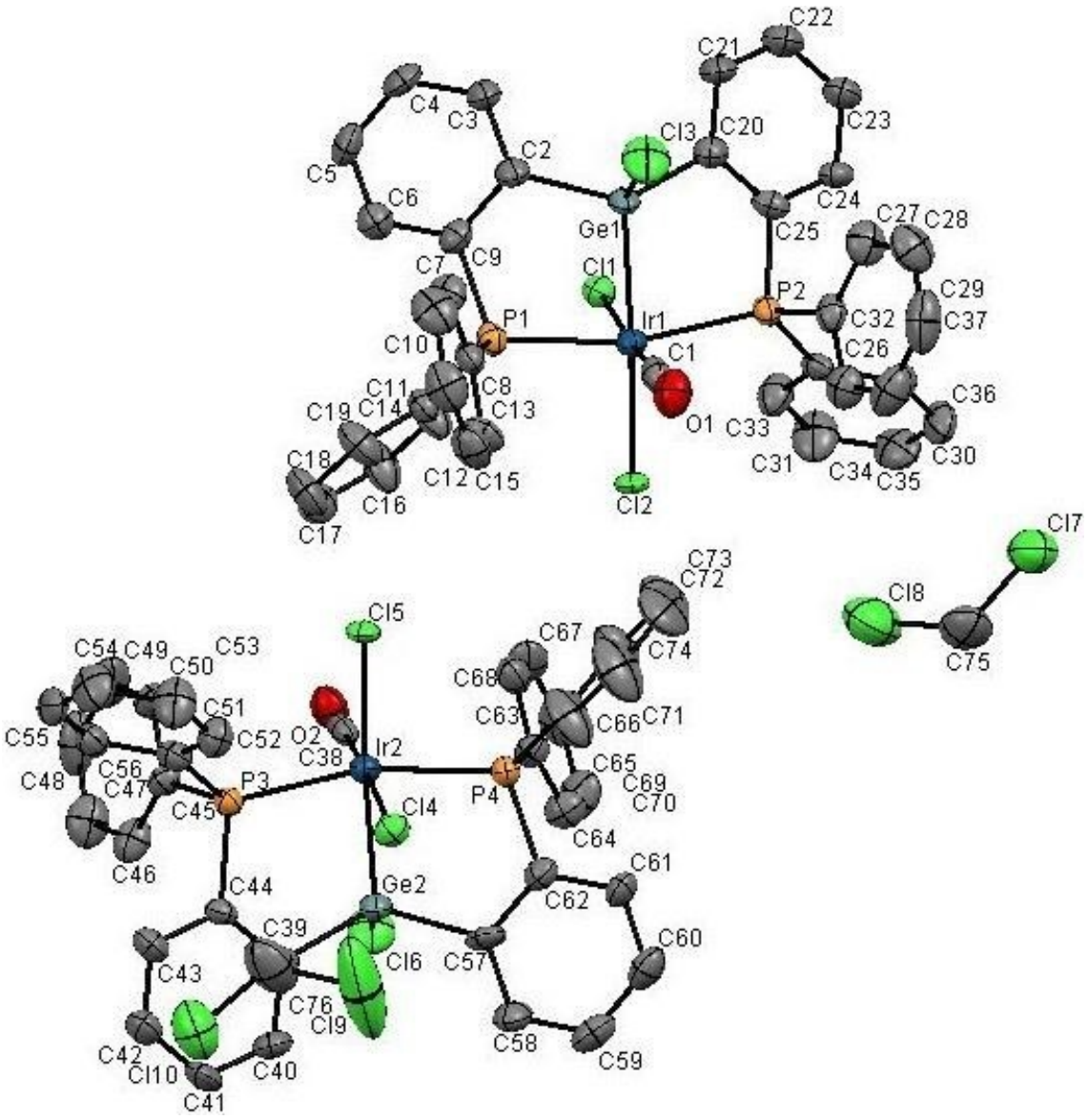


Fig S2 Molecular structure of **7** (Hydrogen atoms are omitted for clarity).

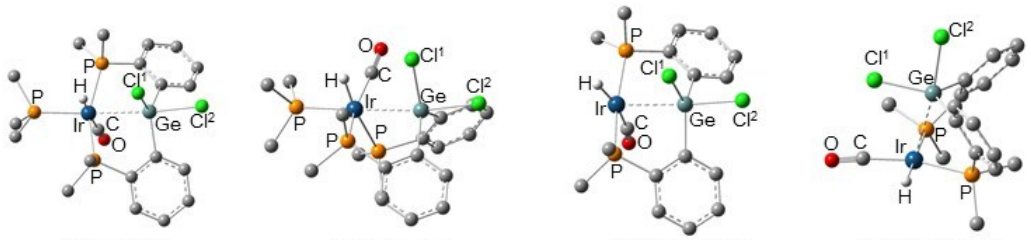
Table S2. Crystal data and structure refinement for 7.

Identification code	crystalclear	
Empirical formula	$C_{37}H_{28}Cl_3GeIrOP_2$, CH_2Cl_2	
Formula weight	1006.60	
Temperature	200(2) K	
Wavelength	0.71070 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 18.3353(9) Å	α= 90°.
	b = 22.6480(9) Å	β= 100.286(2))°.
	c = 18.5245(9) Å	γ = 90°.
Volume	7568.8(6) $Å^3$	
Z	8	
Density (calculated)	1.767 Mg/m^3	
Absorption coefficient	4.775 mm^{-1}	
F(000)	3920	
Crystal size	0.39 x 0.20 x 0.04 mm^3	
Theta range for data collection	2.26 to 26.00°.	
Index ranges	-22<=h<=22, -27<=k<=27, -15<=l<=22	
Reflections collected	52411	
Independent reflections	9688 [R(int) = 0.0446]	
Completeness to theta = 27.48°	99.1 %	
Max. and min. transmission	0.2575 and 0.8320	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14733 / 0 / 865	
Goodness-of-fit on F^2	1.249	
Final R indices [I>2sigma(I)]	R1 = 0.0614, wR2 = 0.0969	
R indices (all data)	R1 = 0.0771, wR2 = 0.1052	
Largest diff. peak and hole	1.933 and -2.169 0 e.$Å^{-3}$	

DFT calculation for activation of Ge−Cl σ-bond in {(*o*-$Me_2P)C_6H_4\}_2Ge(Cl)_2$ by the iridium hydride

Ge−Cl activation in {*o*-$(Me_2P)C_6H_4\}_2Ge(Cl)_2$ were investigated in the same way to Si−Cl activation in {*o*-$(Me_2P)C_6H_4\}_2Si(Cl)_2$. The effective core potentials (ECPs) of the Stuttgart-Dresden-Bonn group were employed for the core electrons of platinum and the corresponding basis set was used for the valence electrons. Usual 6-311G(d,p) basis sets were used for all other atoms. Geometry optimizations were performed by the density functional theory (DFT) with the B3PW91 functional in gas phase. The vibrational frequencies were calculated to identify the structure in the equilibrium state, i.e., the structure that was true minima or transition states. Also, the translational entropy was re-evaluated by the method of Whiteside et al. The polarizable continuum model (PCM) was used to calculate solvation free energies (solvent: toluene), where the gas-phase optimized geometries were employed.

Fig S3 displays optimized structures of {*o*-$Me_2PC_6H_4)_2(Cl)_2Ge\}Ir(H)(CO)(PMe_3)$ (**E1**),. {*o*-$Me_2PC_6H_4)_2(Cl)_2Ge\}Ir(H)(CO)(PMe_3)$ (**F1**), {*o*-$Me_2PC_6H_4)_2(Cl)_2Ge\}$-Ir(H)(CO) (**G1**), and {*o*-$Me_2PC_6H_4)_2(Cl)_2Ge\}Ir(H)(CO)$ (**H1**) with selected distances and Gibbs energy difference ΔG^0 (kcal/mol) relative to that of **E1**. Figs S4 and S5 show S_N2 type oxidative addition (starting from **E1**-**G1**) and σ-bond metathesis pathways (starting from **G1**-**H1**), respectively. Fluorine dissociation modeled by the elongation of the apical Ge−Cl bond in **H1** did not provide any stable species.



	E1, 0.0 (0.0)	**F1**, 1.9 (−0.4)	**G1**, 16.9 (19.7)	**H1**, 13.1 (15.7)
Ir−Ge (Å)	2.780	2.762	2.711	2.786
Ge−Cl^1 (Å)	2.288	2.272	2.235	2.223
Ge−Cl^2 (Å)	2.464	2.439	2.340	2.330

Fig. S3 Optimized structures of {*o*-$Me_2PC_6H_4)_2(Cl)_2Ge\}Ir(H)(CO)(PMe_3)$ (**E1**),. {*o*-$Me_2PC_6H_4)_2(Cl)_2Ge\}Ir(H)(CO)(PMe_3)$ (**F1**), {*o*-$Me_2PC_6H_4)_2(Cl)_2Ge\}Ir(H)(CO)$ (**G1**), and {*o*-$Me_2PC_6H_4)_2(Cl)_2Ge\}Ir(H)(CO)$ (**H1**) at B3PW91 functional with selected bond distances (Å). Hydrogen atoms are omitted for clarity. The Gibbs energy difference ΔG^0 (kcal/mol) relative to that of **E1** in gas phase are provided (kcal/mol). The values in parentheses include solvent effects in toluene (kcal/mol).

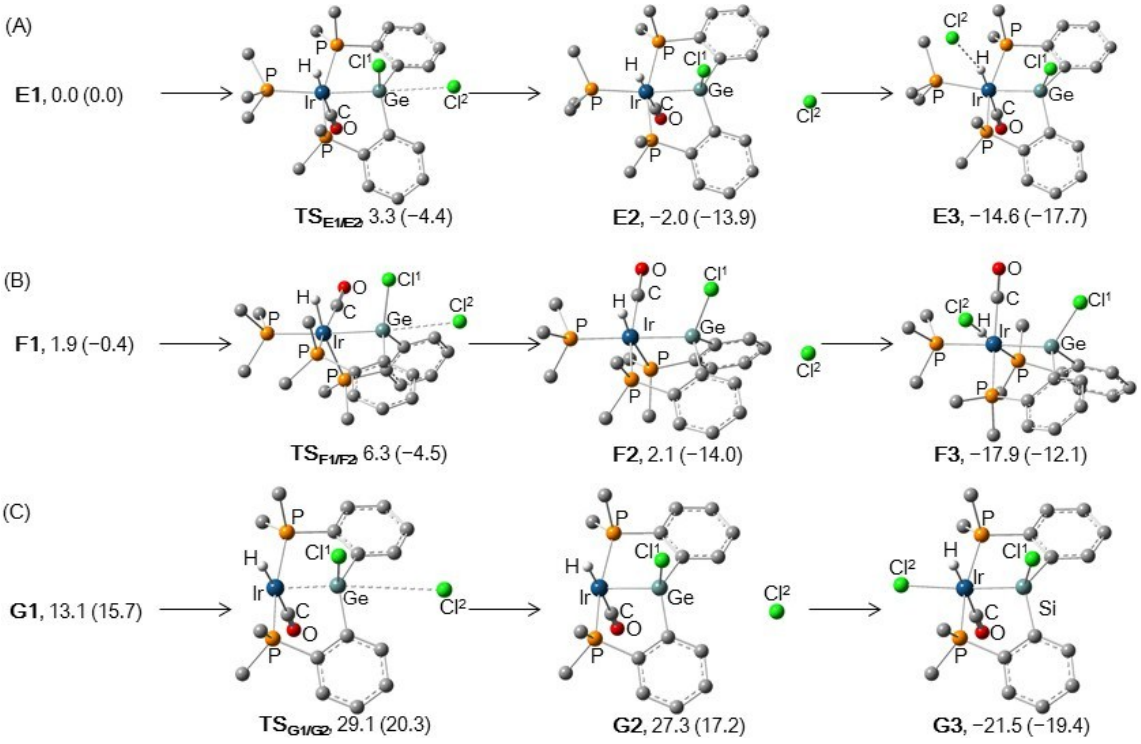


Fig. S4 Gibbs energy changes in the S_N2 type oxidative addition pathways starting from **E1** (A), **F1** (B), and **G1** (C). Hydrogen atoms are omitted for clarity. The Gibbs energies relative to that of **E1** are provided in gas phase are provided (kcal/mol). The values in parentheses include solvent effects in toluene (kcal/mol).

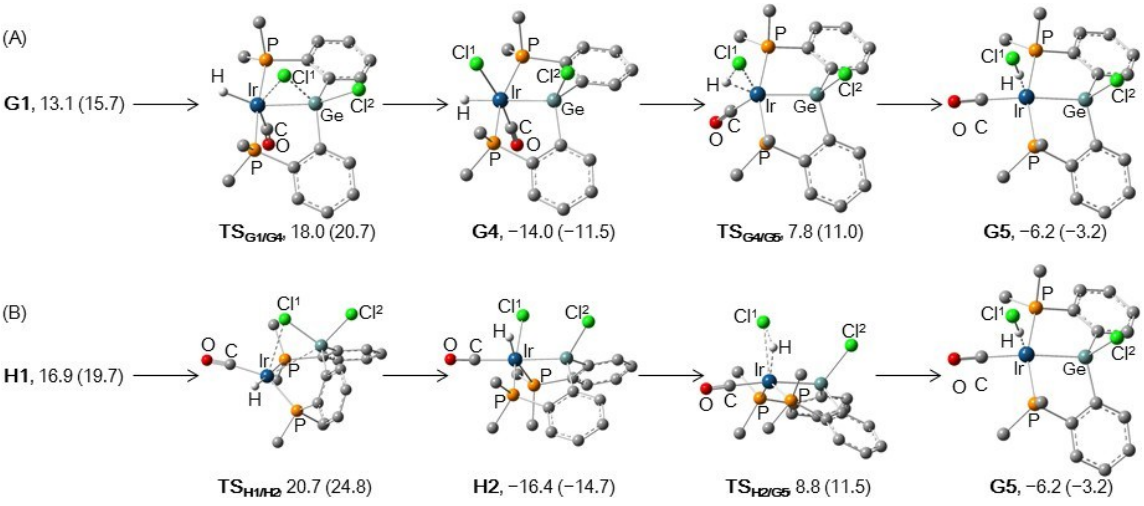


Fig. S5 Gibbs energy changes in the concerted oxidative addition pathways starting from **G1** (A) and **H1** (B). Hydrogen atoms are omitted for clarity. The Gibbs energies relative to that of **E1** are provided in gas phase are provided (kcal/mol). The values in parentheses include solvent effects in toluene (kcal/mol).

