Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Quantification and classification of substituent effects in organic chemistry: a theoretical molecular electrostatic potential study

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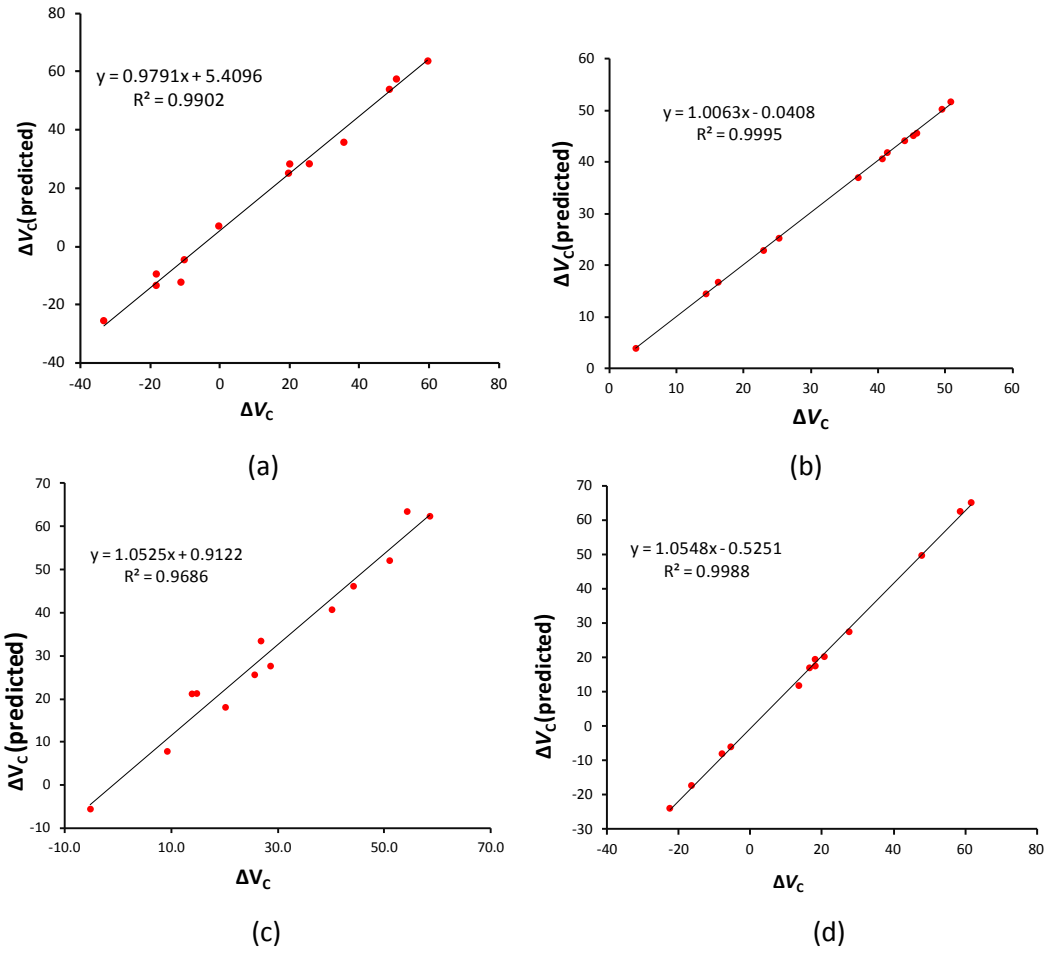
1.Figure S1.Correlation between calculated potential and predicted potential for additivity in (a) pyridine (b) pyrene (c) butadiene (d) butadiyne



2. Table S2.Hammett constant (σ_P) and ΔV_C (kcal/mol) values of all the studied mono substituted benzenes.

substituent	σ_P	ΔV_C	substituent	σ_P	ΔV_C	substituent	σ_P	ΔV_C
SO_2CN	1.26	28.3	$CHCl_2$	0.32	10.0	$NHCOCH_2Cl$	-0.03	2.0
$C(CN)=C(CN)_2$	0.98	27.0	$COOC_6H_5$	0.44	10.0	$P(isopropyl)_2$	0.06	1.8
$SO_2C(CF_3)_3$	1.13	26.4	N=C=S	0.38	10.0	CH_2F	0.11	1.8
N(O)=NCN	0.89	26.3	OCF_2CHFCl	0.28	10.0	$P(C_6H_5)_2$	0.19	1.7
SeO_2CF_3	0.50	26.2	$CHBr_2$	0.32	9.9	$CH_2OC_6H_5$	0.07	1.7
$SO_2CF_2CF_2CF_3$	1.09	25.6	C_6F_5	0.27	9.8	OCOMe	0.31	1.5
N=NCN	1.03	25.4	COMe	0.50	9.7	SH	0.15	1.5
$SO_2CF(CF_3)_2$	1.10	25.3	$SiMeCl_2$	0.39	9.6	$P(CMe_3)_2$	0.15	1.5
SO_2Cl	1.11	25.2	SOMe	0.49	9.6	OCH_2F	0.02	1.4
$C(NO_2)_3$	0.82	25.1	CH_2SCN	0.14	9.6	$P(Et)_2$	0.13	1.3

SO_2CF_3	0.96	24.8	$CONHC_6H_5$	0.41	9.3	NHCHO	0.00	1.3
$SO2CF_2CF_3$	1.08	24.8	$C(OH)(CF_3)_2$	0.30	9.3	C=CMe	0.03	1.3
$CH=NSO_2CF_3$	1.00	23.7	$P(S)Et_2$	0.46	9.2	$NHCSNH_2$	0.16	1.0
SO_2CHF_2	0.86	23.0	$CSNH_2$	0.30	9.2	$CH=CH_2$	-0.04	1.0
$C(CN)_3$	0.96	23.0	$SCHF_2$	0.37	9.1	CH(OH)Me	-0.07	1.0
$CH=C(CN)_2$	0.84	22.8	$CH=NC_6H_5$	0.42	9.0	$Si(Me)_2OMe$	-0.02	0.9
SF_3	0.80	22.5	$N(COMe)_2$	0.33	9.0	OC_6H_4-4F	-0.10	0.8
POF_2	0.89	22.2	COEt	0.48	8.9	$Si(OEt)_3$	-0.01	0.8
PF_4	0.80	22.1	$COCHMe_2$	0.47	8.9	PMe_2	0.06	0.7
GeF_3	0.97	22.0	$SiMeF_2$	0.23	8.9	$Si(NMe_2)_3$	-0.04	0.6
$P(CN)_2$	0.90	21.9	$PO(OMe)_2$	0.53	8.8	$CH=CHC_6H_5$	-0.07	0.7
SF_5	0.68	21.6	CH=CHCOMe	-0.01	8.8	$OCH=CH_2$	-0.09	0.7
NO_2	0.78	21.2	$PO(OC_4H_9)_2$	0.57	8.7	CH_2OMe	0.01	0.6
$P(O)Cl_2$	0.90	20.7	$SCH=NSO_2C_6H_4$-4-Me	0.70	8.7	$Si(C_6H_5)_3$	0.10	0.4
$COCF_2CF_2CF_3$	0.79	20.4	$PO(OPr)_2$	0.50	8.6	$SiH(Me)_2$	0.04	0.3
$P(S)Cl_2$	0.80	19.7	SOC_6H_5	0.44	8.5	$C(OMe)_3$	-0.04	0.3
$COCF_3$	0.80	19.6	$CH=CHCOC_6H_5$	0.05	8.4	$CH_2CH(OH)Me$	-0.25	0.3
$CH=CHSO_2CF_3$	0.55	19.3	COC_6H_5	0.43	8.4	$SiMe(C_6H_5)_2$	0.13	0.2
$N=NCF_3$	0.68	19.3	OCF_3	0.35	8.3	C_6H_5	-0.01	0.2
NO	0.91	19.2	$NHCOCF_3$	0.12	8.2	$P(N(Pr)_2C_6H_4$-3F	0.24	0.1
$N(SO_2CF_3)_2$	0.83	19.2	COOMe	0.45	8.2	$Si(Me)_2OSiMe_3$	-0.01	0.1
COCl	0.61	19.1	$CONH_2$	0.36	8.1	OC_6H_5	-0.03	0.0
SOF	0.83	18.8	$PS(C_6H_5)_2$	0.47	8.1	H	0.00	0.0
COF	0.70	18.4	C_6H_4-3NO_2	0.20	8.1	$C(Me)=CH_2$	0.05	-0.5
CN	0.66	18.0	CH=CHCHO	0.13	8.1	CH_2CH_2COOH	-0.07	-0.3
$CH=CHNO_2$	0.26	17.8	CH_2SCF_3	0.15	8.1	$Si(Me)(OSiMe_3)_2$	-0.01	-0.7
SO_2NH_2	0.60	17.5	$PO(OEt)_2$	0.60	7.8	$OPO(C_3H_7)_2$	0.56	-0.7
$GeCl_3$	0.79	17.3	$P(O)Me_2$	0.50	7.8	$Si(C_6H_5)Me_2$	0.07	-0.7
$P(CF_3)_2$	0.89	17.2	$B(OH)_2$	0.12	7.7	$SiMe_3$	-0.07	-0.9
$SOCF_3$	0.69	17.1	$COC(Me)_3$	0.32	7.6	$CH(OH)C_6H_5$	-0.03	-1.0
SCN	0.52	17.1	Br	0.23	7.6	C_6H_4-4Et	-0.02	-1.1
$CH(CN)_2$	0.52	17.0	$OCHF_2$	0.18	7.5	C_6H_4-4$CHMe_2$	0.01	-1.2
SO_2Me	0.72	16.8	COOEt	0.45	7.5	C_6H_4-4Me	-0.03	-1.2
$C(Me)(NO_2)_2$	0.61	16.5	$SCH=CH_2$	0.20	7.5	C_6H_4-4CMe_3	0.01	-1.2
SeCN	0.66	16.4	$OCHCl_2$	0.26	7.4	$N=CHC_6H_5$	-0.55	-1.3
SC_6H_4-4NO_2	0.24	16.3	C_6Cl_5	0.24	7.4	$GeMe_3$	0.00	-1.4
$NO=NCONH_2$	0.63	16.2	$PS(C_6H_5)C_6H_4$-4Me	0.30	7.3	NHCOMe	0.00	-1.4
SOC_6H_4-4NO_2	0.60	16.2	$PO(Et)_2$	0.47	7.1	$CH(C_6H_5)_2$	-0.05	-1.4
$SOCHF_2$	0.58	16.2	$PO(C_3H_7)_2$	1.10	7.1	SMe	0.00	-1.5
C_6H_2-2,4,6$(NO_2)_3$	0.30	16.2	N=C=O	0.19	7.1	NMeCOMe	0.26	-1.5
SiF_3	0.69	16.1	$PO(C_4H_9)_2$	0.49	7.1	$NHCOC_6H_5$	-0.19	-1.5

cyclo-C_4F_7	0.53	16.1	Cl	0.23	7.0	$CH_2CH=CH_2$	-0.14	-1.6
SO_2Et	0.77	16.1	$C(NO_2)Me_2$	0.20	7.0	$Ge(Et)_3$	0.00	-1.6
SCl	0.48	15.9	CSNHMe	0.34	7.0	$CH_2C_6H_5$	-0.09	-1.8
$SO_2NHC_6H_5$	0.65	15.8	$PO(C_6H_5)_2$	0.53	6.9	$NHCOCH(Me)_2$	-0.10	-1.8
$SC(CF_3)_3$	0.58	15.7	CH_2CONH_2	0.07	6.7	NHCSNHEt	0.07	-1.8
$GeBr_3$	0.73	15.6	CH_2CN	0.18	6.7	$P(N(Me)_2)_2$	0.25	-1.9
$C=CCF_3$	0.51	15.6	CONHMe	0.36	6.4	OH	-0.37	-2.0
PCl_2	0.61	15.6	$PS(C_6H_4\text{-}4Me)_2$	0.23	6.5	$C_6H_4\text{-}4OMe$	-0.08	-2.0
$SeC(CF_3)_3$	0.54	15.5	$PO(isopropyl)_2$	0.41	6.5	$CH_2PO(OEt)_2$	0.06	-2.0
$SCOCF_3$	0.46	15.5	OSO_2Me	0.36	6.3	SEt	0.03	-2.2
$C(Et)(NO_2)_2$	0.64	15.4	$NHSO_2Me$	0.03	6.2	$N(C_6H_5)_2$	-0.22	-2.3
$NO=NSO_2C_6H_5$	0.79	15.4	SCH_2F	0.20	6.2	NHCOOMe	-0.17	-2.4
$(CF_2)_3CF_3$	0.52	15.3	$SN(Me)_2$	0.09	6.1	cyclopropyl	-0.21	-2.4
$CF_2CF_2CF_3$	0.48	15.3	$PO(C_6H_5)C_6H_4\text{-}4Me$	0.30	6.1	$(CH_2)_4NMe_2$	-0.16	-2.4
$N(CF_3)_2$	0.53	15.2	$N=NC_6H_5$	0.39	6.1	$CH_2CH_2Si(Me)_3$	-0.17	-2.4
SOOH	-0.07	15.0	$P(Cl)NMe_2$	0.56	6.1	$CH_2PO(C_6H_5)_2$	0.01	-2.5
PF_2	0.59	14.9	SeCH=CHCl	0.26	6.0	CH_2NMe_2	0.01	-2.6
CF_2CF_3	0.52	14.7	$N=CCl_2$	0.13	5.9	$CH_2C(Me)_3$	-0.17	-2.9
SO_2NMe_2	0.65	14.5	SC_6H_5	0.07	5.9	NHCOOEt	-0.15	-3.0
$SCF_2CF_2CF_3$	0.48	14.5	NHCN	0.06	5.9	$CH_2CH(Me)_2$	-0.12	-3.0
$CH=CHCOC_6H_4\text{-}4NO_2$	0.05	14.4	CH_2CF_3	0.09	5.7	$CH_2CH_2C_6H_5$	-0.12	-3.1
$SiCl_3$	0.56	14.4	C=CH	0.23	5.7	$CH_2CH_2CH_3$	-0.13	-3.1
$SO_2C_6H_5$	0.68	14.4	$PO(N(Me)_2)_2$	0.40	5.6	$(CH_2)_3CH_3$	-0.16	-3.2
NC	0.49	14.3	$PO(CMe_3)_2$	0.41	5.5	CH(Me)(Et)	-0.12	-3.2
$SCF(CF_3)_2$	0.51	14.3	N_3	0.08	5.4	$NHCO_2(CH_2)_3CH_3$	-0.05	-3.2
OCN	0.54	14.2	$PO(C_6H_4\text{-}4Me)_2$	0.30	5.2	$(CH_2)_4CH_3$	-0.15	-3.2
$C(CF_3)_3$	0.55	14.0	F	0.06	5.1	$(CH_2)_6CH_3$	-0.16	-3.2
OSO_2CF_3	1.21	14.0	$SeCH_2CH=CH_2$	-0.07	5.0	Me	-0.17	-3.3
$CF=CFCF_3$	0.46	14.6	CH=CHCOOEt	0.03	4.9	isopropyl	-0.15	-3.3
SSO_2Me	0.54	14.0	$SiClMe_2$	0.21	4.8	$NHCOC_6H_4\text{-}4OMe$	-0.06	-3.4
$C(Me)(CN)_2$	0.57	13.9	$NHSO_2C_6H_5$	0.01	4.8	CH_2NH_2	-0.11	-3.5
SCF_2CF_3	0.48	13.9	$SCH_2CH=CH_2$	0.12	4.8	$NHCONH_2$	-0.24	-3.7
CH=CHCN	0.17	13.9	SeMe	0.00	4.5	cyclopentyl	-0.14	-3.7
$N=NPO(OEt)_2$	0.74	13.8	$OSO_2C_6H_5$	0.33	4.4	$CH_2C(OH)(Me)_2$	-0.17	-3.7
CF_3	0.54	13.7	CH_2OCOMe	0.05	4.4	$N=CHC_6H_4\text{-}4\text{-}OMe$	-0.54	-3.8
$CF(CF_3)_2$	0.53	13.8	$CH=NNHCOC_6H_5$	0.51	4.3	cyclohexyl	-0.15	-3.8
CHO	0.42	13.8	$SCH=CH_2$	0.19	4.1	CH_2OH	0.00	-3.8
$S(O)=NHCF_3$	0.84	13.8	$SCHMe_2$	0.07	4.1	$C(Me)_3$	-0.20	-3.9
$SiBr_3$	0.57	13.6	PH_2	0.05	4.0	cyclobutyl	-0.14	-3.9
ONO_2	0.70	13.4	$N(Me)SO_2Me$	0.24	3.9	$C(Et)_3$	-0.20	-4.0
$CClF_2$	0.46	13.3	$C=CC_6H_5$	0.16	3.9	Et	-0.15	-4.0

$CH_2SO_2CF_3$	0.31	12.5	$CH=NNHCONHNH_2$	0.16	3.8	$C(Et)(Me)_2$	-0.18	-4.2
$CH=NCOC_6H_5$	0.51	12.5	SCH=CHCl	0.24	3.8	$OSiMe_3$	-0.27	-4.2
$N=C(CF_3)_2$	0.23	12.5	CH=NOMe	0.30	3.7	$OCH_2CH=CH_2$	-0.25	-4.8
$CF_2CF_2C_6H_4$-4F	0.39	12.3	C_6H_4-3Br	0.08	3.7	NHC_6H_5	-0.56	-4.8
SCOMe	0.44	12.3	$SeCH=CH_2$	0.21	3.6	$CH_2OSi(CH_3)_3$	-0.05	-4.8
$OCOCF_3$	0.46	12.2	C_6H_4-3Cl	0.10	3.6	$CH_2Si(Me)_3$	-0.21	-4.9
BF_2	0.48	12.1	SiH_3	0.10	3.5	OMe	-0.27	-5.0
OCF_2CF_3	0.28	12.0	C_6H_4-4Br	0.12	3.5	NHOH	-0.34	-5.1
CCl_3	0.46	11.7	$N=NC_6H_3$-5Me,2-OH	0.31	3.3	$N=NNMe_2$	-0.03	-5.6
$N(Me)NO_2$	0.61	11.7	C_6H_4-4Cl	0.12	3.3	OCH_2CH_3	-0.24	-5.8
CBr_3	0.29	11.2	S(SMe)	0.13	3.3	NHCONHEt	-0.26	-5.8
$N(Me)SO_2CF_3$	0.44	11.2	C_6H_4-3F	0.10	3.3	$O(CH_2)_3CH_3$	-0.32	-5.9
CH_2SOCF_3	0.24	11.2	S(OMe)	0.17	3.2	$OCH_2CH_2CH_3$	-0.45	-6.0
$PO(OH)_2$	0.42	11.1	NHCSMe	0.12	3.1	$NHPO(C_3H_7)_2$	0.18	-6.2
$OCCl_3$	0.35	11.1	$SiFMe_2$	0.17	2.9	$O(CH_2)_4CH_3$	-0.34	-6.2
$NHNO_2$	0.57	11.0	CH_2Br	0.14	2.9	$OCHMe_2$	-0.45	-6.5
COOH	0.45	10.9	$OS(=O)CH_3$	0.45	2.8	$N=C(Me)NHC_6H_5$	0.08	-6.6
$N(SO_2Me)_2$	0.49	10.8	CH_2Cl	0.12	2.7	NH_2	-0.66	-9.0
SCF_2CHF_2	0.47	10.7	GeH_3	0.01	2.6	NHMe	-0.70	-11.2
S(O)OMe	0.54	10.7	$CH_2NHCOMe$	-0.05	2.5	$NHNH_2$	-0.55	-11.2
CHF_2	0.32	10.4	C_6H_4-4F	0.06	2.5	NHEt	-0.61	-11.4
$NHSO_2CF_3$	0.39	10.3	$SiMe(OMe)_2$	0.10	2.4	$NH(CH_2)_3CH_3$	-0.51	-11.6
$CH=NNHCSNH_2$	0.40	10.3	$Si(OMe)_3$	0.13	2.4	$N(Et)_2$	-0.72	-11.9
C_6H_4-4NO_2	0.26	10.2	$OCOC_6H_5$	0.13	2.3	$N(Me)_2$	-0.83	-12.3
OCF_2CHF_2	0.25	10.1	OCH_2Cl	0.08	2.2	$N(C_3H_7)_2$	-0.93	-12.9

3. SCF Energies (in au) and Cartesian Coordinates (in Å) of all the optimized structures at B3LYP/6-311+G (d, p) level

SO_2CN			
E(RB3LYP) = -873.182132429			
6	-0.456525000	-0.000331000	-0.192575000
6	-1.118696000	1.221625000	-0.081473000
6	-1.118973000	-1.221855000	-0.078317000
6	-2.489288000	1.212194000	0.160984000
6	-2.489540000	-1.211536000	0.164071000
6	-3.169593000	0.000568000	0.284726000
1	-0.573319000	2.150207000	-0.193416000
1	-3.024884000	2.149842000	0.247913000
1	-4.236840000	0.000914000	0.473924000
1	-3.025346000	-2.148841000	0.253373000
1	-0.573687000	-2.150782000	-0.187867000
16	1.304230000	-0.000844000	-0.493918000
8	1.702866000	1.273141000	-1.067891000
8	1.702623000	-1.276715000	-1.063796000
6	1.947395000	0.001827000	1.179723000
7	2.384832000	0.003687000	2.248490000

SO_2Cl			
E(RB3LYP) = -1240.57729385			
6	0.534054000	-0.000473000	-0.206476000
6	1.192648000	-1.221774000	-0.092421000
6	1.192239000	1.221382000	-0.095947000
6	2.564172000	-1.210839000	0.145925000
6	2.563784000	1.211618000	0.142411000
6	3.245450000	0.000680000	0.263551000
1	0.645464000	-2.149940000	-0.195213000
1	3.099343000	-2.148605000	0.235031000
1	4.313290000	0.001100000	0.449237000
1	3.098623000	2.149827000	0.228796000
1	0.644771000	2.149080000	-0.201420000
16	-1.225980000	-0.001133000	-0.532906000
8	-1.615313000	-1.273422000	-1.112281000
8	-1.615503000	1.268925000	-1.116905000
17	-2.005492000	0.002887000	1.464782000

$C(CN)=C(CN)_2$			
E(RB3LYP) = -586.507233480			
6	-0.821140000	0.205687000	0.052594000
6	-1.363910000	-0.984147000	0.567931000
6	-1.690747000	1.183902000	-0.464627000
6	-2.736570000	-1.195169000	0.540461000
6	-3.060302000	0.958456000	-0.501971000
6	-3.586989000	-0.231684000	-0.001363000
1	-0.724495000	-1.733705000	1.012880000
1	-3.142948000	-2.112104000	0.950131000
1	-4.656909000	-0.403345000	-0.022864000
1	-3.716593000	1.714328000	-0.916303000
1	-1.289443000	2.114732000	-0.846935000
6	0.627854000	0.470125000	0.060375000
6	1.633518000	-0.458069000	-0.047508000
6	1.017653000	1.844663000	0.174113000
7	1.292771000	2.962611000	0.265664000
6	3.010112000	-0.079725000	0.015854000
7	4.130789000	0.196047000	0.063570000
6	1.406696000	-1.850044000	-0.270169000
7	1.278344000	-2.982068000	-0.462242000

SeO_2CF_3			
6	-1.148363844	-0.224777562	0.000013229
6	-1.787175506	-0.046205641	1.223653066
6	-1.787185560	-0.046347989	-1.223640895
6	-3.123230053	0.348387546	1.212441388
6	-3.123241695	0.348245197	-1.212464672
6	-3.784476714	0.546867115	-0.000021167
1	-1.257647413	-0.224424600	2.151474883
1	-3.646939314	0.494136190	2.149720131
1	-4.824514800	0.852135182	-0.000034926
1	-3.646957306	0.493884831	-2.149757174
1	-1.257665934	-0.224677018	-2.151446307
34	0.703758644	-0.795410556	0.000034926
8	1.051279927	-1.477363923	-1.438062458
8	1.051288923	-1.477279784	1.438167235
6	1.714246944	1.005996113	-0.000045509
9	1.384748379	1.706837933	1.087703727
9	3.022093168	0.774844612	-0.000198441
9	1.384485907	1.706881325	-1.087682559

$SO_2C(CF_3)_3$			
E(RB3LYP) = -1831.66301451			
6	-2.027594000	-0.056733000	0.527955000
6	-2.675598000	-1.244114000	0.189872000
6	-2.631681000	1.190542000	0.375074000
6	-3.959397000	-1.170704000	-0.341962000
6	-3.915173000	1.243950000	-0.159610000
6	-4.573421000	0.068549000	-0.521179000
1	-2.189497000	-2.196065000	0.353931000
1	-4.480854000	-2.082162000	-0.608438000
1	-5.573796000	0.118127000	-0.935589000
1	-4.402504000	2.203321000	-0.285352000
1	-2.115971000	2.090217000	0.680663000
16	-0.417809000	-0.156571000	1.321297000
8	-0.247314000	-1.507204000	1.837804000
8	-0.236697000	1.024012000	2.153893000
6	0.972404000	0.010333000	-0.096240000
6	1.235429000	1.522227000	-0.383452000
9	0.079583000	2.196328000	-0.523493000
9	1.929978000	2.092327000	0.601783000
9	1.925996000	1.687729000	-1.525151000
6	2.267125000	-0.659053000	0.480255000

$SO_2CF_2CF_2CF_3$			
E(RB3LYP) = -1593.78763203			
6	1.894238000	0.124218000	-0.318413000
6	1.997998000	-1.143788000	-0.888286000
6	2.808736000	0.594402000	0.624081000
6	3.047761000	-1.966513000	-0.489209000
6	3.847262000	-0.244458000	1.016386000
6	3.964274000	-1.519605000	0.462199000
1	1.282056000	-1.466175000	-1.633128000
1	3.150550000	-2.953430000	-0.924180000
1	4.778173000	-2.166233000	0.769500000
1	4.568720000	0.100762000	1.747206000
1	2.712765000	1.594822000	1.025713000
16	0.568628000	1.205368000	-0.847529000
8	-0.034074000	0.683860000	-2.069217000
8	1.006302000	2.590425000	-0.721914000
6	-0.782222000	1.059878000	0.518793000
9	-1.716050000	1.965195000	0.185981000
9	-0.198242000	1.440903000	1.675722000
6	-1.478675000	-0.310021000	0.808269000
9	-0.539278000	-1.183401000	1.241085000
9	-2.348383000	-0.083573000	1.820720000

9	2.204725000	-1.990955000	0.390724000
9	3.352338000	-0.255487000	-0.206154000
9	2.456187000	-0.330589000	1.761498000
6	0.530043000	-0.717807000	-1.399401000
9	-0.386475000	0.007705000	-2.062738000
9	1.563943000	-0.925349000	-2.227398000
9	-0.016628000	-1.913475000	-1.132117000

6	-2.284329000	-1.011201000	-0.336574000
9	-3.051496000	-1.963367000	0.210795000
9	-3.069779000	-0.145606000	-0.977149000
9	-1.461038000	-1.595416000	-1.210384000

N(O)=NCN

E(RB3LYP) = -509.255249444

6	-0.471599000	0.101862000	-0.000022000
6	-1.325196000	1.202528000	0.000009000
6	-0.951623000	-1.207560000	-0.000083000
6	-2.698240000	0.981028000	-0.000021000
6	-2.327171000	-1.409182000	-0.000118000
6	-3.199823000	-0.320108000	-0.000085000
1	-0.909995000	2.200584000	0.000054000
1	-3.375216000	1.826670000	0.000006000
1	-4.270773000	-0.486417000	-0.000109000
1	-2.717016000	-2.419871000	-0.000171000
1	-0.260155000	-2.037743000	-0.000107000
7	0.966840000	0.365697000	0.000011000
7	1.727128000	-0.683330000	0.000123000
6	3.040338000	-0.436218000	0.000138000
7	4.198420000	-0.373001000	0.000145000
8	1.360792000	1.534639000	-0.000068000

N=NCN

E(RB3LYP) = -434.027359442

6	-0.180477000	-0.534652000	0.000345000
6	-1.388095000	-1.255641000	-0.000292000
6	-0.210558000	0.874275000	0.000770000
6	-2.606807000	-0.591995000	-0.000661000
6	-1.436300000	1.526909000	0.000479000
6	-2.631098000	0.802286000	-0.000271000
1	-1.329777000	-2.337038000	-0.000504000
1	-3.532203000	-1.155353000	-0.001206000
1	-3.579160000	1.328070000	-0.000516000
1	-1.461168000	2.610233000	0.000843000
1	0.696032000	1.460150000	0.001387000
7	0.945404000	-1.387875000	0.000630000
7	2.148829000	-1.026846000	0.000290000
6	2.605984000	0.247325000	-0.000366000
7	3.232966000	1.226563000	-0.000924000

$C(NO_2)_3$

E(RB3LYP) = -885.268804464

6	0.905815000	-0.071955000	-0.024599000
6	1.591504000	1.152987000	-0.012973000
6	1.632221000	-1.267975000	-0.033850000
6	2.978831000	1.176129000	-0.023388000
6	3.024238000	-1.233295000	-0.039898000
6	3.699870000	-0.017364000	-0.037883000
1	1.046178000	2.087794000	0.000260000
1	3.496014000	2.127924000	-0.016062000
1	4.783438000	0.002890000	-0.042232000
1	3.576313000	-2.165338000	-0.044937000
1	1.132508000	-2.225289000	-0.045151000
6	-0.590522000	-0.030093000	-0.000717000
7	-1.253238000	0.536278000	-1.323221000
8	-0.605852000	1.360138000	-1.927481000
8	-2.354736000	0.115908000	-1.589899000
7	-1.272357000	-1.396577000	0.219365000
8	-1.052537000	-2.214630000	-0.650920000
8	-1.952168000	-1.539387000	1.209655000
7	-1.105716000	0.916505000	1.144029000
8	-1.970565000	1.715159000	0.855839000
8	-0.572520000	0.753807000	2.216151000

$C(CN)_3$

E(RB3LYP) = -548.380746119

6	0.452789000	0.039648000	-0.000034000
6	1.150236000	1.244149000	-0.000030000
6	1.137375000	-1.177544000	-0.000026000
6	2.545422000	1.228141000	-0.000020000
6	2.527556000	-1.183934000	-0.000015000
6	3.233873000	0.019227000	-0.000012000
1	0.623344000	2.190174000	-0.000040000
1	3.087700000	2.166133000	-0.000021000
1	4.317509000	0.011493000	-0.000007000
1	3.057865000	-2.128699000	-0.000012000
1	0.593419000	-2.115523000	-0.000031000
6	-1.103937000	0.005393000	-0.000002000
6	-1.588059000	-0.709306000	-1.206170000
7	-1.938691000	-1.270975000	-2.147863000
6	-1.587996000	-0.708824000	1.206479000
7	-1.938565000	-1.270117000	2.148420000
6	-1.690877000	1.362580000	-0.000262000
7	-2.142477000	2.420982000	-0.000462000

SO_2CF_3

E(RB3LYP) = -1118.07839326

6	0.924502000	-0.044521000	-0.342585000
6	1.570774000	-1.229843000	0.006285000
6	1.564559000	1.193395000	-0.294358000
6	2.897192000	-1.165169000	0.423583000
6	2.890841000	1.239655000	0.125852000
6	3.552269000	0.064920000	0.484371000
1	1.047426000	-2.174945000	-0.063446000
1	3.419369000	-2.074947000	0.694697000
1	4.585611000	0.107696000	0.809027000
1	3.408071000	2.190768000	0.166619000
1	1.037054000	2.090347000	-0.593127000
16	-0.781483000	-0.116725000	-0.885789000
8	-1.088439000	-1.467963000	-1.341486000
8	-1.090485000	1.070145000	-1.675384000
6	-1.748761000	0.096955000	0.743038000
9	-1.456562000	1.274357000	1.303355000
9	-3.050418000	0.046532000	0.476231000
9	-1.434206000	-0.878791000	1.600047000

$CH=C(CN)_2$

E(RB3LYP) = -494.256868487

6	0.720665000	-0.399235000	0.000019000
6	1.166018000	0.938393000	-0.000083000
6	1.687012000	-1.426541000	0.000110000
6	2.524702000	1.223742000	-0.000130000
6	3.044408000	-1.134940000	0.000087000
6	3.467042000	0.193569000	-0.000050000
1	0.458908000	1.755360000	-0.000114000
1	2.851639000	2.256896000	-0.000227000
1	4.525595000	0.426950000	-0.000108000
1	3.770265000	-1.939456000	0.000182000
1	1.359483000	-2.460682000	0.000203000
6	-0.670376000	-0.815161000	0.000002000
6	-1.830283000	-0.098968000	-0.000004000
1	-0.813164000	-1.891593000	-0.000014000
6	-1.924202000	1.326048000	0.000008000
7	-2.024198000	2.477387000	0.000196000
6	-3.080746000	-0.796425000	-0.000066000
7	-4.086969000	-1.364582000	-0.000092000

$SO_2CF_2CF_3$

E(RB3LYP) = -1355.93475793

$CH=NSO_2CF_3$

E(RB3LYP) = -1211.55267164

6	1.473648000	-0.285350000	0.221694000
6	1.870749000	0.802416000	0.997339000
6	2.245932000	-0.766340000	-0.835381000
6	3.075733000	1.430221000	0.694165000
6	3.444849000	-0.123345000	-1.127975000
6	3.856048000	0.971150000	-0.366625000
1	1.256557000	1.134178000	1.824347000
1	3.405671000	2.273403000	1.289108000
1	4.792942000	1.464878000	-0.597853000
1	4.060375000	-0.481997000	-1.944257000
1	1.918718000	-1.629402000	-1.400676000
16	-0.054637000	-1.127949000	0.633890000
8	-0.449058000	-0.779445000	1.994936000
8	0.028951000	-2.508364000	0.170862000
6	-1.372318000	-0.345712000	-0.539954000
9	-2.358342000	-1.246864000	-0.651566000
9	-0.796076000	-0.169383000	-1.747248000
6	-1.984623000	1.006137000	-0.079535000
9	-2.720059000	0.850543000	1.017840000
9	-1.010812000	1.897917000	0.164900000
9	-2.765748000	1.495956000	-1.053000000

6	-2.172205000	-0.258303000	0.004747000
6	-2.558629000	0.948539000	-0.602859000
6	-3.136868000	-1.059499000	0.634093000
6	-3.888244000	1.341246000	-0.573454000
6	-4.469192000	-0.660747000	0.661317000
6	-4.843880000	0.538564000	0.057916000
1	-1.806886000	1.556805000	-1.090368000
1	-4.187739000	2.271268000	-1.042162000
1	-5.882029000	0.850499000	0.076583000
1	-5.211675000	-1.281106000	1.148914000
1	-2.837280000	-1.991813000	1.101061000
6	-0.785890000	-0.706797000	0.002849000
7	0.157550000	-0.010888000	-0.526821000
1	-0.576748000	-1.669155000	0.480470000
16	1.704495000	-0.704733000	-0.475855000
8	1.775198000	-1.879725000	0.387797000
8	2.245400000	-0.724069000	-1.822359000
6	2.584166000	0.693429000	0.452456000
9	2.534181000	1.825495000	-0.243433000
9	2.008971000	0.882891000	1.643204000
9	3.855432000	0.339080000	0.631456000