Geometry and Gibbs energy changes in the S_N2-type reaction pathways starting from B1' bearing the silyl ligand *trans* to CO ligand

We investigated an S_N2-type pathway starting from the intermediate {(*o*-$Me_2PC_6H_4)_2(Cl)_2Si$}Ir(H)(CO)(PMe_3) (**B1'**) whose geometry is similar to **B1** except for the positions of the PMe_3 and CO: the PMe_3 ligand in **B1** is *trans* to the silane group but the PMe_3 ligand in **B1**' is *cis* to the silane group. The Gibbs energy changes in the S_N2-type reaction pathway starting from **B1'** are similar to those starting from **B1**.

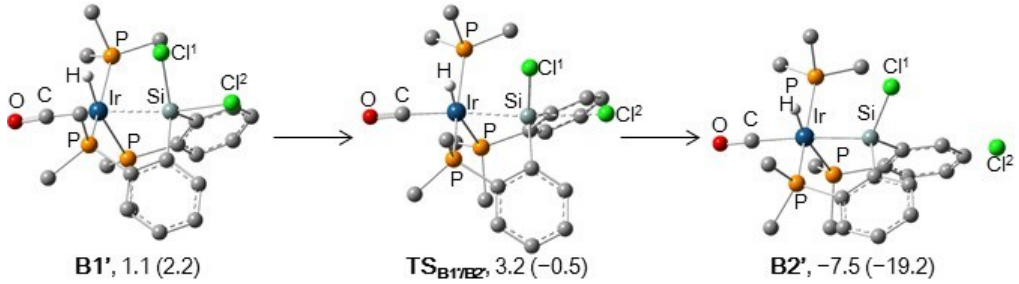


Fig. S6 Gibbs energy changes in the S_N2-type reaction pathway starting from {(*o*-$Me_2PC_6H_4)_2(Cl)_2Si$}Ir(H)(CO)(PMe_3) (**B1'**) bearing the silyl ligand *trans* to CO ligand. Hydrogen atoms are omitted for clarity. The Gibbs energies relative to that of **A1** are provided in gas phase are provided (kcal/mol). The values in parentheses include solvent effects in toluene (kcal/mol).

A1

E(RB3PW91) = -3193.82224163 a.u.

Ir	7.72488	6.82705	8.91352
Cl	10.38995	8.81543	5.02313
Cl	9.53908	6.07540	5.97938
P	6.59790	5.39841	10.48281
P	6.06459	6.88407	7.28130
P	9.90888	6.89991	9.73169
Si	9.07192	8.03194	6.81282
O	7.00712	9.61267	10.01301
C	7.27343	8.57209	9.60972
C	7.52071	8.92721	6.09505
C	7.62484	10.12410	5.37242
C	6.50684	10.76804	4.85716
C	5.24649	10.20288	5.00252
C	5.11384	9.01020	5.69944
C	6.23392	8.39379	6.26679
C	10.22592	9.02964	7.99991
C	10.66902	10.31833	7.67317
C	11.47214	11.05415	8.53524
C	11.91263	10.49325	9.72728
C	11.50121	9.21258	10.07020
C	10.63493	8.50130	9.23350
C	4.32251	6.96902	7.87349
C	5.98478	5.49728	6.08655
C	5.81035	3.91679	9.72438
C	5 .21720	6.12579	11.46257
C	7.52204	4.56031	11.84067
C	11.07049	5.59785	9.17345
C	10.18594	6.85356	11.55009
H	8.16687	5.41664	8.23827
H	8.60403	10.54489	5.18728
H	6.62669	11.70543	4.32345
H	4.37123	10.68628	4.58066
H	4.12654	8.57554	5.80836
H	10.39591	10.74799	6.71895
H	11.76977	12.06170	8.26292
H	12.56522	11.04994	10.39207
H	11.84474	8.78653	11.00573
H	3.60798	6.93719	7.04812
H	4.11959	6.11819	8.52494
H	4.17566	7.88910	8.44236
H	5.75221	4.56968	6.61372
H	5.21877	5.69516	5.33265
H	6.95739	5.3909	5.60609
H	5.30394	3.30474	10.47659
H	5.08678	4.20843	8.96236
H	6.58665	3.32266	9.23773
H	4.45657	6.54076	10.80011
H	4.75415	5.38110	12.11720
H	5.60972	6.94229	12.07302
H	7.87433	5.29660	12.56388
H	6.87163	3.84906	12.35890
H	8.37979	4.01970	11.43551
H	11.07849	5.56236	8.08448
H	12.07688	5.80543	9.54532
H	10.73076	4.62980	9.54930
H	9.85295	5.89127	11.93581
H	11.24630	6.95954	11.78989
H	9.62325	7.65084	12.03905

$TS_{A1/A2}$

E(RB3PW91) = -3193.82859331 a.u.

Ir	7.68287	6.86832	8.93946
Cl	10.45619	9.19386	4.68327
Cl	9.63986	6.36623	5.97235
P	6.59896	5.34058	10.45595
P	6.00057	6.90255	7.30584
P	9.84904	6.98545	9.83489
Si	8.90865	8.04523	7.03162
O	6.82023	9.56034	10.17272
C	7.13973	8.56039	9.71619
C	7.46601	8.96270	6.17700
C	7.59690	10.14664	5.44107
C	6.49059	10.76371	4.86909
C	5.22896	10.19103	4.97621
C	5.07224	9.01035	5.68914
C	6.17709	8.41714	6.30786
C	10.21583	9.03758	8.00709
C	10.76925	10.25151	7.58336
C	11.69491	10.93169	8.36544
C	12.13123	10.39166	9.56886
C	11.60752	9.18278	10.00686
C	10.63397	8.52542	9.24793
C	4.25940	6.95011	7.89234
C	5.99698	5.52043	6.10623
C	5.82732	3.88773	9.63334
C	5.22562	5.99924	11.48883
C	7.58139	4.46299	11.74202
C	10.98237	5.62544	9.37158

C	10.04463	7.05830	11.66020
H	8.18126	5.49627	8.23116
H	8.58916	10.54664	5.27195
H	6.62368	11.68754	4.31561
H	4.36868	10.65968	4.50906
H	4.08432	8.56964	5.76743
H	10.50730	10.62896	6.60312
H	12.09398	11.87853	8.01655
H	12.87371	10.90815	10.16878
H	11.95388	8.77196	10.94835
H	3.55521	6.93085	7.05804
H	4.05648	6.08467	8.52446
H	4.09977	7.85879	8.47576
H	5.78213	4.57829	6.61405
H	5.25000	5.70100	5.32946
H	6.98692	5.45647	5.65197
H	5.33924	3.23602	10.36350
H	5.08896	4.20267	8.89546
H	6.60608	3.32688	9.11231
H	4.44602	6.42678	10.85680
H	4.78835	5.21757	12.11682
H	5.61223	6.79598	12.12829
H	7.87889	5.16074	12.52533
H	6.98331	3.66858	12.19746
H	8.47489	4.02040	11.29815
H	11.00562	5.54448	8.28415
H	11.98881	5.82973	9.74454
H	10.61865	4.68327	9.78809
H	9.68429	6.13156	12.10368
H	11.09440	7.17403	11.93704
H	9.47380	7.89723	12.06190

A2

E(RB3PW91) = -3193.84939739 a.u.

Ir	7.59855	6.83441	8.98511
Cl	10.34224	12.02059	4.75671
Cl	9.73418	6.68446	5.88337
Si	8.77558	8.01382	7.22261
P	6.63945	5.18595	10.45770
P	5.90246	6.92238	7.33308
P	9.71976	7.08368	10.00820
O	6.54405	9.40688	10.32305
C	6.93515	8.45408	9.82871
C	7.48029	8.90213	6.19468
C	7.73298	9.98477	5.34610
C	6.69977	10.53192	4.59004
C	5.41855	9.99564	4.64674
C	5.15335	8.90808	5.47326
C	6.17833	8.37032	6.25486
C	10.16334	8.98435	8.03250
C	10.83332	10.06179	7.44420
C	11.89116	10.67187	8.11260
C	12.31133	10.20349	9.35239
C	11.66514	9.12341	9.94550
C	10.58584	8.52311	9.29310
C	4.18109	7.12258	7.93784
C	5.81607	5.49129	6.19592
C	5.56536	3.92928	9.65708
C	5.58499	5.80042	11.82984
C	7.80604	4.06627	11.33024
C	10.88319	5.68598	9.80620
C	9.70805	7.40801	11.81461
H	8.17902	5.51575	8.23347
H	8.71907	10.45435	5.24938
H	6.92356	11.38565	3.95878
H	4.61831	10.42343	4.05115
H	4.14773	8.50071	5.50476
H	10.55547	10.48126	6.47034
H	12.37458	11.52046	7.63974
H	13.14095	10.67939	9.86558
H	12.00460	8.76896	10.91380
H	3.47278	7.14421	7.10716
H	3.90904	6.29940	8.59962
H	4.10398	8.05994	8.49132
H	5.54925	4.58293	6.73837
H	5.07963	5.68135	5.41162
H	6.79839	5.35750	5.73937
H	5.19581	3.21173	10.39460
H	4.71214	4.39920	9.16713
H	6.14789	3.39689	8.90260
H	4.76126	6.38951	11.42152
H	5.17716	4.97785	12.42411
H	6.17315	6.45260	12.47905
H	8.47240	4.62644	11.98663
H	7.25793	3.33583	11.93171
H	8.41050	3.53406	10.59318
H	11.00045	5.49153	8.73868
H	11.85593	5.94495	10.23116
H	10.49791	4.78820	10.29183
H	9.19151	6.60568	12.34269
H	10.72380	7.48508	12.20771
H	9.18450	8.34694	12.00268

A3

E(RB3PW91) = -3193.85580918 a.u.

Ir	7.57365	6.93075	9.01070
Cl	8.42853	3.20065	8.00367
Cl	9.77856	6.90836	5.84664
P	6.62542	5.24907	10.47799
P	5.93162	6.90713	7.33135
P	9.70914	7.06404	9.98152
Si	8.74316	8.07000	7.27297
C	6.88693	8.54127	9.88573
O	6.48477	9.48846	10.38980
C	7.45528	8.96194	6.21301
C	7.67387	10.04849	5.36072
C	6.64845	10.55812	4.57292
C	5.38994	9.96636	4.60161
C	5.15710	8.86992	5.42329
C	6.17820	8.37411	6.23738
C	10.13820	9.06058	8.07970
C	10.81286	10.15553	7.53162
C	11.88011	10.74546	8.19832
C	12.31165	10.22756	9.41517
C	11.67136	9.12387	9.96613
C	10.58068	8.54680	9.31128
C	4.17789	7.07146	7.84739
C	5.99016	5.46859	6.21391
C	5.51608	4.02615	9.69342
C	5.62266	5.91379	11.86963
C	7.79998	4.11123	11.29510
C	10.81806	5.66375	9.61828
C	9.80235	7.31446	11.79724
H	8.11365	5.55231	8.31515
H	8.65572	10.50588	5.30324
H	6.83175	11.41293	3.93009
H	4.58928	10.35602	3.98169
H	4.17277	8.41368	5.42455
H	10.50977	10.55534	6.56997
H	12.38177	11.60507	7.76595
H	13.14992	10.68022	9.93436
H	12.02801	8.72484	10.90991
H	3.50033	7.00898	6.99318
H	3.92144	6.27603	8.54647
H	4.04203	8.03262	8.34710
H	5.92769	4.54469	6.79139
H	5.19683	5.52104	5.46397
H	6.96699	5.45832	5.72669
H	5.14549	3.32748	10.44874
H	4.66613	4.49925	9.20137
H	6.13127	3.48445	8.96283
H	4.79352	6.50716	11.47751
H	5.22070	5.10388	12.48503
H	6.23779	6.56411	12.49570
H	8.52326	4.63947	11.91636
H	7.24897	3.40293	11.92026
H	8.30781	3.56632	10.48840
H	10.93785	5.59677	8.53535
H	11.79094	5.80268	10.09644
H	10.35380	4.72822	9.93420
H	9.26456	6.51455	12.30549
H	10.83541	7.31475	12.15206
H	9.33284	8.26678	12.05071

B1

E(RB3PW91) = -3193.81947129 a.u.