SO2CHF2

E(RB3LYP) = -1018.80215982

6	0.784060000	-0.206851000	0.189671000
6	1.496860000	-1.082123000	-0.628925000
6	1.382069000	0.906024000	0.779819000
6	2.844803000	-0.825208000	-0.868291000
6	2.729792000	1.149162000	0.530643000
6	3.456507000	0.287709000	-0.291925000
1	1.007982000	-1.954473000	-1.044682000
1	3.417207000	-1.498375000	-1.495431000
1	4.506375000	0.481744000	-0.479623000
1	3.213385000	2.006601000	0.983390000
1	0.803363000	1.552812000	1.426978000
16	-0.956063000	-0.529278000	0.496011000
8	-1.343027000	0.099907000	1.755755000
8	-1.234709000	-1.936026000	0.200778000
6	-1.801582000	0.422636000	-0.897509000
1	-1.546020000	-0.032755000	-1.856467000
9	-1.409235000	1.716093000	-0.869529000
9	-3.128371000	0.360990000	-0.686417000

N=NCF3

E(RB3LYP) = -678.939317758

6	1.095063000	-0.183343000	0.000053000
6	1.967944000	-1.275517000	0.000018000
6	1.592107000	1.128847000	0.000034000
6	3.343268000	-1.061587000	-0.000085000
6	2.963978000	1.331891000	0.000017000
6	3.840022000	0.240168000	-0.000044000
1	1.548329000	-2.274330000	0.000135000
1	4.023437000	-1.905004000	-0.000162000
1	4.910802000	0.409948000	-0.000042000
1	3.359422000	2.341064000	0.000058000
1	0.899597000	1.960543000	0.000050000
7	-0.283090000	-0.517847000	0.000231000
7	-1.070885000	0.442589000	-0.000324000
6	-2.468283000	0.037937000	0.000040000
9	-3.054067000	0.568773000	1.086847000
9	-3.053151000	0.562929000	-1.090207000
9	-2.700378000	-1.277901000	0.003406000

SF_3

E(RB3LYP) = -929.477882010

6	-3.042935000	-0.077842000	0.139317000
6	-2.421669000	1.131559000	-0.162424000
6	-2.280677000	-1.233854000	0.305581000
1	-3.010374000	2.031696000	-0.292627000
1	-2.761377000	-2.175456000	0.542793000
6	-1.036503000	1.199282000	-0.286956000
6	-0.898551000	-1.193440000	0.158245000
1	-0.548644000	2.140225000	-0.492318000
1	-0.305185000	-2.089641000	0.260186000
6	-0.288436000	0.030111000	-0.127694000
1	-4.121020000	-0.121258000	0.243512000
16	1.505868000	0.115829000	-0.355118000
9	2.070947000	-0.279359000	1.123873000
9	1.515882000	1.790850000	0.189804000
9	1.575986000	-1.597460000	-0.728795000

POF_2

E(RB3LYP) = -848.175276951

6	-0.326897000	0.047053000	-0.000005000
6	-0.986071000	-1.189465000	-0.000048000
6	-1.056365000	1.241314000	-0.000036000
6	-2.375911000	-1.224008000	0.000009000
6	-2.448090000	1.194748000	0.000055000
6	-3.105202000	-0.033966000	0.000049000
1	-0.420766000	-2.114020000	-0.000059000
1	-2.890485000	-2.177625000	0.000052000
1	-4.188791000	-0.066662000	0.000080000
1	-3.016720000	2.117105000	0.000104000
1	-0.533299000	2.189928000	-0.000003000
15	1.456731000	0.151653000	-0.000065000
8	2.068195000	1.481515000	-0.000817000
9	1.913750000	-0.793178000	1.195253000
9	1.913444000	-0.794565000	-1.194455000

PF4

E(RB3LYP)=- 972.570287

6	0.55372	0.22104	-0.00022
6	-0.33512	1.29775	-0.0001
6	0.09161	-1.10104	-0.00019
6	-1.70581	1.05485	0.00014
6	-1.27527	-1.33485	-0.00005
6	-2.17237	-0.25904	0.00015
1	0.06742	2.3042	0.
1	-2.40646	1.88144	0.00036

GEF3

E(RB3LYP) = -2608.46209672

6	0.725522000	0.000054000	0.009845000
6	1.420105000	1.215209000	0.005376000
6	1.420206000	-1.215057000	0.005254000
6	2.812838000	1.209473000	-0.009103000
6	2.812928000	-1.209178000	-0.009256000
6	3.506624000	0.000181000	-0.017875000
1	0.885132000	2.157811000	0.020208000
1	3.354211000	2.148305000	-0.011219000

1	-3.23955	-0.45106	0.00027
1	-1.65265	-2.35106	-0.00005
1	0.81107	-1.91077	-0.00032
15	2.36499	0.54488	-0.00041
9	3.08263	-0.80557	0.18088
9	2.19021	0.95523	-1.4744
9	2.67405	0.59645	1.50738
9	3.22555	1.81482	0.13486

1	4.590613000	0.000225000	-0.028607000
1	3.354403000	-2.147951000	-0.011558000
1	0.885268000	-2.157674000	0.020072000
32	-1.192603000	-0.000032000	0.002979000
9	-1.932777000	0.005231000	-1.574643000
9	-1.871623000	-1.401427000	0.783476000
9	-1.872896000	1.395775000	0.792313000

$CH{=}CHNO_2$

E(RB3LYP) = -514.297422793

6	-0.820716000	0.171633000	-0.000124000
6	-1.360330000	-1.127617000	-0.000139000
6	-1.704623000	1.263628000	-0.000031000
6	-2.734444000	-1.321129000	-0.000026000
6	-3.082150000	1.068175000	0.000090000
6	-3.600646000	-0.224602000	0.000098000
1	-0.704348000	-1.989970000	-0.000270000
1	-3.135490000	-2.328055000	-0.000051000
1	-4.673258000	-0.380828000	0.000175000
1	-3.748576000	1.922825000	0.000171000
1	-1.302091000	2.270811000	-0.000039000
6	0.613322000	0.442999000	-0.000185000
6	1.601835000	-0.457661000	0.000266000
1	1.516202000	-1.532910000	0.000672000
1	0.913661000	1.486568000	-0.000557000
7	2.993542000	-0.030611000	0.000122000
8	3.259164000	1.167282000	0.000026000
8	3.829039000	-0.933122000	-0.000107000

SF_5

E(RB3LYP) = -1129.045415

6	0.45835	-0.25877	-0.06656
6	-0.48246	-1.29599	-0.0044
6	0.02299	1.06852	-0.06754
6	-1.84056	-1.00369	0.04482
6	-1.34176	1.34724	-0.013
6	-2.28133	0.32038	0.04012
1	-0.14778	-2.32881	-0.00372
1	-2.55751	-1.81585	0.09221
1	-3.34035	0.54556	0.08161
1	-1.66909	2.38118	-0.00834
1	0.75008	1.86837	-0.094
16	2.23642	-0.63908	-0.1455
9	3.75071	-0.96298	-0.21274
9	1.78654	-0.05403	-1.50852
9	2.68629	-1.22413	1.21752
9	3.07123	0.57937	-0.61557
9	1.40161	-1.85754	0.32456

SOF

E(RB3LYP) = -804.996806772

6	2.841654000	0.094533000	0.125181000
6	2.069454000	1.245217000	0.285626000
6	2.238665000	-1.124539000	-0.187734000
1	2.544198000	2.189282000	0.526315000
1	2.842804000	-2.015648000	-0.311133000
6	0.685874000	1.185331000	0.135521000
6	0.856842000	-1.197321000	-0.340064000
1	0.060615000	2.062818000	0.251115000
1	0.378003000	-2.141112000	-0.577573000
6	0.100074000	-0.038926000	-0.169642000
1	3.918172000	0.147800000	0.240798000
16	-1.691752000	-0.126083000	-0.416950000
8	-2.204509000	1.240851000	-0.208645000
9	-1.977228000	-1.015377000	1.013057000

COF

E(RB3LYP) = -444.963507204

6	0.232922000	0.044308000	0.000002000
6	-0.504788000	1.235867000	0.000002000
6	-0.427162000	-1.190750000	0.000001000
6	-1.893155000	1.189865000	0.000001000
6	-1.817909000	-1.228902000	-0.000001000
6	-2.549994000	-0.041998000	-0.000002000
1	0.023096000	2.181487000	0.000001000
1	-2.464405000	2.110705000	0.000006000
1	-3.633662000	-0.076145000	-0.000006000
1	-2.330528000	-2.183629000	-0.000003000
1	0.147810000	-2.107116000	0.000005000
6	1.705600000	0.143982000	0.000000000
8	2.379072000	1.121327000	-0.000003000
9	2.305781000	-1.090017000	0.000001000

$CH(CN)_2$

E(RB3LYP) = -456.145975588

6	0.215004000	0.000358000	-0.251281000
6	1.143360000	0.002082000	-1.290777000
6	0.650383000	-0.001768000	1.075008000
6	2.508445000	0.001752000	-1.005721000
6	2.013003000	-0.002062000	1.356049000
6	2.943652000	-0.000288000	0.316687000
1	0.807111000	0.003704000	-2.322294000
1	3.226735000	0.003079000	-1.817169000
1	4.004444000	-0.000467000	0.538861000
1	2.348270000	-0.003639000	2.386534000
1	-0.069819000	-0.003200000	1.885841000
6	-1.285010000	0.000726000	-0.579010000
1	-1.400686000	0.001902000	-1.668585000
6	-1.959110000	-1.210034000	-0.079325000
7	-2.466597000	-2.172674000	0.298069000
6	-1.959439000	1.210125000	-0.076590000
7	-2.467373000	2.171714000	0.302871000

SO_2Me

E(RB3LYP) = -820.280464489

6	-0.328929000	0.000007000	-0.080650000
6	-1.006807000	1.216791000	-0.045731000
6	-1.006798000	-1.216782000	-0.045768000
6	-2.397341000	1.210059000	0.039955000
6	-2.397333000	-1.210067000	0.039926000
6	-3.089481000	-0.000007000	0.086121000
1	-0.452620000	2.145353000	-0.109376000
1	-2.939155000	2.148450000	0.060780000
1	-4.171734000	-0.000010000	0.148957000
1	-2.939137000	-2.148464000	0.060734000
1	-0.452618000	-2.145345000	-0.109462000
16	1.474951000	0.000018000	-0.174666000
8	1.895952000	1.278195000	-0.760456000
8	1.895932000	-1.278010000	-0.760772000
6	2.004361000	-0.000189000	1.556442000
1	3.094424000	-0.000190000	1.531731000
1	1.630295000	0.900941000	2.039753000
1	1.630237000	-0.901377000	2.0396000001

$N(SO_2CF_3)_2$

E(RB3LYP) = -2059.18678310

6	-0.124132000	1.533385000	-0.005098000
6	0.351200000	2.262840000	-1.093817000
6	-0.717515000	2.171355000	1.083258000
6	0.224660000	3.648267000	-1.091798000
6	-0.830807000	3.557856000	1.080890000
6	-0.362664000	4.295388000	-0.005579000

C_6H_2-2,4,6$(NO_2)_3$

E(RB3LYP) = -1077.07973572

6	-1.763598000	-0.000134000	0.000000000
6	-2.465950000	-0.637864000	-1.027784000
6	-2.466038000	0.637639000	1.027699000
6	-3.857109000	-0.632362000	-1.027675000
6	-3.857201000	0.632272000	1.027390000
6	-4.554584000	-0.000002000	-0.000197000

1	0.801629000	1.750246000	-1.933611000
1	0.585935000	4.220668000	-1.937735000
1	-0.455583000	5.375274000	-0.005817000
1	-1.284890000	4.060090000	1.926660000
1	-1.073931000	1.589822000	1.923530000
7	-0.000159000	0.086441000	-0.003849000
16	1.255560000	-0.644125000	0.941059000
8	0.861143000	-1.980681000	1.317927000
8	1.682208000	0.357939000	1.893661000
6	2.688466000	-0.813161000	-0.301175000
9	3.015220000	0.390711000	-0.770902000
9	3.722717000	-1.330938000	0.354032000
9	2.349965000	-1.604194000	-1.307172000
16	-1.120843000	-0.848942000	-0.933565000
8	-0.527583000	-2.125928000	-1.252016000
8	-1.672751000	0.042519000	-1.930612000
6	-2.532909000	-1.182600000	0.299215000
9	-3.100339000	-0.029492000	0.650718000
9	-3.426767000	-1.949503000	-0.316789000
9	-2.077402000	-1.799128000	1.379774000

1	-1.928122000	-1.120203000	-1.836465000
1	-4.395016000	-1.120222000	-1.831964000
1	-5.638362000	0.000054000	-0.000299000
1	-4.395162000	1.120185000	1.831612000
1	-1.928286000	1.119903000	1.836472000
6	-0.277012000	-0.000099000	0.000018000
6	0.482683000	-1.179501000	0.055039000
6	0.482460000	1.179420000	-0.054982000
6	1.868166000	-1.210777000	0.023199000
6	1.867974000	1.210915000	-0.023257000
1	2.409733000	-2.146451000	0.038700000
1	2.409385000	2.146678000	-0.038781000
6	2.542498000	0.000135000	-0.000056000
7	-0.187324000	-2.498732000	0.200158000
8	-0.986761000	-2.621589000	1.110358000
8	0.148297000	-3.369859000	-0.588582000
7	4.024808000	0.000241000	-0.000081000
8	4.582993000	-1.085375000	0.044561000
8	4.582847000	1.085936000	-0.044789000
7	-0.187756000	2.498558000	-0.199907000
8	-0.986741000	2.621621000	-1.110454000
8	0.147364000	3.369484000	0.589302000

SC_6H_4-4NO_2
E(RB3LYP) = -1066.19461510

6	2.503902000	0.488237000	-0.000012000
6	2.999677000	-0.002713000	1.211218000
6	2.999588000	-0.002872000	-1.211214000
6	3.980502000	-0.992878000	1.207584000
6	3.980410000	-0.993041000	-1.207524000
6	4.469746000	-1.489164000	0.000045000
1	2.619592000	0.391223000	2.146090000
1	4.363494000	-1.372726000	2.147838000
1	5.234341000	-2.257576000	0.000067000
1	4.363329000	-1.373016000	-2.147756000
1	2.619434000	0.390941000	-2.146110000
16	1.289715000	1.812199000	-0.000055000
6	-0.275501000	0.959931000	-0.000029000
6	-0.414158000	-0.433627000	-0.000033000
6	-1.422914000	1.770860000	-0.000030000
1	0.460687000	-1.069787000	-0.000078000
1	-1.322997000	2.850252000	-0.000030000
6	-1.678418000	-1.008856000	-0.000020000
6	-2.685593000	1.201174000	-0.000010000
1	-1.802708000	-2.083139000	-0.000009000
1	-3.577388000	1.812614000	-0.000022000
6	-2.801644000	-0.187920000	0.000001000
7	-4.139064000	-0.797678000	0.000037000
8	-4.209812000	-2.022484000	0.000019000
8	-5.109357000	-0.046894000	0.000078000

SOC_6H_4-4NO_2
E(RB3LYP) = -1141.38704865

6	-2.379610000	0.113088000	-0.187450000
6	-2.758856000	-0.945231000	-1.008843000
6	-2.813081000	0.207086000	1.130166000
6	-3.558734000	-1.957334000	-0.479921000
6	-3.615887000	-0.807697000	1.647177000
6	-3.982445000	-1.890073000	0.846841000
1	-2.450890000	-0.979652000	-2.048467000
1	-3.860655000	-2.788166000	-1.107154000
1	-4.609905000	-2.674984000	1.253121000
1	-3.960060000	-0.749882000	2.673480000
1	-2.535496000	1.071789000	1.722068000
16	-1.369423000	1.479700000	-0.874923000
8	-1.517311000	2.653171000	0.067038000
6	0.285147000	0.760655000	-0.506413000
6	1.025574000	1.351457000	0.511144000
6	0.803637000	-0.276155000	-1.280667000
1	0.595881000	2.178296000	1.064890000
1	0.226583000	-0.711019000	-2.088465000
6	2.302769000	0.873255000	0.789604000
6	2.077785000	-0.758911000	-1.008135000
1	2.907913000	1.300993000	1.577076000
1	2.513193000	-1.565749000	-1.581064000
6	2.804382000	-0.175940000	0.027120000
7	4.163294000	-0.687000000	0.318485000
8	4.581469000	-1.609811000	-0.369163000
8	4.785473000	-0.157491000	1.229643000

$P(CF_3)_2$
E(RB3LYP) = -1248.56038265

6	1.180643000	-0.000100000	-0.323214000
6	1.555169000	-0.000593000	1.029461000
6	2.176998000	0.000360000	-1.310379000
6	2.902172000	-0.000649000	1.376975000
6	3.524266000	0.000297000	-0.955447000
6	3.886893000	-0.000203000	0.388599000
1	0.804777000	-0.000983000	1.807308000
1	3.183584000	-0.001029000	2.423783000
1	4.934360000	-0.000252000	0.668181000
1	4.284895000	0.000607000	-1.727433000
1	1.897827000	0.000755000	-2.358315000
15	-0.540967000	0.000087000	-0.963675000
6	-1.321531000	1.446440000	0.012495000

$SOCF_3$
E(RB3LYP) = -1042.85258144

6	-0.805284000	0.224296000	-0.375680000
6	-1.461941000	1.100305000	0.481711000
6	-1.428629000	-0.909753000	-0.892309000
6	-2.773394000	0.813144000	0.854210000
6	-2.738701000	-1.187192000	-0.508426000
6	-3.407788000	-0.328010000	0.363615000
1	-0.947571000	1.987386000	0.832709000
1	-3.300219000	1.482830000	1.524034000
1	-4.429384000	-0.544521000	0.654214000
1	-3.237702000	-2.067517000	-0.896317000
1	-0.906091000	-1.567029000	-1.578266000
16	0.883087000	0.655096000	-0.914234000
8	1.168703000	2.050046000	-0.437149000

9	-1.172273000	1.430454000	1.353331000
9	-0.764825000	2.594181000	-0.434069000
9	-2.644851000	1.510130000	-0.237625000
6	-1.321752000	-1.446364000	0.012126000
9	-1.172503000	-1.430650000	1.352939000
9	-2.645250000	-1.509376000	-0.237928000
9	-0.765640000	-2.594242000	-0.434657000

6	1.780210000	-0.508135000	0.321112000
9	1.491086000	-1.787024000	0.027430000
9	3.095478000	-0.323606000	0.174569000
9	1.452893000	-0.267258000	1.589464000

NO_2

E(RB3LYP) = -436.874621477

6	2.515392000	0.000000000	-0.000037000
6	1.821202000	1.210204000	-0.000009000
6	1.821201000	-1.210204000	-0.000009000
1	2.362531000	2.148688000	-0.000021000
1	2.362531000	-2.148688000	-0.000020000
6	0.429822000	1.218803000	0.000028000
6	0.429822000	-1.218803000	0.000028000
1	-0.135406000	2.140447000	0.000044000
1	-0.135406000	-2.140447000	0.000044000
6	-0.241454000	0.000000000	0.000044000
1	3.599321000	0.000000000	-0.000065000
7	-1.722145000	0.000000000	0.000109000
8	-2.290904000	1.084544000	-0.000064000
8	-2.290904000	-1.084544000	-0.000064000

SeCN

E(RB3LYP) = -2726.10902867

6	0.495974000	0.205783000	-0.075441000
6	1.163752000	-0.357064000	-1.162687000
6	1.170698000	0.500922000	1.108818000
6	2.525279000	-0.636987000	-1.054756000
6	2.532387000	0.217340000	1.205365000
6	3.207798000	-0.350833000	0.126513000
1	0.628460000	-0.579072000	-2.077380000
1	3.049366000	-1.079032000	-1.894271000
1	4.266314000	-0.570259000	0.206126000
1	3.061921000	0.440165000	2.124498000
1	0.640748000	0.939800000	1.944913000
34	-1.394474000	0.663893000	-0.241499000
6	-2.103021000	-0.947055000	0.346821000
7	-2.598843000	-1.930944000	0.705611000

SCl

E(RB3LYP) = -1090.13970081

6	0.228305000	0.000614000	-0.381187000
6	0.899880000	1.214012000	-0.184782000
6	0.899291000	-1.213493000	-0.186934000
6	2.235772000	1.209352000	0.205128000
6	2.235133000	-1.210208000	0.203036000
6	2.902122000	-0.000754000	0.399577000
1	0.371370000	2.146913000	-0.338052000
1	2.756532000	2.147858000	0.356291000
1	3.942945000	-0.001255000	0.703074000
1	2.755413000	-2.149240000	0.352551000
1	0.370283000	-2.145830000	-0.341917000
16	-1.449828000	0.001526000	-0.967945000
17	-2.553078000	-0.001177000	0.848597000

PCl_2

E(RB3LYP) = -1493.57865980

6	0.588523000	0.000398000	0.260953000
6	0.996620000	-0.001165000	-1.079130000
6	1.547711000	0.001603000	1.280044000
6	2.350621000	-0.001565000	-1.388883000
6	2.906477000	0.001245000	0.963594000
6	3.306387000	-0.000397000	-0.368965000
1	0.257840000	-0.002059000	-1.871841000
1	2.665321000	-0.002815000	-2.426244000
1	4.361590000	-0.000753000	-0.617733000
1	3.645341000	0.002218000	1.756518000
1	1.237025000	0.002891000	2.320064000
15	-1.152006000	0.000687000	0.835159000
17	-1.913852000	1.626513000	-0.286468000
17	-1.913503000	-1.627131000	-0.283758000

SiF_3

E(RB3LYP) = -821.056275973

6	-0.383161000	0.000162000	-0.014939000
6	-1.096783000	1.209977000	-0.009041000
6	-1.096587000	-1.209795000	-0.009056000
6	-2.488906000	1.208000000	0.007142000
6	-2.488711000	-1.208055000	0.007114000
6	-3.184515000	-0.000083000	0.016629000
1	-0.566673000	2.156082000	-0.025339000
1	-3.029884000	2.147291000	0.009018000
1	-4.268696000	-0.000159000	0.027699000
1	-3.029532000	-2.147436000	0.008973000
1	-0.566324000	-2.155812000	-0.025398000
14	1.452323000	0.000021000	-0.002625000
9	2.045965000	-1.299034000	-0.733547000
9	2.046390000	1.298176000	-0.734858000
9	2.081041000	0.000691000	1.474483000

$GeBr_3$

E(RB3LYP) = -10031.2993027

6	-1.664319000	0.002372000	0.035801000
6	-2.362564000	1.213927000	0.025349000
6	-2.361059000	-1.210252000	0.025399000
6	-3.756031000	1.208635000	0.002620000
6	-3.754369000	-1.206911000	0.002511000
6	-4.450961000	0.000459000	-0.009511000
1	-1.830360000	2.157985000	0.042643000
1	-4.296149000	2.148471000	-0.002646000
1	-5.534941000	-0.000284000	-0.025366000
1	-4.293248000	-2.147454000	-0.002908000
1	-1.827782000	-2.153785000	0.042901000
32	0.285765000	0.001012000	0.011243000
35	1.140620000	1.916762000	1.027317000
35	1.137358000	-1.866157000	1.116935000
35	1.114417000	-0.053082000	-2.170178000

cyclo-C_4F_7

E(RB3LYP) = -1083.23937351

6	-1.386934000	-0.000003000	0.188460000
6	-2.081474000	1.209321000	0.077633000
6	-2.081467000	-1.209328000	0.077603000
6	-3.454258000	1.207090000	-0.150603000
6	-3.454252000	-1.207098000	-0.150634000
6	-4.141350000	-0.000004000	-0.267008000
1	-1.555699000	2.151755000	0.170663000
1	-3.985879000	2.147362000	-0.237605000
1	-5.210135000	-0.000005000	-0.448054000
1	-3.985867000	-2.147371000	-0.237660000
1	-1.555688000	-2.151761000	0.170608000

SO_2Et

E(RB3LYP) = -859.606674474

6	-0.523214000	0.183747000	-0.155403000
6	-1.261881000	1.054454000	0.644265000
6	-1.119691000	-0.893826000	-0.806104000
6	-2.625894000	0.825424000	0.808408000
6	-2.486367000	-1.110000000	-0.637731000
6	-3.235177000	-0.255715000	0.170646000
1	-0.778499000	1.906948000	1.105897000
1	-3.214098000	1.497199000	1.422727000
1	-4.298175000	-0.426856000	0.297278000
1	-2.965689000	-1.940019000	-1.143704000
1	-0.522466000	-1.530711000	-1.446700000

6	0.068008000	0.000003000	0.531106000
6	1.039901000	-1.093068000	-0.060059000
6	1.039891000	1.093067000	-0.060090000
6	2.138298000	0.000001000	-0.295690000
9	0.251178000	0.000023000	1.912269000
9	1.371354000	2.096183000	0.763691000
9	0.609187000	1.610353000	-1.233341000
9	0.609203000	-1.610394000	-1.233296000
9	1.371372000	-2.096157000	0.763752000
9	2.726816000	-0.000013000	-1.499394000
9	3.080343000	0.000019000	0.663848000
16	1.249044000	0.471886000	-0.365015000
8	1.484397000	1.917592000	-0.255691000
8	1.683135000	-0.278816000	-1.551390000
6	2.028294000	-0.294754000	1.098198000
1	3.065247000	0.040229000	1.013424000
1	1.579038000	0.197552000	1.962800000
6	1.913137000	-1.812173000	1.143308000
1	2.337837000	-2.260650000	0.243998000
1	0.874360000	-2.135503000	1.238715000
1	2.462244000	-2.191514000	2.008938000

$SOCHF_2$
E(RB3LYP) = -943.573997576

6	-0.667751000	0.076360000	0.387114000
6	-1.354994000	-1.079989000	0.751807000
6	-1.278477000	1.094136000	-0.336393000
6	-2.681680000	-1.230206000	0.352002000
6	-2.607045000	0.934813000	-0.726236000
6	-3.304700000	-0.224478000	-0.387239000
1	-0.873844000	-1.847754000	1.349689000
1	-3.229566000	-2.123947000	0.627295000
1	-4.338843000	-0.340953000	-0.690398000
1	-3.097756000	1.717828000	-1.292798000
1	-0.713185000	1.988148000	-0.573844000
16	1.058776000	0.314599000	0.934666000
6	1.793985000	-0.758025000	-0.458820000
1	1.295420000	-1.729816000	-0.492900000
9	1.678578000	-0.128496000	-1.643099000
9	3.111617000	-0.925813000	-0.188611000
8	1.438698000	1.739504000	0.638785000

$C{=}CCF_3$
E(RB3LYP) = -645.622312623

6	1.309824000	0.000058000	-0.001793000
6	2.017755000	-1.213754000	-0.000787000
6	2.017867000	1.213804000	-0.000770000
6	3.407818000	-1.208066000	0.000837000
6	3.407928000	1.207984000	0.000874000
6	4.105200000	-0.000075000	0.001725000
1	1.471041000	-2.148776000	-0.001355000
1	3.947880000	-2.147711000	0.001541000
1	5.189129000	-0.000122000	0.003141000
1	3.948082000	2.147577000	0.001620000
1	1.471246000	2.148876000	-0.001307000
6	-0.115065000	0.000142000	-0.002939000
6	-1.319485000	0.000171000	-0.011795000
6	-2.770655000	0.000062000	-0.000845000
9	-3.277348000	1.087802000	-0.624771000
9	-3.277095000	-1.088529000	-0.623678000
9	-3.267168000	0.000527000	1.258373000

$SC(CF_3)_3$
E(RB3LYP) = -1681.24927523

6	1.984268000	-0.028249000	-0.714647000
6	2.619734000	1.195717000	-0.483522000
6	2.673153000	-1.228291000	-0.512165000
6	3.931375000	1.213066000	-0.017168000
6	3.986477000	-1.201300000	-0.050043000
6	4.613776000	0.017218000	0.203001000
1	2.092318000	2.122116000	-0.665943000
1	4.421496000	2.161936000	0.167807000
1	5.635944000	0.035555000	0.563572000
1	4.518138000	-2.132321000	0.108998000
1	2.181451000	-2.170763000	-0.714586000
16	0.356097000	-0.080963000	-1.478952000
6	-0.910271000	-0.004401000	-0.088549000
6	-1.236339000	1.488799000	0.252941000
9	-1.881116000	2.075902000	-0.766266000
9	-2.008722000	1.603731000	1.346713000
9	-0.117940000	2.193622000	0.483513000
6	-2.187895000	-0.696655000	-0.682347000
9	-2.396993000	-0.314456000	-1.951922000
9	-2.057578000	-2.030541000	-0.677582000
9	-3.291831000	-0.391194000	0.016566000
6	-0.463886000	-0.763424000	1.203348000
9	0.080617000	-1.953901000	0.920418000

$SeC(CF_3)_3$
E(RB3LYP) = -3684.58357782

6	-2.070277000	0.075721000	-0.543310000
6	-2.686022000	-1.171160000	-0.403929000
6	-2.744934000	1.243940000	-0.177926000
6	-3.972504000	-1.246156000	0.124867000
6	-4.033081000	1.158735000	0.346392000
6	-4.644927000	-0.083997000	0.500793000
1	-2.165064000	-2.071351000	-0.701973000
1	-4.449710000	-2.212818000	0.238009000
1	-5.647052000	-0.146782000	0.909482000
1	-4.556390000	2.063869000	0.632425000
1	-2.266231000	2.207135000	-0.298310000
6	1.010286000	-0.008780000	0.064069000
6	1.297925000	-1.526708000	0.276829000
9	1.947302000	-2.039526000	-0.780245000
9	2.053965000	-1.751226000	1.367000000
9	0.164076000	-2.228152000	0.434168000
6	2.295610000	0.708540000	-0.458899000
9	2.502616000	0.438500000	-1.761166000
9	2.190808000	2.039527000	-0.337344000
9	3.395947000	0.323792000	0.207022000
6	0.548332000	0.645779000	1.400193000
9	0.008018000	1.857036000	1.207075000
9	-0.369293000	-0.116933000	2.015138000

9	0.443975000	-0.048816000	1.885677000
9	-1.504772000	-0.987232000	2.024916000
9	1.579109000	0.803383000	2.252079000
34	-0.357968000	0.219025000	-1.440813000

$NO=NCONH_2$
E(RB3LYP) = -585.758328115

6	0.884195000	-0.119644000	0.000997000
6	1.763990000	-1.188044000	0.136980000
6	1.331334000	1.192770000	-0.126244000
6	3.131953000	-0.930096000	0.151785000
6	2.701652000	1.433397000	-0.114790000
6	3.601619000	0.376432000	0.026192000
1	1.370619000	-2.191342000	0.222382000
1	3.829423000	-1.752307000	0.258982000
1	4.667821000	0.571523000	0.034425000
1	3.065921000	2.448455000	-0.219906000
1	0.616040000	1.995380000	-0.236953000
7	-0.557974000	-0.418457000	-0.013712000
7	-1.336134000	0.581460000	0.100066000
8	-0.897402000	-1.610428000	-0.117980000
6	-2.735483000	0.286040000	-0.108773000
8	-3.190039000	0.069768000	-1.207060000
7	-3.456490000	0.409655000	1.034386000
1	-3.014378000	0.636141000	1.909224000
1	-4.457282000	0.303695000	0.990110000

$SCOCF_3$
E(RB3LYP) = -1081.02033419

6	-1.078218000	0.713382000	-0.000167000
6	-1.680172000	0.367477000	1.212104000
6	-1.680002000	0.366638000	-1.212278000
6	-2.875408000	-0.347474000	1.207678000
6	-2.875247000	-0.348296000	-1.207516000
6	-3.472135000	-0.706641000	0.000163000
1	-1.216125000	0.653632000	2.147794000
1	-3.339707000	-0.620901000	2.148072000
1	-4.403303000	-1.261528000	0.000287000
1	-3.339425000	-0.622367000	-2.147782000
1	-1.215817000	0.652131000	-2.148100000
16	0.389613000	1.756943000	-0.000396000
6	1.838488000	0.702536000	-0.000051000
8	2.929118000	1.197480000	0.000083000
6	1.694335000	-0.854099000	0.000146000
9	1.029776000	-1.278620000	-1.091021000
9	2.897957000	-1.426666000	0.000191000
9	1.029797000	-1.278384000	1.091380000

$SO_2NHC_6H_5$
E(RB3LYP) = -1067.42933379

6	-1.593464000	-0.043976000	0.143334000
6	-2.525002000	0.217522000	-0.860836000
6	-1.333815000	0.876581000	1.157204000
6	-3.199582000	1.435686000	-0.852353000
6	-2.014892000	2.092048000	1.151909000
6	-2.942807000	2.371697000	0.149737000
1	-2.729603000	-0.530433000	-1.616845000
1	-3.933001000	1.648483000	-1.621407000
1	-3.473211000	3.317098000	0.153855000
1	-1.825077000	2.815627000	1.936056000
1	-0.626370000	0.635322000	1.939629000
16	-0.696929000	-1.605919000	0.117632000
8	-1.467985000	-2.557904000	-0.673991000
8	-0.265246000	-1.888053000	1.480199000
7	0.707030000	-1.351953000	-0.806323000

$NO=NSO_2C_6H_5$
E(RB3LYP) = -1196.72775715

6	2.300089000	-0.442157000	0.369541000
6	3.088800000	-1.242063000	-0.449910000
6	2.613023000	0.881640000	0.650418000
6	4.210476000	-0.676536000	-1.043724000
6	3.755318000	1.424285000	0.065322000
6	4.545290000	0.653569000	-0.784221000
1	2.818269000	-2.275930000	-0.619153000
1	4.826237000	-1.275390000	-1.704004000
1	5.426200000	1.087228000	-1.243085000
1	4.022627000	2.452502000	0.276958000
1	1.986946000	1.474257000	1.303101000
7	1.145772000	-1.083163000	1.029137000
7	-0.064973000	-0.657877000	0.982576000
8	1.415172000	-2.097022000	1.684772000
16	-0.518494000	0.598423000	-0.139853000
8	0.048483000	0.342801000	-1.463238000

6	1.708549000	-0.396907000	-0.471253000
6	2.066715000	0.581514000	-1.404675000
6	2.380823000	-0.467062000	0.753663000
1	1.541788000	0.639192000	-2.352788000
1	2.112191000	-1.236807000	1.464485000
6	3.095439000	1.475920000	-1.120904000
6	3.387916000	0.450802000	1.038305000
1	3.371632000	2.223095000	-1.856204000
1	3.903485000	0.392252000	1.990275000
6	3.754789000	1.420413000	0.105318000
1	4.550521000	2.121088000	0.329549000

$C(Et)(NO_2)_2$
E(RB3LYP) = -759.389385510

6	0.763840000	0.015091000	-0.010614000
6	1.567606000	0.774099000	0.851983000
6	1.379325000	-0.760294000	-0.997490000
6	2.950760000	0.762867000	0.723893000
6	2.768373000	-0.777539000	-1.115490000
6	3.557638000	-0.016513000	-0.260257000
1	1.115644000	1.392371000	1.617101000
1	3.554104000	1.365714000	1.392473000
1	4.636985000	-0.027618000	-0.358300000
1	3.227347000	-1.387372000	-1.884680000
1	0.794821000	-1.354168000	-1.687027000
6	-0.734168000	0.039658000	0.201392000
7	-1.355276000	1.449618000	-0.165428000
8	-0.601678000	2.372520000	-0.382724000
8	-2.571379000	1.496232000	-0.146503000
7	-1.436056000	-0.886623000	-0.825954000
8	-1.435993000	-0.506556000	-1.981704000
8	-1.901537000	-1.933018000	-0.417386000
6	-1.206685000	-0.262952000	1.633704000
1	-0.984820000	0.631088000	2.225051000
1	-2.293008000	-0.354546000	1.607758000
6	-0.572873000	-1.485860000	2.304590000
1	0.509342000	-1.382611000	2.397752000
1	-0.791063000	-2.400826000	1.755720000
1	-0.988232000	-1.587760000	3.310087000

$CF_2CF_2CF_3$
E(RB3LYP) = -1045.17405618

6	-1.212742000	0.417282000	-0.223700000
6	-1.767988000	-0.482530000	-1.135319000
6	-1.898594000	0.743158000	0.949803000
6	-3.008839000	-1.056563000	-0.870523000
6	-3.137062000	0.164200000	1.208050000
6	-3.692514000	-0.736892000	0.300390000
1	-1.239909000	-0.725379000	-2.048296000
1	-3.440749000	-1.750902000	-1.581616000
1	-4.657908000	-1.185693000	0.504500000
1	-3.669346000	0.419622000	2.116760000
1	-1.471112000	1.449204000	1.650231000
6	0.131411000	1.042269000	-0.498669000
9	0.450434000	0.959917000	-1.822792000
9	0.113594000	2.372365000	-0.172518000
6	1.350185000	0.455929000	0.294846000
9	1.155047000	0.689439000	1.617606000
9	2.469869000	1.109479000	-0.088798000
6	1.628555000	-1.070196000	0.136534000
9	1.747828000	-1.408307000	-1.153819000
9	2.769283000	-1.380084000	0.763155000
9	0.641118000	-1.794676000	0.678271000

$SCF_2CF_2CF_3$
E(RB3LYP) = -1443.37741620

6	2.336168000	0.355941000	0.353332000
6	2.954989000	-0.716876000	1.000202000
6	2.947087000	0.970219000	-0.742746000
6	4.184036000	-1.181958000	0.537746000
8	-0.337611000	1.895237000	0.512254000
6	-2.269018000	0.215586000	-0.175303000
6	-3.102459000	0.770388000	0.792495000
6	-2.753972000	-0.621378000	-1.176687000
1	-2.694307000	1.428976000	1.548344000
1	-2.079242000	-1.022831000	-1.921957000
6	-4.461032000	0.468425000	0.755483000
6	-4.115586000	-0.912600000	-1.202032000
1	-5.125028000	0.892071000	1.499689000
1	-4.511603000	-1.558951000	-1.976398000
6	-4.964978000	-0.371666000	-0.237479000
1	-6.023863000	-0.602515000	-0.261551000

$(CF_2)_3CF_3$
E(RB3LYP) = -1283.02909760

6	1.918769000	0.305972000	0.139798000
6	2.313312000	-0.560747000	1.160750000
6	2.568256000	0.277734000	-1.097566000
6	3.357492000	-1.455605000	0.941500000
6	3.609403000	-0.620537000	-1.309418000
6	4.004295000	-1.488289000	-0.291995000
1	1.813829000	-0.530118000	2.120157000
1	3.666225000	-2.123931000	1.736694000
1	4.817137000	-2.185576000	-0.459731000
1	4.115149000	-0.638932000	-2.267640000
1	2.268800000	0.959062000	-1.883671000
6	0.791671000	1.281200000	0.366191000
9	0.592585000	1.508403000	1.695723000
9	1.088319000	2.490877000	-0.204028000
6	-0.603650000	0.894260000	-0.246203000
9	-0.487590000	0.906411000	-1.597293000
9	-1.500225000	1.846539000	0.106239000
6	-1.178133000	-0.499713000	0.168835000
9	-1.021462000	-0.683375000	1.500946000
9	-0.489346000	-1.464534000	-0.479947000
6	-2.695492000	-0.714224000	-0.150270000
9	-2.960062000	-0.419695000	-1.427872000
9	-3.001359000	-2.000363000	0.063127000
9	-3.464936000	0.037870000	0.639157000

SO_2NMe_2
E(RB3LYP) = -914.958138894

6	-0.795347000	0.079736000	0.206615000
6	-1.306679000	-1.211727000	0.329847000
6	-1.603485000	1.153909000	-0.153657000
6	-2.657544000	-1.427188000	0.077484000
6	-2.957219000	0.925324000	-0.400944000
6	-3.481208000	-0.360431000	-0.288312000
1	-0.657859000	-2.027878000	0.621688000
1	-3.068837000	-2.425642000	0.169923000
1	-4.533715000	-0.533874000	-0.481761000
1	-3.598722000	1.753177000	-0.679684000
1	-1.174701000	2.145221000	-0.228675000
16	0.940927000	0.378349000	0.581560000
8	1.275956000	-0.268669000	1.849381000
8	1.184467000	1.813621000	0.406111000
7	1.710540000	-0.537733000	-0.630229000
6	1.630033000	0.057104000	-1.969953000
1	0.599455000	0.333453000	-2.196154000
1	2.267327000	0.943163000	-2.074898000
1	1.942567000	-0.700655000	-2.691324000
6	3.058927000	-1.003788000	-0.269905000
1	3.342330000	-1.774328000	-0.989791000
1	3.804707000	-0.198939000	-0.299866000
1	3.040580000	-1.440406000	0.726184000

$SO_2C_6H_5$
E(RB3LYP) = -1012.05775957

6	-1.432549000	0.215654000	0.000161000
6	-1.975833000	-0.192544000	1.216252000
6	-1.976270000	-0.190900000	-1.216259000
6	-3.079774000	-1.042061000	1.209347000

6	4.176526000	0.499015000	-1.197471000
6	4.793813000	-0.576075000	-0.559709000
1	2.477575000	-1.178666000	1.855270000
1	4.664299000	-2.015553000	1.037025000
1	5.751343000	-0.939016000	-0.915424000
1	4.650755000	0.972789000	-2.049217000
1	2.462236000	1.805648000	-1.231902000
16	0.785379000	1.005959000	0.991649000
6	-0.380261000	-0.037989000	0.033179000
9	-0.096916000	-0.022680000	-1.294591000
9	-0.325253000	-1.344126000	0.421031000
6	-1.840665000	0.475781000	0.226549000
9	-2.076636000	0.650808000	1.549268000
9	-1.962521000	1.671951000	-0.391164000
6	-2.972063000	-0.452773000	-0.324024000
9	-3.049034000	-1.587082000	0.376899000
9	-4.144268000	0.187238000	-0.219947000
9	-2.764268000	-0.750805000	-1.610885000

6	-3.080189000	-1.040461000	-1.210076000
6	-3.627378000	-1.468155000	-0.000534000
1	-3.516704000	-1.362977000	2.147858000
1	-4.487869000	-2.127539000	-0.000801000
1	-3.517423000	-1.360195000	-2.148840000
1	-1.553466000	0.171931000	-2.144689000
1	-1.552518000	0.169066000	2.144931000
16	0.000033000	1.319164000	0.000539000
8	0.000189000	2.033027000	1.283011000
8	-0.000052000	2.033965000	-1.281393000
6	1.432426000	0.215625000	0.000031000
6	1.975985000	-0.191327000	-1.216348000
6	1.976026000	-0.192266000	1.216089000
1	1.552863000	0.171165000	-2.144789000
1	1.552990000	0.169516000	2.144833000
6	3.079923000	-1.040802000	-1.210183000
6	3.079981000	-1.041766000	1.209198000
1	3.516951000	-1.360718000	-2.148986000
1	3.517036000	-1.362367000	2.147757000
6	3.627416000	-1.468157000	-0.000656000
1	4.487942000	-2.127491000	-0.000970000

SOOH

E(RB3LYP) = -780.969011542

6	-0.107625000	0.036574000	0.156544000
6	-0.853005000	1.202052000	0.324020000
6	-0.709071000	-1.182590000	-0.131567000
6	-2.235952000	1.142746000	0.175623000
6	-2.094570000	-1.229673000	-0.280733000
6	-2.854784000	-0.071450000	-0.126756000
1	-0.363349000	2.142517000	0.549272000
1	-2.829589000	2.041878000	0.293735000
1	-3.932190000	-0.113452000	-0.239484000
1	-2.578446000	-2.171047000	-0.514322000
1	-0.091512000	-2.066144000	-0.243323000
16	1.689076000	0.065831000	0.422589000
8	2.180362000	-1.304328000	0.116368000
8	1.949141000	1.094422000	-0.922132000
1	2.863877000	1.406253000	-0.863965000

PF_2

E(RB3LYP) = -772.886869968

6	2.865680000	0.244304000	-0.000114000
6	1.984387000	1.329002000	-0.000193000
6	2.375450000	-1.058791000	0.000113000
1	2.371719000	2.341550000	-0.000370000
1	3.059865000	-1.899236000	0.000172000
6	0.611693000	1.112797000	-0.000050000
6	0.998434000	-1.279971000	0.000261000
1	-0.072191000	1.953629000	-0.000089000
1	0.614849000	-2.295823000	0.000434000
6	0.112266000	-0.197562000	0.000154000
1	3.935761000	0.419011000	-0.000237000
15	-1.671568000	-0.581779000	0.000290000
9	-2.140303000	0.406600000	1.215284000
9	-2.140135000	0.405497000	-1.215870000

$SiCl_3$

E(RB3LYP) = -1902.06231659

6	-0.927632000	0.008426000	0.037439000
6	-1.647055000	1.213333000	0.025047000
6	-1.636779000	-1.203584000	0.024797000
6	-3.039573000	1.205101000	-0.002039000
6	-3.028490000	-1.208463000	-0.002794000
6	-3.731090000	-0.004495000	-0.016061000
1	-1.123747000	2.162463000	0.043122000
1	-3.582871000	2.143116000	-0.008193000
1	-4.815113000	-0.009507000	-0.034953000
1	-3.563391000	-2.151282000	-0.009593000
1	-1.105285000	-2.148645000	0.042935000
14	0.928772000	0.003593000	0.008109000
17	1.684738000	1.763217000	0.774118000
17	1.677834000	-1.572063000	1.109553000
17	1.652212000	-0.197528000	-1.915740000

OCN

E(RB3LYP) = -399.791322794

6	-0.132081000	-0.360593000	0.000014000
6	0.113265000	1.003213000	0.000010000
6	0.882455000	-1.306297000	0.000007000
6	1.441940000	1.430366000	0.000028000
6	2.200989000	-0.860042000	-0.000025000
6	2.483859000	0.506269000	-0.000023000
1	-0.704162000	1.714336000	0.000041000
1	1.654491000	2.492853000	0.000022000
1	3.511923000	0.847851000	-0.000049000
1	3.007271000	-1.583931000	-0.000035000
1	0.635491000	-2.360410000	0.000012000
8	-1.447298000	-0.893777000	0.000028000
6	-2.453663000	-0.090432000	0.000005000
7	-3.392460000	0.586373000	-0.000045000

$SCF(CF_3)_2$

E(RB3LYP) = -1443.38269908

6	1.824321000	0.408059000	0.472316000
6	2.605721000	-0.631620000	0.983179000
6	2.344314000	1.276210000	-0.491716000
6	3.906303000	-0.808309000	0.517453000
6	3.640361000	1.081645000	-0.963052000
6	4.421626000	0.042776000	-0.458876000
1	2.195627000	-1.295990000	1.733395000
1	4.513009000	-1.614083000	0.914222000
1	5.432595000	-0.100304000	-0.822977000
1	4.041508000	1.748363000	-1.717633000
1	1.740273000	2.092378000	-0.866217000
16	0.197773000	0.707289000	1.176848000
6	-0.935671000	0.134118000	-0.170091000

$C(CF_3)_3$

E(RB3LYP) = -1283.04006113

6	1.169667000	0.055999000	-0.036599000
6	1.900992000	-1.142174000	-0.027913000
6	1.883195000	1.261584000	-0.030822000
6	3.292143000	-1.131357000	-0.031614000
6	3.276301000	1.265806000	-0.033955000
6	3.989344000	0.072595000	-0.038076000
1	1.397267000	-2.095288000	-0.014585000
1	3.826996000	-2.073908000	-0.027030000
1	5.073130000	0.080133000	-0.041685000
1	3.798771000	2.215277000	-0.031604000
1	1.382026000	2.215499000	-0.021750000
6	-0.383005000	0.001702000	-0.010108000
6	-1.036088000	1.434498000	0.027002000

9	-0.496446000	0.534449000	-1.410505000
6	-1.063727000	-1.417682000	-0.241421000
9	-1.650527000	-1.898167000	0.864876000
9	-1.788708000	-1.803458000	-1.301691000
9	0.146309000	-1.983736000	-0.357525000
6	-2.309851000	0.838883000	0.061494000
9	-2.736045000	0.663056000	1.322028000
9	-2.187617000	2.152431000	-0.163235000
9	-3.252273000	0.369707000	-0.767956000

9	-0.616457000	2.204745000	-0.991903000
9	-2.372296000	1.395411000	-0.050341000
9	-0.719382000	2.066753000	1.172155000
6	-0.844574000	-0.764184000	1.289896000
9	-0.171186000	-0.317650000	2.359751000
9	-2.152241000	-0.619612000	1.546557000
9	-0.609803000	-2.086315000	1.187978000
6	-0.930144000	-0.737160000	-1.289530000
9	-2.258180000	-0.927613000	-1.236420000
9	-0.659799000	-0.018958000	-2.390779000
9	-0.372343000	-1.946270000	-1.460667000

CF_2CF_3

E(RB3LYP) = -807.319859956

6	-3.425619000	0.046985000	-0.364036000
6	-2.767764000	-1.177889000	-0.267799000
6	-2.733049000	1.231560000	-0.118510000
1	-3.304610000	-2.100699000	-0.453758000
1	-3.242885000	2.185210000	-0.188824000
6	-1.418169000	-1.222479000	0.071423000
6	-1.383926000	1.194823000	0.222039000
1	-0.907331000	-2.173276000	0.153398000
1	-0.846390000	2.113340000	0.420218000
6	-0.727486000	-0.034356000	0.319350000
1	-4.476573000	0.078349000	-0.627873000
6	0.736454000	-0.074316000	0.673869000
9	1.063281000	0.942812000	1.527031000
9	1.061704000	-1.246924000	1.294648000
6	1.702216000	0.054036000	-0.541916000
9	1.504601000	1.221764000	-1.175140000
9	2.980458000	0.000897000	-0.149331000
9	1.487939000	-0.942227000	-1.416062000

OSO_2CF_3

E(RB3LYP) = -1193.31147245

6	1.357225000	-0.181966000	-0.493903000
6	2.113498000	-1.184148000	0.099265000
6	1.844554000	1.105279000	-0.676658000
6	3.399476000	-0.872039000	0.535750000
6	3.135641000	1.398482000	-0.243441000
6	3.911563000	0.413412000	0.365814000
1	1.706038000	-2.178797000	0.220060000
1	4.002388000	-1.640877000	1.004311000
1	4.914620000	0.645543000	0.703687000
1	3.532246000	2.397071000	-0.383854000
1	1.226153000	1.851631000	-1.159122000
8	0.081732000	-0.467708000	-1.035912000
16	-1.197690000	-0.902101000	-0.111536000
8	-2.113211000	-1.566382000	-1.004197000
8	-0.763821000	-1.462525000	1.149576000
6	-1.930134000	0.804643000	0.258796000
9	-3.052778000	0.638438000	0.951756000
9	-1.066886000	1.523415000	0.975567000
9	-2.196663000	1.441480000	-0.877321000

NC

E(RB3LYP) = -324.542985321

6	2.145167000	-0.000005000	0.000033000
6	1.447589000	-1.207477000	0.000024000
6	1.447614000	1.207461000	0.000020000
1	1.986962000	-2.147408000	0.000034000
1	1.986977000	2.147398000	0.000027000
6	0.056441000	-1.215594000	0.000003000
6	0.056449000	1.215597000	-0.000001000
1	-0.499958000	-2.144270000	-0.000004000
1	-0.499908000	2.144298000	-0.000011000
6	-0.634045000	0.000015000	-0.000010000
1	3.228851000	-0.000024000	0.000049000
7	-2.021191000	0.000007000	-0.000031000
6	-3.194980000	-0.000005000	-0.000049000

CHO

E(RB3LYP) = -345.669073013

6	2.216464000	-0.242259000	0.000008000
6	1.332966000	-1.325948000	0.000007000
6	1.729180000	1.063928000	0.000011000
1	1.719725000	-2.338601000	0.000005000
1	2.417294000	1.901267000	0.000012000
6	-0.037858000	-1.104697000	0.000007000
6	0.354619000	1.286796000	0.000013000
1	-0.742032000	-1.928423000	0.000005000
1	-0.035107000	2.300218000	0.000016000
6	-0.534067000	0.206308000	0.000010000
1	3.286426000	-0.418625000	0.000007000
6	-1.992096000	0.463241000	0.000006000
8	-2.848893000	-0.392379000	-0.000041000
1	-2.270408000	1.538992000	-0.000094000

$CF{=}CFCF_3$

E(RB3LYP) = -845.397823052

6	1.379300000	-0.140417000	-0.004464000
6	1.914908000	1.160325000	-0.009892000
6	2.257686000	-1.237630000	0.005645000
6	3.292230000	1.346880000	-0.005625000
6	3.633581000	-1.038342000	0.009833000
6	4.156757000	0.252905000	0.004430000
1	1.263757000	2.021547000	-0.018104000
1	3.691254000	2.354541000	-0.010049000
1	5.229719000	0.406541000	0.007891000
1	4.297063000	-1.895295000	0.017574000
1	1.858896000	-2.242937000	0.010082000
6	-0.060219000	-0.402807000	-0.009028000
6	-1.107163000	0.434303000	-0.009570000
6	-2.558346000	0.007441000	-0.001460000
9	-3.355663000	1.076800000	-0.150047000
9	-2.839929000	-0.857769000	-0.995857000
9	-2.901923000	-0.598282000	1.157598000
9	-0.936127000	1.769152000	0.010726000
9	-0.387813000	-1.716607000	-0.009821000

SSO_2Me

E(RB3LYP) = -1218.49805822

6	-3.539470000	0.298959000	-0.513004000
6	-3.062294000	-1.010685000	-0.483616000
6	-2.752825000	1.340610000	-0.021112000
1	-3.673148000	-1.822692000	-0.861191000
1	-3.123501000	2.358922000	-0.042342000
6	-1.795222000	-1.279921000	0.028364000
6	-1.492833000	1.079574000	0.509687000
1	-1.416116000	-2.294716000	0.051206000
1	-0.879971000	1.883020000	0.896385000
6	-1.008981000	-0.233620000	0.526116000
1	-4.524201000	0.507568000	-0.915438000
16	0.574336000	-0.615899000	1.267805000
16	1.963309000	0.232607000	-0.185708000
8	1.466679000	1.530119000	-0.645039000
8	3.275807000	0.100789000	0.444277000
6	1.888701000	-0.902767000	-1.591791000
1	2.571365000	-0.496072000	-2.338774000
1	2.212698000	-1.885170000	-1.255339000
1	0.868217000	-0.918362000	-1.969836000

$C(Me)(CN)_2$

SCF_2CF_3

E(RB3LYP) = -495.470826034

6	0.355577000	-0.000004000	-0.044639000
6	1.056791000	1.206571000	0.002363000
6	1.056790000	-1.206562000	0.002357000
6	2.447173000	1.204252000	0.091714000
6	2.447185000	-1.204242000	0.091703000
6	3.146022000	0.000000000	0.135220000
1	0.523503000	2.150064000	-0.016950000
1	2.980790000	2.146633000	0.134571000
1	4.227276000	0.000018000	0.209791000
1	2.980783000	-2.146634000	0.134547000
1	0.523523000	-2.150067000	-0.016953000
6	-1.177985000	0.000003000	-0.236826000
6	-1.788737000	-1.191759000	0.385584000
7	-2.268731000	-2.141504000	0.826964000
6	-1.788757000	1.191755000	0.385568000
7	-2.268743000	2.141502000	0.826951000
6	-1.530439000	-0.000008000	-1.758575000
1	-1.101913000	-0.888280000	-2.223149000
1	-2.611519000	0.000041000	-1.902893000
1	-1.101833000	0.888208000	-2.223176000

E(RB3LYP) = -1205.52149053

6	3.788020000	-0.517689000	0.531602000
6	3.241049000	0.687842000	0.969315000
6	3.124271000	-1.277080000	-0.430311000
1	3.758963000	1.283360000	1.712272000
1	3.549059000	-2.212905000	-0.774665000
6	2.031972000	1.139541000	0.446119000
6	1.907640000	-0.839731000	-0.949205000
1	1.611029000	2.082478000	0.770568000
1	1.382954000	-1.429620000	-1.690525000
6	1.359363000	0.365672000	-0.503757000
1	4.732676000	-0.862181000	0.936656000
16	-0.157474000	0.971782000	-1.258542000
6	-1.406353000	0.675823000	0.053141000
9	-0.999049000	1.128626000	1.265870000
9	-2.506702000	1.380963000	-0.313219000
6	-1.861166000	-0.799956000	0.248805000
9	-2.354955000	-1.296682000	-0.892185000
9	-0.834509000	-1.567012000	0.641523000
9	-2.818549000	-0.869913000	1.185579000

CH=CHCOC$_6$H$_4$-4NO$_2$

E(RB3LYP) = -858.769184645

6	-3.749718000	0.118936000	0.009584000
6	-3.825488000	-1.257101000	-0.275610000
6	-4.949375000	0.821033000	0.218503000
6	-5.053446000	-1.900359000	-0.344440000
6	-6.180284000	0.175962000	0.151068000
6	-6.236038000	-1.187203000	-0.130393000
1	-2.919619000	-1.825931000	-0.448737000
1	-5.093980000	-2.960536000	-0.567076000
1	-7.192826000	-1.693776000	-0.185053000
1	-7.093440000	0.735863000	0.316802000
1	-4.907459000	1.882698000	0.437063000
6	-2.491307000	0.853065000	0.097830000
6	-1.238623000	0.371820000	-0.019872000
1	-1.056190000	-0.678589000	-0.207130000
1	-2.578020000	1.921168000	0.283599000
6	-0.077151000	1.282158000	0.075682000
8	-0.204074000	2.495096000	0.163341000
6	1.309952000	0.688651000	0.043042000
6	2.374790000	1.538073000	-0.288525000
6	1.576515000	-0.649075000	0.362552000
1	2.157617000	2.573730000	-0.516716000
1	0.775106000	-1.318463000	0.647139000
6	3.678431000	1.064330000	-0.319494000
6	2.879404000	-1.135649000	0.351376000
1	4.509660000	1.703577000	-0.582902000
1	3.104238000	-2.161773000	0.606979000
6	3.909263000	-0.270368000	0.002493000
7	5.298227000	-0.785410000	-0.023042000
8	5.473869000	-1.959280000	0.277579000
8	6.185928000	-0.006534000	-0.344102000

N=NPO(OEt)$_2$

E(RB3LYP) = -1066.87537020

6	2.284982000	-0.032670000	0.083559000
6	3.189425000	-1.085471000	-0.077275000
6	2.722596000	1.297183000	0.016592000
6	4.533969000	-0.814632000	-0.316740000
6	4.064624000	1.559091000	-0.219479000
6	4.971214000	0.506520000	-0.388240000
1	2.819680000	-2.101728000	-0.007905000
1	5.237524000	-1.629258000	-0.442536000
1	6.018173000	0.721038000	-0.570893000
1	4.413500000	2.584362000	-0.269567000
1	2.005946000	2.096269000	0.156429000
7	0.934428000	-0.421989000	0.324754000
7	0.110381000	0.510271000	0.419934000
15	-1.528411000	0.042161000	0.802241000
8	-1.876780000	0.453431000	2.174383000
8	-1.748897000	-1.504680000	0.494860000
6	-1.677505000	-2.121037000	-0.820457000
1	-0.643087000	-2.067248000	-1.167053000
1	-2.315529000	-1.555685000	-1.503012000
6	-2.140499000	-3.555931000	-0.678947000
1	-3.170170000	-3.597005000	-0.318066000
1	-1.504326000	-4.100070000	0.021992000
1	-2.092534000	-4.054761000	-1.651258000
8	-2.332459000	0.754587000	-0.395715000
6	-2.648656000	2.175063000	-0.366404000
1	-1.740898000	2.730169000	-0.616908000
1	-2.956494000	2.440869000	0.647148000
6	-3.751283000	2.430320000	-1.372630000
1	-4.650463000	1.867942000	-1.112559000
1	-3.436760000	2.142101000	-2.378228000
1	-4.000186000	3.495292000	-1.382111000

CH=CHCN

E(RB3LYP) = -402.000707286

6	-0.361499000	-0.186094000	0.000104000
6	-0.912377000	1.107861000	0.000152000
6	-1.239306000	-1.282657000	0.000040000
6	-2.288268000	1.292047000	0.000102000
6	-2.618616000	-1.097637000	-0.000019000
6	-3.147789000	0.190622000	0.000007000
1	-0.264311000	1.976280000	0.000266000
1	-2.695591000	2.296602000	0.000150000
1	-4.221478000	0.339198000	-0.000030000
1	-3.278172000	-1.957764000	-0.000079000
1	-0.831163000	-2.287834000	0.000023000
6	1.077261000	-0.446617000	0.000124000
6	2.068154000	0.465835000	-0.000226000
1	1.870353000	1.531985000	-0.000596000

CF_3

E(RB3LYP) = -569.460850790

6	2.835657000	0.000027000	0.013476000
6	2.139148000	-1.207419000	0.001795000
6	2.139081000	1.207447000	0.001800000
1	2.678654000	-2.147273000	0.007235000
1	2.678546000	2.147325000	0.007245000
6	0.747013000	-1.211052000	-0.020072000
6	0.746957000	1.211007000	-0.020071000
1	0.202351000	-2.146785000	-0.035090000
1	0.202250000	2.146718000	-0.035090000
6	0.053614000	-0.000045000	-0.033113000
1	3.919579000	0.000060000	0.028662000
6	-1.450512000	-0.000024000	-0.004054000
9	-1.975913000	1.087511000	-0.612692000
9	-1.975950000	-1.088468000	-0.610992000

1	1.360305000	-1.495584000	0.000430000
6	3.440480000	0.097178000	-0.000165000
7	4.564545000	-0.178016000	-0.000125000
9	-1.931152000	0.000991000	1.266848000

$CF(CF_3)_2$
E(RB3LYP) = -1045.18010205

6	-0.991358000	-0.000069000	0.159564000
6	-1.518737000	-0.000346000	-1.136552000
6	-1.854678000	0.000254000	1.257634000
6	-2.898096000	-0.000382000	-1.324686000
6	-3.233357000	0.000226000	1.060085000
6	-3.758745000	-0.000120000	-0.229248000
1	-0.867103000	-0.000538000	-1.999071000
1	-3.297288000	-0.000618000	-2.332170000
1	-4.832075000	-0.000171000	-0.380407000
1	-3.894769000	0.000472000	1.918626000
1	-1.452803000	0.000521000	2.261353000
6	0.512224000	0.000020000	0.407349000
9	0.770366000	0.000134000	1.768504000
6	1.196922000	-1.298926000	-0.121902000
9	1.118698000	-1.388665000	-1.461625000
9	2.490130000	-1.356208000	0.220067000
9	0.586278000	-2.370826000	0.404058000
6	1.196732000	1.298983000	-0.122142000
9	1.119396000	1.387845000	-1.462015000
9	0.585315000	2.370951000	0.402701000
9	2.489662000	1.357046000	0.220650000

$SiBr_3$
E(RB3LYP) = -8243.81528468

6	1.530618000	-0.015162000	0.060316000
6	2.242176000	1.195122000	0.048040000
6	2.246498000	-1.221737000	0.050762000
6	3.634014000	1.196311000	0.025426000
6	3.639199000	-1.216747000	0.028706000
6	4.334074000	-0.009148000	0.015695000
1	1.712795000	2.141184000	0.063000000
1	4.170795000	2.138106000	0.019244000
1	5.418160000	-0.006820000	0.000488000
1	4.179770000	-2.156393000	0.025197000
1	1.720511000	-2.169176000	0.067283000
14	-0.333624000	-0.004389000	0.012254000
35	-1.165235000	-1.906915000	0.849620000
35	-1.072434000	0.205427000	-2.094385000
35	-1.142067000	1.716994000	1.195610000

$CClF_2$
E(RB3LYP) = -929.800759920

6	0.304994000	-0.007461000	0.181502000
6	0.996158000	-1.213550000	0.055297000
6	0.986553000	1.208209000	0.100843000
6	2.373803000	-1.200209000	-0.144872000
6	2.363948000	1.213559000	-0.099505000
6	3.058794000	0.011252000	-0.223186000
1	0.462051000	-2.153090000	0.119506000
1	2.911319000	-2.136661000	-0.237555000
1	4.131526000	0.018531000	-0.378783000
1	2.893977000	2.157070000	-0.157075000
1	0.444862000	2.140475000	0.199701000
6	-1.184926000	-0.016027000	0.378763000
17	-2.086316000	0.045478000	-1.195000000
9	-1.598261000	-1.130302000	1.028312000
9	-1.598664000	1.044292000	1.113483000

$CH{=}NCOC_6H_5$
E(RB3LYP) = -670.265359624

6	2.445572000	0.261340000	0.075085000
6	3.520412000	0.958655000	0.644240000
6	2.674036000	-0.995126000	-0.509146000
6	4.801418000	0.413912000	0.632738000
6	3.952082000	-1.535864000	-0.520548000
6	5.017830000	-0.833604000	0.050719000
1	3.347126000	1.931044000	1.093654000

$S(O){=}NHCF_3$
E(RB3LYP) = -1098.23451665

6	1.100147000	0.404813000	-0.319708000
6	1.595171000	-0.592054000	-1.157456000
6	1.769297000	0.794099000	0.833678000
6	2.780505000	-1.232957000	-0.808819000
6	2.954592000	0.142628000	1.173581000
6	3.458129000	-0.866886000	0.355694000
1	1.057335000	-0.877534000	-2.054108000
1	3.173948000	-2.018609000	-1.443371000
1	4.381152000	-1.368818000	0.622421000
1	3.482851000	0.426806000	2.076316000
1	1.354501000	1.583372000	1.449308000
16	-0.372759000	1.362772000	-0.811726000
8	-0.667111000	2.283742000	0.326264000
7	-1.501123000	0.001249000	-0.911969000
1	-2.255612000	0.248269000	-1.545319000
6	-2.007329000	-0.695382000	0.211997000
9	-2.861691000	0.024922000	0.976702000
9	-2.705079000	-1.773305000	-0.217623000
9	-1.020823000	-1.118513000	1.010059000

ONO_2
E(RB3LYP) = -512.075319040

6	-0.181501000	-0.000178000	0.442773000
6	-0.836480000	1.214650000	0.266942000
6	-0.836678000	-1.214851000	0.266502000
6	-2.181728000	1.209386000	-0.092270000
6	-2.181912000	-1.209249000	-0.092706000
6	-2.853034000	0.000163000	-0.273835000
1	-0.295886000	2.140991000	0.419415000
1	-2.705291000	2.148376000	-0.228560000
1	-3.900105000	0.000287000	-0.553710000
1	-2.705653000	-2.148090000	-0.229326000
1	-0.296212000	-2.141320000	0.418639000
8	1.139200000	-0.000379000	0.888973000
7	2.156659000	0.000045000	-0.197828000
8	1.749897000	0.000490000	-1.324402000
8	3.265219000	-0.000121000	0.242167000

CCl_3
E(RB3LYP) = -1650.48245753

6	3.411814000	-0.009218000	0.000109000
6	2.690448000	1.185727000	0.000491000
6	2.730400000	-1.220528000	-0.000054000
1	3.210127000	2.136793000	0.000628000
1	3.278455000	-2.155536000	-0.000335000
6	1.302634000	1.164787000	0.000723000
6	1.335360000	-1.247055000	0.000146000
1	0.752686000	2.097499000	0.000988000
1	0.822276000	-2.197822000	0.000023000
6	0.611085000	-0.055065000	0.000550000
1	4.495576000	0.008384000	-0.000046000
6	-0.906650000	-0.019941000	0.000327000
17	-1.665667000	-1.652502000	0.002567000
17	-1.507954000	0.862804000	-1.470469000
17	-1.509300000	0.867254000	1.467019000

$CF_2CF_2C_6H_4$-4F
E(RB3LYP) = -1038.41972473

6	-1.811269000	0.199675000	0.319047000
6	-1.387305000	1.256344000	1.127794000
6	-2.789205000	0.414419000	-0.655965000
6	-1.942459000	2.523018000	0.961839000
6	-3.338347000	1.683272000	-0.818748000
6	-2.915745000	2.738849000	-0.011755000
1	-0.637580000	1.086347000	1.889730000
1	-1.616225000	3.338995000	1.596240000

1	6.014414000	-1.260585000	0.039905000
1	4.125188000	-2.505312000	-0.973808000
1	1.838083000	-1.525916000	-0.947780000
6	1.113800000	0.868158000	0.099217000
1	1.044436000	1.867976000	0.544445000
7	0.069911000	0.292872000	-0.364610000
6	-1.132602000	1.041609000	-0.362447000
8	-1.160047000	2.239055000	-0.583072000
6	-2.368119000	0.241934000	-0.116429000
6	-3.592765000	0.916561000	-0.018534000
6	-2.333909000	-1.150382000	0.031996000
1	-3.602865000	1.993049000	-0.137527000
1	-1.387573000	-1.667415000	-0.056095000
6	-4.763561000	0.209491000	0.226790000
6	-3.509128000	-1.856087000	0.277689000
1	-5.708153000	0.736168000	0.302270000
1	-3.478361000	-2.934103000	0.388693000
6	-4.723475000	-1.178510000	0.375818000
1	-5.637986000	-1.729598000	0.565611000

1	-3.347370000	3.725256000	-0.138406000
1	-4.100512000	1.845374000	-1.572117000
1	-3.123920000	-0.408227000	-1.274753000
6	-1.211679000	-1.174821000	0.486375000
9	-0.742226000	-1.345037000	1.765519000
9	-2.166841000	-2.134100000	0.286524000
6	-0.018830000	-1.510810000	-0.470085000
9	-0.511643000	-1.443077000	-1.749525000
9	0.318448000	-2.818279000	-0.245767000
6	1.196825000	-0.630232000	-0.326763000
6	1.356354000	0.488428000	-1.147424000
6	2.163780000	-0.930739000	0.636682000
1	0.613288000	0.717883000	-1.899800000
1	2.046209000	-1.802723000	1.266663000
6	2.475171000	1.305092000	-1.012604000
6	3.284807000	-0.119955000	0.782180000
1	2.622607000	2.173344000	-1.642103000
1	4.049484000	-0.336536000	1.517279000
6	3.416078000	0.983788000	-0.047011000
9	4.505035000	1.774082000	0.089459000

$CH_2SO_2CF_3$
E(RB3LYP) = -1157.40606166

6	-1.337103000	0.464087000	0.619605000
6	-2.003326000	1.223846000	-0.349310000
6	-1.899802000	-0.742446000	1.048349000
6	-3.211343000	0.780342000	-0.878246000
6	-3.111384000	-1.182734000	0.520563000
6	-3.767974000	-0.422846000	-0.444808000
1	-1.568682000	2.153891000	-0.696596000
1	-3.718649000	1.374733000	-1.629284000
1	-4.710486000	-0.764708000	-0.856934000
1	-3.540311000	-2.117163000	0.863501000
1	-1.392975000	-1.336864000	1.801015000
6	-0.042418000	0.938465000	1.212892000
1	-0.052619000	2.003783000	1.460566000
1	0.253902000	0.380598000	2.101032000
16	1.427946000	0.875227000	0.103237000
8	2.603786000	1.204159000	0.903394000
6	1.600068000	-0.979725000	-0.321247000
9	0.669707000	-1.362055000	-1.191850000
9	2.804937000	-1.180825000	-0.843702000
9	1.477292000	-1.709105000	0.798194000
8	1.140583000	1.557846000	-1.154102000