Ir	-0.13354	0.60587	-0.88382
Cl	1.07087	-4.16978	0.37372
Cl	0.16550	-2.63211	-2.07777
P	2.17589	0.65221	-1.19013
P	-0.31345	0.83687	1.48039
P	-0.70400	2.80637	-1.65326
Si	0.54305	-1.93752	-0.06656
O	-2.89670	-0.62973	-1.16623
C	-0.76779	-1.92641	1.35041
C	-1.46378	-3.07884	1.73558
C	-0.99074	-0.75349	2.09974
C	-2.32239	-3.08284	2.82861
C	-1.79870	-0.78027	3.24055
C	-2.46816	-1.94087	3.60576
C	2.29196	-1.42772	0.61204
C	2.86573	-2.11040	1.69554
C	3.00432	-0.33287	0.10014
C	4.08610	-1.72472	2.23852
C	4.25976	0.02047	0.60464
C	4.80071	-0.67150	1.67965
C	-1.85900	-0.16876	-1.00628
C	3.07359	2.25978	-1.18919
C	2.75915	-0.05823	-2.77765
C	-1.54933	2.07619	2.05640
C	1.10459	1.24536	2.57718
C	-0.33125	3.11392	-3.42810
C	-2.50760	3.17054	-1.61320
C	-0.02524	4.33709	-0.87868

H	-1.31255	-3.99308	1.17570
H	-2.86205	-3.98937	3.08344
H	-1.93522	0.11266	3.84159
H	-3.11014	-1.94526	4.48079
H	2.34769	-2.96394	2.11292
H	4.48573	-2.26260	3.09238
H	4.81548	0.84868	0.17914
H	5.76715	-0.38416	2.08134
H	-0.05419	0.21695	-2.44782
H	2.64994	2.88985	-1.97377
H	2.95499	2.76269	-0.22795
H	4.13721	2.12955	-1.40224
H	2.38460	0.54707	-3.60639
H	3.85149	-0.08626	-2.80364
H	2.36136	-1.06827	-2.88091
H	-1.61791	2.12007	3.14566
H	-1.25511	3.06340	1.69458
H	-2.52933	1.82805	1.64561
H	0.78524	1.21694	3.62216
H	1.91084	0.52753	2.43184
H	1.47295	2.24719	2.34222
H	-0.67711	4.10138	-3.74775
H	0.74402	3.03810	-3.60212
H	-0.82171	2.34468	-4.02766
H	-2.73034	4.13928	-2.07050
H	-3.04598	2.38791	-2.15175
H	-2.86240	3.17461	-0.58096
H	1.05681	4.37470	-1.01108
H	-0.46728	5.23402	-1.32347
H	-0.23324	4.33637	0.19260

$TS_{B1/B2}$

E(RB3PW91) = -3193.82449231 a.u.

Ir	-0.16764	0.61866	-0.85059
Cl	1.06464	-4.60408	0.69933
Cl	0.13083	-2.79934	-1.81138
P	2.15913	0.73046	-1.12750
P	-0.36095	0.90255	1.52703
P	-0.71626	2.80000	-1.72546
Si	0.45072	-1.71213	-0.05040
O	-2.98418	-0.49806	-1.12364
C	-0.77004	-1.86021	1.40794
C	-1.39421	-3.04384	1.81569
C	-1.01429	-0.68981	2.15706
C	-2.21192	-3.07061	2.94011
C	-1.79008	-0.73674	3.31945
C	-2.39054	-1.92685	3.70948
C	2.25387	-1.44759	0.56104
C	2.85507	-2.24240	1.54658
C	2.98699	-0.34959	0.07844
C	4.13325	-1.95954	2.01680
C	4.28810	-0.09010	0.51987
C	4.86128	-0.89672	1.49423
C	-1.93480	-0.07115	-0.97195
C	3.01489	2.35050	-0.99118
C	2.73012	0.13272	-2.76352
C	-1.58422	2.15144	2.09830
C	1.08549	1.30859	2.58307
C	-0.12630	3.10089	-3.44008
C	-2.52029	3.09081	-1.92076
C	-0.19819	4.34877	-0.87358
H	-1.18960	-3.95311	1.26212
H	-2.69304	-4.00005	3.22675
H	-1.95108	0.15419	3.91765
H	-3.00515	-1.95452	4.60366
H	2.31400	-3.11177	1.90671
H	4.56634	-2.58861	2.78787
H	4.85639	0.74453	0.12339
H	5.86717	-0.68986	1.84584
H	-0.06118	0.16088	-2.39371
H	2.58338	3.04586	-1.71328
H	2.88806	2.75599	0.01356
H	4.08085	2.25723	-1.20874
H	2.33766	0.77421	-3.55558
H	3.82218	0.11966	-2.80318
H	2.34941	-0.87885	-2.91360
H	-1.67216	2.16600	3.18672
H	-1.26319	3.14176	1.77009
H	-2.56108	1.93108	1.66488
H	0.79670	1.26292	3.63616
H	1.88639	0.59107	2.40384
H	1.44562	2.31465	2.35362
H	-0.49658	4.05463	-3.82694
H	0.96492	3.10796	-3.47243
H	-0.47770	2.28913	-4.07969
H	-2.71624	4.06180	-2.38412
H	-2.95031	2.30462	-2.54471
H	-3.01024	3.05595	-0.94589
H	0.87910	4.34609	-0.70427
H	-0.46620	5.22937	-1.46486
H	-0.69439	4.41786	0.09570

B2

E(RB3PW91) = -3193.84562082 a.u.

Ir	-0.23676	0.67461	-0.92863
Cl	1.27017	-5.45954	2.34288
Cl	-0.25595	-3.11772	-1.33243
Si	0.26288	-1.54586	-0.07394
P	2.13766	0.81849	-0.95296
P	-0.69614	1.06269	1.41740
P	-0.65900	2.87814	-1.83463
O	-3.04297	-0.37409	-1.45247
C	-0.67325	-1.71372	1.54924
C	-0.87079	-2.94722	2.17993
C	-1.05778	-0.53697	2.21773
C	-1.45208	-3.00168	3.44318
C	-1.64339	-0.59939	3.48493
C	-1.84672	-1.83570	4.08950
C	2.10712	-1.63493	0.29449
C	2.68172	-2.74531	0.92692
C	2.90793	-0.51843	0.01153
C	4.02935	-2.72282	1.27177
C	4.26410	-0.50557	0.35260
C	4.81779	-1.61079	0.98902
C	-2.00267	0.03384	-1.22069
C	2.96728	2.36886	-0.42512
C	2.83173	0.56904	-2.63288
C	-2.17365	2.09673	1.77133
C	0.58995	1.82896	2.47932
C	0.17289	3.26443	-3.42494
C	-2.42011	3.15306	-2.27116
C	-0.28123	4.37988	-0.84288
H	0.05113	0.18464	-2.44164
H	-0.51378	-3.87749	1.73848
H	-1.56294	-3.96865	3.92136
H	-1.94324	0.30206	4.01113
H	-2.30128	-1.88316	5.07391
H	2.09567	-3.63375	1.20067
H	4.44784	-3.58734	1.77665
H	4.89492	0.34948	0.13011
H	5.86772	-1.60015	1.26440
H	2.67415	3.18876	-1.08366
H	2.69444	2.61523	0.60068
H	4.05200	2.25989	-0.48456
H	2.45236	1.31959	-3.32762
H	3.92281	0.61569	-2.59667
H	2.52982	-0.41841	-2.98457
H	-2.36818	2.14493	2.84473
H	-2.02706	3.11326	1.40215
H	-3.04401	1.66002	1.27856
H	0.23925	1.88218	3.51280
H	1.48886	1.20966	2.45327
H	0.82767	2.83599	2.12820
H	-0.20234	4.20296	-3.84251
H	1.25095	3.35629	-3.27992
H	-0.01218	2.45471	-4.13296
H	-2.57070	4.15379	-2.68504
H	-2.73224	2.41224	-3.01003
H	-3.04577	3.03494	-1.38454
H	0.76324	4.37172	-0.52981
H	-0.47304	5.28658	-1.42342
H	-0.90366	4.40266	0.05278

B3

E(RB3PW91) = -3193.85405932 a.u.

Ir	-0.26234	0.70635	-0.82833
Cl	-0.00102	0.33298	-4.56405
Cl	-0.45785	-3.18381	-1.05043
P	2.10811	0.80905	-0.95379
P	-0.60687	1.16119	1.54801
P	-0.68852	2.82569	-1.93009
Si	0.18009	-1.48605	-0.00150
O	-3.09318	-0.27316	-1.34671
C	-2.04019	0.11474	-1.13297
C	-0.62961	-1.63169	1.71322
C	-0.89555	-2.85182	2.34700
C	-0.91876	-0.44354	2.40454
C	-1.41682	-2.89484	3.63379
C	-1.42841	-0.49028	3.70594
C	-1.67594	-1.71131	4.31924
H	-0.06990	0.28106	-2.41198
H	-0.70967	-3.78022	1.81582
H	-1.62538	-3.85087	4.10318
H	-1.64698	0.42318	4.25079
H	-2.08057	-1.73922	5.32567
C	2.04435	-1.70148	0.24918
C	2.62663	-2.84489	0.81004
C	2.87447	-0.63412	-0.11091
C	3.99658	-2.91661	1.02129
C	4.25595	-0.70701	0.09929
C	4.81267	-1.84324	0.66990
C	2.97185	2.25339	-0.20809
C	2.82805	0.73624	-2.63129
C	-2.08598	2.16418	1.98684

C	0.67573	1.92860	2.62560
C	0.57614	3.45358	-3.08991
C	-2.15242	2.71303	-3.01702
C	-1.05522	4.30598	-0.89866
H	2.00112	-3.69029	1.07951
H	4.43308	-3.80937	1.45729
H	4.90682	0.11321	-0.18773
H	5.88419	-1.89694	0.83208
H	2.53725	3.17453	-0.59974
H	2.85747	2.24559	0.87517
H	4.03591	2.24067	-0.45462
H	2.77308	1.71636	-3.10599
H	3.87226	0.42212	-2.56323
H	2.24694	0.04889	-3.25203
H	-2.28609	2.14591	3.06050
H	-1.92118	3.19927	1.68301
H	-2.95705	1.77630	1.45620
H	0.32159	1.99865	3.65743
H	1.57501	1.31010	2.61059
H	0.92167	2.92977	2.26484
H	0.20184	4.35361	-3.58583
H	1.50610	3.69745	-2.57322
H	0.73982	2.66543	-3.83481
H	-2.31562	3.66244	-3.53409
H	-1.94362	1.92464	-3.74924
H	-3.04314	2.45782	-2.43959
H	-0.23497	4.50558	-0.20566
H	-1.20236	5.18420	-1.53384
H	-1.96751	4.13660	-0.32451

C1

E(RB3PW91) = -2732.76492719 a.u.

Ir	7.75827	6.32840	8.71532
Cl	9.96565	6.69662	5.44844
Cl	8.40287	4.15840	7.81871
P	6.00412	6.46711	7.16341
P	9.84623	6.53003	9.76591
Si	8.88728	7.62043	7.01599
O	6.69702	8.70058	10.21405
C	7.11340	7.80521	9.62625
C	7.51683	8.58059	6.10580
C	7.69028	9.72665	5.32256
C	6.61742	10.32976	4.67642
C	5.34425	9.78012	4.78277
C	5.14903	8.62703	5.53347
C	6.22213	8.02930	6.19928
C	10.21687	8.62561	7.93724
C	10.85078	9.78059	7.46743
C	11.83561	10.41852	8.21252
C	12.22455	9.89567	9.44117
C	11.62837	8.73478	9.91938
C	10.62478	8.10174	9.18152
C	4.30789	6.53771	7.84847
C	5.91494	5.15019	5.90497
C	11.07783	5.23552	9.40049
C	9.83970	6.62999	11.59388
H	6.99160	5.41901	9.86604
H	8.67935	10.15830	5.20913
H	6.77385	11.22706	4.08636
H	4.50376	10.24610	4.27899
H	4.15186	8.20354	5.59877
H	10.57637	10.19113	6.50130
H	12.30329	11.32178	7.83410
H	12.99420	10.38846	10.02607
H	11.94966	8.33286	10.87497
H	3.54626	6.58365	7.06669
H	4.15618	5.63377	8.44177
H	4.20927	7.40371	8.50512
H	5.73222	4.19529	6.40007
H	5.11792	5.37380	5.19138
H	6.87386	5.08232	5.39043
H	11.19375	5.14996	8.31968
H	12.03375	5.49112	9.86479
H	10.71202	4.27812	9.77458
H	9.37111	5.71869	11.97096
H	10.84722	6.71133	12.00809
H	9.24270	7.48481	11.91601

$TS_{C1/C2}$

E(RB3PW91) = -2732.71660821 a.u.

Ir	7.68546	6.99419	8.80019
Cl	10.66763	10.22559	4.34895
Cl	9.70289	6.77573	5.84291
P	5.90598	6.95637	7.27980
P	9.76434	7.00986	9.87942
Si	8.82526	8.17951	7.09000
O	6.74102	9.60334	10.15567
C	7.10908	8.66155	9.62696
C	7.40082	9.02536	6.17195
C	7.57926	10.14740	5.35696
C	6.49680	10.70008	4.67629
C	5.23108	10.13857	4.77869

C	5.03835	9.00655	5.56379
C	6.11139	8.45498	6.26392
C	10.17516	9.07894	8.06734
C	10.82456	10.22224	7.59236
C	11.83761	10.81640	8.34141
C	12.23158	10.27582	9.55796
C	11.61499	9.12376	10.03573
C	10.58692	8.53031	9.30290
C	4.21964	7.00879	7.99323
C	5.84808	5.54721	6.11931
C	10.89841	5.62954	9.50103
C	9.73298	7.06789	11.70986
H	8.10957	5.54626	8.19053
H	8.58445	10.54160	5.18656
H	6.66074	11.56882	4.04752
H	4.39263	10.57095	4.24220
H	4.04857	8.56537	5.62727
H	10.59687	10.60190	6.59359
H	12.32951	11.70083	7.95062
H	13.02483	10.74036	10.13476
H	11.93925	8.70075	10.98137
H	3.45676	6.98871	7.21168
H	4.07963	6.13817	8.63805
H	4.09942	7.91414	8.59019
H	5.67368	4.62391	6.67632
H	5.05502	5.69147	5.38185
H	6.80942	5.47411	5.60871
H	11.01393	5.55942	8.41848
H	11.87520	5.79975	9.95993
H	10.47126	4.69511	9.87191
H	9.21310	6.18305	12.08429
H	10.74331	7.07776	12.12458
H	9.19850	7.95914	12.04227

C2

E(RB3PW91) = -2732.72218899 a.u.