$N{=}C(CF_3)_2$
E(RB3LYP) = -1000.04956227

6	1.503000000	-0.568608000	0.110568000
6	2.361730000	-1.378029000	-0.645702000
6	2.028448000	0.480046000	0.877302000
6	3.720569000	-1.091621000	-0.693369000
6	3.396926000	0.729854000	0.854695000
6	4.244173000	-0.040497000	0.060111000
1	1.945967000	-2.213062000	-1.196200000
1	4.375525000	-1.704556000	-1.301615000
1	5.307684000	0.166518000	0.040094000
1	3.800439000	1.532977000	1.460437000
1	1.377877000	1.074588000	1.505308000
7	0.149178000	-0.945341000	0.148493000
6	-0.870833000	-0.216820000	0.029677000
6	-2.238827000	-0.899789000	0.183318000
9	-3.042054000	-0.172921000	0.990533000
9	-2.857490000	-1.019914000	-1.010085000
9	-2.124847000	-2.119031000	0.708259000
6	-0.913056000	1.290605000	-0.294669000
9	0.073931000	1.633824000	-1.136090000
9	-2.074202000	1.635927000	-0.872285000
9	-0.780285000	2.034347000	0.826438000

SCOMe
E(RB3LYP) = -783.217728392

6	-0.466794000	-0.492988000	-0.010077000
6	-1.134087000	-0.249247000	-1.214944000
6	-1.134133000	-0.298804000	1.203741000
6	-2.449946000	0.209173000	-1.202585000
6	-2.449975000	0.159723000	1.210360000
6	-3.108207000	0.417612000	0.008669000
1	-0.623702000	-0.423232000	-2.154916000
1	-2.961517000	0.397976000	-2.139644000
1	-4.132779000	0.771575000	0.015869000
1	-2.961561000	0.309621000	2.154407000
1	-0.623739000	-0.511391000	2.135737000
16	1.210606000	-1.140547000	-0.022962000
6	2.302625000	0.326054000	0.006716000
8	3.486214000	0.116763000	0.003376000
6	1.682917000	1.703095000	0.033178000
1	1.048386000	1.824833000	0.913422000
1	2.487960000	2.437227000	0.050059000
1	1.053130000	1.860341000	-0.844906000

$OCOCF_3$
E(RB3LYP) = -758.058561375

6	1.214708000	0.174102000	0.190954000
6	1.960546000	1.287025000	-0.168120000
6	1.799016000	-1.060345000	0.438402000
6	3.342579000	1.155085000	-0.291143000
6	3.181345000	-1.177694000	0.309153000
6	3.953350000	-0.075081000	-0.054670000
1	1.462909000	2.233236000	-0.340708000
1	3.938612000	2.015932000	-0.570320000
1	5.028016000	-0.174636000	-0.151278000
1	3.653334000	-2.135118000	0.495780000
1	1.191167000	-1.909858000	0.721213000
8	-0.170348000	0.370249000	0.378356000
6	-1.048855000	-0.335026000	-0.346993000
8	-0.826106000	-1.158096000	-1.181321000
6	-2.484199000	0.088978000	0.069726000
9	-2.671906000	1.405247000	-0.135791000
9	-3.391354000	-0.580926000	-0.640405000
9	-2.693778000	-0.165326000	1.374547000

BF_2
E(RB3LYP) = -456.454090790

6	2.615094000	0.000185000	0.000073000
6	1.919907000	-1.209539000	-0.000118000
6	1.919520000	1.209689000	0.000129000
1	2.463189000	-2.147674000	-0.000165000
1	2.462507000	2.147998000	0.000177000

CBr_3
E(RB3LYP) = -7992.24013233

6	-1.207891000	0.101119000	0.000020000
6	-1.905413000	1.310475000	0.000950000
6	-1.936647000	-1.099603000	-0.000699000
6	-3.300826000	1.321360000	0.000826000
6	-3.323702000	-1.083676000	-0.000824000

6	0.528635000	-1.208604000	0.000011000
6	0.528254000	1.208280000	-0.000074000
1	-0.010594000	-2.149434000	-0.000059000
1	-0.011322000	2.148896000	-0.000100000
6	-0.189760000	-0.000314000	-0.000126000
1	3.699617000	0.000364000	0.000136000
5	-1.730461000	-0.000025000	-0.000052000
9	-2.438160000	-1.130708000	0.000140000
9	-2.437505000	1.130908000	-0.000040000

OCF_2CF_3
E(RB3LYP) = -882.559345580

6	4.036285000	0.001703000	0.078678000
6	3.352811000	1.213305000	-0.013645000
6	3.344959000	-1.201420000	-0.055954000
1	3.888453000	2.150203000	0.084833000
1	3.874680000	-2.144566000	0.009415000
6	1.977004000	1.228661000	-0.236296000
6	1.969197000	-1.200729000	-0.280010000
1	1.427427000	2.157698000	-0.318237000
1	1.414960000	-2.123224000	-0.395389000
6	1.309429000	0.018017000	-0.358753000
1	5.106233000	-0.004814000	0.250574000
8	-0.072392000	0.033102000	-0.661079000
6	-0.952679000	-0.033661000	0.357847000
9	-0.831615000	-1.180674000	1.082645000
9	-0.808772000	0.989742000	1.243805000
6	-2.392629000	0.024163000	-0.230032000
9	-2.600073000	-1.002822000	-1.062483000
9	-3.292627000	-0.039574000	0.758575000
9	-2.577900000	1.166622000	-0.901829000

$N(Me)SO_2CF_3$
E(RB3LYP) = -1212.76131053

6	1.366403000	0.362587000	0.292338000
6	1.878965000	-0.750700000	0.961930000
6	2.110825000	0.981254000	-0.712843000
6	3.138318000	-1.241159000	0.626651000
6	3.362335000	0.474626000	-1.053310000
6	3.880688000	-0.632364000	-0.383668000
1	1.297908000	-1.233828000	1.738194000
1	3.533490000	-2.104450000	1.149425000
1	4.858505000	-1.018645000	-0.647079000
1	3.935586000	0.952901000	-1.838970000
1	1.702737000	1.841590000	-1.226032000
7	0.085386000	0.907148000	0.675785000
6	-0.149136000	1.216482000	2.100153000
1	0.690439000	1.818937000	2.448290000
1	-1.063826000	1.797418000	2.191169000
1	-0.230157000	0.315116000	2.712796000
16	-1.214398000	0.795621000	-0.352553000
8	-2.283657000	1.622371000	0.179753000
8	-0.751677000	0.890040000	-1.723657000
6	-1.848765000	-0.985251000	-0.172254000
9	-2.984517000	-1.131024000	-0.849688000
9	-0.946120000	-1.853661000	-0.632062000
9	-2.074601000	-1.248776000	1.123950000

$PO(OH)_2$
E(RB3LYP) = -800.117575058

6	-0.341768000	-0.034531000	-0.015648000
6	-1.073402000	-1.226340000	-0.037064000
6	-1.007354000	1.197070000	0.026490000
6	-2.466291000	-1.184793000	-0.018215000
6	-2.397865000	1.230878000	0.044175000
6	-3.127144000	0.040989000	0.022114000
1	-0.547218000	-2.172974000	-0.071096000
1	-3.032781000	-2.108718000	-0.036807000
1	-4.210929000	0.071545000	0.035739000

6	-4.014689000	0.129608000	-0.000128000
1	-1.368675000	2.247928000	0.001772000
1	-3.822380000	2.271443000	0.001412000
1	-5.098532000	0.140247000	-0.000190000
1	-3.867507000	-2.021212000	-0.001493000
1	-1.413646000	-2.047410000	-0.001140000
6	0.304113000	0.026146000	0.000065000
35	0.937347000	-0.960248000	1.613673000
35	0.937356000	-0.959384000	-1.613832000
35	1.207614000	1.781815000	0.000113000

$N(Me)NO_2$
E(RB3LYP) = -531.541837240

6	0.338358000	0.143457000	0.190564000
6	0.995024000	0.971505000	-0.719992000
6	1.050678000	-0.801830000	0.926167000
6	2.372235000	0.851716000	-0.892209000
6	2.425218000	-0.924042000	0.743176000
6	3.087539000	-0.096575000	-0.162982000
1	0.432146000	1.698837000	-1.293797000
1	2.883106000	1.493862000	-1.600286000
1	4.158404000	-0.191414000	-0.301409000
1	2.978987000	-1.663101000	1.310378000
1	0.522845000	-1.437571000	1.626293000
7	-1.074163000	0.292193000	0.411407000
6	-1.639445000	1.560797000	0.868678000
1	-2.523341000	1.373201000	1.475991000
1	-0.876935000	2.045529000	1.475865000
1	-1.919110000	2.213562000	0.035519000
7	-1.927871000	-0.539786000	-0.304804000
8	-1.436708000	-1.519058000	-0.847839000
8	-3.115731000	-0.234682000	-0.301559000

$N(SO2Me)_2$
E(RB3LYP) = -1463.60942690

6	3.955692000	-0.080278000	0.036942000
6	3.309385000	0.116975000	-1.182400000
6	3.210427000	-0.259010000	1.201519000
1	3.886952000	0.258748000	-2.088362000
1	3.710596000	-0.419672000	2.149402000
6	1.919042000	0.132344000	-1.241232000
6	1.819869000	-0.234495000	1.150336000
1	1.404038000	0.292911000	-2.179815000
1	1.234034000	-0.386735000	2.048893000
6	1.177322000	-0.039746000	-0.073038000
1	5.038734000	-0.096075000	0.079630000
7	-0.262874000	-0.006680000	-0.146175000
16	-1.080972000	1.520261000	-0.132287000
8	-2.361470000	1.303063000	-0.796421000
8	-0.125487000	2.488166000	-0.647703000
6	-1.386703000	1.870895000	1.605511000
1	-1.923720000	2.819278000	1.630666000
1	-1.988528000	1.058259000	2.007364000
1	-0.424001000	1.960488000	2.105824000
16	-1.167337000	-1.472961000	0.123866000
8	-2.154709000	-1.205738000	1.165603000
8	-0.169919000	-2.517925000	0.299003000
6	-2.021813000	-1.733424000	-1.435424000
1	-2.608654000	-2.642575000	-1.301808000
1	-2.654167000	-0.868534000	-1.621127000
1	-1.268873000	-1.866238000	-2.209838000

$OCCl_3$
E(RB3LYP) = -1725.71604818

6	-1.083178000	0.000108000	-0.512661000
6	-1.742004000	-1.214501000	-0.371360000
6	-1.741909000	1.214722000	-0.371101000
6	-3.096304000	-1.206963000	-0.042956000
6	-3.096250000	1.207233000	-0.042735000
6	-3.772438000	0.000158000	0.127082000
1	-1.204767000	-2.140977000	-0.522945000
1	-3.622320000	-2.147442000	0.072047000
1	-4.826207000	0.000148000	0.380156000

1	-2.913461000	2.183902000	0.074699000
1	-0.441663000	2.121020000	0.042679000
15	1.456022000	-0.138564000	-0.021992000
8	2.010194000	-1.512665000	-0.024894000
8	1.998309000	0.764736000	1.227386000
1	2.260001000	0.213056000	1.974801000
8	1.834430000	0.832744000	-1.258020000
1	2.785205000	0.952463000	-1.377018000

CH_2SOCF_3
E(RB3LYP) = -1082.18015830

6	-1.251225000	0.553094000	-0.493761000
6	-1.719371000	-0.674367000	-0.975604000
6	-2.030785000	1.257422000	0.432927000
6	-2.942683000	-1.183179000	-0.546513000
6	-3.250111000	0.745939000	0.867225000
6	-3.709155000	-0.476538000	0.378039000
1	-1.127102000	-1.230668000	-1.693825000
1	-3.295820000	-2.131947000	-0.934009000
1	-4.660690000	-0.873520000	0.712636000
1	-3.843668000	1.303145000	1.582910000
1	-1.685841000	2.215147000	0.809477000
6	0.058491000	1.110215000	-0.964752000
1	0.448616000	0.622373000	-1.857523000
1	0.011686000	2.186004000	-1.146918000
16	1.445250000	1.051774000	0.302771000
8	2.643181000	1.667348000	-0.361014000
6	1.721092000	-0.845596000	0.247446000
9	0.777185000	-1.466254000	0.968874000
9	1.712999000	-1.349610000	-0.995191000
9	2.912688000	-1.092984000	0.793094000

COOH
E(RB3LYP) = -420.948152275

6	2.567706000	-0.045292000	0.000007000
6	1.838661000	-1.234276000	0.000024000
6	1.904925000	1.182741000	0.000006000
1	2.354499000	-2.187573000	0.000025000
1	2.471847000	2.106518000	-0.000007000
6	0.447367000	-1.200120000	0.000038000
6	0.515263000	1.222224000	0.000020000
1	-0.124302000	-2.118853000	0.000051000
1	-0.018641000	2.164458000	0.000020000
6	-0.219670000	0.030940000	0.000038000
1	3.651623000	-0.075547000	-0.000004000
6	-1.703151000	0.125074000	0.000057000
8	-2.333977000	1.156636000	-0.000060000
8	-2.312916000	-1.088674000	-0.000074000
1	-3.266497000	-0.920442000	-0.000155000

S(O)OMe
E(RB3LYP) = -820.279693058

6	3.179359000	0.264048000	0.280112000
6	2.439117000	1.321094000	-0.251867000
6	2.566362000	-0.958732000	0.550180000
1	2.918638000	2.270200000	-0.462051000
1	3.145086000	-1.778221000	0.960726000
6	1.081224000	1.158099000	-0.513552000
6	1.207715000	-1.133121000	0.290534000
1	0.497438000	1.975339000	-0.921863000
1	0.703424000	-2.072737000	0.484364000
6	0.482745000	-0.067070000	-0.227882000
1	4.236941000	0.393962000	0.480099000
16	-1.271779000	-0.326110000	-0.622885000
8	-1.782842000	0.749208000	0.599482000
6	-3.205567000	0.950820000	0.626541000
1	-3.578286000	1.289772000	-0.346285000
1	-3.723778000	0.036290000	0.925514000
1	-3.378557000	1.726772000	1.371186000
8	-1.589429000	-1.728513000	-0.230723000

$NHSO_2CF_3$
E(RB3LYP) = -1173.44653093

1	-3.622151000	2.147758000	0.072451000
1	-1.204656000	2.141233000	-0.522426000
8	0.259578000	0.000148000	-0.948384000
6	1.295819000	-0.000134000	-0.077464000
17	1.311582000	1.467041000	1.005002000
17	2.779539000	-0.000654000	-1.078206000
17	1.310117000	-1.466718000	1.005848000

SCF_2CHF_2
E(RB3LYP) = -1106.24498244

6	3.645493000	0.293066000	-0.425163000
6	3.054888000	-0.943286000	-0.683487000
6	2.963502000	1.247921000	0.326947000
1	3.585609000	-1.690011000	-1.262986000
1	3.420588000	2.209199000	0.531832000
6	1.785197000	-1.230669000	-0.188275000
6	1.687554000	0.973937000	0.814187000
1	1.329187000	-2.194897000	-0.372512000
1	1.148271000	1.715866000	1.389807000
6	1.096610000	-0.264115000	0.549768000
1	4.637071000	0.510037000	-0.805824000
16	-0.501537000	-0.648736000	1.283023000
6	-1.641650000	-0.540168000	-0.147676000
9	-1.193915000	-1.251474000	-1.222156000
9	-2.808861000	-1.114042000	0.264489000
6	-2.009571000	0.863570000	-0.671729000
9	-2.518428000	1.614859000	0.337482000
9	-0.904802000	1.488602000	-1.156225000
1	-2.754225000	0.786543000	-1.468415000

CHF_2
E(RB3LYP) = -470.179286818

6	0.168117000	-0.189065000	0.000126000
6	-0.349471000	1.110100000	-0.000111000
6	-0.696006000	-1.282827000	0.000258000
6	-1.725810000	1.305949000	-0.000213000
6	-2.076531000	-1.084318000	0.000150000
6	-2.590813000	0.209445000	-0.000080000
1	0.325167000	1.958081000	-0.000207000
1	-2.126983000	2.312918000	-0.000393000
1	-3.663543000	0.366264000	-0.000163000
1	-2.745378000	-1.937168000	0.000260000
1	-0.293816000	-2.290674000	0.000440000
6	1.650133000	-0.412838000	0.000191000
1	1.930186000	-1.468107000	0.000663000
9	2.238649000	0.172809000	-1.100266000
9	2.238758000	0.173858000	1.099986000

OCF_2CHF_2
E(RB3LYP) = -783.282783047

6	-1.112309000	-0.092332000	-0.390688000
6	-1.817307000	1.098128000	-0.512754000
6	-1.724611000	-1.271059000	0.012897000
6	-3.177075000	1.104498000	-0.205509000
6	-3.085067000	-1.251681000	0.313817000
6	-3.811096000	-0.066181000	0.207694000
1	-1.310459000	1.995960000	-0.841730000
1	-3.739718000	2.026546000	-0.293904000
1	-4.868984000	-0.055631000	0.442668000
1	-3.575552000	-2.164730000	0.630479000
1	-1.141093000	-2.180209000	0.084797000
8	0.247997000	-0.142174000	-0.765823000
6	1.184946000	0.257780000	0.128797000
9	1.104089000	1.602417000	0.382323000
9	1.051850000	-0.358217000	1.330997000
6	2.573769000	-0.031249000	-0.476290000
9	3.534641000	0.411920000	0.373143000
1	2.688210000	0.461931000	-1.443225000
9	2.728990000	-1.370997000	-0.633162000

$CH{=}NNHCSNH_2$
E(RB3LYP) = -872.861558494

6	-1.491433000	-0.263227000	0.338411000
6	-1.718522000	1.047861000	-0.078951000
6	-2.562443000	-1.141284000	0.513894000
6	-3.020250000	1.469445000	-0.333653000
6	-3.863412000	-0.701185000	0.284330000
6	-4.096149000	0.602958000	-0.146860000
1	-0.888328000	1.729509000	-0.205945000
1	-3.192737000	2.486214000	-0.666800000
1	-5.107772000	0.941755000	-0.336387000
1	-4.691697000	-1.384754000	0.430066000
1	-2.378447000	-2.164128000	0.824974000
7	-0.168657000	-0.718588000	0.647783000
1	-0.111404000	-1.524492000	1.259978000
16	1.100718000	-0.743152000	-0.440735000
8	1.831976000	-1.981793000	-0.236655000
8	0.674434000	-0.260512000	-1.738476000
6	2.216477000	0.606072000	0.274074000
9	2.546274000	0.309099000	1.531058000
9	3.320722000	0.688434000	-0.464318000
9	1.588850000	1.785917000	0.256033000
6	1.783319000	-0.346759000	0.000526000
6	2.135014000	1.013651000	0.001363000
6	2.804281000	-1.308756000	-0.000745000
6	3.470417000	1.392173000	0.000785000
6	4.142822000	-0.925739000	-0.001318000
6	4.480134000	0.425621000	-0.000601000
1	1.352829000	1.762337000	0.002616000
1	3.730387000	2.444754000	0.001437000
1	5.521295000	0.727216000	-0.001057000
1	4.919965000	-1.681369000	-0.002315000
1	2.545507000	-2.362734000	-0.001297000
6	0.393376000	-0.798123000	0.000865000
7	-0.602929000	0.011593000	0.000347000
1	0.230492000	-1.881750000	0.001446000
7	-1.848042000	-0.523758000	0.001043000
1	-1.997558000	-1.528668000	0.001793000
6	-2.977950000	0.255486000	-0.000302000
16	-4.491749000	-0.460600000	-0.000014000
7	-2.757112000	1.583743000	-0.001876000
1	-3.552055000	2.198753000	-0.001582000
1	-1.814767000	1.944700000	-0.000860000

C_6H_4-4NO_2
E(RB3LYP) = -667.986850637

6	1.890473000	0.000004000	0.000004000
6	2.608939000	1.105244000	-0.480135000
6	2.608934000	-1.105242000	0.480137000
6	4.000808000	1.103788000	-0.482531000
6	4.000803000	-1.103799000	0.482519000
6	4.702181000	-0.000008000	-0.000010000
1	2.074553000	1.959776000	-0.879406000
1	4.537906000	1.962756000	-0.868598000
1	5.786125000	-0.000014000	-0.000015000
1	4.537897000	-1.962772000	0.868580000
1	2.074545000	-1.959770000	0.879411000
6	0.407196000	0.000008000	0.000008000
6	-0.313190000	1.157620000	0.338385000
6	-0.313193000	-1.157602000	-0.338368000
1	0.220676000	2.054738000	0.627277000
1	0.220668000	-2.054721000	-0.627265000
6	-1.701445000	1.166136000	0.340456000
6	-1.701446000	-1.166106000	-0.340432000
1	-2.261226000	2.051377000	0.609268000
1	-2.261233000	-2.051346000	-0.609243000
6	-2.379581000	0.000014000	0.000017000
7	-3.855423000	-0.000006000	0.000006000
8	-4.425341000	1.041324000	0.304513000
8	-4.425261000	-1.041366000	-0.304557000

$COOC_6H_5$
E(RB3LYP) = -652.039162040

6	1.844992000	0.166130000	-0.061084000
6	2.234347000	-1.096894000	0.400862000
6	2.818776000	1.108411000	-0.413083000
6	3.586383000	-1.409714000	0.508822000
6	4.167978000	0.790493000	-0.305259000
6	4.553366000	-0.468722000	0.156121000
1	1.479854000	-1.823096000	0.672331000
1	3.885800000	-2.387760000	0.867666000
1	5.605725000	-0.716157000	0.240320000
1	4.918985000	1.522285000	-0.579756000
1	2.499501000	2.080480000	-0.767977000
6	0.416139000	0.563457000	-0.197081000
8	0.031510000	1.642674000	-0.566958000
8	-0.425677000	-0.460796000	0.148156000
6	-1.809291000	-0.261596000	0.090728000
6	-2.535218000	-1.055859000	-0.787781000
6	-2.438150000	0.640033000	0.941755000
1	-2.011984000	-1.750534000	-1.433604000
1	-1.850804000	1.249513000	1.616371000
6	-3.924273000	-0.942832000	-0.816400000
6	-3.826317000	0.747388000	0.901903000
1	-4.497319000	-1.560053000	-1.498771000
1	-4.325221000	1.450357000	1.559114000
6	-4.571950000	-0.041384000	0.026031000
1	-5.651871000	0.046471000	0.001510000

$CHCl_2$
E(RB3LYP) = -1190.87700970

6	-0.362649000	-0.000217000	0.227398000
6	-1.268915000	0.000190000	1.289305000
6	-0.839623000	-0.000636000	-1.087395000
6	-2.641501000	0.000453000	1.042380000
6	-2.207279000	-0.000583000	-1.331448000
6	-3.111922000	0.000066000	-0.267267000
1	-0.904465000	0.000168000	2.311248000
1	-3.337846000	0.000999000	1.872972000
1	-4.178364000	0.000350000	-0.461722000
1	-2.571073000	-0.001061000	-2.352494000
1	-0.138580000	-0.000974000	-1.913783000
6	1.104515000	0.000040000	0.534012000
1	1.288953000	0.000363000	1.602343000
17	1.935627000	-1.482494000	-0.102570000
17	1.935291000	1.482746000	-0.103340000

N=C=S
E(RB3LYP) = -722.803162453

6	0.440301000	-0.227627000	0.000077000
6	1.361027000	-1.281298000	0.000264000
6	0.888234000	1.101134000	0.000053000
6	2.724023000	-1.003277000	0.000425000
6	2.253709000	1.363143000	0.000216000
6	3.175671000	0.315944000	0.000402000
1	0.996701000	-2.301042000	0.000280000
1	3.435025000	-1.821323000	0.000569000
1	4.238424000	0.527416000	0.000528000
1	2.598224000	2.390942000	0.000196000
1	0.166331000	1.908874000	-0.000092000
7	-0.914639000	-0.514711000	-0.000085000
6	-2.060290000	-0.184711000	-0.000263000
16	-3.608018000	0.149891000	-0.000495000

OCF_2CHFCl
E(RB3LYP) = -1143.62997524

6	-1.330615000	0.106958000	0.357078000
6	-2.141061000	-0.951967000	0.744596000
6	-1.844554000	1.235624000	-0.267273000

$SiMeCl_2$
E(RB3LYP) = -1481.73107251

6	-3.600489000	-0.066642000	-0.115921000
6	-2.851170000	-1.212217000	-0.374004000
6	-2.957338000	1.116775000	0.244960000

6	-3.508667000	-0.878548000	0.485403000
6	-3.213628000	1.296765000	-0.520285000
6	-4.045282000	0.241774000	-0.147179000
1	-1.706391000	-1.810871000	1.239480000
1	-4.153122000	-1.698074000	0.781399000
1	-5.109463000	0.294450000	-0.345200000
1	-3.628369000	2.171107000	-1.008171000
1	-1.181136000	2.045073000	-0.543871000
8	0.042548000	0.078598000	0.683224000
6	0.905749000	-0.489607000	-0.194039000
9	0.653239000	-1.828709000	-0.349887000
9	0.813395000	0.046833000	-1.438223000
6	2.336017000	-0.351287000	0.364859000
9	3.194222000	-1.017190000	-0.457421000
1	2.381033000	-0.786039000	1.361669000
17	2.833037000	1.358171000	0.489396000

1	-3.347114000	-2.134136000	-0.656279000
1	-3.535573000	2.012059000	0.444141000
6	-1.461523000	-1.178122000	-0.270595000
6	-1.569514000	1.150118000	0.348460000
1	-0.892900000	-2.078082000	-0.474175000
1	-1.088996000	2.084377000	0.622290000
6	-0.798241000	0.003109000	0.092316000
1	-4.681430000	-0.094063000	-0.196646000
14	1.059050000	0.110494000	0.264128000
17	1.885501000	-1.786192000	0.017574000
17	1.823456000	1.321580000	-1.254302000
6	1.638116000	0.806126000	1.892388000
1	1.252676000	1.818661000	2.038767000
1	1.286327000	0.180177000	2.716704000
1	2.728990000	0.847623000	1.926161000

$CHBr_2$

E(RB3LYP) = -5418.71804195

6	-1.005020000	0.000287000	0.250478000
6	-1.935378000	0.000429000	1.293696000
6	-1.458387000	-0.000033000	-1.073617000
6	-3.302498000	0.000383000	1.019179000
6	-2.820538000	-0.000101000	-1.344865000
6	-3.747002000	0.000153000	-0.299408000
1	-1.592436000	0.000611000	2.322981000
1	-4.014815000	0.000550000	1.836146000
1	-4.809283000	-0.000003000	-0.515292000
1	-3.163374000	-0.000363000	-2.373148000
1	-0.741760000	-0.000195000	-1.886523000
6	0.448571000	0.000078000	0.594608000
1	0.613679000	-0.000055000	1.664606000
35	1.380175000	-1.627290000	-0.052605000
35	1.380668000	1.627070000	-0.052800000

COMe

E(RB3LYP) = -385.001693251

6	-0.204467000	-0.057594000	-0.000006000
6	0.430523000	1.191338000	0.000110000
6	0.579969000	-1.219778000	-0.000091000
6	1.821092000	1.276386000	0.000133000
6	1.966564000	-1.134773000	-0.000133000
6	2.590390000	0.114519000	-0.000033000
1	-0.153768000	2.103449000	0.000233000
1	2.302787000	2.247543000	0.000242000
1	3.672678000	0.181189000	-0.000041000
1	2.564249000	-2.039305000	-0.000231000
1	0.077202000	-2.179094000	-0.000158000
6	-1.698907000	-0.204331000	0.000046000
8	-2.213276000	-1.307034000	0.000259000
6	-2.558561000	1.046259000	-0.000214000
1	-2.355147000	1.660624000	0.881690000
1	-2.355405000	1.660120000	-0.882578000
1	-3.606013000	0.749585000	-0.000088000

C_6F_5

E(RB3LYP) = -959.726275098

6	0.000000000	0.000000000	-1.652332000
6	0.967128000	-0.722386000	-2.362325000
6	-0.967128000	0.722386000	-2.362325000
6	0.966673000	-0.719977000	-3.754204000
6	-0.966673000	0.719977000	-3.754204000
6	0.000000000	0.000000000	-4.453798000
1	1.724157000	-1.281347000	-1.825601000
1	1.723231000	-1.280393000	-4.291315000
1	0.000000000	0.000000000	-5.537783000
1	-1.723231000	1.280393000	-4.291315000
1	-1.724157000	1.281347000	-1.825601000
6	0.000000000	0.000000000	-0.164746000
6	-0.011489000	1.186618000	0.574689000
6	0.011489000	-1.186618000	0.574689000
6	-0.010745000	1.200142000	1.963912000
6	0.010745000	-1.200142000	1.963912000
6	0.000000000	0.000000000	2.663416000
9	0.000000000	-2.372314000	-0.054454000
9	0.009986000	-2.358840000	2.630737000
9	0.000000000	0.000000000	3.997603000
9	-0.009986000	2.358840000	2.630737000
9	0.000000000	2.372314000	-0.054454000

$C(OH)(CF_3)_2$

E(RB3LYP) = -1021.16058904

6	-0.995029000	0.000049000	-0.183971000
6	-1.511348000	0.000496000	1.116681000
6	-1.871354000	-0.000369000	-1.271452000
6	-2.888769000	0.000546000	1.320788000
6	-3.248063000	-0.000310000	-1.059403000
6	-3.761216000	0.000146000	0.234985000
1	-0.852477000	0.000833000	1.973970000
1	-3.276757000	0.000890000	2.332762000
1	-4.833044000	0.000164000	0.397200000
1	-3.918511000	-0.000610000	-1.911156000
1	-1.475377000	-0.000743000	-2.276931000
6	0.513524000	-0.000050000	-0.440627000
8	0.744503000	-0.000287000	-1.828106000
1	1.695949000	0.000121000	-1.993697000
6	1.175281000	-1.294048000	0.138866000
9	1.157748000	-1.352536000	1.480163000
9	0.548601000	-2.380365000	-0.331212000
9	2.469505000	-1.379719000	-0.251687000
6	1.175443000	1.293984000	0.138522000
9	1.157962000	1.352874000	1.479718000
9	2.469753000	1.379315000	-0.252126000
9	0.549028000	2.380318000	-0.331926000

SOMe

E(RB3LYP) = -745.047820785

6	-0.128391000	0.058490000	-0.188022000
6	-0.697129000	-1.154262000	0.182049000
6	-0.909697000	1.191819000	-0.406891000
6	-2.078475000	-1.225573000	0.363530000
6	-2.288168000	1.111066000	-0.221297000
6	-2.871588000	-0.096266000	0.166321000
1	-0.054304000	-2.017989000	0.311777000
1	-2.534316000	-2.165513000	0.653688000
1	-3.945125000	-0.157115000	0.303980000

CH_2SCN

E(RB3LYP) = -762.100854874

6	-0.703753000	0.311064000	-0.000153000
6	-1.647013000	1.347725000	0.000287000
6	-1.159606000	-1.007638000	-0.000395000
6	-3.009736000	1.070283000	0.000253000
6	-2.527421000	-1.287089000	-0.000408000
6	-3.455770000	-0.251687000	-0.000099000
1	-1.310367000	2.379710000	0.000562000
1	-3.723394000	1.886321000	0.000525000
1	-4.517450000	-0.469651000	-0.000131000

1	-2.906224000	1.986316000	-0.386265000
1	-0.456407000	2.124748000	-0.726808000
16	1.679316000	0.108032000	-0.473927000
8	2.190203000	-1.306700000	-0.296324000
6	2.118103000	1.016388000	1.064117000
1	1.648727000	2.000928000	1.051247000
1	1.785069000	0.430430000	1.920855000
1	3.203972000	1.113303000	1.066106000

$CONHC_6H_5$
E(RB3LYP) = -632.172790651

6	-1.904373000	-0.183428000	-0.037452000
6	-2.289498000	1.102510000	-0.436011000
6	-2.885367000	-1.088993000	0.382032000
6	-3.629950000	1.480944000	-0.396974000
6	-4.221470000	-0.706350000	0.431770000
6	-4.597162000	0.580117000	0.044105000
1	-1.557879000	1.806313000	-0.818353000
1	-3.918363000	2.474452000	-0.720835000
1	-5.639666000	0.875861000	0.076743000
1	-4.971895000	-1.412591000	0.768416000
1	-2.579667000	-2.089442000	0.661980000
6	-0.481761000	-0.675015000	-0.074719000
8	-0.221515000	-1.859929000	-0.210458000
7	0.473271000	0.306903000	0.069956000
1	0.128076000	1.227260000	0.294863000
6	1.879795000	0.192534000	0.049126000
6	2.555177000	-1.000889000	-0.238177000
6	2.619263000	1.353073000	0.322725000
1	1.990983000	-1.897535000	-0.441160000
1	2.100773000	2.280812000	0.546889000
6	3.948838000	-1.011095000	-0.249092000
6	4.008274000	1.325728000	0.308585000
1	4.461866000	-1.939963000	-0.472371000
1	4.561580000	2.233179000	0.522531000
6	4.684220000	0.140287000	0.021563000
1	5.767506000	0.116232000	0.010379000

$CSNH_2$
E(RB3LYP) = -724.024651588

6	-0.106470000	0.127854000	0.048328000
6	-0.963205000	1.186570000	-0.291174000
6	-0.662282000	-1.127375000	0.328868000
6	-2.341371000	0.993802000	-0.343042000
6	-2.039431000	-1.312470000	0.292547000
6	-2.883980000	-0.254023000	-0.043876000
1	-0.552915000	2.153238000	-0.561014000
1	-2.988890000	1.815879000	-0.626137000
1	-3.957104000	-0.403541000	-0.080130000
1	-2.455434000	-2.286617000	0.522978000
1	0.000805000	-1.947288000	0.573758000
6	1.369907000	0.321649000	0.098408000
16	2.462242000	-0.858162000	-0.333360000
7	1.773981000	1.550361000	0.496182000
1	2.764259000	1.731220000	0.558901000
1	1.136520000	2.199119000	0.931762000

$P(S)Et_2$
E(RB3LYP) = -1129.83774424

6	0.789336000	0.000357000	0.011035000
6	1.409871000	0.000725000	1.262261000
6	1.579592000	0.000342000	-1.146522000
6	2.801023000	0.001118000	1.356073000
6	2.968792000	0.000718000	-1.050890000
6	3.581470000	0.001124000	0.202269000
1	0.792424000	0.000731000	2.153513000
1	3.273147000	0.001426000	2.332082000
1	4.663189000	0.001411000	0.276544000
1	3.571490000	0.000704000	-1.952224000
1	1.121453000	0.000022000	-2.129872000
15	-1.051256000	-0.000352000	-0.098817000
6	-1.472937000	-1.452237000	-1.164003000
1	-2.545791000	-1.363736000	-1.359711000

1	-2.861068000	-2.318430000	-0.000615000
1	-0.460431000	-1.836331000	-0.000624000
6	0.758206000	0.705068000	-0.000296000
1	0.998185000	1.293781000	-0.886678000
1	0.998089000	1.294821000	0.885427000
16	1.895801000	-0.765283000	0.000725000
6	3.370586000	0.072204000	0.000098000
7	4.398666000	0.607817000	-0.000827000

$CH{=}NC_6H_5$
E(RB3LYP) = -556.883349179

6	1.554776000	-0.634478000	-0.056723000
6	1.171966000	0.680137000	-0.371834000
6	2.907610000	-0.889724000	0.220385000
6	2.117930000	1.699562000	-0.396291000
6	3.849730000	0.133595000	0.209799000
6	3.455274000	1.433773000	-0.099686000
1	0.141548000	0.905569000	-0.605167000
1	1.809328000	2.707994000	-0.647545000
1	4.185434000	2.235079000	-0.116041000
1	4.887653000	-0.083353000	0.435107000
1	3.217988000	-1.904301000	0.448859000
6	0.642234000	-1.802247000	-0.028152000
7	-0.626962000	-1.902833000	-0.029207000
6	-1.534992000	-0.831253000	0.022382000
6	-1.781380000	-0.155872000	1.226780000
6	-2.305488000	-0.517747000	-1.106292000
1	-1.208254000	-0.418818000	2.108366000
1	-2.138124000	-1.064644000	-2.026933000
6	-2.754722000	0.837637000	1.285231000
6	-3.266762000	0.487074000	-1.040093000
1	-2.933752000	1.352031000	2.223201000
1	-3.846159000	0.728067000	-1.924740000
6	-3.497714000	1.171668000	0.153237000
1	-4.254306000	1.945906000	0.203202000
1	1.176594000	-2.756454000	-0.006318000