Ir	7.66075	6.95654	8.83488
Cl	10.28871	12.03607	4.82646
Cl	9.70141	6.77281	5.82080
P	5.88368	6.92857	7.29323
P	9.75091	6.99320	9.91546
Si	8.78786	8.11245	7.14222
O	6.69424	9.56220	10.19636
C	7.06155	8.61569	9.67887
C	7.41941	8.96550	6.17930
C	7.64104	10.07754	5.36450
C	6.59056	10.61483	4.62273
C	5.32446	10.04553	4.67090
C	5.09063	8.92989	5.47107
C	6.12923	8.39200	6.23020
C	10.17201	9.00766	8.04222
C	10.82046	10.12552	7.51395
C	11.88922	10.69717	8.20162
C	12.33007	10.15582	9.40248
C	11.69935	9.03484	9.93689
C	10.61813	8.46280	9.26699
C	4.19388	7.04782	7.98922
C	5.80079	5.48073	6.18202
C	10.84739	5.56360	9.61320
C	9.72140	7.15051	11.73980
H	8.11891	5.53951	8.18779
H	8.61890	10.57226	5.27772
H	6.78910	11.48756	4.00947
H	4.51128	10.46770	4.08924
H	4.09570	8.49631	5.50147
H	10.52435	10.59877	6.56720
H	12.36480	11.57368	7.77417
H	13.16463	10.60415	9.93191
H	12.05311	8.62370	10.87748
H	3.44035	7.03775	7.19847
H	4.01703	6.19610	8.64998
H	4.09638	7.96952	8.56483
H	5.60174	4.58087	6.76841
H	5.01558	5.61613	5.43453
H	6.76295	5.36822	5.68017
H	10.96653	5.43549	8.53635
H	11.82653	5.72966	10.06866
H	10.39480	4.66023	10.02825
H	9.18979	6.29623	12.16521
H	10.73312	7.17072	12.15079
H	9.20221	8.06769	12.02185

C3

E(RB3PW91) = -2732.78128532 a.u.

Ir	7.65422	6.93492	8.84374
Cl	6.55366	5.40617	10.50646
Cl	9.77726	6.95673	5.68453
P	5.90290	6.94382	7.31107
P	9.71891	7.01990	9.91250
Si	8.76457	8.08984	7.17400
O	6.57259	9.42003	10.33854
C	6.97536	8.50601	9.78439

C	7.43507	8.98936	6.15830
C	7.62899	10.09142	5.32034
C	6.57798	10.63195	4.58743
C	5.31224	10.06042	4.66036
C	5.09938	8.94952	5.46866
H	8.17622	5.58757	8.11755
H	8.61352	10.53974	5.23366
H	6.74665	11.49834	3.95613
H	4.49054	10.47845	4.08827
H	4.10764	8.51014	5.51486
C	6.14644	8.41642	6.22286
C	10.19294	9.02268	8.00885
C	10.88751	10.11652	7.48418
C	11.95738	10.68417	8.16706
C	12.37016	10.14794	9.38213
C	11.71045	9.04539	9.91310
C	10.62162	8.48504	9.24154
C	4.21647	7.07208	8.00167
C	5.81283	5.50950	6.18358
C	10.82848	5.59496	9.63908
C	9.68319	7.21215	11.72875
H	10.59481	10.53509	6.52668
H	12.47274	11.54320	7.74981
H	13.20658	10.58644	9.91632
H	12.04603	8.63302	10.85979
H	3.44579	6.96952	7.23422
H	4.11169	6.27287	8.73980
H	4.10071	8.02883	8.51355
H	5.64009	4.61470	6.78574
H	5.00843	5.62957	5.45378
H	6.76764	5.40521	5.66625
H	10.97138	5.45854	8.56621
H	11.79586	5.74798	10.12385
H	10.34374	4.70425	10.04500
H	9.04683	6.41534	12.12195
H	10.67895	7.14213	12.17217
H	9.23213	8.17150	11.98740

D1

E(RB3PW91) = -2732.69898109 a.u.

Ir	0.00978	3.39560	-0.59182
Cl	-1.70041	0.52680	0.13222
Cl	0.66247	-1.48023	0.77355
P	2.30201	3.30614	-0.98565
P	-0.08226	3.78199	1.70909
Si	0.50557	0.78094	0.23186
O	-2.96547	3.54667	-1.17222
C	-1.85949	3.44843	-0.89649
C	1.30112	1.37874	1.97997
C	2.21063	0.52570	2.61457
C	1.01164	2.61168	2.58838
C	2.81857	0.88322	3.81375
C	1.59606	2.94624	3.81358
C	2.50188	2.08939	4.42538
C	1.74617	0.59996	-1.32824
C	1.85336	-0.61639	-2.00366
C	2.60242	1.65203	-1.69771
C	2.79619	-0.79294	-3.01171
C	3.57847	1.45160	-2.67579
C	3.67683	0.23156	-3.33384
C	3.61051	3.54888	0.28280
C	2.80885	4.50976	-2.27259
C	-1.70639	3.59037	2.54274
C	0.43766	5.45512	2.26790
H	0.09764	3.12242	-2.20395
H	2.43946	-0.43502	2.17146
H	3.53182	0.20698	4.27373
H	1.35649	3.89029	4.29174
H	2.95845	2.36525	5.37035
H	1.20227	-1.43774	-1.73241
H	2.84701	-1.74160	-3.53602
H	4.25323	2.25652	-2.94921
H	4.42816	0.08973	-4.10370
H	3.56847	4.57595	0.65456
H	3.45724	2.86539	1.11820
H	4.59674	3.36862	-0.15260
H	2.55776	5.51337	-1.92199
H	3.88187	4.46570	-2.47343
H	2.24688	4.31330	-3.18574
H	-1.61193	3.72231	3.62344
H	-2.40565	4.33013	2.14489
H	-2.09720	2.59379	2.33156
H	0.29489	5.60553	3.34074
H	1.48519	5.62374	2.01358
H	-0.16818	6.18829	1.73035

$TS_{D1/D2}$

E(RB3PW91) = -2732.71246619 a.u.

Ir	0.03963	3.25226	-0.57906
Cl	-0.02962	-0.24042	-0.93002
Cl	1.01342	-2.08859	1.84727
P	2.34206	3.37789	-0.98648

P	-0.05119	3.94592	1.72041
Si	0.53215	1.15152	0.47275
O	-2.94171	2.64417	-0.76252
C	-1.83474	2.88789	-0.64711
C	-0.55378	1.24475	2.02081
C	-1.14620	0.13141	2.62580
C	-0.73876	2.51333	2.61112
C	-1.89367	0.28238	3.79050
C	-1.46487	2.65079	3.79486
C	-2.04375	1.53110	4.38222
C	2.40802	1.27076	0.79657
C	3.04717	0.39484	1.68433
C	3.18306	2.27277	0.17919
C	4.40949	0.52178	1.94226
C	4.55167	2.38466	0.43139
C	5.16436	1.50881	1.31977
C	3.10507	5.03835	-0.83954
C	2.86393	2.82862	-2.65102
C	-1.20002	5.34623	2.01123
C	1.44168	4.45255	2.65839
H	0.02235	2.76817	-2.12732
H	-0.96564	-0.85656	2.20891
H	-2.34813	-0.59237	4.24339
H	-1.59939	3.62466	4.25542
H	-2.61725	1.63850	5.29730
H	2.47136	-0.42023	2.12892
H	4.88042	-0.17131	2.63167
H	5.14452	3.15255	-0.05609
H	6.22722	1.59807	1.52038
H	2.59840	5.72353	-1.52314
H	2.99666	5.41001	0.17916
H	4.16517	5.00851	-1.10090
H	2.42278	3.48109	-3.40768
H	3.95320	2.84345	-2.73695
H	2.50188	1.81212	-2.81201
H	-1.24672	5.61375	3.06927
H	-0.85341	6.21519	1.44682
H	-2.19928	5.07922	1.66389
H	1.19644	4.56662	3.71708
H	2.21326	3.68832	2.55434
H	1.82108	5.40414	2.27751

D2

E(RB3PW91) = -2732.72016393 a.u.

Ir	0.07705	3.28633	-0.65509
Cl	-0.22085	-0.36296	-0.62255
Cl	1.13620	-2.47683	2.66946
P	2.42801	3.44463	-0.85637
P	-0.28118	4.09326	1.59404
Si	0.47538	1.24852	0.44726
O	-2.86281	2.63975	-1.12717
C	-0.45046	1.37777	2.07991
C	-0.75806	0.24184	2.83573
C	-0.78806	2.64994	2.58156
C	-1.40199	0.38027	4.06289
C	-1.43766	2.77744	3.80978
C	-1.75114	1.63719	4.54361
C	2.34646	1.13140	0.64457
C	2.90127	0.05210	1.34076
C	3.19377	2.12985	0.13317
C	4.27944	-0.01092	1.52883
C	4.57561	2.05451	0.32156
C	5.11364	0.98374	1.02732
C	-1.77499	2.89655	-0.90845
C	3.23199	5.02821	-0.39821
C	3.02551	3.18459	-2.56685
C	-1.62772	5.33241	1.72448
C	1.06153	4.86616	2.57693
H	-0.44431	-0.75655	2.51428
H	-1.61818	-0.51091	4.64215
H	-1.70541	3.75421	4.20174
H	-2.26140	1.73572	5.49639
H	2.27482	-0.75814	1.74831
H	4.69201	-0.85346	2.07397
H	5.23636	2.81885	-0.07716
H	6.18667	0.92566	1.17942
H	0.24905	2.69106	-2.15114
H	2.77160	5.84389	-0.96077
H	3.11501	5.21891	0.66772
H	4.29741	4.99849	-0.63837
H	2.61337	3.95314	-3.22465
H	4.11703	3.22029	-2.59952
H	2.68461	2.20779	-2.91153
H	-1.78889	5.63476	2.76173
H	-1.36529	6.21692	1.13916
H	-2.55287	4.91098	1.32840
H	0.71725	5.04065	3.59911
H	1.92044	4.19338	2.61232
H	1.35813	5.81983	2.13437

D3

E(RB3PW91) = -2732.78733570 a.u.

Ir	0.13995	3.32447	-0.70798
Cl	-0.55694	-0.44895	-0.27757
Cl	0.25749	5.68193	-1.59101
P	2.48824	3.40735	-0.59940
P	-0.53904	4.18012	1.42270
Si	0.39002	1.30241	0.41267
O	-2.65678	2.71798	-1.73034
C	-0.24689	1.52030	2.19894
C	-0.34076	0.46057	3.11017
C	-0.60402	2.80697	2.63998
C	-0.75736	0.66998	4.41844
C	-1.02370	3.01572	3.95772
C	-1.09591	1.95135	4.84599
C	2.23986	0.86439	0.48974
C	2.73847	-0.35659	0.95989
C	3.15884	1.84469	0.08376
C	4.10569	-0.58845	1.04088
C	4.53506	1.61288	0.16879
C	5.00681	0.39919	0.65036
C	-1.62952	2.97186	-1.30279
C	3.31445	4.75025	0.32990
C	3.22057	3.57641	-2.26500
C	-2.23311	4.87791	1.39007
C	0.40080	5.52688	2.23449
H	-0.09608	-0.54676	2.78757
H	-0.82310	-0.16644	5.10689
H	-1.30218	4.00936	4.29649
H	-1.42320	2.11806	5.86701
H	2.04886	-1.14224	1.25281
H	4.47270	-1.54262	1.40518
H	5.24454	2.37153	-0.14840
H	6.07500	0.21887	0.71168
H	0.53419	2.70494	-2.14754
H	2.87929	5.69818	0.00605
H	3.15703	4.61916	1.40013
H	4.38800	4.75482	0.12809
H	2.80179	4.47714	-2.71956
H	4.30930	3.65324	-2.21401
H	2.93769	2.71271	-2.86717
H	-2.53506	5.25255	2.37104
H	-2.24283	5.69569	0.66506
H	-2.93888	4.11146	1.06644
H	-0.14774	5.92660	3.09078
H	1.36789	5.15911	2.57631
H	0.55395	6.31976	1.49854

$TS_{C1/C4}$

E(RB3PW91) = -2732.71496998 a.u.

Ir	7.87765	6.89931	8.51942
Cl	9.29276	6.04377	6.43595
Cl	10.24653	8.65602	4.99040
P	6.00999	6.94207	7.14460
P	9.84905	7.00378	9.73849
Si	9.01950	8.29208	6.80033
O	6.81543	9.24950	10.03098
C	7.26732	8.39934	9.38470
C	7.44079	9.08876	6.03492
C	7.52082	10.28745	5.31433
C	6.39410	10.88274	4.75949
C	5.15680	10.25873	4.85979
C	5.05302	9.05383	5.54274
C	6.17250	8.48270	6.15318
C	10.29059	9.14072	7.97356
C	10.89495	10.35330	7.61687
C	11.80695	10.98792	8.45189
C	12.18810	10.39128	9.64728
C	11.62860	9.17342	10.01200
C	10.66629	8.56216	9.20424
C	4.38829	7.04843	7.98341
C	5.78415	5.58854	5.93677
C	11.08663	5.67875	9.50445
C	9.67455	7.11598	11.55532
H	7.62255	5.28784	8.94169
H	8.48563	10.75940	5.17050
H	6.48795	11.82667	4.23243
H	4.27656	10.70577	4.40965
H	4.08419	8.56877	5.61076
H	10.65943	10.80538	6.66060
H	12.23352	11.94146	8.15796
H	12.91679	10.86953	10.29349
H	11.93760	8.71051	10.94407
H	3.56092	7.10083	7.27229
H	4.27284	6.15638	8.60237
H	4.36805	7.92642	8.63066
H	5.59388	4.66127	6.48108
H	4.94876	5.80686	5.26672
H	6.69828	5.47158	5.35454
H	11.29107	5.56333	8.43992
H	12.01319	5.92028	10.03124
H	10.67356	4.74248	9.88545
H	9.16568	6.21266	11.89776
H	10.64179	7.19353	12.05664

H	9.06058	7.98030	11.81257

C4

E(RB3PW91) = -2732.76492719 a.u.