$SCHF_2$
E(RB3LYP) = -868.385326026

6	-0.429090000	-0.040657000	-0.531763000
6	-1.100073000	-1.227536000	-0.226834000
6	-1.053953000	1.193134000	-0.332337000
6	-2.393590000	-1.176235000	0.288334000
6	-2.346602000	1.235996000	0.185545000
6	-3.016542000	0.053441000	0.495633000
1	-0.609971000	-2.179086000	-0.390224000
1	-2.912831000	-2.097263000	0.527543000
1	-4.023521000	0.090039000	0.895568000
1	-2.829417000	2.193507000	0.344263000
1	-0.529371000	2.107608000	-0.578872000
16	1.219898000	-0.107435000	-1.249592000
6	2.252982000	0.003681000	0.242839000
1	3.297015000	-0.043416000	-0.072057000
9	2.012957000	-1.010522000	1.125708000
9	2.054926000	1.165703000	0.934153000

$N(COMe)_2$
E(RB3LYP) = -593.064710899

6	0.664239000	-0.000085000	0.000001000
6	1.351922000	0.000373000	1.207754000
6	1.351882000	-0.000388000	-1.207775000
6	2.744410000	0.000362000	1.206292000
6	2.744369000	-0.000400000	-1.206359000
6	3.442440000	-0.000025000	-0.000045000
1	0.800561000	0.000653000	2.140669000
1	3.282752000	0.000667000	2.147127000

1	-0.954235000	-1.333750000	-2.121106000
6	-1.474036000	1.450554000	-1.164901000
1	-0.953809000	1.332776000	-2.121253000
1	-2.546472000	1.360251000	-1.362085000
6	-1.150255000	-2.806057000	-0.526464000
1	-0.077141000	-2.922574000	-0.357146000
1	-1.659488000	-2.913601000	0.433017000
1	-1.477575000	-3.617486000	-1.181473000
6	-1.154475000	2.805070000	-0.527253000
1	-1.482179000	3.615778000	-1.182965000
1	-1.665226000	2.911988000	0.431479000
1	-0.081791000	2.923378000	-0.356446000
16	-1.967466000	-0.000145000	1.654392000

6	-2.879839000	1.489138000	-0.000011000
1	-3.046340000	2.564289000	-0.000297000
1	-3.351437000	1.058685000	-0.883730000
1	-3.350990000	1.059221000	0.884214000
6	-1.377144000	-1.296139000	0.000335000
8	-0.647112000	-2.263317000	0.000735000
6	-2.880062000	-1.488675000	0.000113000
1	-3.350950000	-1.058636000	-0.884172000
1	-3.047206000	-2.563756000	0.000397000
1	-3.351327000	-1.058106000	0.883932000

COEt

E(RB3LYP) = -424.325972017

6	0.276583000	0.114041000	-0.000155000
6	0.813254000	-1.180363000	-0.000477000
6	1.150173000	1.210720000	0.000350000
6	2.192954000	-1.373625000	-0.000329000
6	2.526201000	1.017945000	0.000557000
6	3.051092000	-0.275723000	0.000203000
1	0.161244000	-2.044960000	-0.000871000
1	2.596843000	-2.379659000	-0.000634000
1	4.124894000	-0.426545000	0.000346000
1	3.192283000	1.873420000	0.000994000
1	0.724669000	2.206738000	0.000559000
6	-1.202862000	0.383440000	-0.000359000
8	-1.619881000	1.526340000	-0.000992000
6	-2.164037000	-0.799565000	0.000404000
1	-1.936733000	-1.423926000	-0.872132000
1	-1.936274000	-1.423109000	0.873416000
6	-3.634006000	-0.387945000	0.000555000
1	-3.873756000	0.213466000	0.879314000
1	-3.874170000	0.212578000	-0.878705000
1	-4.276070000	-1.272278000	0.001146000

$COCHMe_2$

E(RB3LYP) = -463.648559625

6	-0.522820000	0.210553000	-0.065217000
6	-0.974923000	-1.089488000	-0.329633000
6	-1.467827000	1.211962000	0.203757000
6	-2.337589000	-1.380343000	-0.324293000
6	-2.826363000	0.922141000	0.209933000
6	-3.265229000	-0.376503000	-0.054605000
1	-0.272135000	-1.884729000	-0.543604000
1	-2.673752000	-2.389870000	-0.531961000
1	-4.325465000	-0.603860000	-0.051099000
1	-3.545609000	1.705726000	0.420133000
1	-1.109075000	2.213890000	0.404440000
6	0.932345000	0.598838000	-0.059392000
8	1.248088000	1.763296000	0.102766000
6	2.006855000	-0.482047000	-0.212295000
1	1.644224000	-1.237388000	-0.916398000
6	2.227289000	-1.165984000	1.155188000
1	2.598151000	-0.441656000	1.885589000
1	1.308332000	-1.605039000	1.550457000
1	2.970546000	-1.962158000	1.060659000
6	3.310983000	0.106750000	-0.758556000
1	3.159881000	0.567504000	-1.737725000
1	3.700358000	0.875637000	-0.089135000
1	4.063515000	-0.679693000	-0.862802000

$PO(OMe)_2$

E(RB3LYP) = -878.734321776

6	0.801654000	-0.075428000	-0.104175000
6	1.628723000	0.283229000	-1.173527000
6	1.366926000	-0.486009000	1.109863000
6	3.014023000	0.228038000	-1.029428000
6	2.750468000	-0.540744000	1.247145000
6	3.573921000	-0.183880000	0.178131000
1	1.179042000	0.600346000	-2.107017000
1	3.653720000	0.505188000	-1.859568000
1	4.651807000	-0.227406000	0.288395000
1	3.187257000	-0.861896000	2.185972000
1	0.726943000	-0.763835000	1.938956000
15	-0.986459000	0.027522000	-0.327276000
8	-1.413499000	0.546338000	-1.650684000
8	-1.465345000	-1.452175000	0.081393000
6	-2.862583000	-1.807211000	0.043558000
1	-3.413622000	-1.249368000	0.803430000
1	-3.279691000	-1.609029000	-0.945721000
1	-2.909177000	-2.873039000	0.258718000
8	-1.577222000	0.871268000	0.931681000
6	-1.656990000	2.307248000	0.868585000
1	-0.657967000	2.748397000	0.927923000
1	-2.146743000	2.623897000	-0.053746000
1	-2.243008000	2.619016000	1.731763000

CH=CHCOMe

E(RB3LYP) = -462.425337796

6	-0.889588000	-0.185222000	-0.000014000
6	-1.398844000	1.126164000	0.000022000
6	-1.804916000	-1.251259000	-0.000033000
6	-2.767871000	1.356772000	0.000029000
6	-3.177514000	-1.020628000	-0.000027000
6	-3.663868000	0.284623000	0.000006000
1	-0.719423000	1.970292000	0.000040000
1	-3.141905000	2.374408000	0.000053000
1	-4.732169000	0.468761000	0.000015000
1	-3.865622000	-1.858288000	-0.000046000
1	-1.428467000	-2.268709000	-0.000059000
6	0.540004000	-0.490891000	-0.000023000
6	1.573360000	0.369444000	0.000020000
1	1.422443000	1.444340000	0.000058000
1	0.799692000	-1.547432000	-0.000033000
6	2.977897000	-0.116477000	0.000042000
8	3.259986000	-1.302260000	0.000077000
6	4.053156000	0.952991000	-0.000046000
1	3.947396000	1.596591000	0.879670000
1	5.038719000	0.490061000	0.000960000
1	3.948549000	1.594948000	-0.881129000

$PO(OC_4H_9)_2$

E(RB3LYP) = -1114.68976966

6	0.120011000	1.838643000	-0.073816000
6	0.308084000	2.876049000	-0.993486000

6	0.192880000	2.107102000	1.299906000
6	0.566699000	4.169983000	-0.543146000
6	0.451461000	3.400392000	1.744774000
6	0.638698000	4.432168000	0.823480000
1	0.248880000	2.657138000	-2.053147000
1	0.711697000	4.971170000	-1.259072000
1	0.840064000	5.438894000	1.172559000
1	0.506979000	3.604785000	2.808136000
1	0.046637000	1.306007000	2.015697000
15	-0.212706000	0.162807000	-0.689153000
8	-0.248459000	0.103726000	-2.172072000
8	0.840470000	-0.808149000	0.051031000
6	2.209937000	-0.883243000	-0.416934000
1	2.207322000	-1.047833000	-1.498065000
1	2.708263000	0.070786000	-0.209958000
8	-1.524910000	-0.355317000	0.088656000
6	-2.848793000	0.008586000	-0.380806000
1	-3.015233000	1.070077000	-0.169536000
1	-2.894324000	-0.146668000	-1.462558000
6	2.896147000	-2.023888000	0.314452000
1	2.832835000	-1.841937000	1.392811000
1	2.344336000	-2.948776000	0.116369000
6	4.362209000	-2.185786000	-0.105147000
1	4.902389000	-1.250344000	0.084270000
1	4.415475000	-2.355947000	-1.186991000
6	5.064451000	-3.334257000	0.625023000
1	4.570246000	-4.289976000	0.425661000
1	5.057177000	-3.177390000	1.708045000
1	6.106975000	-3.426813000	0.309128000
6	-3.865525000	-0.854974000	0.345995000
1	-3.763817000	-0.688836000	1.424563000
1	-4.862661000	-0.492193000	0.065590000
6	-3.747364000	-2.350245000	0.032385000
1	-2.737001000	-2.685786000	0.282613000
1	-3.864281000	-2.500133000	-1.047686000
6	-4.777873000	-3.197249000	0.783757000
1	-5.800842000	-2.901576000	0.528826000
1	-4.663230000	-3.090155000	1.867186000
1	-4.670229000	-4.258365000	0.543318000
6	3.701724000	0.496984000	1.231175000
6	4.992489000	0.058484000	-1.205658000
6	4.883909000	-0.237774000	1.188903000
6	5.529343000	-0.456451000	-0.027236000
1	3.382995000	1.189098000	-2.086448000
1	5.491096000	-0.113172000	-2.152621000
1	6.448997000	-1.029557000	-0.056511000
1	5.298144000	-0.640293000	2.106029000
1	3.195114000	0.668329000	2.172914000
16	1.664171000	1.991745000	0.095996000
6	0.389503000	0.778757000	0.041295000
1	-0.596628000	1.252594000	0.063823000
7	0.595941000	-0.472001000	-0.013341000
16	-0.706056000	-1.581315000	-0.056362000
8	-0.616045000	-2.335486000	1.188715000
8	-0.610417000	-2.244457000	-1.351522000
6	-2.246123000	-0.648097000	-0.027276000
6	-2.826469000	-0.246158000	-1.228908000
6	-2.838870000	-0.336745000	1.195388000
1	-2.360834000	-0.515866000	-2.168876000
1	-2.383025000	-0.675832000	2.117538000
6	-4.015249000	0.477007000	-1.198265000
6	-4.027155000	0.387304000	1.206437000
1	-4.472397000	0.785985000	-2.132316000
1	-4.493705000	0.626544000	2.156259000
6	-4.633534000	0.804479000	0.014732000
6	-5.940253000	1.557017000	0.037226000
1	-6.785689000	0.860650000	0.048339000
1	-6.023348000	2.185961000	0.926225000
1	-6.050400000	2.192217000	-0.844051000

$PO(OPr)_2$

E(RB3LYP) = -1036.04091458

6	0.000685000	1.323957000	0.127362000
6	0.000343000	1.765493000	-1.202772000
6	0.001912000	2.258917000	1.168142000
6	0.001227000	3.128540000	-1.484548000
6	0.002797000	3.623295000	0.880941000
6	0.002458000	4.057803000	-0.442955000
1	-0.000628000	1.043694000	-2.011700000
1	0.000947000	3.467150000	-2.514567000
1	0.003141000	5.119200000	-0.665127000
1	0.003738000	4.344705000	1.690280000
1	0.002132000	1.905829000	2.192671000
15	-0.000362000	-0.446136000	0.530402000
8	-0.000548000	-0.692415000	1.994397000
8	1.203431000	-1.102620000	-0.316438000
8	-1.204868000	-1.101197000	-0.316488000
6	2.563358000	-1.044896000	0.179300000
1	2.918185000	-0.008980000	0.127274000
1	2.575039000	-1.364795000	1.225006000
6	3.419057000	-1.953857000	-0.686429000
1	3.336767000	-1.627810000	-1.727927000
1	3.009258000	-2.967112000	-0.638042000
6	4.885251000	-1.950654000	-0.243502000
1	4.992220000	-2.295855000	0.789280000
1	5.321810000	-0.949078000	-0.306880000
1	5.482576000	-2.611278000	-0.876208000
6	-2.564614000	-1.042918000	0.179648000
1	-2.576216000	-1.363440000	1.225163000
1	-2.918806000	-0.006747000	0.128365000
6	-3.421141000	-1.950789000	-0.686407000

$PS(C_6H_5)_2$

E(RB3LYP) = -1434.74232739

6	1.539280000	0.696493000	0.087207000
6	2.144862000	1.789391000	0.718652000
6	2.112577000	0.168937000	-1.075035000
6	3.298289000	2.355749000	0.183517000
6	3.271607000	0.736182000	-1.604542000
6	3.863197000	1.831070000	-0.979062000
1	1.719621000	2.178075000	1.636879000
1	3.761151000	3.201401000	0.679599000
1	4.765737000	2.269244000	-1.390285000
1	3.712983000	0.316783000	-2.501728000
1	1.666096000	-0.687996000	-1.564748000
15	0.000298000	0.000751000	0.823733000
16	0.002105000	0.000455000	2.801418000
6	-0.166695000	-1.680416000	0.088442000
6	0.493800000	-2.746748000	0.710344000
6	-0.925685000	-1.918368000	-1.062550000
1	1.056118000	-2.568992000	1.619840000
1	-1.456254000	-1.106411000	-1.544896000
6	0.408126000	-4.029500000	0.177049000
6	-1.013577000	-3.206678000	-1.590129000
1	0.922144000	-4.849542000	0.665687000
1	-1.609559000	-3.383346000	-2.478518000
6	-0.345049000	-4.261869000	-0.974040000
1	-0.416343000	-5.263210000	-1.383807000
6	-1.372850000	0.985406000	0.089149000
6	-1.202155000	1.754618000	-1.066883000
6	-2.624088000	0.952974000	0.716246000
1	-0.235399000	1.803157000	-1.553153000
1	-2.748567000	0.382831000	1.629711000

1	-3.012071000	-2.964370000	-0.638667000	6	-2.274359000	2.474013000	-1.594498000
1	-3.338834000	-1.624229000	-1.727743000	6	-3.692757000	1.667757000	0.182944000
6	-4.887240000	-1.946749000	-0.243176000	1	-2.131542000	3.073108000	-2.486882000
1	-5.323084000	-0.944824000	-0.305974000	1	-4.658109000	1.637567000	0.675535000
1	-4.994250000	-2.292374000	0.789460000	6	-3.520213000	2.428980000	-0.973276000
1	-5.485177000	-2.606630000	-0.876081000	1	-4.352089000	2.990846000	-1.383127000
SOC_6H_5				COC_6H_5			
E(RB3LYP) = -936.825682346				E(RB3LYP) = -576.782062372			
6	1.384760000	0.228641000	0.315025000	6	-1.299692000	0.348353000	-0.026234000
6	1.825946000	-0.935639000	0.938685000	6	-1.442090000	-0.890896000	-0.663548000
6	2.020157000	0.734492000	-0.812554000	6	-2.426200000	0.957077000	0.544480000
6	2.906126000	-1.627890000	0.394192000	6	-2.688656000	-1.510714000	-0.725380000
6	3.101153000	0.035983000	-1.348558000	6	-3.663800000	0.326200000	0.502794000
6	3.540500000	-1.144590000	-0.750425000	6	-3.797825000	-0.908897000	-0.134380000
1	1.343233000	-1.299715000	1.839260000	1	-0.585954000	-1.359352000	-1.133509000
1	3.257637000	-2.536725000	0.869281000	1	-2.793018000	-2.461428000	-1.235838000
1	4.384315000	-1.682131000	-1.167763000	1	-4.765360000	-1.396777000	-0.174350000
1	3.603879000	0.418165000	-2.229872000	1	-4.526689000	0.797459000	0.959675000
1	1.670925000	1.666530000	-1.242318000	1	-2.310898000	1.926607000	1.013660000
16	-0.000008000	1.197259000	1.033450000	6	0.000025000	1.098114000	-0.000118000
8	-0.000126000	2.528539000	0.310657000	8	-0.000003000	2.318571000	-0.000319000
6	-1.384739000	0.228499000	0.315091000	6	1.299746000	0.348362000	0.026138000
6	-2.020735000	0.734734000	-0.811970000	6	1.441917000	-0.891194000	0.663095000
6	-1.825306000	-0.936248000	0.938319000	6	2.426348000	0.957125000	-0.544107000
1	-1.671950000	1.667090000	-1.241407000	1	0.585616000	-1.359654000	1.132733000
1	-1.342103000	-1.300670000	1.838489000	1	2.311271000	1.926788000	-1.013094000
6	-3.101728000	0.036161000	-1.347911000	6	2.688378000	-1.511021000	0.725057000
6	-2.905497000	-1.628541000	0.393906000	6	3.664015000	0.326258000	-0.502159000
1	-3.604913000	0.418640000	-2.228835000	1	2.792661000	-2.461961000	1.235100000
1	-3.256528000	-2.537735000	0.868663000	1	4.527020000	0.797775000	-0.958546000
6	-3.540480000	-1.144848000	-0.750210000	6	3.797843000	-0.908951000	0.134680000
1	-4.384294000	-1.682435000	-1.167488000	1	4.765323000	-1.396920000	0.174814000
$SiMeF_2$				COOMe			
E(RB3LYP) = -761.057773772				E(RB3LYP) = -460.258108263			
6	3.210642000	0.000212000	0.084544000	6	0.231973000	0.123114000	-0.000114000
6	2.513675000	1.207166000	0.054686000	6	0.750286000	-1.177266000	-0.000270000
6	2.513834000	-1.206842000	0.055539000	6	1.103495000	1.218159000	0.000159000
1	3.053820000	2.147241000	0.068300000	6	2.127990000	-1.376134000	-0.000134000
1	3.054144000	-2.146816000	0.069820000	6	2.479223000	1.014898000	0.000239000
6	1.121657000	1.206666000	-0.000487000	6	2.993176000	-0.282256000	0.000101000
6	1.121802000	-1.206623000	0.000368000	1	0.073416000	-2.021278000	-0.000466000
1	0.593184000	2.153713000	-0.038176000	1	2.526963000	-2.384072000	-0.000222000
1	0.593470000	-2.153759000	-0.036663000	1	4.065982000	-0.440141000	0.000190000
6	0.403215000	-0.000021000	-0.025596000	1	3.151019000	1.865634000	0.000436000
1	4.294257000	0.000286000	0.125073000	1	0.685043000	2.217039000	0.000290000
14	-1.454003000	-0.000167000	-0.048024000	6	-1.233549000	0.396940000	-0.000153000
6	-2.324479000	0.002459000	1.589110000	8	-1.725359000	1.502691000	-0.000432000
1	-3.408530000	0.001999000	1.447848000	8	-1.972001000	-0.735040000	0.000220000
1	-2.054076000	-0.880836000	2.173784000	6	-3.398903000	-0.553011000	0.000273000
1	-2.054446000	0.888278000	2.170168000	1	-3.713281000	-0.004071000	0.888963000
9	-1.948993000	1.302615000	-0.882791000	1	-3.713391000	-0.004496000	-0.888640000
9	-1.948546000	-1.305489000	-0.879077000	1	-3.819021000	-1.556483000	0.000539000
OCF_3				$CONH_2$			
E(RB3LYP) = -644.699445350				E(RB3LYP) = -401.070258290			
6	3.207559000	-0.353776000	0.004114000	6	2.577052000	0.047730000	0.022310000
6	2.840162000	0.991765000	0.002543000	6	1.906607000	-1.168577000	0.154732000
6	2.220009000	-1.334240000	0.000016000	6	1.851433000	1.226550000	-0.139976000
1	3.599003000	1.765462000	0.005721000	1	2.468585000	-2.087775000	0.275173000
1	2.494020000	-2.382825000	0.001191000	1	2.368766000	2.171392000	-0.262003000
6	1.497153000	1.352565000	-0.002934000	6	0.516474000	-1.205644000	0.127383000
6	0.866948000	-0.991139000	-0.006077000	6	0.458797000	1.191834000	-0.157196000
1	1.188288000	2.390369000	-0.003521000	1	-0.021329000	-2.141671000	0.213841000
1	0.113894000	-1.765675000	-0.009751000	1	-0.090806000	2.112811000	-0.316279000
6	0.525722000	0.356699000	-0.007405000	6	-0.219605000	-0.024720000	-0.016538000
1	4.254033000	-0.634122000	0.008470000	1	3.660807000	0.075836000	0.038020000
8	-0.789677000	0.848030000	-0.015242000	6	-1.718709000	-0.136738000	-0.037507000
6	-1.863090000	0.037980000	0.000747000	8	-2.284975000	-1.181250000	-0.314952000
9	-2.951749000	0.808013000	-0.003063000	7	-2.418911000	1.008056000	0.252838000
9	-1.924705000	-0.779674000	-1.073922000	1	-1.986586000	1.771072000	0.746908000
9	-1.912279000	-0.752403000	1.096298000	1	-3.419563000	0.909336000	0.334839000

$CH{=}CHCOC_6H_5$ E(RB3LYP) = -654.207604255 6 2.602498000 0.232108000 -0.012231000 6 2.834492000 -1.136415000 0.217902000 6 3.715477000 1.070661000 -0.193676000 6 4.127211000 -1.640849000 0.260577000 6 5.011609000 0.565325000 -0.152254000 6 5.222040000 -0.792798000 0.074886000 1 1.998773000 -1.809466000 0.368819000 1 4.286420000 -2.698083000 0.440628000 1 6.229878000 -1.190654000 0.108891000 1 5.855282000 1.230678000 -0.296008000 1 3.553890000 2.128904000 -0.369365000 6 1.266822000 0.823053000 -0.068289000 6 0.080244000 0.197193000 0.034041000 1 0.024238000 -0.873876000 0.178744000 1 1.229983000 1.900647000 -0.210328000 6 -1.185306000 0.970436000 -0.023178000 8 -1.183761000 2.193937000 -0.061468000 6 -2.489656000 0.223741000 -0.013576000 6 -3.655991000 0.948042000 0.272668000 6 -2.596918000 -1.143173000 -0.303406000 1 -3.563548000 2.006374000 0.482886000 1 -1.717920000 -1.724474000 -0.552135000 6 -4.894991000 0.319813000 0.283295000 6 -3.841301000 -1.770186000 -0.306814000 1 -5.788031000 0.889230000 0.515123000 1 -3.912257000 -2.825597000 -0.544318000 6 -4.990983000 -1.042365000 -0.007804000 1 -5.958112000 -1.532692000 -0.004043000	$C_6H_4\text{-}3NO_2$ E(RB3LYP) = -667.986126905 6 -1.654343000 0.118111000 -0.035588000 6 -2.614770000 0.903910000 0.617705000 6 -2.067271000 -1.081874000 -0.632139000 6 -3.946693000 0.502334000 0.672251000 6 -3.399596000 -1.482024000 -0.579124000 6 -4.344409000 -0.691753000 0.073321000 1 -2.312799000 1.821996000 1.109068000 1 -4.672448000 1.118555000 1.190912000 1 -5.381498000 -1.004226000 0.115450000 1 -3.700684000 -2.408980000 -1.053914000 1 -1.345817000 -1.694527000 -1.160807000 6 -0.233340000 0.546559000 -0.093074000 6 0.111825000 1.890577000 -0.306791000 6 0.800020000 -0.384311000 0.065335000 1 -0.673751000 2.622026000 -0.456245000 1 0.591513000 -1.428153000 0.254201000 6 1.443152000 2.297008000 -0.357298000 6 2.120899000 0.042126000 0.008225000 1 1.682714000 3.339353000 -0.530958000 6 2.469957000 1.372189000 -0.198358000 1 3.511691000 1.658105000 -0.233262000 7 3.198312000 -0.959664000 0.186260000 8 4.355188000 -0.559120000 0.163361000 8 2.869850000 -2.128833000 0.343506000
$NHCOCF_3$ E(RB3LYP) = -738.201559385 6 -1.283366000 0.196843000 -0.007960000 6 -1.848437000 -1.083052000 -0.005077000 6 -2.111023000 1.326837000 -0.003117000 6 -3.236273000 -1.210892000 0.002774000 6 -3.492677000 1.181351000 0.004804000 6 -4.063643000 -0.090835000 0.007830000 1 -1.212255000 -1.954668000 -0.008908000 1 -3.669751000 -2.204421000 0.004793000 1 -5.141022000 -0.205736000 0.014005000 1 -4.121923000 2.063789000 0.008983000 1 -1.671314000 2.319501000 -0.004699000 7 0.115422000 0.426308000 -0.015191000 1 0.398121000 1.396219000 -0.024944000 6 1.119228000 -0.488271000 -0.009581000 8 1.028335000 -1.695357000 -0.004225000 6 2.541502000 0.146870000 0.001637000 9 3.184847000 -0.175905000 1.132125000 9 3.260401000 -0.297923000 -1.035077000 9 2.513824000 1.506151000 -0.074488000	CH_2SCF_3 E(RB3LYP) = -1006.98982418 6 -1.452242000 0.000165000 -0.399467000 6 -2.140175000 1.205051000 -0.220665000 6 -2.139649000 -1.205015000 -0.220537000 6 -3.489889000 1.205502000 0.123008000 6 -3.489355000 -1.206027000 0.123122000 6 -4.167573000 -0.000398000 0.295728000 1 -1.616291000 2.145950000 -0.353624000 1 -4.012066000 2.146518000 0.253573000 1 -5.218515000 -0.000617000 0.561543000 1 -4.011130000 -2.147255000 0.253776000 1 -1.615332000 -2.145688000 -0.353381000 6 0.006446000 0.000451000 -0.772649000 1 0.269729000 -0.889755000 -1.342706000 1 0.269346000 0.890582000 -1.343004000 16 1.022822000 0.000883000 0.785193000 6 2.677986000 -0.000150000 0.040815000 9 2.911825000 1.079861000 -0.738444000 9 3.592244000 0.000038000 1.025087000 9 2.911022000 -1.081159000 -0.737241000
$PO(OEt)_2$ E(RB3LYP) = -957.393674387 6 -1.261080000 -0.163857000 0.119851000 6 -2.259416000 -0.062848000 1.094248000 6 -1.611796000 -0.233458000 -1.234313000 6 -3.600727000 -0.036528000 0.715993000 6 -2.952495000 -0.207088000 -1.606248000 6 -3.946855000 -0.108423000 -0.631743000 1 -1.975313000 -0.007047000 2.138488000 1 -4.372887000 0.039830000 1.473069000 1 -4.990677000 -0.087968000 -0.924938000 1 -3.223061000 -0.263611000 -2.654602000 1 -0.839511000 -0.311090000 -1.990527000 15 0.464694000 -0.175854000 0.654295000 8 0.653794000 0.014791000 2.114596000 8 1.252468000 0.919767000 -0.255311000 6 1.263155000 2.317822000 0.129822000 1 0.258880000 2.729171000 -0.018328000	$COC(Me)_3$ E(RB3LYP) = -502.965361432 6 -3.449250000 0.383195000 -0.062256000 6 -3.029826000 -0.939500000 -0.205990000 6 -2.506190000 1.384356000 0.156305000 1 -3.757059000 -1.725406000 -0.376299000 1 -2.824170000 2.413566000 0.278965000 6 -1.678771000 -1.253805000 -0.125679000 6 -1.149831000 1.070685000 0.218027000 1 -1.343178000 -2.278992000 -0.218047000 1 -0.445595000 1.870559000 0.393424000 6 -0.713882000 -0.254416000 0.079990000 1 -4.503379000 0.631002000 -0.117983000 6 0.723915000 -0.717743000 0.169350000 8 0.929302000 -1.889405000 0.427305000 6 1.929074000 0.228475000 -0.079015000 6 3.190090000 -0.637319000 -0.261461000 1 3.378715000 -1.257513000 0.615110000

1	1.514426000	2.388539000	1.190696000
8	1.013379000	-1.538519000	0.005487000
6	2.384647000	-1.980607000	0.206517000
1	2.869523000	-1.346382000	0.952582000
1	2.312861000	-2.989604000	0.616497000
6	3.131241000	-1.968575000	-1.113775000
1	3.195043000	-0.954947000	-1.513637000
1	4.146099000	-2.351236000	-0.968112000
1	2.628140000	-2.603166000	-1.847005000
6	2.278112000	3.036639000	-0.735924000
1	2.021158000	2.947644000	-1.793868000
1	2.301588000	4.098418000	-0.474693000
1	3.277464000	2.622482000	-0.584795000
1	3.092756000	-1.304222000	-1.121089000
1	4.055454000	0.011330000	-0.425080000
6	1.733487000	1.076768000	-1.354658000
1	1.560405000	0.437178000	-2.225044000
1	0.900623000	1.775862000	-1.286972000
1	2.641364000	1.656295000	-1.546121000
6	2.144269000	1.129099000	1.162265000
1	1.317653000	1.815145000	1.350476000
1	2.286344000	0.521495000	2.059931000
1	3.047149000	1.730166000	1.019019000

$P(O)Me_2$

E(RB3LYP) = -728.222511052

6	0.362365000	-0.027672000	-0.000115000
6	1.107901000	-1.211086000	-0.000145000
6	1.027872000	1.204737000	-0.000143000
6	2.501219000	-1.161611000	0.000010000
6	2.419803000	1.251663000	-0.000079000
6	3.157533000	0.067479000	0.000060000
1	0.582150000	-2.159297000	-0.000251000
1	3.072932000	-2.082912000	-0.000031000
1	4.241183000	0.105139000	0.000124000
1	2.928379000	2.209270000	-0.000100000
1	0.468846000	2.135101000	-0.000316000
15	-1.464099000	-0.187011000	-0.000070000
8	-1.909196000	-1.620114000	-0.001834000
6	-2.043228000	0.765242000	-1.450712000
1	-3.135358000	0.757775000	-1.461909000
1	-1.687939000	1.797817000	-1.434314000
1	-1.680518000	0.274421000	-2.355374000
6	-2.042506000	0.762556000	1.452676000
1	-1.685278000	1.794511000	1.438439000
1	-3.134618000	0.757174000	1.463905000
1	-1.680477000	0.269230000	2.356237000

C_6Cl_5

E(RB3LYP) = -2761.50174378

6	2.136119000	0.000000000	0.000000000
6	2.840458000	-0.000521000	-1.206824000
6	2.840458000	0.000521000	1.206824000
6	4.233251000	-0.000523000	-1.205712000
6	4.233251000	0.000523000	1.205712000
6	4.932226000	0.000000000	0.000000000
1	2.298643000	-0.000959000	-2.145938000
1	4.771054000	-0.000952000	-2.146974000
1	6.016287000	0.000000000	0.000000000
1	4.771054000	0.000952000	2.146974000
1	2.298643000	0.000959000	2.145938000
6	0.641123000	0.000000000	0.000000000
6	-0.080802000	1.201118000	-0.000087000
6	-0.080802000	-1.201118000	0.000086000
6	-1.481527000	1.213490000	-0.000046000
6	-1.481527000	-1.213490000	0.000046000
6	-2.182097000	0.000000000	0.000000000
17	0.793904000	-2.709630000	0.000214000
17	-2.348106000	-2.718488000	0.000018000
17	-3.918446000	0.000000000	0.000000000
17	-2.348106000	2.718488000	-0.000018000
17	0.793904000	2.709630000	-0.000214000

Br

E(RB3LYP) = -2805.85388222

6	2.881288000	0.000070000	0.000040000
6	2.181610000	-1.205541000	0.000031000
6	2.181765000	1.205372000	0.000027000
1	2.718318000	-2.147528000	0.000038000
1	2.717885000	2.147662000	0.000033000
6	0.787648000	-1.214023000	0.000012000
6	0.787213000	1.213968000	0.000007000
1	0.239498000	-2.147426000	0.000006000
1	0.240696000	2.148209000	-0.000002000
6	0.106437000	0.000241000	0.000001000
1	3.964926000	-0.000289000	0.000055000
35	-1.812488000	-0.000033000	-0.000024000

Cl

E(RB3LYP) = -691.934214822

6	2.272325000	-0.000032000	0.000032000
6	1.572289000	-1.205579000	0.000024000
6	1.572689000	1.205304000	0.000020000
1	2.108906000	-2.147498000	0.000032000
1	2.108991000	2.147398000	0.000026000
6	0.178656000	-1.213464000	0.000004000
6	0.178543000	1.213472000	0.000000000
1	-0.373508000	-2.144674000	-0.000002000
1	-0.372077000	2.145480000	-0.000011000
6	-0.502516000	0.000275000	-0.000007000
1	3.355947000	-0.000396000	0.000049000
17	-2.262363000	-0.000010000	-0.000031000

$OCHF_2$

E(RB3LYP) = -545.421640026

6	-0.317481000	-0.285984000	0.137982000
6	-0.711713000	1.040898000	-0.018721000
6	-1.254113000	-1.316475000	0.170214000
6	-2.069959000	1.326238000	-0.170784000
6	-2.604457000	-1.013910000	0.031929000
6	-3.017715000	0.307390000	-0.145143000
1	0.014917000	1.842710000	0.002413000
1	-2.381794000	2.356850000	-0.295293000
1	-4.070213000	0.539168000	-0.256591000
1	-3.335093000	-1.814158000	0.057080000
1	-0.910683000	-2.335130000	0.301258000
8	1.009435000	-0.670910000	0.309884000
6	1.987487000	0.060680000	-0.296101000
1	1.707167000	0.434868000	-1.283685000
9	2.349352000	1.135061000	0.477729000
9	3.075973000	-0.731733000	-0.395563000

$OCHCl_2$

E(RB3LYP) = -1266.10821236

6	0.898052000	0.291417000	0.143752000
6	1.298173000	-0.900866000	-0.453776000
6	1.832782000	1.232488000	0.571097000
6	2.662665000	-1.133731000	-0.640935000
6	3.186732000	0.980934000	0.384136000
6	3.608235000	-0.201470000	-0.226848000
1	0.580208000	-1.655360000	-0.746085000
1	2.978954000	-2.060911000	-1.104747000
1	4.664331000	-0.394352000	-0.372481000
1	3.914614000	1.713225000	0.713861000
1	1.483324000	2.144868000	1.038019000
8	-0.429737000	0.635736000	0.387636000
6	-1.429474000	0.005377000	-0.293532000
1	-1.137528000	-0.306154000	-1.293084000
17	-2.797146000	1.147663000	-0.456476000
17	-1.990442000	-1.510727000	0.560009000

CH=CHCHO
E(RB3LYP) = -423.083572768

6	0.286565000	0.538418000	-0.000005000
6	0.383392000	-0.867222000	-0.000058000
6	1.483316000	1.287133000	0.000047000
6	1.629724000	-1.483980000	-0.000070000
6	2.724764000	0.665817000	0.000050000
6	2.801282000	-0.726982000	-0.000014000
1	-0.520814000	-1.458666000	-0.000092000
1	1.686024000	-2.566702000	-0.000115000
1	3.767829000	-1.218460000	-0.000017000
1	3.629403000	1.263044000	0.000092000
1	1.428375000	2.370859000	0.000092000
6	-0.955241000	1.305009000	-0.000005000
6	-2.280311000	1.001974000	-0.000051000
1	-2.950525000	1.858104000	-0.000114000
1	-0.764084000	2.376922000	0.000009000
6	-3.012364000	-0.268436000	-0.000053000
8	-2.566291000	-1.401437000	0.000169000
1	-4.112636000	-0.123986000	-0.000255000

SCH=CH_2
E(RB3LYP) = -707.938253019

6	-0.099337000	-0.107213000	-0.442135000
6	-0.762151000	1.121092000	-0.513308000
6	-0.773196000	-1.236759000	0.030199000
6	-2.092524000	1.217621000	-0.108792000
6	-2.103846000	-1.134879000	0.432730000
6	-2.764170000	0.090991000	0.363973000
1	-0.236182000	1.992063000	-0.885487000
1	-2.603748000	2.171961000	-0.166661000
1	-3.799912000	0.167522000	0.675084000
1	-2.623723000	-2.013875000	0.796838000
1	-0.255816000	-2.187409000	0.078134000
16	1.597264000	-0.249091000	-1.017941000
6	2.546146000	0.103954000	0.438920000
6	2.122619000	0.403092000	1.665963000
1	3.606183000	0.047179000	0.208606000
1	2.843249000	0.593732000	2.452387000
1	1.072491000	0.466889000	1.922872000

$B(OH)_2$
E(RB3LYP) = -408.390248587

6	0.193724000	0.000073000	0.000123000
6	-0.536221000	-1.179941000	-0.221984000
6	-0.536356000	1.179997000	0.222195000
6	-1.929343000	-1.183568000	-0.229591000
6	-1.929475000	1.183494000	0.229526000
6	-2.629311000	-0.000060000	-0.000111000
1	-0.011789000	-2.111475000	-0.416161000
1	-2.468391000	-2.105986000	-0.415400000
1	-3.713624000	-0.000082000	-0.000244000
1	-2.468641000	2.105853000	0.415294000
1	-0.012013000	2.111546000	0.416530000
5	1.769864000	-0.000009000	0.000034000
8	2.505126000	1.077254000	-0.412534000
1	1.972609000	1.783562000	-0.785895000
8	2.505073000	-1.077221000	0.412387000
1	1.972825000	-1.783615000	0.785937000

N=C=O
E(RB3LYP) = -399.843673147

6	-0.092325000	-0.257947000	0.000009000
6	0.848991000	-1.290524000	0.000199000
6	0.331977000	1.076506000	-0.000022000
6	2.207577000	-0.987683000	0.000356000
6	1.692644000	1.366716000	0.000137000
6	2.635412000	0.338909000	0.000326000
1	0.504255000	-2.317115000	0.000220000
1	2.933048000	-1.793041000	0.000503000
1	3.693867000	0.570975000	0.000449000
1	2.015871000	2.401457000	0.000112000
1	-0.400995000	1.875329000	-0.000169000
7	-1.450111000	-0.597879000	-0.000147000
6	-2.535851000	-0.080151000	-0.000333000
8	-3.640728000	0.306574000	-0.000515000

COOEt
E(RB3LYP) = -499.586857911

6	-0.654319000	0.151631000	-0.082055000
6	-1.118396000	-1.168895000	-0.097343000
6	-1.564294000	1.205222000	0.061193000
6	-2.480188000	-1.428738000	0.029017000
6	-2.924083000	0.941399000	0.186219000
6	-3.383740000	-0.375853000	0.170715000
1	-0.412182000	-1.980918000	-0.208313000
1	-2.836925000	-2.452355000	0.016654000
1	-4.443979000	-0.581231000	0.268636000
1	-3.625477000	1.760592000	0.296061000
1	-1.187470000	2.220467000	0.071318000
6	0.792860000	0.490638000	-0.214288000
8	1.230654000	1.619527000	-0.202256000
8	1.567200000	-0.607232000	-0.356513000
6	2.995963000	-0.397785000	-0.491588000
1	3.163350000	0.509141000	-1.073340000
1	3.338074000	-1.262801000	-1.060675000
6	3.677496000	-0.319648000	0.864473000
1	3.476134000	-1.217077000	1.454284000
1	4.759502000	-0.237180000	0.725738000
1	3.338338000	0.555182000	1.421726000

$C(NO_2)Me_2$
E(RB3LYP) = -554.848188994

6	0.467472000	0.188624000	0.172783000
6	0.980501000	-1.104450000	0.342076000
6	1.349189000	1.216476000	-0.169940000
6	2.337605000	-1.360389000	0.175193000
6	2.711965000	0.962335000	-0.326860000
6	3.210951000	-0.325079000	-0.155864000
1	0.314549000	-1.922610000	0.591958000
1	2.712331000	-2.369607000	0.302657000
1	4.269125000	-0.522670000	-0.283437000
1	3.379754000	1.775020000	-0.589559000
1	0.986330000	2.224816000	-0.319249000
6	-1.027025000	0.442386000	0.394266000
7	-1.765493000	-0.519266000	-0.609216000
8	-2.285584000	-1.529438000	-0.161890000
8	-1.751467000	-0.204951000	-1.786914000
6	-1.495329000	1.854905000	0.038154000
1	-1.042541000	2.572614000	0.724786000
1	-1.236519000	2.121477000	-0.984910000
1	-2.579469000	1.924883000	0.148913000
6	-1.451324000	0.076394000	1.818488000
1	-1.192148000	-0.949014000	2.073868000
1	-0.932983000	0.745593000	2.509184000
1	-2.527589000	0.202267000	1.950955000

$PS(C_6H_5)C_6H_4$-4Me
E(RB3LYP) = -1474.07054180

6	1.168665000	1.454142000	0.040397000

$PO(C_6H_5)C_6H_4$-4Me
E(RB3LYP) = -1151.10230579

6	1.182341000	1.469592000	0.198982000

6	1.085042000	2.699489000	0.674828000
6	1.834467000	1.350225000	-1.185503000
6	1.645756000	3.826546000	0.081113000
6	2.401011000	2.481129000	-1.773696000
6	2.304397000	3.719712000	-1.144062000
1	0.597813000	2.774958000	1.640153000
1	1.576916000	4.786751000	0.579878000
1	2.747306000	4.597536000	-1.601207000
1	2.921851000	2.390002000	-2.720322000
1	1.921491000	0.390608000	-1.680253000
15	0.390585000	-0.000258000	0.862965000
16	0.616760000	-0.008471000	2.828533000
6	1.127769000	-1.474148000	0.037129000
6	2.304064000	-2.016872000	0.566615000
6	0.548071000	-2.058852000	-1.094259000
1	2.734213000	-1.583235000	1.462102000
1	-0.372812000	-1.660950000	-1.503536000
6	2.899801000	-3.120260000	-0.038074000
6	1.145473000	-3.167371000	-1.693708000
1	3.809943000	-3.535432000	0.380006000
1	0.686050000	-3.618933000	-2.565921000
6	2.322572000	-3.696831000	-1.169376000
1	2.783993000	-4.560703000	-1.634716000
6	-1.366783000	0.026968000	0.322911000
6	-1.803898000	0.778543000	-0.770977000
6	-2.299014000	-0.739726000	1.033263000
1	-1.105236000	1.390302000	-1.328944000
1	-1.976800000	-1.305315000	1.900160000
6	-3.145911000	0.755215000	-1.150020000
6	-3.632485000	-0.761074000	0.643982000
1	-3.467226000	1.348712000	-2.000000000
1	-4.339776000	-1.363237000	1.205684000
6	-4.081358000	-0.012524000	-0.452437000
6	-5.537731000	-0.019691000	-0.845858000
1	-5.683244000	0.391504000	-1.846728000
1	-5.948379000	-1.032747000	-0.830726000
1	-6.132475000	0.581861000	-0.150246000

6	1.123992000	2.668573000	0.921314000
6	1.834209000	1.443780000	-1.038536000
6	1.692537000	3.828100000	0.401148000
6	2.403515000	2.607021000	-1.556200000
6	2.329508000	3.799765000	-0.839562000
1	0.647549000	2.680324000	1.895033000
1	1.645114000	4.751861000	0.966903000
1	2.774952000	4.702855000	-1.241860000
1	2.911267000	2.578037000	-2.513870000
1	1.913991000	0.516602000	-1.594274000
15	0.389696000	0.002157000	0.963096000
8	0.505879000	-0.003104000	2.460819000
6	1.176413000	-1.468136000	0.198297000
6	2.250349000	-2.044158000	0.888306000
6	0.750918000	-2.034141000	-1.008681000
1	2.556360000	-1.622376000	1.838865000
1	-0.099186000	-1.618555000	-1.537533000
6	2.900086000	-3.160156000	0.366434000
6	1.404019000	-3.150876000	-1.528337000
1	3.728931000	-3.602683000	0.907589000
1	1.066130000	-3.586998000	-2.461845000
6	2.480680000	-3.712044000	-0.843659000
1	2.985398000	-4.582863000	-1.247107000
6	-1.349604000	0.013881000	0.393789000
6	-2.300377000	-0.587000000	1.227993000
6	-1.771459000	0.585375000	-0.810572000
1	-1.984492000	-1.007193000	2.176172000
1	-1.059012000	1.080727000	-1.460852000
6	-3.638640000	-0.627888000	0.851860000
6	-3.114414000	0.538571000	-1.179674000
1	-4.362376000	-1.097851000	1.510428000
1	-3.424931000	0.987555000	-2.117819000
6	-4.069019000	-0.068106000	-0.357410000
6	-5.527872000	-0.088722000	-0.742079000
1	-5.658327000	0.024138000	-1.820440000
1	-6.006803000	-1.021933000	-0.435845000
1	-6.070134000	0.730238000	-0.257004000

$PO(C_3H_7)_2$

E(RB3LYP) = -885.514326209

6	0.972459000	-0.000023000	-0.014787000
6	1.593971000	-0.000046000	1.238102000
6	1.762167000	-0.000031000	-1.171729000
6	2.985236000	-0.000079000	1.332173000
6	3.151515000	-0.000063000	-1.076401000
6	3.764356000	-0.000087000	0.177075000
1	0.973495000	-0.000039000	2.127153000
1	3.459465000	-0.000097000	2.307299000
1	4.846196000	-0.000111000	0.250647000
1	3.755320000	-0.000068000	-1.977080000
1	1.301232000	-0.000012000	-2.154212000
15	-0.865194000	0.000018000	-0.049099000
8	-1.435160000	0.000027000	1.343930000
6	-1.341586000	-1.451716000	-1.079359000
1	-2.412426000	-1.348976000	-1.288811000
1	-0.819963000	-1.357359000	-2.038040000
6	-1.341524000	1.451777000	-1.079353000
1	-0.819928000	1.357386000	-2.038046000
1	-2.412374000	1.349094000	-1.288781000
6	-1.050036000	2.823665000	-0.440073000
1	-0.020480000	2.840571000	-0.066121000
1	-1.094871000	3.580406000	-1.230850000
6	-2.019860000	3.203717000	0.684373000
1	-2.000325000	2.466467000	1.488551000
1	-3.046691000	3.262437000	0.308674000
6	-1.050188000	-2.823617000	-0.440066000
1	-1.095038000	-3.580359000	-1.230840000
1	-0.020644000	-2.840575000	-0.066082000
6	-2.020063000	-3.203615000	0.684354000
1	-3.046887000	-3.262287000	0.308625000
1	-2.000516000	-2.466360000	1.488528000

$PO(C_6H_5)_2$

E(RB3LYP) = -1111.77433682

6	0.440631000	1.633240000	0.220478000
6	0.099220000	2.760486000	0.978137000
6	1.094136000	1.800062000	-1.005489000
6	0.391670000	4.037089000	0.504647000
6	1.384709000	3.079635000	-1.476687000
6	1.030432000	4.198331000	-0.724612000
1	-0.377804000	2.626664000	1.942343000
1	0.127141000	4.905161000	1.098024000
1	1.260366000	5.192813000	-1.090596000
1	1.895693000	3.201110000	-2.425311000
1	1.394577000	0.936206000	-1.587636000
15	-0.001288000	-0.002211000	0.922703000
8	-0.002212000	-0.000525000	2.424587000
6	1.195861000	-1.200842000	0.221192000
6	2.348410000	-1.458309000	0.974297000
6	1.011788000	-1.856039000	-1.001287000
1	2.473300000	-0.972655000	1.935396000
1	0.110567000	-1.689948000	-1.580349000
6	3.310443000	-2.346542000	0.500373000
6	1.977375000	-2.744635000	-1.472871000
1	4.198604000	-2.543816000	1.090168000
1	1.825854000	-3.252580000	-2.418807000
6	3.127944000	-2.987537000	-0.724810000
1	3.876142000	-3.681735000	-1.091057000
6	-1.638242000	-0.437599000	0.220640000
6	-2.441055000	-1.303113000	0.974179000
6	-2.112304000	0.052446000	-1.001315000
1	-2.083891000	-1.656404000	1.934801000
1	-1.514344000	0.746772000	-1.580586000
6	-3.694010000	-1.684975000	0.501321000
6	-3.366588000	-0.333363000	-1.472446000

1	-1.762400000	4.182212000	1.099285000
1	-1.762664000	-4.182119000	1.099281000

1	-4.311827000	-2.352620000	1.091365000
1	-3.729708000	0.053997000	-2.417862000
6	-4.156170000	-1.204216000	-0.723709000
1	-5.133140000	-1.500318000	-1.089366000

$PS(C_6H_4\text{-}4Me)_2$

E(RB3LYP) = -1513.39875091

6	-1.468349000	-0.515847000	0.308898000
6	-1.963089000	-1.574989000	1.079771000
6	-2.100021000	-0.207116000	-0.898906000
6	-3.054576000	-2.313743000	0.640141000
6	-3.198822000	-0.951015000	-1.328667000
6	-3.693970000	-2.014492000	-0.570291000
1	-1.498175000	-1.804893000	2.031756000
1	-3.422436000	-3.132197000	1.251040000
1	-3.678787000	-0.693929000	-2.267516000
1	-1.746065000	0.616543000	-1.507565000
15	-0.003038000	0.408283000	0.925411000
16	-0.007790000	0.678373000	2.886321000
6	0.004676000	1.985662000	-0.027495000
6	-0.801442000	3.038414000	0.423095000
6	0.786600000	2.161761000	-1.173894000
1	-1.383144000	2.915911000	1.329491000
1	1.428504000	1.363160000	-1.525290000
6	-0.835225000	4.242642000	-0.273679000
6	0.754526000	3.372825000	-1.865835000
1	-1.461669000	5.052282000	0.083535000
1	1.369365000	3.502317000	-2.749543000
6	-0.057971000	4.412156000	-1.419924000
1	-0.080440000	5.353588000	-1.957444000
6	1.453164000	-0.536736000	0.317837000
6	1.378653000	-1.399724000	-0.779849000
6	2.680233000	-0.379375000	0.972069000
1	0.437258000	-1.550605000	-1.294867000
1	2.741881000	0.266070000	1.840860000
6	2.512607000	-2.082634000	-1.216504000
6	3.806704000	-1.061333000	0.526037000
1	2.434383000	-2.750256000	-2.068713000
1	4.749853000	-0.924589000	1.045731000
6	3.743747000	-1.926709000	-0.573317000
6	4.963094000	-2.690940000	-1.026184000
1	4.867045000	-3.018485000	-2.063479000
1	5.867566000	-2.083469000	-0.941972000
1	5.112582000	-3.584512000	-0.410457000
6	-4.897210000	-2.804505000	-1.022236000
1	-5.788767000	-2.516336000	-0.455081000
1	-5.110206000	-2.637992000	-2.080093000
1	-4.748504000	-3.876662000	-0.869106000

$PO(C_6H_4\text{-}4Me)_2$

E(RB3LYP) = -1190.43046307

6	-0.021318000	2.014511000	0.158108000
6	0.598779000	3.085045000	0.814552000
6	-0.624529000	2.227376000	-1.086360000
6	0.631794000	4.345241000	0.222901000
6	-0.588621000	3.490289000	-1.676441000
6	0.042304000	4.548397000	-1.024704000
1	1.035055000	2.925267000	1.794037000
1	1.111044000	5.170012000	0.738452000
1	0.065834000	5.530865000	-1.483047000
1	-1.061522000	3.648774000	-2.639323000
1	-1.137828000	1.416274000	-1.590269000
15	-0.000170000	0.391551000	1.014445000
8	0.000213000	0.535378000	2.510067000
6	1.478379000	-0.492342000	0.393975000
6	2.052142000	-0.269972000	-0.861622000
6	2.059089000	-1.440967000	1.244603000
1	1.638177000	0.478210000	-1.528292000
1	1.636802000	-1.599125000	2.230538000
6	3.172335000	-0.995358000	-1.262536000
6	3.177384000	-2.160093000	0.836148000
1	3.605429000	-0.809072000	-2.240256000
1	3.614266000	-2.891945000	1.508355000
6	3.752622000	-1.951545000	-0.423191000
6	4.986276000	-2.710937000	-0.845600000
1	5.891880000	-2.222022000	-0.470140000
1	4.980343000	-3.730523000	-0.452897000
1	5.069425000	-2.764740000	-1.933291000
6	-1.454011000	-0.536275000	0.400491000
6	-1.443306000	-1.329844000	-0.750613000
6	-2.635697000	-0.442415000	1.145897000
1	-0.533499000	-1.441760000	-1.329720000
1	-2.644923000	0.148023000	2.055146000
6	-2.596201000	-1.999811000	-1.155365000
6	-3.781490000	-1.115250000	0.734773000
1	-2.568912000	-2.612052000	-2.051317000
1	-4.688624000	-1.030534000	1.324978000
6	-3.783005000	-1.904185000	-0.421939000
6	-5.020076000	-2.659316000	-0.841582000
1	-5.081345000	-3.623312000	-0.324738000
1	-5.928047000	-2.101847000	-0.599598000
1	-5.019814000	-2.862079000	-1.914791000

$PO(Et)_2$

E(RB3LYP) = -806.868290020

6	-0.632050000	0.000067000	0.035768000
6	-1.386223000	0.000002000	1.213676000
6	-1.290154000	0.000182000	-1.200750000
6	-2.779265000	0.000038000	1.155485000
6	-2.681912000	0.000225000	-1.257065000
6	-3.427670000	0.000150000	-0.077880000
1	-0.866585000	-0.000086000	2.165280000
1	-3.356965000	-0.000021000	2.073109000
1	-4.511084000	0.000179000	-0.122729000
1	-3.184161000	0.000311000	-2.218067000
1	-0.724757000	0.000235000	-2.127293000
15	1.196565000	-0.000052000	0.201969000
8	1.624876000	-0.000061000	1.643277000
6	1.793581000	1.455619000	-0.751974000
1	2.882900000	1.353760000	-0.800502000
1	1.417533000	1.385818000	-1.778168000
6	1.793515000	-1.455837000	-0.751852000
1	1.417973000	-1.385838000	-1.778221000
1	2.882881000	-1.354191000	-0.799854000
6	1.407639000	2.792954000	-0.108444000

$PO(isopropyl)_2$

E(RB3LYP) = -885.512066246

6	-0.989423000	-0.105375000	-0.092940000
6	-1.496436000	-0.234328000	1.207143000
6	-1.880653000	-0.069190000	-1.171750000
6	-2.870809000	-0.313417000	1.423217000
6	-3.255067000	-0.146297000	-0.953361000
6	-3.751806000	-0.266575000	0.343156000
1	-0.827765000	-0.283344000	2.059033000
1	-3.253084000	-0.415742000	2.432821000
1	-4.820986000	-0.329144000	0.512797000
1	-3.936810000	-0.118060000	-1.796139000
1	-1.478801000	0.006765000	-2.175730000
15	0.801226000	0.004252000	-0.498585000
8	1.034563000	-0.131132000	-1.980471000
6	1.628188000	-1.328654000	0.495421000
1	1.326437000	-1.191798000	1.540141000
6	1.138879000	-2.703978000	0.011462000
1	0.057335000	-2.814939000	0.116814000
1	1.392551000	-2.852437000	-1.040702000
1	1.617940000	-3.495673000	0.595203000
6	3.158249000	-1.216205000	0.394189000

1	0.323199000	2.926180000	-0.085047000
1	1.776322000	2.848128000	0.917605000
1	1.835804000	3.625927000	-0.671764000
6	1.406969000	-2.793130000	-0.108641000
1	1.835189000	-3.626152000	-0.671852000
1	1.775200000	-2.848516000	0.917561000
1	0.322488000	-2.926091000	-0.085744000

1	3.627523000	-2.045015000	0.932509000
1	3.481621000	-1.266865000	-0.648603000
1	3.539343000	-0.286890000	0.824260000
6	1.414605000	1.644294000	0.128701000
1	2.473519000	1.620049000	-0.155490000
6	0.741397000	2.777256000	-0.662891000
1	0.839519000	2.619142000	-1.738150000
1	-0.323133000	2.850656000	-0.421823000
1	1.207200000	3.734996000	-0.411677000
6	1.314086000	1.867121000	1.644007000
1	1.783629000	2.820232000	1.906393000
1	0.273091000	1.918393000	1.973033000
1	1.818719000	1.087038000	2.219725000

CSNHMe

E(RB3LYP) = -763.342828205

6	-0.442561000	0.010908000	-0.007004000
6	-1.204455000	-1.082454000	-0.438559000
6	-1.106643000	1.169163000	0.424358000
6	-2.592646000	-1.009853000	-0.460670000
6	-2.498397000	1.233437000	0.416441000
6	-3.245209000	0.147024000	-0.032997000
1	-0.692006000	-1.983382000	-0.751130000
1	-3.168045000	-1.860451000	-0.808083000
1	-4.328130000	0.197056000	-0.041855000
1	-2.997145000	2.127925000	0.772182000
1	-0.539702000	2.008589000	0.811880000
6	1.048156000	-0.072322000	0.006986000
16	1.868406000	-1.463130000	0.429665000
7	1.678520000	1.071398000	-0.331664000
6	3.123254000	1.232327000	-0.363839000
1	3.576299000	0.559467000	-1.097103000
1	3.348030000	2.266649000	-0.626352000
1	3.552287000	0.998380000	0.612445000
1	1.115284000	1.826679000	-0.693272000

CONHMe

E(RB3LYP) = -440.387359463

6	0.245011000	0.106173000	-0.048893000
6	0.798964000	-1.169304000	-0.210863000
6	1.095657000	1.197472000	0.157575000
6	2.179198000	-1.351227000	-0.151173000
6	2.472809000	1.013719000	0.226860000
6	3.017983000	-0.261302000	0.074174000
1	0.163385000	-2.022602000	-0.420644000
1	2.598799000	-2.341167000	-0.290258000
1	4.091777000	-0.403559000	0.122143000
1	3.122600000	1.865076000	0.395337000
1	0.656128000	2.182302000	0.256736000
6	-1.233445000	0.379911000	-0.114752000
8	-1.671725000	1.481800000	-0.417124000
7	-2.057521000	-0.671053000	0.176551000
1	-1.661564000	-1.484494000	0.618456000
6	-3.503469000	-0.507483000	0.202936000
1	-3.820912000	0.045301000	-0.680849000
1	-3.972405000	-1.492208000	0.198546000
1	-3.837620000	0.046569000	1.086476000

CH_2CN

E(RB3LYP) = -363.899159093

6	2.522572000	-0.571127000	-0.000039000
6	2.288337000	0.804244000	-0.000029000
6	1.444695000	-1.451372000	-0.000029000
1	3.120953000	1.498604000	-0.000037000
1	1.615800000	-2.521849000	-0.000036000
6	0.984444000	1.289895000	-0.000008000
6	0.136587000	-0.964593000	-0.000008000
1	0.810903000	2.361707000	0.000000000
1	-0.695621000	-1.659228000	0.000000000
6	-0.102704000	0.409153000	0.000003000
1	3.537818000	-0.950853000	-0.000055000
6	-1.508479000	1.000183000	0.000025000
1	-1.642124000	1.643395000	0.876722000
1	-1.642150000	1.643400000	-0.876665000
6	-2.591108000	0.020554000	0.000039000
7	-3.450236000	-0.748114000	0.000049000

SCH_2F

E(RB3LYP) = -769.113340793

6	-0.250699000	-0.362317000	0.177965000
6	-1.272695000	-1.257255000	-0.152018000
6	-0.541765000	0.995050000	0.354693000
6	-2.578722000	-0.795862000	-0.307434000
6	-1.845723000	1.450784000	0.172332000
6	-2.867027000	0.558665000	-0.152658000
1	-1.043303000	-2.306971000	-0.292716000
1	-3.367142000	-1.495490000	-0.561253000
1	-3.881786000	0.917346000	-0.281574000
1	-2.065116000	2.504819000	0.300826000
1	0.244076000	1.685181000	0.634549000
16	1.403981000	-1.011741000	0.440201000
6	2.389434000	0.026304000	-0.662120000
1	3.330253000	-0.499144000	-0.830396000
1	1.860959000	0.201754000	-1.598623000
9	2.695728000	1.276460000	-0.110954000

OSO_2Me

E(RB3LYP) = -895.520707695

6	-0.782693000	-0.000093000	0.469551000
6	-1.434618000	1.215059000	0.293338000
6	-1.434723000	-1.215161000	0.293224000
6	-2.780426000	1.207933000	-0.067039000
6	-2.780539000	-1.207879000	-0.067152000
6	-3.453785000	0.000063000	-0.246621000
1	-0.889912000	2.139896000	0.433490000
1	-3.301417000	2.147901000	-0.207470000
1	-4.500791000	0.000125000	-0.526714000
1	-3.301610000	-2.147791000	-0.207668000
1	-0.890116000	-2.140071000	0.433281000
8	0.554239000	-0.000192000	0.903121000
16	1.756140000	0.000064000	-0.259328000
8	1.716355000	1.260512000	-0.984245000
8	1.716202000	-1.259966000	-0.984965000
6	3.123619000	-0.000354000	0.899411000

$NHSO_2Me$

E(RB3LYP) = -875.651479623

6	0.802978000	-0.285059000	0.392386000
6	1.233426000	1.044189000	0.313227000
6	1.710320000	-1.323381000	0.151790000
6	2.557046000	1.317977000	-0.021914000
6	3.037390000	-1.036251000	-0.155293000
6	3.465885000	0.286148000	-0.252323000
1	0.536534000	1.845172000	0.520461000
1	2.882358000	2.350337000	-0.083358000
1	4.496922000	0.509932000	-0.499230000
1	3.732555000	-1.849868000	-0.328493000
1	1.377885000	-2.354916000	0.212260000
7	-0.532133000	-0.607972000	0.761219000
1	-0.701338000	-1.583518000	0.975612000
16	-1.912095000	0.076566000	0.062138000
8	-3.016236000	-0.713207000	0.594767000
8	-1.844066000	1.520460000	0.243089000

1	4.029038000	-0.000325000	0.293341000
1	3.060701000	0.900342000	1.505929000
1	3.060486000	-0.901333000	1.505492000

6	-1.778547000	-0.245795000	-1.710779000
1	-1.811542000	-1.321738000	-1.873909000
1	-2.634808000	0.241899000	-2.175921000
1	-0.848699000	0.188450000	-2.075579000

$PO(C_4H_9)_2$
E(RB3LYP) = -964.163423993

6	0.000185000	1.198110000	0.075444000
6	0.000306000	1.706088000	-1.227702000
6	0.000251000	2.087647000	1.157581000
6	0.000488000	3.083328000	-1.445833000
6	0.000434000	3.463039000	0.938235000
6	0.000552000	3.962104000	-0.364698000
1	0.000257000	1.008450000	-2.057640000
1	0.000581000	3.468495000	-2.459451000
1	0.000694000	5.033146000	-0.533969000
1	0.000483000	4.144778000	1.781471000
1	0.00159000	1.717063000	2.177629000
15	-0.000061000	-0.629949000	0.266142000
8	-0.000085000	-1.314072000	-1.074784000
6	-1.449906000	-1.017651000	1.335015000
1	-1.342456000	-2.064223000	1.641721000
1	-1.354821000	-0.410559000	2.241696000
6	1.449595000	-1.018023000	1.335123000
1	1.354582000	-0.410961000	2.241831000
1	1.341867000	-2.064588000	1.641757000
6	2.823052000	-0.791010000	0.675831000
1	2.840747000	0.191278000	0.189162000
1	3.579019000	-0.745783000	1.468974000
6	3.221216000	-1.874382000	-0.335659000
1	2.454119000	-1.944840000	-1.111139000
1	3.235006000	-2.846078000	0.173984000
6	4.590456000	-1.611302000	-0.967673000
1	5.379913000	-1.561106000	-0.210039000
1	4.597322000	-0.663796000	-1.515903000
1	4.858326000	-2.402116000	-1.673583000
6	-2.823266000	-0.790335000	0.675620000
1	-3.579228000	-0.744659000	1.468742000
1	-2.840623000	0.191844000	0.188717000
6	-3.221807000	-1.873829000	-0.335597000
1	-3.235894000	-2.845395000	0.174285000
1	-2.454760000	-1.944722000	-1.111083000
6	-4.590988000	-1.610470000	-0.967626000
1	-4.597569000	-0.663098000	-1.516091000
1	-5.380404000	-1.559833000	-0.209978000
1	-4.859133000	-2.401374000	-1.673330000

P(isopropyl)$_2$
E(RB3LYP) = -810.229478986

6	-0.961438000	0.000565000	0.220177000
6	-1.434584000	0.018497000	-1.100279000
6	-1.900158000	-0.021767000	1.258626000
6	-2.800289000	0.014967000	-1.372515000
6	-3.270133000	-0.024087000	0.990721000
6	-3.723039000	-0.005399000	-0.325615000
1	-0.734175000	0.030525000	-1.928842000
1	-3.145952000	0.027548000	-2.400686000
1	-4.786550000	-0.006684000	-0.537284000
1	-3.980085000	-0.039822000	1.810483000
1	-1.552485000	-0.035481000	2.286206000
15	0.843497000	0.016445000	0.676844000
6	1.513382000	-1.459699000	-0.316117000
1	1.552926000	-1.178415000	-1.375981000
6	2.932987000	-1.810435000	0.164453000
1	3.630664000	-0.975462000	0.091184000
1	2.914348000	-2.132286000	1.210066000
1	3.338424000	-2.635218000	-0.431401000
6	0.608409000	-2.692090000	-0.163640000
1	1.062605000	-3.551887000	-0.667419000
1	0.483553000	-2.958854000	0.891151000
1	-0.384072000	-2.537686000	-0.587917000
6	1.393157000	1.514410000	-0.350258000
1	1.019429000	1.378694000	-1.371789000
6	0.754745000	2.782214000	0.238667000
1	-0.335731000	2.724702000	0.254932000
1	1.098528000	2.953377000	1.263675000
1	1.035097000	3.657274000	-0.357091000
6	2.919524000	1.663588000	-0.412093000
1	3.180816000	2.602824000	-0.911090000
1	3.361403000	1.689518000	0.589245000
1	3.393423000	0.856079000	-0.972852000

$SO_2CF(CF_3)_2$
E(RB3LYP) = -1593.79550880

6	-1.892188000	-0.311829000	0.262652000
6	-2.444378000	-1.190982000	-0.668816000
6	-2.576878000	0.812213000	0.721040000
6	-3.716100000	-0.920312000	-1.164300000
6	-3.851140000	1.063212000	0.220222000
6	-4.414921000	0.203213000	-0.722010000
1	-1.896512000	-2.070062000	-0.982376000
1	-4.163039000	-1.590748000	-1.888523000
1	-5.407073000	0.405725000	-1.108799000
1	-4.403249000	1.927456000	0.569533000
1	-2.125650000	1.460389000	1.460391000
16	-0.284915000	-0.695519000	0.962571000
8	-0.096587000	-2.140218000	0.901337000
8	-0.089635000	0.064660000	2.190760000
6	0.968677000	0.024886000	-0.345537000
9	0.400903000	-0.153526000	-1.574725000
6	1.204352000	1.550579000	-0.156376000
9	0.035440000	2.189566000	0.023026000
9	1.989644000	1.790017000	0.894804000
9	1.775729000	2.072810000	-1.249900000
6	2.293814000	-0.798548000	-0.303476000
9	2.113015000	-1.990576000	-0.869237000

$COCF_2CF_2CF_3$
E(RB3LYP) = -1158.52019662

6	2.081327000	-0.253212000	0.122180000
6	2.593911000	0.989062000	-0.283182000
6	2.954865000	-1.344319000	0.266102000
6	3.954442000	1.130175000	-0.538477000
6	4.309879000	-1.197543000	0.006805000
6	4.812390000	0.041413000	-0.396054000
1	1.946840000	1.846704000	-0.397952000
1	4.343905000	2.092600000	-0.848633000
1	5.871314000	0.156874000	-0.598047000
1	4.976154000	-2.044927000	0.118225000
1	2.548490000	-2.296970000	0.581849000
6	0.648436000	-0.505090000	0.433335000
8	0.234930000	-1.558895000	0.855470000
6	-0.367241000	0.665908000	0.223013000
9	-0.031568000	1.674859000	1.078374000
9	-0.268907000	1.154040000	-1.048614000
6	-1.878834000	0.358842000	0.484706000
9	-2.021883000	-0.205774000	1.698631000
9	-2.531160000	1.549401000	0.500619000
6	-2.613688000	-0.523197000	-0.581298000
9	-3.810564000	-0.876017000	-0.098967000

9	3.266530000	-0.166660000	-0.985475000
9	2.709460000	-0.963253000	0.956115000
9	-1.928944000	-1.630748000	-0.878401000

$COCF_3$
E(RB3LYP) = -682.810496540

6	-3.350763000	-0.469373000	-0.000022000
6	-3.019230000	0.887301000	-0.000097000
6	-2.345923000	-1.434891000	0.000084000
1	-3.800597000	1.638221000	-0.000220000
1	-2.603243000	-2.487495000	0.000141000
6	-1.686946000	1.274292000	-0.000033000
6	-1.007765000	-1.053122000	0.000131000
1	-1.410203000	2.321215000	-0.000070000
1	-0.242375000	-1.816833000	0.000198000
6	-0.667168000	0.308188000	0.000089000
1	-4.391773000	-0.772394000	-0.000036000
6	0.731496000	0.806992000	0.000220000
8	1.032128000	1.975994000	0.000230000
6	1.899951000	-0.232720000	0.000041000
9	1.839137000	-1.030405000	-1.092031000
9	3.084863000	0.371630000	0.000235000
9	1.839251000	-1.031299000	1.091315000

$GeCl_3$
E(RB3LYP) = -3689.53265211

6	-1.149768000	0.011797000	0.017607000
6	-1.856980000	1.217605000	0.011786000
6	-1.836547000	-1.207532000	0.009842000
6	-3.250937000	1.200361000	-0.004340000
6	-3.228999000	-1.215905000	-0.006355000
6	-3.935219000	-0.013362000	-0.013894000
1	-1.330692000	2.164767000	0.024356000
1	-3.799170000	2.135410000	-0.007322000
1	-5.019191000	-0.023250000	-0.025372000
1	-3.760782000	-2.160388000	-0.010969000
1	-1.295873000	-2.147314000	0.021792000
32	0.789407000	0.007526000	0.005610000
17	1.596545000	1.965817000	0.464995000
17	1.598720000	-0.574043000	-1.922344000
17	1.598581000	-1.401648000	1.441473000