Ir	7.75827	6.32840	8.71532
Cl	9.96565	6.69662	5.44844
Cl	8.40287	4.15840	7.81871
P	6.00412	6.46711	7.16341
P	9.84623	6.53003	9.76591
Si	8.88728	7.62043	7.01599
O	6.69702	8.70058	10.21405
C	7.11340	7.80521	9.62625
C	7.51683	8.58059	6.10580
C	7.69028	9.72665	5.32256
C	6.61742	10.32976	4.67642
C	5.34425	9.78012	4.78277
C	5.14903	8.62703	5.53347
C	6.22213	8.02930	6.19928
C	10.21687	8.62561	7.93724
C	10.85078	9.78059	7.46743
C	11.83561	10.41852	8.21252
C	12.22455	9.89567	9.44117
C	11.62837	8.73478	9.91938
C	10.62478	8.10174	9.18152
C	4.30789	6.53771	7.84847
C	5.91494	5.15019	5.90497
C	11.07783	5.23552	9.40049
C	9.83970	6.62999	11.59388
H	6.99160	5.41901	9.86604
H	8.67935	10.15830	5.20913
H	6.77385	11.22706	4.08636
H	4.50376	10.24610	4.27899
H	4.15186	8.20354	5.59877
H	10.57637	10.19113	6.50130
H	12.30329	11.32178	7.83410
H	12.99420	10.38846	10.02607
H	11.94966	8.33286	10.87497
H	3.54626	6.58365	7.06669
H	4.15618	5.63377	8.44177
H	4.20927	7.40371	8.50512
H	5.73222	4.19529	6.40007
H	5.11792	5.37380	5.19138
H	6.87386	5.08232	5.39043
H	11.19375	5.14996	8.31968
H	12.03375	5.49112	9.86479
H	10.71202	4.27812	9.77458
H	9.37111	5.71869	11.97096
H	10.84722	6.71133	12.00809
H	9.24270	7.48481	11.91601

$TS_{C4/C5}$

E(RB3PW91) = -2732.72384837 a.u.

Ir	7.73281	6.33120	8.73972
Cl	9.90508	6.62052	5.44161
Cl	8.25072	3.72129	8.09264
P	6.00195	6.53944	7.18215
P	9.79401	6.63934	9.79583
Si	8.87414	7.60725	7.01709
O	6.11127	7.41094	11.03247
C	6.71831	6.92319	10.17908
C	7.53607	8.59871	6.10110
C	7.74043	9.73562	5.31260
C	6.68149	10.36264	4.66621
C	5.39457	9.84642	4.77752
C	5.17031	8.70224	5.53402
C	6.23046	8.08301	6.19982
C	10.24433	8.60728	7.87114
C	10.92800	9.69918	7.32548
C	11.93995	10.33953	8.03046
C	12.30547	9.88161	9.29250
C	11.66129	8.78031	9.84272
C	10.63171	8.14662	9.14232
C	4.29806	6.63321	7.84735
C	5.90349	5.21191	5.92825
C	11.02061	5.30533	9.54553
C	9.76273	6.85622	11.61457
H	7.46101	4.76823	9.22277
H	8.73914	10.14309	5.19760
H	6.85933	11.25365	4.07270
H	4.56570	10.33243	4.27337
H	4.16283	8.30503	5.60407
H	10.67621	10.05421	6.33176
H	12.44835	11.19361	7.59477
H	13.09668	10.37732	9.84533
H	11.96718	8.42428	10.82122
H	3.55003	6.68870	7.05342
H	4.11719	5.73378	8.43956
H	4.20457	7.50341	8.49918
H	5.70805	4.26146	6.42799
H	5.11741	5.43001	5.20105
H	6.86677	5.13311	5.42196
H	11.15991	5.14975	8.47476

H	11.97410	5.56849	10.01047
H	10.63330	4.37798	9.97140
H	9.29198	5.97377	12.05289
H	10.76652	6.96445	12.03122
H	9.16547	7.73289	11.87031

C5

E(RB3PW91) = -2732.74625477 a.u.

Ir	7.69541	6.46000	8.78609
Si	8.86232	7.61202	7.03141
Cl	9.83378	6.50114	5.50585
Cl	8.32141	3.28392	8.02224
P	5.96725	6.65659	7.24976
P	9.72362	6.78282	9.86356
O	6.07584	5.44387	11.17330
C	6.69063	5.79742	10.27030
C	7.56029	8.62420	6.08727
C	7.79636	9.72983	5.26367
C	6.75495	10.36932	4.60171
C	5.45235	9.89925	4.73614
C	5.19484	8.78988	5.53251
C	6.23831	8.15626	6.21140
C	10.26719	8.61009	7.82902
C	10.99982	9.63762	7.22426
C	12.02283	10.28742	7.90373
C	12.34848	9.90499	9.20170
C	11.65578	8.86704	9.81222
C	10.61788	8.22165	9.13477
C	4.27177	6.83939	7.92400
C	5.79693	5.29190	6.03937
C	10.92807	5.40789	9.73492
C	9.65742	7.12413	11.66460
H	8.07717	4.65468	8.31756
H	8.80664	10.10298	5.13437
H	6.95805	11.23396	3.97804
H	4.63706	10.39478	4.21923
H	4.17502	8.42978	5.62153
H	10.77860	9.93211	6.20372
H	12.57116	11.09000	7.42104
H	13.14771	10.40925	9.73499
H	11.93210	8.56762	10.81810
H	3.51996	6.92071	7.13569
H	4.04868	5.95893	8.53036
H	4.22796	7.72231	8.56382
H	5.57039	4.36566	6.57129
H	5.00937	5.51237	5.31432
H	6.74804	5.15957	5.52119
H	11.10534	5.19295	8.68001
H	11.87204	5.66839	10.22038
H	10.50337	4.51321	10.19449
H	9.17224	6.27839	12.15654
H	10.65193	7.25780	12.09653
H	9.05963	8.01957	11.84259

$TS_{D1/D4}$

E(RB3PW91) = -2732.71089618 a.u.

Ir	-0.05501	3.66948	-0.64096
Cl	0.54897	-1.54707	0.95149
Cl	-1.34423	0.76329	-0.15074
P	2.18298	3.27206	-1.02070
P	-0.16105	3.70782	1.67826
Si	0.64446	0.47900	0.34686
O	-2.69488	5.04949	-1.16839
C	-1.72598	4.47859	-0.92586
C	3.49503	3.50710	0.25237
C	2.80284	4.39859	-2.33197
C	-1.77201	3.31453	2.47987
C	0.20795	5.34271	2.43969
C	1.32826	1.29558	1.92638
C	2.31720	0.51922	2.55476
C	0.99680	2.53692	2.51309
C	2.95716	0.93409	3.71613
C	1.61894	2.92121	3.70456
C	2.59404	2.13505	4.30583
C	1.81358	0.45426	-1.14807
C	2.03172	-0.78991	-1.75740
C	2.50941	1.57265	-1.66257
C	2.90202	-0.94055	-2.83083
C	3.39958	1.40173	-2.72424
C	3.59954	0.15693	-3.30956
H	2.60017	-0.43795	2.13270
H	3.72638	0.31019	4.15866
H	1.35617	3.86435	4.16880
H	3.06929	2.46692	5.22316
H	1.50969	-1.66551	-1.39224
H	3.03086	-1.91722	-3.28513
H	3.93693	2.25529	-3.12045
H	4.28926	0.05388	-4.14094
H	0.00433	3.60330	-2.27520
H	3.45258	4.53994	0.60724
H	3.34142	2.83892	1.09869
H	4.48049	3.31718	-0.18092

H	2.54051	5.41267	-2.02519
H	3.88565	4.33434	-2.46819
H	2.28388	4.18751	-3.26718
H	-1.68877	3.35542	3.56910
H	-2.51778	4.03927	2.14414
H	-2.10047	2.31954	2.17922
H	0.00802	5.38011	3.51380
H	1.24408	5.62175	2.24193
H	-0.43481	6.06940	1.93833

D4

E(RB3PW91) = -2732.77336845 a.u.

Ir	-0.15766	3.51218	-0.46492
Cl	-2.29519	2.88440	0.57134
Cl	-0.54987	-0.35687	-0.97128
P	1.74378	3.67813	-1.71077
P	0.64605	3.70692	1.80000
Si	0.52349	1.24913	-0.15704
O	-1.18772	6.37670	-1.00414
C	0.65184	0.91503	1.70621
C	0.70188	-0.36058	2.27854
C	0.73907	2.03140	2.55378
C	0.85073	-0.52564	3.65029
C	0.89721	1.86357	3.93174
C	0.95461	0.58788	4.47860
C	2.27785	1.08143	-0.88996
C	3.06399	-0.07422	-0.80652
C	2.82415	2.20780	-1.52370
C	4.35373	-0.10442	-1.32068
C	4.12109	2.17828	-2.04793
C	4.88581	1.02473	-1.93964
C	-0.80156	5.32622	-0.77531
C	2.82982	5.13232	-1.44307
C	1.43227	3.76753	-3.51446
C	-0.44329	4.67936	2.90236
C	2.30932	4.40734	2.15868
H	0.60060	-1.23581	1.64396
H	0.87753	-1.52330	4.07679
H	0.96046	2.72373	4.59170
H	1.06598	0.46330	5.55076
H	2.65972	-0.96367	-0.33299
H	4.94877	-1.00860	-1.24105
H	4.54191	3.04763	-2.54428
H	5.89332	1.00346	-2.34190
H	-0.84417	3.03121	-1.83627
H	2.23412	6.03840	-1.57429
H	3.23387	5.12153	-0.43143
H	3.65513	5.14790	-2.15856
H	0.82624	4.64951	-3.73275
H	2.37080	3.81823	-4.07217
H	0.87502	2.88064	-3.81761
H	-0.12441	4.62283	3.94530
H	-0.42696	5.72279	2.57848
H	-1.45840	4.29345	2.79772
H	2.52822	4.36165	3.22839
H	3.06806	3.83248	1.62390
H	2.34888	5.44960	1.83343

$TS_{D4/C5}$

E(RB3PW91) = -2732.72400663 a.u.

Ir	0.36861	3.86020	-0.26302
Cl	-2.35485	3.57172	-0.54198
Cl	-0.58466	0.11029	-0.81779
P	1.87335	3.61673	-1.94436
P	0.42174	3.75993	2.12697
Si	0.77908	1.50743	-0.01063
O	0.22557	6.91451	-0.58931
C	0.89460	1.03784	1.82782
C	1.08100	-0.26565	2.30621
C	0.79872	2.07919	2.76187
C	1.20689	-0.51938	3.66569
C	0.92242	1.82441	4.13144
C	1.13629	0.52859	4.58087
C	2.40827	1.10305	-0.90174
C	3.13655	-0.08602	-0.78501
C	2.88357	2.09093	-1.77480
C	4.31033	-0.27951	-1.50239
C	4.05570	1.89221	-2.51018
C	4.77100	0.71036	-2.36695
C	0.25602	5.77657	-0.44806
C	3.10012	4.97687	-2.05680
C	1.24498	3.51531	-3.66845
C	-1.18015	4.17918	2.91145
C	1.61742	4.86675	2.97244
H	1.10900	-1.09558	1.60689
H	1.35394	-1.53580	4.01666
H	0.84362	2.63014	4.85554
H	1.23286	0.33258	5.64374
H	2.78505	-0.87294	-0.12564
H	4.86788	-1.20412	-1.39204
H	4.42106	2.65168	-3.19461
H	5.68554	0.55988	-2.93124

H	-0.88042	3.58331	-1.33051
H	2.57383	5.91805	-2.22817
H	3.64441	5.04613	-1.11433
H	3.80458	4.81485	-2.87593
H	0.68159	4.42286	-3.89689
H	2.06038	3.39785	-4.38725
H	0.56982	2.66131	-3.74365
H	-1.15194	4.01881	3.99206
H	-1.41999	5.22321	2.69884
H	-1.95541	3.55643	2.46220
H	1.56180	4.76518	4.05923
H	2.62721	4.62464	2.63855
H	1.39715	5.90077	2.69944

E1

E(RB3PW91) = -4981.33339458

Ir	7.69914	6.84679	8.94016
Ge	9.05763	8.04246	6.82939
Cl	10.39318	8.84463	4.91988
Cl	9.59460	6.00127	5.94703
P	6.59624	5.37317	10.46763
P	6.03648	6.90968	7.29948
P	9.87918	6.95411	9.78296
O	6.93204	9.60424	10.08146
C	7.21530	8.57484	9.66184
C	7.45071	8.95491	6.05648
C	7.55868	10.11990	5.29236
C	6.42995	10.74916	4.78068
C	5.17086	10.19578	4.97959
C	5.04591	9.02589	5.71625
C	6.17682	8.41873	6.27452
C	10.30959	9.05669	8.02459
C	10.84248	10.29099	7.64531
C	11.66287	11.01134	8.50563
C	12.01394	10.48114	9.74092
C	11.51590	9.24241	10.12305
C	10.64449	8.54121	9.28170
C	4.29595	6.97044	7.89678
C	5.98904	5.52774	6.09893
C	5.80894	3.91181	9.67186
C	5.22541	6.06277	11.48641
C	7.55124	4.49964	11.77931
C	11.04062	5.64824	9.23658
C	10.13078	6.92010	11.60487
H	8.16862	5.45501	8.24705
H	8.54060	10.52160	5.07809
H	6.53884	11.66630	4.21061
H	4.28805	10.67047	4.56363
H	4.05879	8.60039	5.85790
H	10.62633	10.68105	6.65932
H	12.04009	11.98241	8.20119
H	12.67218	11.02801	10.40830
H	11.80339	8.84060	11.08765
H	3.58028	6.92915	7.07290
H	4.10591	6.11755	8.54912
H	4.13831	7.88834	8.46640
H	5.76531	4.59353	6.61790
H	5.23033	5.71821	5.33589
H	6.97084	5.43903	5.63189
H	5.30667	3.28045	10.41061
H	5.08187	4.22059	8.92023
H	6.58513	3.33179	9.16825
H	4.45220	6.48904	10.84581
H	4.77749	5.29683	12.12673
H	5.62014	6.86587	12.11290
H	7.88075	5.21034	12.53786
H	6.92648	3.74258	12.26257
H	8.42440	4.00947	11.34439
H	11.04843	5.60795	8.14696
H	12.04663	5.85634	9.60898
H	10.69862	4.68209	9.61508
H	9.79833	5.95847	11.99242
H	11.18737	7.03198	11.85758
H	9.55795	7.71722	12.08213