$N(CF_3)_2$
E(RB3LYP) = -961.962117722

6	3.684003000	0.047123000	-0.100833000
6	2.896839000	0.088126000	-1.250528000
6	3.084001000	-0.006371000	1.156340000
1	3.362160000	0.129380000	-2.228313000
1	3.694561000	-0.039180000	2.051010000
6	1.507787000	0.073903000	-1.148200000
6	1.695861000	-0.018323000	1.266199000
1	0.888241000	0.101826000	-2.036037000
1	1.211075000	-0.059696000	2.233661000
6	0.916715000	0.023358000	0.113214000
1	4.764669000	0.056578000	-0.184786000
7	-0.531377000	0.003600000	0.257347000
6	-1.263124000	1.209234000	0.049782000
9	-0.440304000	2.256525000	0.182666000
9	-1.829837000	1.290459000	-1.181014000
9	-2.261242000	1.355449000	0.937294000
6	-1.175307000	-1.241178000	0.018243000
9	-2.480690000	-1.180663000	0.304467000
9	-1.071505000	-1.662861000	-1.268998000
9	-0.614390000	-2.199948000	0.774222000

$SN(Me)_2$
E(RB3LYP) = -764.513444414

6	-3.087193000	-0.000053000	-0.540771000
6	-2.442385000	1.207107000	-0.274102000
6	-2.442321000	-1.207185000	-0.274048000
1	-2.945556000	2.147360000	-0.470808000
1	-2.945474000	-2.147451000	-0.470747000
6	-1.152703000	1.208313000	0.254614000
6	-1.152644000	-1.208344000	0.254650000
1	-0.654462000	2.144290000	0.478293000
1	-0.654389000	-2.144299000	0.478378000
6	-0.495699000	0.000003000	0.515301000
1	-4.092294000	-0.000109000	-0.947470000
16	1.170128000	0.000145000	1.229675000
7	2.264998000	0.000026000	-0.104677000
6	2.289521000	1.219855000	-0.909321000
1	1.400470000	1.333853000	-1.548981000
1	2.365599000	2.087142000	-0.252938000
1	3.172457000	1.194307000	-1.555348000
6	2.289679000	-1.219984000	-0.909039000
1	1.400761000	-1.334111000	-1.548858000
1	3.172765000	-1.194637000	-1.554865000
1	2.365560000	-2.087118000	-0.252427000

CH_2CONH_2
E(RB3LYP) = -440.395287950

6	0.252405000	-0.031542000	0.536565000
6	0.939777000	1.179266000	0.383686000
6	0.930651000	-1.222031000	0.245466000
6	2.263098000	1.201617000	-0.053750000
6	2.253786000	-1.203760000	-0.191508000
6	2.924073000	0.009167000	-0.344130000
1	0.434632000	2.111951000	0.614356000
1	2.778917000	2.149327000	-0.161088000
1	3.954488000	0.024364000	-0.680536000
1	2.762489000	-2.136705000	-0.407382000
1	0.417827000	-2.170978000	0.366367000
6	-1.189002000	-0.053478000	0.987175000
1	-1.401484000	-0.956921000	1.564491000
1	-1.397698000	0.787361000	1.654642000
6	-2.280345000	0.004905000	-0.096370000
8	-3.457821000	-0.068767000	0.207504000
7	-1.859371000	0.150202000	-1.382676000
1	-0.883011000	0.196250000	-1.623543000
1	-2.554649000	0.189220000	-2.111420000

$NHNO_2$
E(RB3LYP) = -492.226107056

6	2.935767000	0.224656000	-0.181692000
6	2.433993000	-1.071144000	-0.281279000
6	2.075644000	1.274282000	0.138634000
1	3.092107000	-1.895326000	-0.530451000
1	2.460229000	2.284043000	0.222966000
6	1.078684000	-1.313320000	-0.076639000
6	0.722858000	1.042225000	0.368742000
1	0.684745000	-2.319759000	-0.172652000
1	0.060482000	1.854819000	0.628839000
6	0.223076000	-0.256862000	0.249320000
1	3.989007000	0.415203000	-0.350640000
7	-1.135886000	-0.566684000	0.532353000
1	-1.381160000	-1.540357000	0.657859000
7	-2.208012000	0.078449000	-0.089085000
8	-3.264448000	-0.539919000	-0.063963000
8	-2.025335000	1.192417000	-0.543701000

$N{=}NC_6H_5$
E(RB3LYP) = -572.883489760

6	-1.426847000	-0.757527000	0.069178000
6	-2.526245000	-0.687011000	-0.791989000
6	-1.263250000	0.201626000	1.075449000

$P(Cl)NMe_2$
E(RB3LYP) = -1167.95511214

6	0.808701000	-0.033047000	0.305355000
6	1.581117000	-1.113386000	-0.132821000
6	1.432875000	1.208100000	0.510311000

6	-3.414043000	0.379991000	-0.698102000
6	-2.178640000	1.243725000	1.186935000
6	-3.245021000	1.346989000	0.293347000
1	-2.667231000	-1.470360000	-1.527792000
1	-4.251371000	0.444465000	-1.383680000
1	-3.949372000	2.166173000	0.380482000
1	-2.057294000	1.979358000	1.974131000
1	-0.436452000	0.123630000	1.770125000
7	-0.621359000	-1.943853000	-0.011527000
7	0.621555000	-1.943809000	0.012122000
6	1.426994000	-0.757721000	-0.069069000
6	2.526048000	-0.686586000	0.792581000
6	1.263586000	0.200674000	-1.075925000
1	2.666790000	-1.469519000	1.528844000
1	0.437193000	0.122080000	-1.770986000
6	3.413604000	0.380523000	0.698425000
6	2.178874000	1.242987000	-1.187666000
1	4.250710000	0.445694000	1.384207000
1	2.057743000	1.978095000	-1.975375000
6	3.244761000	1.346960000	-0.293702000
1	3.948989000	2.166252000	-0.380898000

6	2.944367000	-0.950655000	-0.379366000
6	2.792115000	1.368081000	0.257493000
6	3.552714000	0.287316000	-0.188504000
1	1.118047000	-2.078369000	-0.292712000
1	3.528759000	-1.795980000	-0.725331000
1	4.612219000	0.410384000	-0.382849000
1	3.257109000	2.335584000	0.411027000
1	0.851794000	2.054389000	0.860820000
15	-0.955863000	-0.158460000	0.849880000
17	-1.501274000	-2.057658000	-0.111927000
7	-1.663316000	1.037482000	-0.110698000
6	-3.010829000	1.466169000	0.277539000
1	-3.786473000	0.906646000	-0.261083000
1	-3.155489000	1.318248000	1.348648000
1	-3.133679000	2.530572000	0.055194000
6	-1.399646000	1.207034000	-1.541625000
1	-0.367106000	0.950136000	-1.771260000
1	-2.062749000	0.573515000	-2.143995000
1	-1.568100000	2.251904000	-1.819313000

SeCH=CHCl

E(RB3LYP) = -3170.89082671

6	1.347362000	-0.180732000	-0.048733000
6	1.323028000	1.152446000	-0.464215000
6	2.532891000	-0.743691000	0.430156000
6	2.482868000	1.921477000	-0.385692000
6	3.693474000	0.026727000	0.483801000
6	3.670793000	1.361234000	0.082428000
1	0.408790000	1.587413000	-0.849955000
1	2.458026000	2.958196000	-0.702667000
1	4.571976000	1.961117000	0.135018000
1	4.611614000	-0.415295000	0.854404000
1	2.548933000	-1.772856000	0.770286000
6	-1.544058000	-0.047146000	0.382353000
1	-1.351058000	0.484698000	1.306520000
6	-2.677576000	0.093049000	-0.295315000
1	-2.902021000	-0.404070000	-1.228918000
34	-0.220745000	-1.317562000	-0.173719000
17	-3.989036000	1.111630000	0.265474000

$N{=}CCl_2$

E(RB3LYP) = -1245.02094122

6	3.554448000	-0.178698000	-0.017953000
6	3.048723000	0.973738000	-0.619015000
6	2.698948000	-1.015340000	0.696784000
1	3.708772000	1.635917000	-1.167568000
1	3.086562000	-1.905411000	1.179257000
6	1.699463000	1.292017000	-0.504274000
6	1.342168000	-0.719724000	0.797623000
1	1.299586000	2.197201000	-0.944814000
1	0.681423000	-1.367231000	1.360060000
6	0.837271000	0.432498000	0.184987000
1	4.608600000	-0.417237000	-0.097250000
7	-0.511394000	0.820022000	0.314085000
6	-1.520851000	0.154086000	0.040967000
17	-3.122855000	0.796091000	0.313147000
17	-1.569275000	-1.473436000	-0.666264000

NHCN

E(RB3LYP) = -379.938935394

6	-0.126450000	-0.366180000	-0.000240000
6	0.150309000	1.002031000	-0.000200000
6	0.917134000	-1.295297000	-0.000043000
6	1.475116000	1.430870000	-0.000077000
6	2.235742000	-0.851761000	0.000251000
6	2.523224000	0.512392000	0.000160000
1	-0.661116000	1.720289000	-0.000268000
1	1.684503000	2.494386000	-0.000126000
1	3.550958000	0.854705000	0.000382000
1	3.039979000	-1.578473000	0.000470000
1	0.699422000	-2.358563000	-0.000198000
7	-1.460882000	-0.842720000	-0.000624000
1	-1.610869000	-1.840832000	0.001589000
6	-2.538442000	-0.062087000	0.000093000
7	-3.470929000	0.626816000	0.000407000

C=CH

E(RB3LYP) = -308.477248610

6	-0.593787000	-0.000074000	0.000001000
6	0.119282000	-1.210909000	0.000000000
6	0.119222000	1.210884000	0.000000000
6	1.510014000	-1.206510000	0.000000000
6	1.509887000	1.206587000	0.000000000
6	2.209616000	0.000036000	-0.000001000
1	-0.426884000	-2.146438000	0.000001000
1	2.049053000	-2.147127000	-0.000001000
1	3.293655000	0.000134000	-0.000002000
1	2.048948000	2.147192000	0.000000000
1	-0.427104000	2.146318000	0.000001000
6	-2.021947000	-0.000055000	0.000003000
6	-3.226988000	0.000017000	-0.000001000
1	-4.289461000	0.000076000	-0.000012000

SC_6H_5

E(RB3LYP) = -861.629361281

6	-1.400167000	0.552936000	-0.051443000
6	-1.636673000	-0.286783000	-1.145721000
6	-2.337728000	0.627251000	0.981635000
6	-2.794568000	-1.057438000	-1.192189000
6	-3.506063000	-0.133194000	0.919590000
6	-3.733930000	-0.979621000	-0.162398000
1	-0.915960000	-0.332256000	-1.953347000
1	-2.970399000	-1.709896000	-2.040204000
1	-4.638879000	-1.574851000	-0.206713000
1	-4.231055000	-0.068551000	1.723202000
1	-2.148975000	1.275158000	1.829285000

CH=CHCOOEt

E(RB3LYP) = -576.998750223

6	1.255570000	0.883261000	-0.023226000
6	1.112235000	-0.072660000	0.993012000
6	2.398914000	0.826784000	-0.835449000
6	2.066742000	-1.068660000	1.169571000
6	3.344530000	-0.181028000	-0.671845000
6	3.180634000	-1.133855000	0.332162000
1	0.261721000	-0.020484000	1.660974000
1	1.946456000	-1.791725000	1.968705000
1	3.922266000	-1.912287000	0.471515000
1	4.213043000	-0.216119000	-1.319818000
1	2.537997000	1.574260000	-1.609724000

16	0.043116000	1.619983000	0.005359000
6	1.419173000	0.467785000	0.046754000
6	1.338175000	-0.800987000	0.628450000
6	2.639175000	0.913349000	-0.473922000
1	0.399904000	-1.152032000	1.039681000
1	2.702188000	1.891518000	-0.937459000
6	2.467411000	-1.615231000	0.676555000
6	3.767215000	0.099037000	-0.404449000
1	2.393419000	-2.600060000	1.124730000
1	4.707625000	0.455197000	-0.810233000
6	3.686276000	-1.170040000	0.166192000
1	4.562497000	-1.806334000	0.210996000

N3

E(RB3LYP) = -395.943085051

6	-0.148484000	0.361457000	0.000183000
6	0.880205000	1.308030000	-0.000028000
6	0.153998000	-1.004637000	0.000220000
6	2.205043000	0.886555000	-0.000186000
6	1.485349000	-1.413008000	0.000059000
6	2.515168000	-0.473858000	-0.000135000
1	0.625257000	2.360669000	-0.000128000
1	2.998921000	1.624685000	-0.000356000
1	3.548878000	-0.798549000	-0.000247000
1	1.715314000	-2.472442000	0.000091000
1	-0.639201000	-1.744196000	0.000375000
7	-1.472394000	0.877223000	0.000395000
7	-2.415933000	0.086216000	-0.000067000
7	-3.368364000	-0.528782000	-0.000387000

$PO(N(Me)_2)_2$

E(RB3LYP) = -917.599438749

6	1.018444000	-0.041070000	0.155577000
6	1.907749000	0.382286000	1.151257000
6	1.526719000	-0.451214000	-1.084800000
6	3.280025000	0.401821000	0.907947000
6	2.898695000	-0.432067000	-1.324721000
6	3.777102000	-0.003672000	-0.329319000
1	1.509206000	0.683173000	2.113095000
1	3.960352000	0.727868000	1.686829000
1	4.844985000	0.009286000	-0.517401000
1	3.282829000	-0.755724000	-2.285837000
1	0.852599000	-0.800375000	-1.858096000
15	-0.771343000	0.059582000	0.533405000
8	-0.991470000	0.323595000	1.988544000
7	-1.412061000	-1.351324000	-0.154031000
1	-3.291006000	-0.486230000	-0.565454000
6	-2.871951000	-1.449066000	-0.277905000
1	-3.342134000	-1.768195000	0.661641000
1	-3.114218000	-2.183395000	-1.052359000
1	-1.025156000	-3.379066000	-0.526395000
6	-0.811877000	-2.630711000	0.243051000
1	-1.212513000	-2.991727000	1.199587000
1	0.269521000	-2.538920000	0.335650000
7	-1.483387000	1.267046000	-0.412288000
1	-1.776037000	2.485786000	1.267910000
6	-1.671991000	2.588273000	0.189397000
1	-2.585491000	3.039866000	-0.211678000
1	-0.831181000	3.262501000	-0.027450000
1	-0.439858000	1.808629000	-2.195388000
6	-1.350438000	1.287984000	-1.865715000
1	-2.212317000	1.806537000	-2.298614000
6	0.299178000	1.984215000	-0.226452000
6	-1.039882000	2.017747000	-0.125941000
1	-1.537289000	2.976039000	-0.229207000
1	0.769226000	2.931385000	-0.485661000
6	-2.010760000	0.925889000	0.131602000
8	-3.088745000	1.120673000	0.651020000
8	-1.610541000	-0.279980000	-0.316062000
6	-2.530959000	-1.381311000	-0.117802000
1	-3.490958000	-1.119873000	-0.568231000
1	-2.693092000	-1.511965000	0.955265000
6	-1.915788000	-2.610443000	-0.755183000
1	-0.951791000	-2.847585000	-0.300386000
1	-1.763639000	-2.460162000	-1.826260000
1	-2.582144000	-3.466665000	-0.619512000

F

E(RB3LYP) = -331.580111910

6	-1.833211000	0.000044000	0.000028000
6	-1.134223000	1.206869000	0.000019000
6	-1.134443000	-1.206675000	0.000016000
1	-1.672723000	2.147566000	0.000029000
1	-1.672868000	-2.147420000	0.000022000
6	0.260070000	1.215831000	-0.000002000
6	0.260065000	-1.215940000	-0.000006000
1	0.826352000	2.138813000	-0.000009000
1	0.825736000	-2.139281000	-0.000016000
6	0.925889000	-0.000170000	-0.000014000
1	-2.916687000	0.000197000	0.000045000
9	2.282812000	0.000042000	-0.000036000

$PO(CMe_3)_2$

E(RB3LYP) = -964.148181826

6	1.242867000	-0.001447000	-0.118167000
6	2.107376000	0.082261000	-1.216678000
6	1.791531000	-0.104635000	1.167748000
6	3.489180000	0.069306000	-1.033789000
6	3.173207000	-0.120435000	1.348639000
6	4.024955000	-0.031852000	0.248214000
1	1.676903000	0.150874000	-2.209198000
1	4.146004000	0.135802000	-1.894114000
1	5.099802000	-0.043431000	0.391171000
1	3.583598000	-0.202157000	2.349115000
1	1.153274000	-0.175153000	2.039359000
15	-0.559957000	0.013335000	-0.526936000
8	-0.742864000	0.041672000	-2.024707000
6	-1.266321000	1.604676000	0.227583000
6	-1.303101000	-1.593510000	0.161764000
6	-0.641038000	2.743175000	-0.609667000
1	0.444494000	2.786624000	-0.488775000
1	-0.862112000	2.620894000	-1.670692000
1	-1.053975000	3.699638000	-0.271756000
6	-0.340770000	-2.728018000	-0.255349000
1	-0.804036000	-3.690741000	-0.014666000
1	-0.145703000	-2.708167000	-1.329899000
1	0.615024000	-2.674552000	0.269152000
6	-1.511660000	-1.631464000	1.684811000
1	-1.885967000	-2.622378000	1.964903000
1	-0.586123000	-1.470786000	2.241674000
1	-2.251277000	-0.901899000	2.020530000
6	-2.652204000	-1.823395000	-0.553348000
1	-2.534841000	-1.773932000	-1.636552000
1	-3.026890000	-2.817441000	-0.286813000
1	-3.409446000	-1.095013000	-0.259533000
6	-2.793773000	1.619867000	0.020197000
1	-3.059897000	1.389879000	-1.013531000
1	-3.306268000	0.915280000	0.679090000
1	-3.175195000	2.619969000	0.252391000
6	-0.935838000	1.840136000	1.711261000
1	-1.390109000	2.786685000	2.024427000
1	-1.330046000	1.061503000	2.366033000

			1 0.138599000 1.927118000 1.880062000
$SiClMe_2$			
E(RB3LYP) = -1061.39312126			$SCH_2CH{=}CH_2$
6 -0.640605000	-0.095293000	-0.072572000	E(RB3LYP) = -747.261246459
6 -1.270274000	1.136455000	-0.319939000	6 -0.619171000 -0.372108000 0.369473000
6 -1.451211000	-1.189411000	0.267566000	6 -1.170122000 0.748499000 0.998594000
6 -2.653279000	1.269566000	-0.232349000	6 -1.324598000 -0.995484000 -0.666598000
6 -2.837559000	-1.061598000	0.354542000	6 -2.409777000 1.242002000 0.591925000
6 -3.440681000	0.168311000	0.103780000	6 -2.553673000 -0.488792000 -1.081326000
1 -0.675401000	2.009171000	-0.570987000	6 -3.100454000 0.629567000 -0.451497000
1 -3.117216000	2.231017000	-0.423371000	1 -0.624957000 1.228880000 1.802184000
1 -4.518059000	0.270580000	0.172413000	1 -2.830352000 2.109674000 1.087982000
1 -3.443823000	-1.920695000	0.620210000	1 -4.061661000 1.017066000 -0.769594000
1 -1.003244000	-2.156273000	0.471621000	1 -3.091664000 -0.976752000 -1.886546000
14 1.224436000	-0.271483000	-0.236459000	1 -0.915820000 -1.882384000 -1.137120000
6 1.807254000	0.190185000	-1.957898000	16 0.947208000 -1.036739000 0.948603000
1 1.492682000	1.201733000	-2.225840000	6 2.062896000 -0.655382000 -0.488697000
1 2.897484000	0.146207000	-2.026453000	1 2.946077000 -1.275128000 -0.320536000
1 1.387958000	-0.499463000	-2.697405000	1 1.562881000 -1.015761000 -1.390510000
6 1.813106000	-1.979140000	0.264013000	6 2.426759000 0.789772000 -0.600399000
1 2.904033000	-2.028129000	0.214364000	1 1.603345000 1.474634000 -0.787952000
1 1.513366000	-2.225173000	1.285549000	6 3.665929000 1.264229000 -0.487719000
1 1.412425000	-2.745298000	-0.407131000	1 3.877959000 2.323224000 -0.580053000
17 2.120423000	1.110743000	1.085564000	1 4.512127000 0.610549000 -0.298039000
$NHSO_2C_6H_5$			$OSO_2C_6H_5$
E(RB3LYP) = -1067.42933381			E(RB3LYP) = -1087.29760571
6 1.708708000	-0.396705000	-0.471202000	6 -1.920817000 0.000268000 -0.460257000
6 2.381136000	-0.467050000	0.753582000	6 -2.597433000 -1.214604000 -0.456805000
6 2.066750000	0.581796000	-1.404593000	6 -2.597913000 1.214848000 -0.456138000
6 3.388344000	0.450748000	1.038158000	6 -3.990613000 -1.207885000 -0.453595000
6 3.095581000	1.476096000	-1.120902000	6 -3.991106000 1.207556000 -0.452940000
6 3.755127000	1.420411000	0.105220000	6 -4.687975000 -0.000300000 -0.451918000
1 2.112548000	-1.236787000	1.464418000	1 -2.035124000 -2.139470000 -0.453975000
1 3.904054000	0.392042000	1.990041000	1 -4.530080000 -2.147993000 -0.451940000
1 4.550936000	2.121019000	0.329384000	1 -5.771830000 -0.000522000 -0.449638000
1 3.371704000	2.223348000	-1.856149000	1 -4.530947000 2.147449000 -0.450762000
1 1.541659000	0.639625000	-2.352599000	1 -2.036022000 2.139967000 -0.452816000
7 0.707072000	-1.351661000	-0.806278000	8 -0.518288000 0.000570000 -0.538405000
1 0.467279000	-1.384055000	-1.790798000	16 0.342400000 -0.000034000 0.899255000
16 -0.696702000	-1.605808000	0.117631000	8 0.100840000 -1.264141000 1.578249000
8 -1.467662000	-2.557974000	-0.673892000	8 0.101146000 1.263676000 1.579099000
8 -0.264926000	-1.887743000	1.480227000	6 1.975175000 -0.000009000 0.173159000
6 -1.593609000	-0.044061000	0.143306000	6 2.592002000 1.218778000 -0.097903000
6 -2.525568000	0.217040000	-0.860574000	6 2.592302000 -1.218740000 -0.097257000
6 -1.333848000	0.876756000	1.156914000	1 2.089011000 2.146717000 0.142160000
1 -2.730270000	-0.531099000	-1.616373000	1 2.089501000 -2.146662000 0.143262000
1 -0.626056000	0.635838000	1.939134000	6 3.863053000 1.210554000 -0.666229000
6 -3.200437000	1.435044000	-0.852077000	6 3.863393000 -1.210478000 -0.665578000
6 -2.015232000	2.092047000	1.151657000	1 4.360419000 2.148711000 -0.882112000
1 -3.934161000	1.647512000	-1.620933000	1 4.360984000 -2.148634000 -0.880949000
1 -1.825316000	2.815799000	1.935621000	6 4.495025000 0.000027000 -0.949953000
6 -2.943575000	2.371295000	0.149762000	1 5.485541000 0.000051000 -1.390376000
1 -3.474217000	3.316561000	0.153909000	
CH_2CF_3			SeMe
E(RB3LYP) = -608.790247742			E(RB3LYP) = -2673.17974393
6 -0.558717000	-0.021351000	-0.547470000	6 -0.341690000 0.022037000 0.161340000
6 -1.247950000	-1.214229000	-0.310206000	6 -1.026853000 -1.196266000 0.169614000
6 -1.215723000	1.193348000	-0.328813000	6 -1.050120000 1.214290000 -0.009341000
6 -2.565984000	-1.194326000	0.140468000	6 -2.409964000 -1.220340000 -0.006061000
6 -2.533385000	1.215539000	0.122339000	6 -2.434264000 1.185700000 -0.180966000
6 -3.211824000	0.021161000	0.358585000	6 -3.115035000 -0.030430000 -0.182110000
1 -0.751469000	-2.164076000	-0.478051000	1 -0.479695000 -2.119533000 0.318872000
1 -3.087966000	-2.127631000	0.318796000	1 -2.935984000 -2.168658000 0.000256000
1 -4.238212000	0.037594000	0.707105000	1 -4.190909000 -0.051105000 -0.314545000
1 -3.029949000	2.165113000	0.286822000	1 -2.978328000 2.114552000 -0.312200000
1 -0.694058000	2.126811000	-0.510904000	1 -0.519974000 2.159171000 -0.004468000
6 0.875138000	-0.045403000	-1.029945000	34 1.583266000 0.063633000 0.430712000
1 1.079939000	-0.952296000	-1.603272000	6 2.132409000 -0.201148000 -1.451728000
6 1.905615000	-0.000730000	0.084288000	1 3.222623000 -0.196274000 -1.453639000
9 1.793992000	-1.045333000	0.934154000	1 1.766643000 -1.159302000 -1.815908000

9	3.162600000	-0.038427000	-0.423807000
9	1.815936000	1.126235000	0.825482000
1	1.085944000	0.808154000	-1.678423000

$SeCH_2CH=CH_2$
E(RB3LYP) = -2750.59406210

6	1.011553000	-0.074020000	-0.219580000
6	1.652950000	1.166255000	-0.292779000
6	1.707542000	-1.185792000	0.263586000
6	2.976357000	1.293781000	0.127458000
6	3.032790000	-1.054483000	0.678389000
6	3.667487000	0.184681000	0.613521000
1	1.120039000	2.025072000	-0.683444000
1	3.468222000	2.258466000	0.068481000
1	4.697725000	0.285203000	0.935992000
1	3.567347000	-1.921177000	1.051271000
1	1.213534000	-2.148865000	0.311187000
6	-1.749934000	0.277911000	0.879406000
1	-1.686359000	-0.555527000	1.577566000
6	-3.159366000	0.653339000	0.577606000
1	-3.298622000	1.572878000	0.013799000
34	-0.824871000	-0.266723000	-0.825622000
1	-1.176298000	1.123646000	1.258874000
6	-4.223729000	-0.066251000	0.933205000
1	-4.123760000	-0.995232000	1.486278000
1	-5.230105000	0.251590000	0.686267000

$PO(C_6H_4\text{-}4Me)_2$
E(RB3LYP) = -1190.43046307

6	-0.021318000	2.014511000	0.158108000
6	0.598779000	3.085045000	0.814552000
6	-0.624529000	2.227376000	-1.086360000
6	0.631794000	4.345241000	0.222901000
6	-0.588621000	3.490289000	-1.676441000
6	0.042304000	4.548397000	-1.024704000
1	1.035055000	2.925267000	1.794037000
1	1.111044000	5.170012000	0.738452000
1	0.065834000	5.530865000	-1.483047000
1	-1.061522000	3.648774000	-2.639323000
1	-1.137828000	1.416274000	-1.590269000
15	-0.000170000	0.391551000	1.014445000
8	0.000213000	0.535378000	2.510067000
6	1.478379000	-0.492342000	0.393975000
6	2.052142000	-0.269972000	-0.861622000
6	2.059089000	-1.440967000	1.244603000
1	1.638177000	0.478210000	-1.528292000
1	1.636802000	-1.599125000	2.230538000
6	3.172335000	-0.995358000	-1.262536000
6	3.177384000	-2.160093000	0.836148000
1	3.605429000	-0.809072000	-2.240256000
1	3.614266000	-2.891945000	1.508355000
6	3.752622000	-1.951545000	-0.423191000
6	4.986276000	-2.710937000	-0.845600000
1	5.891880000	-2.222022000	-0.470140000
1	4.980343000	-3.730523000	-0.452897000
1	5.069425000	-2.764740000	-1.933291000
6	-1.454011000	-0.536275000	0.400491000
6	-1.443306000	-1.329844000	-0.750613000
6	-2.635697000	-0.442415000	1.145897000
1	-0.533499000	-1.441760000	-1.329720000
1	-2.644923000	0.148023000	2.055146000
6	-2.596201000	-1.999811000	-1.155365000
6	-3.781490000	-1.115250000	0.734773000
1	-2.568912000	-2.612052000	-2.051317000
1	-4.688624000	-1.030534000	1.324978000
6	-3.783005000	-1.904185000	-0.421939000
6	-5.020076000	-2.659316000	-0.841582000
1	-5.081345000	-3.623312000	-0.324738000
1	-5.928047000	-2.101847000	-0.599598000
1	-5.019814000	-2.862079000	-1.914791000

1	1.757667000	0.614565000	-2.067057000

CH_2OCOMe
E(RB3LYP) = -499.583004675

6	0.847594000	-0.006506000	0.436477000
6	1.519924000	1.200990000	0.226001000
6	1.522306000	-1.206930000	0.195552000
6	2.839262000	1.210130000	-0.220863000
6	2.841690000	-1.202051000	-0.251308000
6	3.502421000	0.007540000	-0.461126000
1	1.006786000	2.138453000	0.414335000
1	3.350160000	2.153430000	-0.378009000
1	4.530393000	0.012896000	-0.805752000
1	3.354491000	-2.140031000	-0.432311000
1	1.011032000	-2.149886000	0.359968000
6	-0.581836000	-0.013722000	0.898651000
1	-0.816296000	-0.905766000	1.482368000
1	-0.817048000	0.860918000	1.507874000
8	-1.438076000	0.002945000	-0.279403000
6	-2.769880000	-0.001000000	-0.047251000
8	-3.252396000	-0.018919000	1.059185000
6	-3.542552000	0.022580000	-1.341815000
1	-3.255660000	-0.827110000	-1.965076000
1	-4.608809000	-0.012985000	-1.128406000
1	-3.304842000	0.931674000	-1.899157000

$CH=NNHCOC_6H_5$
E(RB3LYP) = -725.616079604

6	-3.079494000	-0.341607000	0.083263000
6	-3.562318000	0.942400000	-0.220763000
6	-3.996667000	-1.373213000	0.327066000
6	-4.929228000	1.177756000	-0.276847000
6	-5.367341000	-1.132733000	0.269528000
6	-5.837237000	0.143169000	-0.032719000
1	-2.852360000	1.738548000	-0.408251000
1	-5.293124000	2.171739000	-0.511745000
1	-6.903527000	0.333669000	-0.078167000
1	-6.065704000	-1.939698000	0.460233000
1	-3.633108000	-2.368562000	0.562732000
6	-1.646153000	-0.630799000	0.151110000
7	-0.759405000	0.266526000	-0.065167000
1	-1.364876000	-1.664039000	0.396757000
7	0.540422000	-0.111995000	0.009627000
1	0.764992000	-1.069183000	0.265396000
6	1.567390000	0.815907000	-0.099672000
8	1.377612000	2.008327000	-0.213931000
6	2.944449000	0.214867000	-0.045990000
6	3.240937000	-1.075995000	-0.500838000
6	3.977953000	1.019746000	0.446679000
1	2.468002000	-1.698784000	-0.937727000
1	3.741185000	2.025841000	0.770285000
6	4.547244000	-1.558419000	-0.446790000
6	5.278816000	0.532445000	0.510674000
1	4.769256000	-2.553781000	-0.814403000
1	6.070834000	1.160468000	0.902461000
6	5.566392000	-0.758394000	0.065795000
1	6.581959000	-1.135329000	0.109675000

$SCHMe_2$

E(RB3LYP) = -707.938253019

6	-0.099337000	-0.107213000	-0.442135000
6	-0.762151000	1.121092000	-0.513308000
6	-0.773196000	-1.236759000	0.030199000
6	-2.092524000	1.217621000	-0.108792000
6	-2.103846000	-1.134879000	0.432730000
6	-2.764170000	0.090991000	0.363973000
1	-0.236182000	1.992063000	-0.885487000
1	-2.603748000	2.171961000	-0.166661000
1	-3.799912000	0.167522000	0.675084000
1	-2.623723000	-2.013875000	0.796838000
1	-0.255816000	-2.187409000	0.078134000
16	1.597264000	-0.249091000	-1.017941000
6	2.546146000	0.103954000	0.438920000
6	2.122619000	0.403092000	1.665963000
1	3.606183000	0.047179000	0.208606000
1	2.843249000	0.593732000	2.452387000
1	1.072491000	0.466889000	1.922872000

E(RB3LYP) = -748.497993483

6	0.481293000	-0.000355000	-0.541564000
6	1.136742000	-1.207646000	-0.272015000
6	1.136332000	1.207336000	-0.272764000
6	2.416600000	-1.205621000	0.280147000
6	2.416174000	1.206100000	0.279418000
6	3.057356000	0.000434000	0.559631000
1	0.643407000	-2.143458000	-0.504815000
1	2.914823000	-2.146717000	0.485239000
1	4.054526000	0.000742000	0.985269000
1	2.914073000	2.147493000	0.483935000
1	0.642692000	2.142829000	-0.506198000
16	-1.146095000	-0.000896000	-1.307314000
6	-2.312772000	0.000095000	0.153274000
1	-3.273211000	-0.000169000	-0.372249000
6	-2.204940000	-1.270181000	0.995261000
1	-2.976577000	-1.269091000	1.772776000
1	-2.335688000	-2.165819000	0.384880000
1	-1.233587000	-1.331533000	1.492832000
6	-2.204753000	1.271385000	0.993725000
1	-2.335365000	2.166275000	0.382230000
1	-2.976377000	1.271360000	1.771254000
1	-1.233386000	1.333143000	1.491199000

PH_2

E(RB3LYP) = -574.280366764

6	0.487853000	-0.006306000	-0.013182000
6	-0.219228000	1.204029000	-0.005115000
6	-0.234854000	-1.205222000	-0.016627000
6	-1.611811000	1.212292000	0.004698000
6	-1.629833000	-1.198000000	0.003093000
6	-2.320795000	0.010712000	0.012560000
1	0.319391000	2.145292000	-0.006377000
1	-2.144260000	2.157116000	0.008364000
1	-3.404943000	0.018885000	0.021671000
1	-2.173320000	-2.136338000	0.003275000
1	0.295617000	-2.151371000	-0.039562000
15	2.340531000	-0.112384000	-0.033794000
1	2.579841000	0.408820000	1.271153000
1	2.591711000	1.138316000	-0.664184000

SiH_3

E(RB3LYP) = -523.029744770

6	2.350416000	0.000059000	0.010350000
6	1.650713000	1.205765000	0.003135000
6	1.651119000	-1.205409000	0.003157000
1	2.189766000	2.146860000	0.003780000
1	2.190140000	-2.146518000	0.003742000
6	0.257145000	1.203344000	-0.009639000
6	0.257098000	-1.203290000	-0.009709000
1	-0.269444000	2.152848000	-0.021940000
1	-0.269692000	-2.152540000	-0.021921000
6	-0.466224000	-0.000199000	-0.012759000
1	3.434773000	0.000283000	0.017692000
14	-2.348752000	-0.000090000	0.005627000
1	-2.855089000	-1.251463000	-0.615562000
1	-2.862560000	1.174358000	-0.746343000
1	-2.876970000	0.075806000	1.394556000

C_6H_4-3Cl

E(RB3LYP) = -923.045598369

6	-1.421907000	0.094274000	-0.031426000
6	-2.350940000	0.927029000	0.609372000
6	-1.885560000	-1.092967000	-0.616546000
6	-3.699271000	0.583851000	0.663036000
6	-3.234104000	-1.435572000	-0.563942000
6	-4.146681000	-0.598702000	0.076236000
1	-2.010322000	1.837200000	1.089914000
1	-4.399701000	1.237061000	1.171447000
1	-5.196528000	-0.865672000	0.117536000
1	-3.573295000	-2.353588000	-1.030758000
1	-1.188785000	-1.739904000	-1.137489000
6	0.016219000	0.463000000	-0.089257000
6	0.414753000	1.783492000	-0.341810000
6	1.006953000	-0.509737000	0.107668000
1	-0.336165000	2.543574000	-0.521246000
1	0.732962000	-1.532868000	0.330112000
6	1.763748000	2.120759000	-0.395948000
6	2.348934000	-0.154718000	0.048101000
1	2.056505000	3.144221000	-0.601282000
6	2.748110000	1.153994000	-0.201330000
1	3.799417000	1.407107000	-0.242788000
17	3.573788000	-1.393256000	0.308214000