$TS_{E1/E2}$

E(RB3PW91) = -4981.34036193

Ir	7.65005	6.88075	8.98200
Ge	8.87802	8.09077	7.07368
Cl	10.53318	9.53694	4.48031
Cl	9.71339	6.44013	5.86518
P	6.59686	5.31116	10.45274
P	5.96685	6.93278	7.33570
P	9.81661	7.03741	9.89380
O	6.72843	9.52812	10.27016
C	7.06906	8.54528	9.79338
C	7.39147	8.99473	6.13556
C	7.52947	10.12573	5.32963
C	6.40991	10.71168	4.74721
C	5.14708	10.16109	4.93008
C	4.99715	9.02104	5.70967
C	6.11386	8.44803	6.32711

C	10.29554	9.06423	8.04335
C	10.94310	10.20362	7.56380
C	11.90012	10.84571	8.34307
C	12.24824	10.34195	9.59024
C	11.63009	9.19353	10.06903
C	10.64064	8.56236	9.30746
C	4.22549	6.94377	7.92001
C	6.00651	5.56271	6.12397
C	5.83606	3.87070	9.60079
C	5.22438	5.93632	11.50506
C	7.60040	4.41954	11.71065
C	10.94734	5.67709	9.42671
C	9.99038	7.11448	11.72015
H	8.18142	5.53624	8.24380
H	8.52897	10.49654	5.11403
H	6.53417	11.59642	4.13129
H	4.27722	10.61260	4.46372
H	4.00759	8.59516	5.83423
H	10.73278	10.53752	6.54992
H	12.38674	11.73670	7.95983
H	13.00400	10.83626	10.19236
H	11.92256	8.80792	11.03899
H	3.52397	6.91940	7.08373
H	4.03705	6.06897	8.54346
H	4.04775	7.84384	8.51158
H	5.81271	4.60938	6.61895
H	5.26320	5.73292	5.34142
H	7.00261	5.53070	5.67833
H	5.35565	3.20121	10.3197
H	5.09260	4.19451	8.87206
H	6.61767	3.32614	9.06695
H	4.43797	6.37057	10.88616
H	4.79748	5.13661	12.11694
H	5.60717	6.72168	12.16058
H	7.88850	5.10175	12.51084
H	7.01719	3.60408	12.14763
H	8.49916	4.00344	11.25239
H	10.97430	5.60895	8.33774
H	11.95325	5.87469	9.80440
H	10.57929	4.73115	9.83022
H	9.61597	6.19332	12.16341
H	11.03754	7.22233	12.00929
H	9.42214	7.96012	12.11155

E2

E(RB3PW91) = -4981.35326752

Ir	7.58806	6.84708	8.99850
Ge	8.79444	8.07878	7.19954
Cl	10.31270	11.99840	4.80431
Cl	9.80490	6.65513	5.82453
P	6.64665	5.18938	10.44484
P	5.90648	6.93107	7.32502
P	9.71746	7.10124	10.01342
O	6.50245	9.39307	10.36102
C	6.90719	8.45159	9.85519
C	7.42409	8.93740	6.11268
C	7.64584	10.00860	5.24684
C	6.58457	10.51464	4.50030
C	5.31822	9.94793	4.59246
C	5.09279	8.87227	5.44558
C	6.14407	8.37097	6.21894
C	10.24692	9.04058	8.07296
C	10.93815	10.11618	7.51475
C	11.98908	10.69430	8.22226
C	12.36869	10.19494	9.46333
C	11.68948	9.11692	10.02174
C	10.61650	8.54338	9.33248
C	4.18109	7.11211	7.92576
H	8.18182	5.53969	8.23661
H	8.62486	10.49530	5.14241
H	6.77006	11.36180	3.84825
H	4.49700	10.34422	4.00373
H	4.09711	8.44439	5.50273
H	10.67268	10.55261	6.54279
H	12.50179	11.54348	7.78264
H	13.19323	10.64625	10.00601
H	12.00055	8.74182	10.99161
H	3.46942	7.09612	7.09801
H	3.92911	6.30219	8.61116
H	4.08625	8.06205	8.45483
H	5.58584	4.58386	6.74246
H	5.11556	5.66812	5.40420
H	6.83520	5.36705	5.75022
H	5.20677	3.21412	10.37273
H	4.72149	4.40431	9.14842
H	6.15980	3.40606	8.88240
H	4.76501	6.37533	11.42563
H	5.19584	4.95958	12.41582
H	6.18197	6.44068	12.47628
H	8.48816	4.61918	11.96129
H	7.27213	3.33032	11.90140
H	8.41878	3.53793	10.55933

H	10.99138	5.51787	8.72617
H	11.84766	5.94981	10.22495
H	10.48382	4.79883	10.27042
H	9.16030	6.60567	12.33586
H	10.71229	7.45346	12.22846
H	9.19344	8.35044	12.01965

E3

E(RB3PW91) = -4981.35934177

Ir	7.60654	7.03079	8.95360
Ge	8.75952	8.34103	7.23086
Cl	9.89712	7.27722	5.65850
Cl	8.55128	3.37146	7.73845
P	6.73848	5.26011	10.32785
P	5.96431	7.04468	7.26572
P	9.74685	7.19984	9.92009
O	6.41646	9.46124	10.47127
C	6.86174	8.56728	9.90937
C	7.36062	9.22751	6.17831
C	7.51011	10.34761	5.35969
C	6.43756	10.82904	4.61754
C	5.21062	10.17519	4.66641
C	5.05421	9.04476	5.45990
C	6.12192	8.57078	6.22795
C	10.18257	9.33400	8.14778
C	10.84416	10.46969	7.67914
C	11.88142	11.03618	8.41120
C	12.28519	10.45318	9.60799
C	11.65078	9.30786	10.07482
C	10.59059	8.74792	9.35529
C	4.20833	7.10639	7.79803
C	6.08507	5.66697	6.07930
C	5.65073	4.04785	9.49937
C	5.74355	5.81868	11.77166
C	7.96146	4.11695	11.06019
C	10.89634	5.86088	9.46272
C	9.83603	7.33784	11.74854
H	8.18849	5.70429	8.19173
H	8.46912	10.85085	5.29371
H	6.55933	11.70982	3.99552
H	4.37356	10.54282	4.08220
H	4.09273	8.54274	5.47279
H	10.55482	10.91809	6.73443
H	12.38025	11.92797	8.04597
H	13.09965	10.88752	10.17820
H	11.99109	8.86213	11.00345
H	3.52622	7.02302	6.94937
H	4.00243	6.28625	8.48458
H	4.02668	8.04935	8.31755
H	6.07878	4.71389	6.61151
H	5.28306	5.71448	5.33835
H	7.05629	5.73225	5.58472
H	5.30998	3.30577	10.22673
H	4.78208	4.52001	9.04093
H	6.26969	3.55692	8.73659
H	4.88133	6.39550	11.42939
H	5.38980	4.96238	12.35301
H	6.34640	6.46126	12.41713
H	8.68623	4.63237	11.68988
H	7.44112	3.36624	11.66151
H	8.46301	3.62592	10.21518
H	11.00701	5.86576	8.37659
H	11.86934	6.00147	9.93987
H	10.46549	4.89291	9.72394
H	9.29118	6.51254	12.20589
H	10.86740	7.30998	12.10698
H	9.37071	8.27574	12.05804

F1

E(RB3PW91) = -4981.32955132

Ir	-0.15534	0.62017	-0.88722
Ge	0.50858	-1.93607	-0.07865
Cl	0.17599	-2.68060	-2.19978
Cl	0.97519	-4.28930	0.36119
P	2.16910	0.68412	-1.13762
P	-0.37885	0.85723	1.47649
P	-0.70442	2.80925	-1.67820
O	-2.91208	-0.61970	-1.21571
C	-0.82416	-1.91936	1.42962
C	-1.46956	-3.07788	1.86730
C	-1.05092	-0.72324	2.13173
C	-2.30407	-3.06103	2.97926
C	-1.84217	-0.72692	3.28625
C	-2.47144	-1.89041	3.70863
C	2.35643	-1.47166	0.58470
C	2.97938	-2.23944	1.57393
C	3.02177	-0.33217	0.11767
C	4.21748	-1.87486	2.09266
C	4.28693	0.01000	0.60799
C	4.88142	-0.75645	1.60182
C	-1.87753	-0.15757	-1.04428
C	3.04915	2.29952	-1.09139

C	2.76261	0.00803	-2.73586
C	-1.61500	2.10353	2.03420
C	1.04230	1.26513	2.56856
C	-0.24645	3.11957	-3.43244
C	-2.51079	3.15300	-1.72810
C	-0.08170	4.34645	-0.87095
H	-1.29722	-4.00564	1.33629
H	-2.80984	-3.97162	3.28434
H	-1.99204	0.18338	3.85717
H	-3.09816	-1.87638	4.59453
H	2.48821	-3.13653	1.92973
H	4.66841	-2.47615	2.87579
H	4.81313	0.87980	0.23063
H	5.85655	-0.47958	1.98963
H	-0.03721	0.22860	-2.44757
H	2.61751	2.94828	-1.85570
H	2.92761	2.77214	-0.11540
H	4.11337	2.18583	-1.30985
H	2.39466	0.63063	-3.55461
H	3.85496	-0.02317	-2.75486
H	2.36056	-0.99846	-2.86115
H	-1.68601	2.15948	3.12257
H	-1.32074	3.08664	1.66250
H	-2.59409	1.85021	1.62420
H	0.72701	1.24457	3.61486
H	1.84134	0.53846	2.42346
H	1.41990	2.26183	2.32649
H	-0.59383	4.10020	-3.77088
H	0.83725	3.06444	-3.55388
H	-0.69240	2.34090	-4.05411
H	-2.71850	4.11995	-2.19569
H	-3.01353	2.36617	-2.29413
H	-2.91712	3.15331	-0.71507
H	1.00549	4.39525	-0.94274
H	-0.50719	5.23725	-1.34313
H	-0.34944	4.34815	0.18676

$TS_{F1/F2}$

E(RB3PW91) = -4981.33460623

Ir	-0.18087	0.63475	-0.85918
Ge	0.42915	-1.72220	-0.02927
Cl	0.99095	-4.83938	0.92158
Cl	0.06691	-2.96883	-1.78719
P	2.16278	0.77563	-1.04631
P	-0.44367	0.93391	1.51323
P	-0.7137	2.79717	-1.75744
O	-2.98553	-0.49514	-1.19550
C	-0.81413	-1.84682	1.50698
C	-1.38429	-3.03357	1.96913
C	-1.08901	-0.64571	2.18640
C	-2.20434	-3.02788	3.09303
C	-1.87521	-0.65964	3.34413
C	-2.43462	-1.84921	3.79299
C	2.33543	-1.51422	0.50944
C	2.99499	-2.41777	1.34724
C	3.01552	-0.35854	0.09771
C	4.29673	-2.16465	1.76920
C	4.33269	-0.12066	0.50640
C	4.96914	-1.02228	1.35004
C	-1.94113	-0.06427	-1.02687
C	2.98408	2.40335	-0.81666
C	2.77106	0.26119	-2.69697
C	-1.67487	2.19005	2.04723
C	1.00002	1.36047	2.56360
C	-0.05962	3.10653	-3.44622
C	-2.51255	3.06010	-2.02075
C	-0.25091	4.35048	-0.88385
H	-1.13308	-3.96287	1.46624
H	-2.64816	-3.95835	3.43174
H	-2.07257	0.25390	3.89516
H	-3.05601	-1.85021	4.68289
H	2.47677	-3.33508	1.62929
H	4.78826	-2.87542	2.42589
H	4.86900	0.76364	0.17916
H	5.98736	-0.83128	1.67410
H	-0.01108	0.16257	-2.39318
H	2.55960	3.11875	-1.52298
H	2.82064	2.76712	0.19871
H	4.05743	2.34017	-1.00598
H	2.37393	0.92319	-3.46924
H	3.86341	0.27393	-2.72048
H	2.41676	-0.75283	-2.89053
H	-1.76652	2.23288	3.13442
H	-1.35904	3.17286	1.69340
H	-2.64867	1.95155	1.61639
H	0.72329	1.29902	3.61893
H	1.81303	0.66000	2.36894
H	1.33901	2.37505	2.33937
H	-0.43745	4.05026	-3.84980
H	1.03151	3.14227	-3.43482
H	-0.36493	2.28577	-4.09778
H	-2.70459	4.03024	-2.48733

H	-2.90583	2.27079	-2.66458
H	-3.03933	3.01364	-1.06553
H	0.81450	4.35407	-0.65228
H	-0.48862	5.22642	-1.49442
H	-0.80314	4.42242	0.05415

F2

E(RB3PW91) = -4981.34795187

Ir	-0.23286	0.68075	-0.94891
Ge	0.27116	-1.60607	-0.07704
Cl	1.29809	-5.41767	2.33110
Cl	-0.28802	-3.24170	-1.40233
P	2.14730	0.81164	-0.94494
P	-0.73967	1.04068	1.39932
P	-0.64126	2.87898	-1.82428
O	-3.02177	-0.38147	-1.53098
C	-0.71563	-1.74896	1.60632
C	-0.91921	-2.96534	2.26086
C	-1.10925	-0.55061	2.22201
C	-1.52819	-2.98172	3.51240
C	-1.71805	-0.57884	3.48149
C	-1.93365	-1.79672	4.11680
C	2.19421	-1.67610	0.27994
C	2.79811	-2.77549	0.89576
C	2.94735	-0.52983	-0.00170
C	4.14875	-2.71554	1.22644
C	4.30715	-0.48282	0.32757
C	4.90002	-1.57783	0.94561
C	-1.98788	0.02942	-1.27656
C	2.96655	2.36003	-0.39519
C	2.84568	0.58554	-2.62686
C	-2.23192	2.06454	1.72134
C	0.52226	1.82297	2.47925
C	0.19898	3.28195	-3.40575
C	-2.39951	3.16046	-2.26675
C	-0.26785	4.36880	-0.81342
H	-0.54390	-3.90322	1.84972
H	-1.65442	-3.93312	4.01744
H	-2.02611	0.33640	3.97802
H	-2.40720	-1.81518	5.09319
H	2.22918	-3.67497	1.17136
H	4.60039	-3.56979	1.72010
H	4.91203	0.39160	0.10918
H	5.95228	-1.53835	1.20904
H	0.07845	0.21353	-2.46296
H	2.66203	3.18678	-1.03968
H	2.69360	2.58738	0.63503
H	4.05201	2.26507	-0.45955
H	2.46392	1.34219	-3.31346
H	3.93647	0.63579	-2.58805
H	2.54852	-0.39914	-2.99045
H	-2.44453	2.12202	2.79063
H	-2.08910	3.07879	1.34502
H	-3.09040	1.61521	1.21905
H	0.15684	1.87596	3.50761
H	1.42786	1.21300	2.46773
H	0.75538	2.83084	2.12765
H	-0.17447	4.22518	-3.81417
H	1.27633	3.37214	-3.25501
H	0.01654	2.48029	-4.12353
H	-2.54692	4.16762	-2.66584
H	-2.70695	2.43151	-3.01924
H	-3.03072	3.02853	-1.38609
H	0.77433	4.35746	-0.49338
H	-0.45527	5.28093	-1.38684
H	-0.89655	4.38384	0.07797

F3

E(RB3PW91) = -4981.35387620

Ir	-0.24493	0.53527	-0.83537
Ge	0.11609	-1.63652	0.24257
Cl	-0.95056	-3.47128	-0.33832
Cl	1.19774	-0.63779	-3.92110
P	2.09923	0.68842	-0.43329
P	-1.18983	1.11534	1.33614
P	-0.44260	2.62210	-1.96559
O	-2.71582	-0.56708	-2.21651
C	-0.35288	-1.42481	2.15983
C	-0.17238	-2.44870	3.09463
C	-0.82791	-0.18170	2.59937
C	-0.43542	-2.23982	4.44246
C	-1.09857	0.02286	3.95803
C	-0.89460	-0.99875	4.87591
C	2.02757	-2.05204	0.16161
C	2.59284	-3.30718	0.38777
C	2.85805	-0.95521	-0.08117
C	3.97342	-3.46604	0.38751
C	4.24686	-1.11427	-0.05905
C	4.80033	-2.36665	0.17442
C	-1.80201	-0.14425	-1.67298
C	2.67474	1.69919	0.99430
C	3.09542	1.32774	-1.82460

C	-3.03268	1.11239	1.35034
C	-0.83960	2.70266	2.20569
C	-0.00045	2.60481	-3.73632
C	-2.15798	3.28423	-2.00952
C	0.46566	4.08694	-1.32025
H	0.17792	-3.42208	2.76505
H	-0.28309	-3.04264	5.15677
H	-1.47490	0.97734	4.31257
H	-1.10107	-0.82950	5.92773
H	1.94922	-4.16755	0.54209
H	4.40714	-4.44789	0.54739
H	4.90843	-0.27356	-0.24301
H	5.87853	-2.48765	0.17165
H	0.44501	-0.08201	-2.28940
H	2.35067	2.73468	0.86902
H	2.24842	1.29786	1.91591
H	3.76437	1.67351	1.07278
H	2.85451	2.37594	-2.00905
H	4.16226	1.25053	-1.60675
H	2.84072	0.73303	-2.71032
H	-3.42065	1.27537	2.35931
H	-3.41539	1.88853	0.68432
H	-3.38457	0.14448	0.98891
H	-1.38618	2.78852	3.14808
H	0.22870	2.79376	2.40493
H	-1.14600	3.52997	1.56137
H	-0.14616	3.59494	-4.17788
H	1.02819	2.26877	-3.86809
H	-0.61787	1.86510	-4.24917
H	-2.20365	4.19369	-2.61528
H	-2.82823	2.53949	-2.44225
H	-2.50306	3.51648	-0.99992
H	1.54325	3.92698	-1.37167
H	0.22042	4.97428	-1.91078
H	0.19382	4.26712	-0.27885

G1

E(RB3PW91) = -4520.22813590

Ir	7.74451	7.07896	8.71020
Ge	9.09040	8.29249	6.69430
Cl	10.32175	9.07317	4.86382
Cl	9.56605	6.20671	6.04617
P	5.98690	6.96526	7.22075
P	9.78504	7.02418	9.78826
O	6.92011	9.77143	9.87717
C	7.28808	8.81704	9.35082
C	7.37452	9.06437	5.98152
C	7.43114	10.25145	5.24712
C	6.28431	10.82006	4.70257
C	5.05764	10.18618	4.84404
C	4.98204	9.00045	5.56327
C	6.12135	8.44744	6.15440
C	10.36456	9.11723	8.01403
C	10.99232	10.31818	7.67406
C	11.90451	10.92502	8.53122
C	12.24350	10.31669	9.73184
C	11.63813	9.11710	10.08329
C	10.68474	8.52521	9.25016
C	4.29902	7.01775	7.93815
C	5.90048	5.53664	6.08229
C	10.90839	5.61926	9.45888
C	9.74549	7.09472	11.62118
H	7.93619	5.46128	8.45718
H	8.38693	10.73070	5.07833
H	6.35849	11.75304	4.15350
H	4.16225	10.61209	4.40348
H	4.01852	8.51429	5.67644
H	10.78318	10.77850	6.71698
H	12.36028	11.86794	8.24731
H	12.97031	10.77302	10.39574
H	11.90342	8.65123	11.02673
H	3.52108	6.93232	7.17578
H	4.20282	6.17868	8.63085
H	4.16455	7.94564	8.49628
H	5.72243	4.63163	6.66726
H	5.09835	5.67293	5.35266
H	6.85564	5.43496	5.56685
H	11.03002	5.50755	8.38130
H	11.88209	5.78517	9.92668
H	10.45543	4.70760	9.85474
H	9.15640	6.24630	11.97665
H	10.74387	7.03409	12.06039
H	9.25774	8.01560	11.94471

$TS_{G1/G2}$

E(RB3PW91) = -4520.21911773

Ir	7.66816	7.03521	8.82326
Ge	8.84253	8.27210	7.06039
Cl	10.57258	10.83376	4.44599
Cl	9.75874	6.77768	5.75613
P	5.90049	6.97245	7.29009
P	9.75134	7.03189	9.89300

O	6.70693	9.62904	10.19264
C	7.07844	8.68837	9.66313
C	7.32384	9.06140	6.08738
C	7.47147	10.15602	5.23808
C	6.36456	10.64659	4.54784
C	5.11919	10.04776	4.68524
C	4.96900	8.94177	5.51555
C	6.06396	8.44570	6.22579
C	10.28481	9.11521	8.10057
C	10.98902	10.22368	7.63508
C	12.02598	10.75284	8.40122
C	12.37519	10.17877	9.61638
C	11.69088	9.05860	10.07712
C	10.63977	8.52356	9.32955
C	4.21126	7.01225	7.99810
C	5.86888	5.53813	6.15904
C	10.84888	5.62114	9.51615
C	9.71967	7.09042	11.7237
H	8.11690	5.60873	8.18133
H	8.46196	10.59699	5.06614
H	6.49465	11.49936	3.88982
H	4.26157	10.43266	4.14299
H	3.99313	8.47539	5.60659
H	10.77071	10.64570	6.64573
H	12.56569	11.61586	8.02572
H	13.18533	10.59365	10.20736
H	11.98234	8.61229	11.02267
H	3.44916	6.95453	7.21777
H	4.08896	6.15730	8.66703
H	4.07240	7.93083	8.57037
H	5.70936	4.62419	6.73567
H	5.07582	5.65193	5.41622
H	6.83353	5.47068	5.65363
H	10.96188	5.54664	8.43348
H	11.82990	5.76441	9.97518
H	10.39585	4.69908	9.88736
H	9.16448	6.22579	12.09467
H	10.72780	7.06046	12.14256
H	9.21795	8.00075	12.0556

G2

E(RB3PW91) = -4520.22222928

Ir	7.65282	7.00264	8.84512
Ge	8.81715	8.21798	7.09630
Cl	10.28535	11.92508	4.83476
Cl	9.76068	6.77012	5.74054
P	5.88770	6.95224	7.29451
P	9.74657	7.01875	9.91361
O	6.66928	9.58539	10.22894
C	7.04380	8.64563	9.70206
C	7.34416	9.02009	6.09120
C	7.52337	10.11498	5.25011
C	6.43856	10.59937	4.52065
C	5.19229	9.99298	4.61562
C	5.01155	8.89345	5.45020
C	6.08254	8.40285	6.19911
C	10.27868	9.06725	8.07765
C	10.96995	10.16803	7.57875
C	12.04262	10.68547	8.30324
C	12.43315	10.10540	9.50357
C	11.74894	8.99995	10.00157
C	10.66268	8.47648	9.29763
C	4.19516	7.04365	7.98913
C	5.83386	5.49282	6.19631
C	10.81967	5.57512	9.59320
C	9.71821	7.15247	11.74022
H	8.12688	5.59993	8.17570
H	8.49367	10.62494	5.14453
H	6.58999	11.46048	3.87831
H	4.35272	10.37426	4.04340
H	4.03090	8.43252	5.51531
H	10.69444	10.65771	6.63170
H	12.56456	11.55072	7.90835
H	13.27093	10.51166	10.06105
H	12.06704	8.55980	10.94160
H	3.43923	6.99738	7.20210
H	4.04341	6.20090	8.66742
H	4.07558	7.97322	8.54780
H	5.65286	4.59522	6.79196
H	5.04683	5.60482	5.44683
H	6.79907	5.39463	5.69711
H	10.93398	5.45733	8.51456
H	11.80218	5.71882	10.04889
H	10.35143	4.67520	9.99835
H	9.15906	6.30816	12.14996
H	10.72757	7.13583	12.15677
H	9.22387	8.07983	12.03366

G3

E(RB3PW91) = -4520.28364233

Ir	7.64240	6.95676	8.85955
Ge	8.78301	8.15667	7.14269

Cl	6.55735	5.42417	10.50114
Cl	9.84270	6.97518	5.57434
P	5.90144	6.95891	7.31135
P	9.71455	7.04062	9.91854
O	6.54985	9.43288	10.35790
C	6.95859	8.52323	9.79992
C	7.36785	9.03539	6.08679
C	7.52322	10.12280	5.22647
C	6.44154	10.62213	4.50835
C	5.19259	10.02188	4.62602
C	5.02542	8.92407	5.46253
C	6.10228	8.42795	6.20197
C	10.28567	9.06695	8.03746
C	11.02222	10.14066	7.53560
C	12.09431	10.66411	8.25045
C	12.45712	10.10166	9.46958
C	11.74792	9.01723	9.97312
C	10.65754	8.49655	9.27034
C	4.21105	7.05827	7.99795
C	5.84064	5.52040	6.18687
C	10.80914	5.60520	9.63809
C	9.67817	7.22127	11.73642
H	8.17109	5.61347	8.12904
H	8.49585	10.58994	5.11038
H	6.57358	11.47815	3.85458
H	4.34710	10.40728	4.06588
H	4.04546	8.46355	5.54028
H	10.76320	10.57630	6.57596
H	12.64931	11.50857	7.85488
H	13.29462	10.50529	10.02887
H	12.04909	8.58526	10.92252
H	3.44263	6.93238	7.23185
H	4.12333	6.26267	8.74222
H	4.07442	8.01619	8.50262
H	5.68097	4.62415	6.79045
H	5.03777	5.62513	5.45301
H	6.79958	5.43157	5.67410
H	10.95132	5.47260	8.56460
H	11.77774	5.74549	10.12422
H	10.31410	4.71789	10.03898
H	9.02824	6.43124	12.12110
H	10.67066	7.13161	12.18337
H	9.24116	8.18548	12.00134

$TS_{G1/G4}$

E(RB3PW91) = -4520.22031070

Ir	7.86576	6.93156	8.53474
Ge	9.01744	8.40246	6.79964
Cl	10.29346	8.83948	4.91499
Cl	9.33107	6.08678	6.37803
P	6.00395	6.95963	7.15005
P	9.84362	7.02259	9.74558
O	6.80476	9.28569	10.04164
C	7.26229	8.44412	9.38784
C	7.35249	9.14990	5.98222
C	7.40365	10.31734	5.21712
C	6.25507	10.84794	4.64052
C	5.04063	10.18607	4.77509
C	4.97849	9.00611	5.50532
C	6.11815	8.49204	6.13169
C	10.37024	9.20530	8.03378
C	11.03024	10.38672	7.68745
C	11.97410	10.95583	8.53513
C	12.31473	10.31981	9.72280
C	11.69229	9.12658	10.06640
C	10.70463	8.57374	9.24530
C	4.38218	7.04601	7.99252
C	5.79952	5.59524	5.95114
C	11.06745	5.68736	9.49904
C	9.66546	7.11691	11.56395
H	7.64701	5.30812	8.90512
H	8.35534	10.81010	5.05546
H	6.31419	11.77033	4.07199
H	4.14402	10.58365	4.31117
H	4.02626	8.49230	5.59297
H	10.81663	10.85985	6.73608
H	12.45499	11.88819	8.25772
H	13.06502	10.74787	10.37936
H	11.97686	8.63325	10.99056
H	3.55074	7.07322	7.28488
H	4.28656	6.15977	8.62308
H	4.34749	7.93129	8.62920
H	5.61960	4.67013	6.50258
H	4.96450	5.79725	5.27566
H	6.71939	5.48644	5.37630
H	11.26656	5.57870	8.43271
H	11.99737	5.91482	10.02612
H	10.64434	4.75279	9.87308
H	9.14020	6.21818	11.89344
H	10.63150	7.17211	12.07034
H	9.06471	7.98798	11.82953

G4

E(RB3PW91) = -4520.27161550

Ir	7.74572	6.33815	8.73456
Ge	8.91805	7.62714	6.97026
Cl	10.06429	6.71767	5.30134
Cl	8.35353	4.13847	7.89182
P	5.99906	6.47608	7.16438
P	9.84769	6.53902	9.77029
O	6.71450	8.74845	10.19124
C	7.12170	7.84105	9.61582
C	7.47132	8.59998	6.03273
C	7.61910	9.73390	5.23179
C	6.52087	10.31933	4.61139
C	5.25633	9.76207	4.76889
C	5.09263	8.61956	5.54325
C	6.19098	8.03519	6.18155
C	10.30163	8.64745	7.95123
C	10.96309	9.79067	7.49902
C	11.93198	10.41213	8.27917
C	12.26761	9.88219	9.52044
C	11.63742	8.73064	9.97744
C	10.65163	8.10973	9.20403
C	4.29952	6.52788	7.84297
C	5.93181	5.15231	5.91138
C	11.06655	5.23850	9.38370
C	9.84913	6.61717	11.59938
H	6.97159	5.47609	9.89562
H	8.60267	10.16865	5.08564
H	6.65077	11.20869	4.00310
H	4.39625	10.21407	4.28595
H	4.10017	8.19286	5.64596
H	10.72344	10.20414	6.52468
H	12.42727	11.30808	7.91891
H	13.02371	10.36218	10.13295
H	11.92106	8.32567	10.94339
H	3.53902	6.55011	7.05922
H	4.16220	5.62849	8.44654
H	4.18399	7.39976	8.48902
H	5.74804	4.19862	6.40827
H	5.14250	5.36967	5.18746
H	6.89694	5.08688	5.40791
H	11.16907	5.15752	8.30106
H	12.02946	5.48728	9.83693
H	10.69993	4.28142	9.75759
H	9.36637	5.70860	11.96493
H	10.85858	6.67469	12.01257
H	9.26714	7.47718	11.93497

$TS_{G4/G5}$

E(RB3PW91) = -4520.23162120

Ir	7.72365	6.34263	8.75442
Ge	8.91098	7.60259	6.96402
Cl	10.01876	6.63533	5.29069
Cl	8.20594	3.70771	8.15481
P	5.99621	6.54902	7.18365
P	9.79960	6.64350	9.79825
O	6.11829	7.46423	11.03112
C	6.72257	6.97230	10.17836
C	7.49772	8.60818	6.01983
C	7.68032	9.72902	5.20826
C	6.59654	10.34630	4.59322
C	5.31487	9.83393	4.76644
C	5.11818	8.70308	5.55051
C	6.20294	8.08893	6.18294
C	10.32613	8.62537	7.88302
C	11.02676	9.71342	7.35927
C	12.01773	10.34567	8.10156
C	12.33518	9.88077	9.37395
C	11.66589	8.78211	9.89964
C	10.65832	8.15225	9.16245
C	4.29129	6.62650	7.84752
C	5.91406	5.21355	5.93682
C	11.01381	5.30153	9.53093
C	9.77268	6.84037	11.61913
H	7.43170	4.80013	9.25961
H	8.67644	10.13003	5.05174
H	6.75072	11.22667	3.97760
H	4.46680	10.31241	4.28775
H	4.11302	8.31081	5.66512
H	10.80331	10.07229	6.35988
H	12.54539	11.19899	7.68781
H	13.10932	10.36970	9.95613
H	11.93743	8.42464	10.88754
H	3.54167	6.66101	7.05403
H	4.12555	5.73029	8.44890
H	4.18426	7.50150	8.49081
H	5.73450	4.26313	6.44248
H	5.12266	5.41747	5.21134
H	6.87613	5.14572	5.42654
H	11.14853	5.15350	8.45850
H	11.97084	5.55434	9.99432
H	10.62031	4.37395	9.95053

H	9.28652	5.96031	12.04518
H	10.77759	6.92503	12.03816
H	9.18994	7.72347	11.88615

G5

E(RB3PW91) = -4520.25258923

Ir	7.69087	6.47255	8.79598
Ge	8.89911	7.61691	6.98040
Cl	9.95328	6.51659	5.35851
Cl	8.21075	3.24344	8.16226
P	5.96644	6.66604	7.24593
P	9.73975	6.77480	9.85392
O	6.05000	5.63630	11.21723
C	6.67603	5.91970	10.29614
C	7.52212	8.63568	6.00184
C	7.73481	9.72374	5.15357
C	6.66815	10.35107	4.51961
C	5.37220	9.88378	4.71433
C	5.14419	8.78850	5.53916
C	6.21222	8.16245	6.18841
C	10.34542	8.63856	7.84685
C	11.08414	9.67624	7.27488
C	12.08851	10.31465	7.99320
C	12.37873	9.90842	9.29214
C	11.66952	8.86140	9.86805
C	10.65071	8.22355	9.15337
C	4.26649	6.82555	7.91321
C	5.81986	5.29295	6.04137
C	10.93128	5.39241	9.68668
C	9.69212	7.07677	11.66225
H	8.00636	4.62376	8.41108
H	8.74180	10.09017	4.98263
H	6.84632	11.20383	3.87239
H	4.53724	10.37005	4.22061
H	4.12778	8.43236	5.67080
H	10.88090	9.98929	6.25595
H	12.64794	11.12709	7.54068
H	13.16305	10.40281	9.85586
H	11.91981	8.54913	10.87663
H	3.51475	6.88275	7.12291
H	4.06040	5.94654	8.52754
H	4.20337	7.71328	8.54472
H	5.60076	4.36703	6.57693
H	5.03328	5.50190	5.31196
H	6.77402	5.16856	5.52672
H	11.10044	5.19661	8.62669
H	11.88056	5.63726	10.16995
H	10.50314	4.49251	10.13268
H	9.19694	6.22679	12.13652
H	10.69116	7.18337	12.09071
H	9.10931	7.97653	11.86632

H1

E(RB3PW91) = -4520.22156812

Ir	0.00978	3.39560	-0.59182
Ge	0.50557	0.78094	0.23186
Cl	-1.70041	0.52680	0.13222
Cl	0.66247	-1.48023	0.77355
P	2.30201	3.30614	-0.98565
P	-0.08226	3.78199	1.70909
O	-2.96547	3.54667	-1.17222
C	1.30112	1.37874	1.97997
C	2.21063	0.52570	2.61457
C	1.01164	2.61168	2.58838
C	2.81857	0.88322	3.81375
C	1.59606	2.94624	3.81358
C	2.50188	2.08939	4.42538
C	1.74617	0.59996	-1.32824
C	1.85336	-0.61639	-2.00366
C	2.60242	1.65203	-1.69771
C	2.79619	-0.79294	-3.01171
C	3.57847	1.45160	-2.67579
C	3.67683	0.23156	-3.33384
C	-1.85949	3.44843	-0.89649
C	3.61051	3.54888	0.28280
C	2.80885	4.50976	-2.27259
C	-1.70639	3.59037	2.54274
C	0.43766	5.45512	2.26790
H	2.43946	-0.43502	2.17146
H	3.53182	0.20698	4.27373
H	1.35649	3.89029	4.29174
H	2.95845	2.36525	5.37035
H	1.20227	-1.43774	-1.73241
H	2.84701	-1.74160	-3.53602
H	4.25323	2.25652	-2.94921
H	4.42816	0.08973	-4.10370
H	0.09764	3.12242	-2.20395
H	3.56847	4.57595	0.65456
H	3.45724	2.86539	1.11820
H	4.59674	3.36862	-0.15260
H	2.55776	5.51337	-1.92199
H	3.88187	4.46570	-2.47343

H	2.24688	4.31330	-3.18574
H	-1.61193	3.72231	3.62344
H	-2.40565	4.33013	2.14489
H	-2.09720	2.59379	2.33156
H	0.29489	5.60553	3.34074
H	1.48519	5.62374	2.01358
H	-0.16818	6.18829	1.73035

$TS_{H1/H2}$

E(RB3PW91) = -4520.21332929

Ir	-0.07746	3.50808	-0.60164
Ge	0.62296	0.58031	0.28708
Cl	-1.50618	0.76667	-0.18081
Cl	0.49897	-1.58763	0.86013
P	2.13547	3.26605	-1.08632
P	-0.10649	3.70903	1.71657
O	-2.60889	5.09713	-1.14243
C	-1.70352	4.43699	-0.88915
C	1.31450	1.29005	2.01007
C	2.21596	0.44336	2.66575
C	1.02009	2.53950	2.58169
C	2.82555	0.82167	3.85687
C	1.61359	2.89157	3.79793
C	2.51646	2.04644	4.43131
C	1.86100	0.47490	-1.25240
C	2.11117	-0.77856	-1.81499
C	2.55362	1.59605	-1.74052
C	3.03018	-0.92573	-2.84913
C	3.49449	1.42906	-2.75856
C	3.73212	0.17705	-3.31455
C	3.46414	3.57686	0.15140
C	2.63521	4.42114	-2.42250
C	-1.71656	3.38918	2.54985
C	0.32764	5.36212	2.39382
H	-0.08840	3.30104	-2.22301
H	2.44404	-0.53008	2.24851
H	3.53216	0.15140	4.33482
H	1.38180	3.84623	4.25659
H	2.97524	2.34726	5.36750
H	1.58319	-1.64956	-1.44723
H	3.19426	-1.90544	-3.28539
H	4.03817	2.28580	-3.14128
H	4.45639	0.06942	-4.11540
H	3.38966	4.61114	0.49653
H	3.35027	2.91157	1.00749
H	4.44882	3.41974	-0.29663
H	2.33746	5.42413	-2.11223
H	3.71301	4.40697	-2.60460
H	2.09127	4.17301	-3.33421
H	-1.61886	3.44977	3.63693
H	-2.44507	4.12800	2.20688
H	-2.07711	2.39788	2.27167
H	0.15047	5.44549	3.46910
H	1.37031	5.59290	2.17097
H	-0.29780	6.09357	1.87783

H2

E(RB3PW91) = -4520.27775777

Ir	-0.17308	3.53324	-0.47315
Ge	0.50503	1.19777	-0.16926
Cl	-2.32725	2.96150	0.55310
Cl	-0.55678	-0.54230	-0.98987
P	1.74107	3.66992	-1.71738
P	0.63571	3.68459	1.80627
O	-1.08283	6.42704	-0.95459
C	-0.74329	5.35464	-0.75055
C	0.63003	0.87777	1.77188
C	0.66998	-0.38558	2.36416
C	0.70772	2.01629	2.58555
C	0.79984	-0.51933	3.74172
C	0.84949	1.87692	3.96963
C	0.89614	0.61325	4.54490
C	2.32761	1.05205	-0.93938
C	3.12999	-0.09082	-0.88498
C	2.83938	2.20570	-1.54718
C	4.41772	-0.08248	-1.40661
C	4.13555	2.21306	-2.07683
C	4.92322	1.07236	-1.99959
C	2.82173	5.12753	-1.44669
C	1.42282	3.76012	-3.51966
C	-0.43892	4.68508	2.89778
C	2.30899	4.36522	2.15649
H	-0.87141	3.09658	-1.85116
H	0.57716	-1.27155	1.74360
H	0.81951	-1.50685	4.19160
H	0.90928	2.75017	4.61230
H	0.99391	0.51319	5.62091
H	2.74228	-0.99819	-0.43223
H	5.03106	-0.97633	-1.35300
H	4.53810	3.10064	-2.55556
H	5.92847	1.08139	-2.40782
H	2.21892	6.03125	-1.55966

H	3.23813	5.10659	-0.44011
H	3.63814	5.15752	-2.17159
H	0.81541	4.64169	-3.73547
H	2.35985	3.81063	-4.07977
H	0.86536	2.87269	-3.82111
H	-0.12356	4.63305	3.94184
H	-0.40269	5.72501	2.56441
H	-1.46090	4.31776	2.79373
H	2.53015	4.32474	3.22589
H	3.05954	3.77772	1.62377
H	2.35960	5.40435	1.82289

$TS_{H2/G5}$

E(RB3PW91) = -4520.22948598

Ir	-0.18482	3.07301	-0.59865
Ge	1.04142	1.02041	0.01548
Cl	0.15019	-1.00022	-0.15309
Cl	-2.65311	1.99565	-0.06889
P	0.96813	2.76782	-2.53743
P	0.35824	3.61957	1.67856
O	-1.27951	5.80420	-1.42572
C	1.60867	1.12742	1.90234
C	2.26703	0.10928	2.59763
C	1.32127	2.32602	2.56506
C	2.65925	0.29167	3.91789
C	1.71719	2.50762	3.89500
C	2.39024	1.49530	4.56563
C	2.58457	0.92067	-1.21137
C	3.70889	0.10653	-1.06068
C	2.49259	1.75223	-2.33295
C	4.73348	0.13290	-1.99955
C	3.51600	1.76599	-3.28652
C	4.63656	0.96304	-3.11325
C	-0.88735	4.77684	-1.09559
C	1.55075	4.32207	-3.31855
C	0.10322	1.92934	-3.92551
C	-1.12189	3.86448	2.72969
C	1.32235	5.16238	1.92549
H	2.45761	-0.84097	2.10860
H	3.17001	-0.50609	4.44767
H	1.49412	3.43193	4.42005
H	2.69282	1.63885	5.59771
H	3.78940	-0.55364	-0.20297
H	5.60860	-0.49522	-1.86669
H	3.45230	2.39918	-4.16582
H	5.43353	0.98298	-3.84936
H	-1.47598	2.24041	-1.23694
H	2.21864	4.84373	-2.63180
H	2.07141	4.12908	-4.25913
H	0.68852	4.96019	-3.52188
H	0.75481	1.82108	-4.79677
H	-0.21806	0.94213	-3.58875
H	-0.78274	2.50784	-4.19694
H	-1.75321	2.97817	2.64907
H	-0.84871	4.03386	3.77389
H	-1.68783	4.71873	2.35191
H	1.51215	5.35461	2.98452
H	2.27367	5.07579	1.39867
H	0.76437	6.00119	1.50433