C_6H_4-4Cl

E(RB3LYP) = -923.045603262

6	1.615224000	0.000001000	-0.000001000
6	2.335342000	1.127682000	-0.421317000
6	2.335342000	-1.127682000	0.421317000
6	3.727674000	1.127882000	-0.421224000
6	3.727673000	-1.127883000	0.421225000
6	4.430168000	0.000000000	0.000000000
1	1.800232000	2.001796000	-0.775065000
1	4.264345000	2.007271000	-0.759580000
1	5.514201000	-0.000001000	0.000001000
1	4.264344000	-2.007272000	0.759581000
1	1.800229000	-2.001795000	0.775064000
6	0.130378000	0.000000000	0.000000000
6	-0.593066000	1.125586000	0.419625000
6	-0.593065000	-1.125585000	-0.419626000
1	-0.062659000	2.002374000	0.772543000
1	-0.062659000	-2.002373000	-0.772544000
6	-1.984755000	1.133354000	0.422685000
6	-1.984755000	-1.133354000	-0.422685000
1	-2.530380000	2.005961000	0.758862000
1	-2.530380000	-2.005961000	-0.758862000
6	-2.671209000	0.000000000	0.000000000
17	-4.429823000	0.000000000	0.000000000

C6H4-3F

E(RB3LYP) = -562.691658258

6	-1.074185000	0.070143000	-0.024168000
6	-1.909931000	1.052238000	0.527471000
6	-1.665537000	-1.093108000	-0.538198000
6	-3.290656000	0.876762000	0.564296000

C_6H_4-4F

E(RB3LYP) = -562.691307808

6	-1.178473000	0.000000000	0.000000000
6	-1.899133000	1.125976000	0.425032000
6	-1.899133000	-1.125976000	-0.425032000
6	-3.291552000	1.126521000	0.424409000

6	-3.046336000	-1.268247000	-0.502551000
6	-3.864985000	-0.284186000	0.049221000
1	-1.472470000	1.948236000	0.952947000
1	-3.917734000	1.644385000	1.003963000
1	-4.940007000	-0.420823000	0.077490000
1	-3.483649000	-2.171183000	-0.913911000
1	-1.041155000	-1.855060000	-0.991020000
6	0.398840000	0.258550000	-0.063044000
6	0.960829000	1.504801000	-0.379265000
6	1.259870000	-0.812773000	0.215249000
1	0.311275000	2.337145000	-0.621715000
1	0.876702000	-1.787321000	0.490490000
6	2.342065000	1.675705000	-0.416438000
6	2.628773000	-0.612202000	0.169596000
1	2.758336000	2.643470000	-0.671619000
6	3.199294000	0.611991000	-0.139905000
1	4.276361000	0.718760000	-0.161366000
9	3.444900000	-1.659518000	0.451240000

6	-3.291551000	-1.126521000	-0.424409000
6	-3.994287000	0.000000000	0.000000000
1	-1.364165000	1.998859000	0.782090000
1	-3.828081000	2.005055000	0.765301000
1	-5.078327000	-0.000001000	0.000000000
1	-3.828081000	-2.005055000	-0.765301000
1	-1.364164000	-1.998858000	-0.782090000
6	0.306844000	0.000000000	0.000000000
6	1.028989000	1.125832000	-0.422996000
6	1.028988000	-1.125832000	0.422997000
1	0.496523000	2.000543000	-0.777740000
1	0.496522000	-2.000542000	0.777740000
6	2.421217000	1.134929000	-0.426197000
6	2.421217000	-1.134929000	0.426197000
1	2.981815000	1.998539000	-0.761750000
1	2.981815000	-1.998539000	0.761750000
6	3.091975000	0.000000000	0.000000000
9	4.448393000	0.000000000	0.000000000

C_6H_4-3Br
E(RB3LYP) = -3036.96527868

6	-2.038427000	0.100607000	-0.037258000
6	-2.366289000	-1.112585000	-0.659985000
6	-3.047742000	0.788452000	0.652138000
6	-3.660798000	-1.621176000	-0.595472000
6	-4.342090000	0.279403000	0.717424000
6	-4.654117000	-0.927577000	0.093807000
1	-1.608005000	-1.648936000	-1.219263000
1	-3.895358000	-2.556457000	-1.091398000
1	-5.661834000	-1.323915000	0.144471000
1	-5.105442000	0.821976000	1.263938000
1	-2.810463000	1.715703000	1.161304000
6	-0.657471000	0.644320000	-0.105776000
6	0.448278000	-0.207710000	0.034460000
6	-0.427072000	2.012068000	-0.311230000
1	0.300152000	-1.263439000	0.220345000
1	-1.268357000	2.681626000	-0.445180000
6	1.735707000	0.310419000	-0.034919000
6	0.869586000	2.512892000	-0.376054000
6	1.968596000	1.666550000	-0.238687000
1	2.978573000	2.051625000	-0.289406000
35	3.230567000	-0.877821000	0.170547000
1	1.031939000	3.571549000	-0.544652000

C_6H_4-4Br
E(RB3LYP) = -3036.96529250

6	2.350919000	0.000001000	-0.000001000
6	3.070985000	1.127515000	-0.421890000
6	3.070985000	-1.127515000	0.421890000
6	4.463294000	1.127663000	-0.421926000
6	4.463292000	-1.127664000	0.421927000
6	5.165733000	0.000000000	0.000000000
1	2.535860000	2.001530000	-0.775854000
1	4.999967000	2.006832000	-0.760822000
1	6.249761000	-0.000002000	0.000000000
1	4.999967000	-2.006832000	0.760823000
1	2.535857000	-2.001528000	0.775854000
6	0.866031000	0.000000000	0.000000000
6	0.142820000	1.125521000	0.420040000
6	0.142820000	-1.125520000	-0.420040000
1	0.673346000	2.002111000	0.773322000
1	0.673346000	-2.002111000	-0.773324000
6	-1.249229000	1.133309000	0.423112000
6	-1.249229000	-1.133309000	-0.423112000
1	-1.790538000	2.008137000	0.760230000
1	-1.790538000	-2.008137000	-0.760230000
6	-1.936237000	0.000000000	0.000000000
35	-3.854289000	0.000000000	0.000000000

N(Me)SO_2Me
E(RB3LYP) = -914.960470358

6	0.859703000	0.182599000	0.327583000
6	1.468789000	-0.991073000	0.772963000
6	1.599668000	1.112300000	-0.406539000
6	2.807633000	-1.235995000	0.482910000
6	2.943995000	0.870689000	-0.681676000
6	3.550365000	-0.303635000	-0.240396000
1	0.885292000	-1.706038000	1.339459000
1	3.272429000	-2.152673000	0.827541000
1	4.594916000	-0.492182000	-0.460379000
1	3.513090000	1.596758000	-1.251069000
1	1.128051000	2.017676000	-0.769018000
7	-0.521730000	0.422365000	0.670497000
6	-0.856241000	1.773046000	1.154992000
1	-0.839102000	2.532731000	0.368816000
1	-1.852554000	1.768040000	1.599723000
1	-0.137532000	2.030775000	1.933070000
16	-1.690566000	-0.249327000	-0.394642000
8	-2.343661000	0.818851000	-1.154364000
8	-1.061516000	-1.372175000	-1.080320000
6	-2.906597000	-0.910904000	0.760460000
1	-3.289360000	-0.106681000	1.386144000
1	-3.707915000	-1.324245000	0.148270000
1	-2.428618000	-1.687066000	1.353926000

C=CC_6H_5
E(RB3LYP) = -539.598697986

6	-2.028762000	0.000000000	0.000024000
6	-2.745808000	1.210924000	0.000018000
6	-2.745811000	-1.210928000	-0.000006000
6	-4.135984000	1.206286000	-0.000008000
6	-4.135984000	-1.206287000	-0.000018000
6	-4.836687000	0.000001000	-0.000023000
1	-2.200816000	2.147202000	0.000036000
1	-4.674856000	2.147116000	-0.000005000
1	-5.920683000	0.000001000	-0.000038000
1	-4.674860000	-2.147115000	-0.000039000
1	-2.200816000	-2.147204000	-0.000015000
6	-0.605457000	-0.000010000	0.000027000
6	0.605456000	0.000028000	0.000027000
6	2.028763000	0.000052000	0.000006000
6	2.745786000	-1.210913000	0.000019000
6	2.745836000	1.210941000	-0.000005000
1	2.200741000	-2.147161000	0.000043000
1	2.200886000	2.147247000	-0.000007000
6	4.135945000	-1.206313000	-0.000006000
6	4.136020000	1.206261000	-0.000016000
1	4.674804000	-2.147151000	0.000001000
1	4.674908000	2.147083000	-0.000033000
6	4.836689000	-0.000033000	-0.000023000
1	5.920683000	-0.000070000	-0.000037000

SCH=CHCl
E(RB3LYP) = -1167.55562749

CH=NOMe
E(RB3LYP) = -440.302913069

6	0.604172000	-0.699308000	-0.017739000
6	0.956431000	-0.129477000	1.208300000
6	1.459185000	-0.580554000	-1.114847000
6	2.151584000	0.574126000	1.324808000
6	2.665274000	0.106584000	-0.983555000
6	3.011904000	0.690431000	0.232523000
1	0.298634000	-0.231625000	2.062979000
1	2.416473000	1.023076000	2.275610000
1	3.944859000	1.233475000	0.330282000
1	3.325378000	0.195753000	-1.839033000
1	1.176858000	-1.012916000	-2.067455000
16	-0.866681000	-1.718704000	-0.200296000
6	-2.182015000	-0.782962000	0.529689000
6	-2.503909000	0.505659000	0.412160000
1	-2.844139000	-1.395628000	1.133332000
1	-3.357245000	0.923164000	0.929391000
17	-1.651158000	1.685705000	-0.539319000

6	0.552311000	-0.280759000	-0.000001000
6	0.938010000	1.070196000	-0.000006000
6	1.546928000	-1.268350000	0.000002000
6	2.283244000	1.413778000	-0.000002000
6	2.895821000	-0.920156000	0.000004000
6	3.267928000	0.421710000	0.000003000
1	0.173035000	1.836715000	-0.000012000
1	2.570176000	2.459479000	-0.000003000
1	4.316703000	0.696333000	0.000006000
1	3.653108000	-1.695907000	0.000006000
1	1.259624000	-2.314809000	0.000003000
6	-0.853272000	-0.696289000	0.000003000
7	-1.808654000	0.152285000	0.000001000
1	-1.074836000	-1.765330000	-0.000007000
8	-3.049937000	-0.482122000	-0.000017000
6	-4.089255000	0.494250000	0.000011000
1	-5.019292000	-0.074152000	-0.000038000
1	-4.034389000	1.121137000	0.894413000
1	-4.034339000	1.121241000	-0.894314000

S(SMe)
E(RB3LYP) = -1068.06837168

6	3.171324000	-0.575488000	-0.251260000
6	2.831843000	0.737669000	-0.569598000
6	2.209824000	-1.419177000	0.305285000
1	3.568736000	1.400367000	-1.009521000
1	2.466025000	-2.442100000	0.558344000
6	1.537969000	1.204253000	-0.342715000
6	0.920161000	-0.956263000	0.553424000
1	1.271135000	2.220134000	-0.612111000
1	0.178067000	-1.612595000	0.991269000
6	0.580496000	0.357675000	0.224108000
1	4.174850000	-0.940243000	-0.437316000
16	-1.027223000	1.087038000	0.589262000
16	-2.407531000	-0.468675000	0.357565000
6	-2.667966000	-0.503780000	-1.456266000
1	-3.416500000	-1.278756000	-1.636240000
1	-3.043410000	0.455806000	-1.809306000
1	-1.744761000	-0.765748000	-1.972205000

S(OMe)
E(RB3LYP) = -745.057725125

6	2.875490000	-0.484198000	-0.183371000
6	2.498987000	0.823006000	-0.486526000
6	1.924240000	-1.379917000	0.306351000
1	3.228699000	1.523235000	-0.877524000
1	2.210521000	-2.398314000	0.545109000
6	1.177688000	1.232068000	-0.315992000
6	0.608835000	-0.973104000	0.512251000
1	0.880884000	2.239411000	-0.587194000
1	-0.127235000	-1.659326000	0.912577000
6	0.233036000	0.335770000	0.194256000
1	3.900256000	-0.804516000	-0.331337000
16	-1.422281000	0.936109000	0.500820000
8	-2.341878000	-0.469055000	0.314860000
6	-2.690643000	-0.794382000	-1.040066000
1	-3.262878000	0.014708000	-1.502426000
1	-1.798015000	-1.003328000	-1.637498000
1	-3.306506000	-1.692639000	-0.975125000

CH_2Br
E(RB3LYP) = -2845.17832277

6	3.302680000	-0.572312000	-0.000045000
6	3.076333000	0.804352000	-0.000038000
6	2.217818000	-1.443168000	-0.000031000
1	3.912375000	1.494701000	-0.000049000
1	2.381136000	-2.515013000	-0.000036000
6	1.775642000	1.297238000	-0.000016000
6	0.912627000	-0.948063000	-0.000009000
1	1.612149000	2.370889000	-0.000011000
1	0.076569000	-1.635571000	0.000002000
6	0.676615000	0.425908000	-0.000002000
1	4.315382000	-0.959064000	-0.000062000
6	-0.693794000	1.065576000	0.000022000
1	-0.839017000	1.682121000	0.885555000
1	-0.839037000	1.682145000	-0.885491000
35	-2.235060000	-0.168497000	0.000023000

CH_2Cl
E(RB3LYP) = -731.257358982

6	2.685773000	-0.480160000	-0.000037000
6	2.382205000	0.881688000	-0.000031000
6	1.652104000	-1.411455000	-0.000022000
1	3.178097000	1.617953000	-0.000042000
1	1.876442000	-2.472233000	-0.000027000
6	1.055611000	1.299819000	-0.000010000
6	0.320673000	-0.991910000	-0.000001000
1	0.830489000	2.362348000	-0.000005000
1	-0.475666000	-1.724857000	0.000011000
6	0.009651000	0.366798000	0.000006000
1	3.718749000	-0.808938000	-0.000053000
6	-1.399650000	0.917659000	0.000031000
1	-1.574796000	1.529291000	0.884863000
1	-1.574815000	1.529322000	-0.884776000
17	-2.718630000	-0.325148000	0.000024000

$CH{=}NNHCONHNH_2$
E(RB3LYP) = -605.228768826

6	1.883614000	-0.343236000	0.000097000
6	2.173306000	1.029918000	0.066219000
6	2.942905000	-1.258842000	-0.063249000
6	3.491523000	1.465298000	0.068800000
6	4.264177000	-0.817795000	-0.060227000
6	4.542240000	0.545335000	0.005820000
1	1.354241000	1.736987000	0.113529000
1	3.705393000	2.527064000	0.119705000
1	5.569458000	0.891935000	0.008091000
1	5.073596000	-1.537334000	-0.109546000
1	2.729708000	-2.322019000	-0.115075000
6	0.507243000	-0.843541000	-0.005663000
7	-0.501652000	-0.059347000	0.055777000

$SiMe(OMe)_2$
E(RB3LYP) = -716.317036779

6	0.598008000	-0.154674000	-0.075662000
6	1.401323000	-1.084991000	0.602889000
6	1.240276000	0.941529000	-0.678039000
6	2.786362000	-0.933718000	0.673784000
6	2.622742000	1.100763000	-0.608505000
6	3.399814000	0.160459000	0.067467000
1	0.946028000	-1.942965000	1.087444000
1	3.384711000	-1.667374000	1.203351000
1	4.476214000	0.281191000	0.122167000
1	3.094114000	1.956503000	-1.079951000
1	0.650720000	1.685974000	-1.204910000
14	-1.277835000	-0.343261000	-0.228614000
6	-1.907599000	-1.606562000	1.018082000

1	0.380566000	-1.933098000	-0.064193000
7	-1.734521000	-0.622300000	0.061301000
1	-1.824820000	-1.625501000	-0.080252000
6	-2.872531000	0.174902000	-0.040310000
8	-2.869257000	1.376312000	-0.184082000
7	-4.039183000	-0.589340000	0.025544000
1	-4.022320000	-1.394214000	0.636846000
7	-5.280122000	0.083175000	0.073825000
1	-5.583024000	0.251129000	-0.880980000
1	-5.135267000	0.996996000	0.500474000

$SiFMe_2$
E(RB3LYP) = -701.053952943

6	0.414547000	0.004240000	0.000042000
6	1.117026000	1.221021000	-0.000294000
6	1.159508000	-1.185792000	0.000320000
6	2.509961000	1.250126000	-0.000373000
6	2.553751000	-1.160948000	0.000243000
6	3.231227000	0.056640000	-0.000106000
1	0.577560000	2.164404000	-0.000475000
1	3.032141000	2.200727000	-0.000633000
1	4.315488000	0.076810000	-0.000162000
1	3.110283000	-2.091903000	0.000477000
1	0.643308000	-2.139778000	0.000628000
14	-1.462929000	-0.036441000	0.000014000
9	-1.869956000	-1.630409000	0.001512000
6	-2.188008000	0.715636000	-1.553101000
1	-1.807078000	0.210449000	-2.444501000
1	-3.279046000	0.636634000	-1.555142000
1	-1.928750000	1.775915000	-1.634356000
6	-2.187866000	0.718576000	1.551779000
1	-3.278907000	0.639711000	1.554167000
1	-1.806814000	0.214920000	2.443998000
1	-1.928453000	1.778966000	1.631132000

$N{=}NC_6H_3$-5Me,2-OH
E(RB3LYP) = -687.454829289

6	-1.801469000	0.304377000	-0.723190000
6	-3.027510000	0.718973000	-0.193106000
6	-1.437666000	-1.046038000	-0.670082000
6	-3.851761000	-0.196726000	0.450150000
6	-2.286320000	-1.963164000	-0.055209000
6	-3.485000000	-1.541948000	0.519406000
1	-3.309671000	1.760824000	-0.286788000
1	-4.791128000	0.133369000	0.879292000
1	-4.138290000	-2.260275000	1.001464000
1	-2.010433000	-3.011475000	-0.028188000
1	-0.513165000	-1.379058000	-1.123271000
7	-1.063481000	1.284880000	-1.458786000
7	0.171106000	1.421094000	-1.396866000
6	1.010885000	0.730915000	-0.457084000
6	2.158294000	0.118917000	-0.969886000
6	0.851381000	0.830271000	0.934381000
1	2.287134000	0.120153000	-2.047413000
6	3.107373000	-0.485412000	-0.146660000
6	1.809183000	0.255939000	1.768766000
1	1.689442000	0.331483000	2.846020000
6	2.913033000	-0.403253000	1.236742000
1	3.641566000	-0.841248000	1.910796000
8	-0.227018000	1.518271000	1.414590000
1	-0.207428000	1.522699000	2.377098000
6	4.301692000	-1.202888000	-0.729151000
1	4.096620000	-2.270473000	-0.864849000

1	-1.626187000	-1.353485000	2.044352000
1	-2.999382000	-1.663838000	0.974022000
1	-1.518852000	-2.607193000	0.805077000
6	-1.774736000	-0.806036000	-1.974506000
1	-2.862666000	-0.875945000	-2.062855000
1	-1.427056000	-0.055678000	-2.689538000
1	-1.345237000	-1.769872000	-2.263490000
8	-1.992933000	1.149509000	0.027207000
6	-1.908544000	1.918751000	1.217045000
1	-2.388551000	1.408877000	2.061394000
1	-0.867848000	2.136969000	1.485152000
1	-2.428734000	2.863298000	1.045390000

$CH_2NHCOMe$
E(RB3LYP) = -479.709017596

6	0.863957000	-0.397965000	0.058189000
6	1.124151000	0.947906000	0.338259000
6	1.935261000	-1.243292000	-0.240282000
6	2.429195000	1.433540000	0.326942000
6	3.243560000	-0.760039000	-0.248646000
6	3.493666000	0.580275000	0.035411000
1	0.299296000	1.617176000	0.556778000
1	2.615839000	2.479197000	0.544834000
1	4.509091000	0.959760000	0.024403000
1	4.063656000	-1.428997000	-0.484322000
1	1.746222000	-2.287192000	-0.470584000
6	-0.550089000	-0.948289000	0.108400000
1	-0.557065000	-1.955820000	-0.326323000
1	-0.858511000	-1.056108000	1.150480000
7	-1.511247000	-0.084264000	-0.564429000
1	-1.265800000	0.248189000	-1.488321000
6	-2.810317000	0.184373000	-0.215636000
8	-3.534552000	0.830957000	-0.956946000
6	-3.298179000	-0.336998000	1.125473000
1	-3.277769000	-1.429912000	1.158914000
1	-2.684665000	0.035238000	1.950609000
1	-4.322375000	0.003593000	1.261445000

$P(C_6H_5)_2$
E(RB3LYP) = -1036.49864718

6	-1.140882000	1.219459000	-0.406929000
6	-2.402648000	1.392558000	-0.995432000
6	-0.812188000	1.993646000	0.712264000
6	-3.320420000	2.295136000	-0.464446000
6	-1.726828000	2.907440000	1.236545000
6	-2.983404000	3.057669000	0.653877000
1	-2.666152000	0.817744000	-1.877736000
1	-4.292900000	2.411714000	-0.930097000
1	-3.693009000	3.768112000	1.063072000
1	-1.455144000	3.500863000	2.102909000
1	0.160947000	1.887081000	1.176536000
15	0.000664000	0.000822000	-1.214662000
6	1.626557000	0.377071000	-0.404421000
6	2.425984000	1.355636000	-1.013638000
6	2.112905000	-0.269011000	0.739049000
1	2.074535000	1.850445000	-1.913492000
1	1.519885000	-1.037974000	1.220044000
6	3.666322000	1.697701000	-0.480701000
6	3.360694000	0.064995000	1.265738000
1	4.268518000	2.459967000	-0.962796000
1	3.723811000	-0.446885000	2.150403000
6	4.138154000	1.050826000	0.661205000
1	5.107823000	1.308767000	1.072239000
6	-0.486159000	-1.596355000	-0.406690000
6	-0.015565000	-2.777003000	-1.000292000
6	-1.309211000	-1.696139000	0.721552000
1	0.606501000	-2.719440000	-1.887931000
1	-1.694448000	-0.798393000	1.190072000
6	-0.337689000	-4.022336000	-0.466550000
6	-1.642595000	-2.943821000	1.248623000
1	0.040124000	-4.923924000	-0.936160000
1	-2.283100000	-3.003304000	2.122003000

NHCSMe			
E(RB3LYP) = -763.340684770			
6	0.607830000	0.368938000	0.003392000
6	0.951056000	-0.987227000	-0.026634000
6	1.627072000	1.335405000	0.026029000
6	2.297200000	-1.351248000	-0.032625000
6	2.962428000	0.957553000	0.019363000
6	3.307111000	-0.394112000	-0.009747000
1	0.175565000	-1.736110000	-0.043293000
1	2.550901000	-2.405111000	-0.055824000
1	4.348517000	-0.693584000	-0.014632000
1	3.733149000	1.719514000	0.037139000
1	1.367290000	2.390087000	0.048943000
7	-0.715486000	0.870397000	0.010224000
1	-0.737446000	1.881315000	0.012222000
6	-1.946524000	0.294130000	0.012926000
16	-2.303735000	-1.328311000	0.030116000
6	-3.060445000	1.322857000	-0.045251000
1	-3.313732000	1.522459000	-1.091584000
1	-3.950005000	0.932261000	0.443338000
1	-2.780447000	2.271584000	0.425548000
OCH_2Cl			
E(RB3LYP) = -806.493112407			
6	2.914232000	0.681519000	-0.101959000
6	1.808037000	1.453239000	0.237860000
6	2.749215000	-0.684064000	-0.341581000
1	1.920421000	2.516947000	0.414280000
1	3.602098000	-1.296710000	-0.610717000
6	0.538685000	0.880282000	0.344365000
6	1.493753000	-1.270033000	-0.236741000
1	-0.311835000	1.506745000	0.575792000
1	1.345655000	-2.327805000	-0.416745000
6	0.393402000	-0.486115000	0.112408000
1	3.893740000	1.137013000	-0.185353000
8	-0.807334000	-1.170711000	0.199702000
6	-1.922552000	-0.553992000	0.720635000
1	-2.635173000	-1.333115000	0.969553000
1	-1.697347000	0.082789000	1.575615000
17	-2.794559000	0.526754000	-0.489997000
$Si(OMe)_3$			
E(RB3LYP) = -866.856288445			
6	-0.952851000	0.087304000	-0.155297000
6	-1.671364000	-0.960176000	-0.753799000
6	-1.680311000	1.132212000	0.438424000
6	-3.065240000	-0.963669000	-0.762057000
6	-3.073689000	1.132696000	0.432270000
6	-3.768166000	0.083222000	-0.168052000
1	-1.135331000	-1.777541000	-1.224759000
1	-3.602017000	-1.780169000	-1.232736000
1	-4.852714000	0.082401000	-0.173944000
1	-3.617275000	1.950596000	0.892623000
1	-1.152719000	1.958203000	0.904424000
14	0.912316000	0.101568000	-0.163322000
8	1.504271000	0.818081000	1.208282000
6	1.284976000	0.492960000	2.572900000
1	0.239830000	0.225848000	2.766902000
1	1.926567000	-0.337297000	2.886584000
1	1.535954000	1.369179000	3.174191000
8	1.446482000	0.991237000	-1.430001000
6	2.807268000	1.249469000	-1.765374000
1	3.321023000	1.765427000	-0.948272000
1	3.336314000	0.319436000	-1.995222000
1	2.813208000	1.889421000	-2.649060000
8	1.509366000	-1.430586000	-0.363891000
6	1.493642000	-2.525924000	0.538438000
1	2.261916000	-2.408602000	1.310073000
1	0.517800000	-2.643259000	1.024352000
1	1.708485000	-3.434012000	-0.028488000
6	-1.155061000	-4.109014000	0.660100000
1	-1.415144000	-5.077843000	1.071725000
OS(=O)CH3			
E(RB3LYP) = -820.289779357			
6	-0.621703000	-0.274809000	0.283599000
6	-1.105559000	1.029832000	0.380729000
6	-1.469964000	-1.332001000	-0.040472000
6	-2.456987000	1.270364000	0.138469000
6	-2.821135000	-1.079915000	-0.265918000
6	-3.317224000	0.220857000	-0.181445000
1	-0.430192000	1.833604000	0.645462000
1	-2.838270000	2.282674000	0.210039000
1	-4.368231000	0.414650000	-0.361525000
1	-3.485155000	-1.900811000	-0.512111000
1	-1.064416000	-2.334656000	-0.103516000
8	0.707676000	-0.567599000	0.563774000
16	1.896972000	0.109342000	-0.510201000
8	2.184671000	1.516528000	-0.128018000
6	3.191340000	-0.901360000	0.275504000
1	4.138485000	-0.595012000	-0.168741000
1	3.175267000	-0.684887000	1.343268000
1	2.989584000	-1.954265000	0.081503000
CH_2F			
E(RB3LYP) = -370.901456299			
6	2.290751000	-0.321781000	-0.000035000
6	1.862061000	1.006059000	-0.000026000
6	1.349731000	-1.347978000	-0.000023000
1	2.586944000	1.812341000	-0.000035000
1	1.674843000	-2.382412000	-0.000030000
6	0.501669000	1.299597000	-0.000005000
6	-0.014695000	-1.055256000	-0.000002000
1	0.176536000	2.336079000	0.000002000
1	-0.746069000	-1.853395000	0.000007000
6	-0.446344000	0.270804000	0.000007000
1	3.350108000	-0.551903000	-0.000051000
6	-1.912305000	0.626545000	0.000030000
1	-2.178211000	1.205759000	0.889626000
1	-2.178239000	1.205762000	-0.889555000
9	-2.719014000	-0.515575000	0.000040000
$OCOC_6H_5$			
E(RB3LYP) = -652.039162040			
6	1.809295000	-0.261457000	-0.090617000
6	2.535271000	-1.056580000	0.787061000
6	2.438125000	0.640901000	-0.940900000
6	3.924346000	-0.943679000	0.815623000
6	3.826296000	0.748108000	-0.901115000
6	4.571991000	-0.041507000	-0.026034000
1	2.012062000	-1.751803000	1.432313000
1	4.497425000	-1.561568000	1.497362000
1	5.651920000	0.046240000	-0.001538000
1	4.325156000	1.451639000	-1.557754000
1	1.850761000	1.251112000	-1.614846000
8	0.425697000	-0.460739000	-0.148104000
6	-0.416177000	0.563538000	0.196975000
8	-0.031548000	1.642780000	0.566792000
6	-1.845014000	0.166155000	0.061015000
6	-2.818818000	1.108364000	0.413125000
6	-2.234337000	-1.096859000	-0.401008000
1	-2.499568000	2.080427000	0.768050000
1	-1.479833000	-1.823004000	-0.672577000
6	-4.168010000	0.790363000	0.305407000
6	-3.586365000	-1.409741000	-0.508913000
1	-4.919036000	1.522080000	0.580049000
1	-3.885759000	-2.387766000	-0.867832000
6	-4.553367000	-0.468834000	-0.156046000
1	-5.605720000	-0.716321000	-0.240161000

$SiFMe_2$			
E(RB3LYP) = -701.053952943			
6	0.414547000	0.004240000	0.000042000
6	1.117026000	1.221021000	-0.000294000
6	1.159508000	-1.185792000	0.000320000
6	2.509961000	1.250126000	-0.000373000
6	2.553751000	-1.160948000	0.000243000
6	3.231227000	0.056640000	-0.000106000
1	0.577560000	2.164404000	-0.000475000
1	3.032141000	2.200727000	-0.000633000
1	4.315488000	0.076810000	-0.000162000
1	3.110283000	-2.091903000	0.000477000
1	0.643308000	-2.139778000	0.000628000
14	-1.462929000	-0.036441000	0.000014000
9	-1.869956000	-1.630409000	0.001512000
6	-2.188008000	0.715636000	-1.553101000
1	-1.807078000	0.210449000	-2.444501000
1	-3.279046000	0.636634000	-1.555142000
1	-1.928750000	1.775915000	-1.634356000
6	-2.187866000	0.718576000	1.551779000
1	-3.278907000	0.639711000	1.554167000
1	-1.806814000	0.214920000	2.443998000
1	-1.928453000	1.778966000	1.631132000

$NHCOCH_2Cl$			
E(RB3LYP) = -900.011572818			
6	-0.960768000	-0.112788000	0.000048000
6	-1.591763000	-1.364212000	0.000169000
6	-1.734369000	1.053788000	-0.000094000
6	-2.978536000	-1.451228000	0.000073000
6	-3.124235000	0.948950000	-0.000205000
6	-3.754752000	-0.292769000	-0.000101000
1	-0.992637000	-2.269622000	0.000328000
1	-3.451460000	-2.426632000	0.000180000
1	-4.836323000	-0.359073000	-0.000163000
1	-3.716958000	1.856816000	-0.000329000
1	-1.250129000	2.018078000	-0.000062000
7	0.453964000	-0.106653000	0.000023000
1	0.896661000	-1.015972000	-0.000111000
6	1.301600000	0.955169000	0.000074000
8	0.984627000	2.132306000	0.000424000
6	2.802870000	0.652089000	-0.000334000
1	3.239538000	1.104736000	-0.887919000
1	3.240106000	1.105296000	0.886670000
17	3.297421000	-1.097618000	0.000004000

NHEt			
E(RB3LYP) = -366.328858962			
6	0.080596000	-0.227728000	0.055825000
6	1.001320000	-1.292802000	0.005780000
6	0.583287000	1.084427000	0.051214000
6	2.366876000	-1.051435000	-0.041177000
6	1.958386000	1.312462000	0.008621000
6	2.861980000	0.255113000	-0.038111000
1	0.631495000	-2.313887000	0.011488000
1	3.052302000	-1.891344000	-0.079612000
1	3.928729000	0.440561000	-0.073777000
1	2.320998000	2.334902000	0.008111000
1	-0.093320000	1.928641000	0.082855000
7	-1.280025000	-0.502305000	0.142818000
1	-1.535626000	-1.430796000	-0.160362000
6	-2.298401000	0.509706000	-0.096970000
1	-2.200451000	1.295352000	0.659639000
1	-2.160958000	0.992878000	-1.077162000
6	-3.692746000	-0.102144000	-0.010959000
1	-3.864932000	-0.546024000	0.972863000
1	-3.830571000	-0.880999000	-0.768183000
1	-4.455272000	0.661262000	-0.180926000

$CH_2OC_6H_5$			
E(RB3LYP) = -577.974868305			
6	-1.589358000	0.552966000	-0.385040000
6	-1.758117000	0.570687000	1.001771000
6	-2.475891000	-0.192194000	-1.166913000
6	-2.795193000	-0.146767000	1.594266000
6	-3.518500000	-0.904183000	-0.575976000
6	-3.679918000	-0.883907000	0.808075000
1	-1.069145000	1.140726000	1.613952000
1	-2.912653000	-0.129896000	2.672145000
1	-4.486108000	-1.441690000	1.270993000
1	-4.197995000	-1.479351000	-1.195080000
1	-2.350833000	-0.219582000	-2.245474000
6	-0.505029000	1.377796000	-1.051273000
1	-0.228902000	0.942627000	-2.018266000
1	-0.875182000	2.388810000	-1.241136000
8	0.656006000	1.583938000	-0.249250000
6	1.588102000	0.585468000	-0.134777000
6	2.746850000	0.926247000	0.572990000
6	1.450608000	-0.698117000	-0.668039000
1	2.831559000	1.928076000	0.976875000
1	0.552296000	-0.991432000	-1.193449000
6	3.760329000	-0.008405000	0.738511000
6	2.480526000	-1.626175000	-0.495682000
1	4.654457000	0.267847000	1.286402000
1	2.364916000	-2.621648000	-0.910096000
6	3.635866000	-1.292656000	0.202816000
1	4.427889000	-2.020544000	0.332759000

$P(CMe_3)_2$			
E(RB3LYP) = -888.864290718			
6	-1.185939000	-0.027958000	-0.250030000
6	-1.672298000	-0.224939000	1.052436000
6	-2.126588000	0.131518000	-1.279032000
6	-3.040772000	-0.263244000	1.312484000
6	-3.497324000	0.102678000	-1.022338000
6	-3.958758000	-0.097375000	0.275875000
1	-0.984040000	-0.349712000	1.877340000
1	-3.390558000	-0.420381000	2.327265000
1	-5.023371000	-0.125905000	0.480064000
1	-4.201055000	0.230724000	-1.837630000
1	-1.774686000	0.275517000	-2.294900000
15	0.600039000	0.029733000	-0.780608000
6	1.393297000	-1.557794000	-0.024009000
6	2.731214000	-1.766881000	-0.768625000
1	3.462902000	-0.990460000	-0.538550000
1	2.585494000	-1.780713000	-1.851502000
1	3.166779000	-2.728224000	-0.472724000

P(N(Pr)2C6H4-3F			
E(RB3LYP) = -1195.96794843			
6	-0.097180000	1.729960000	0.658095000
6	0.875691000	2.466742000	-0.028494000
6	-1.262259000	2.391278000	1.077511000
6	0.679280000	3.818200000	-0.311444000
6	-1.457292000	3.740815000	0.796203000
6	-0.487859000	4.459679000	0.096812000
1	1.791707000	1.976891000	-0.335281000
1	1.442072000	4.369723000	-0.850560000
1	-0.640312000	5.510272000	-0.123320000
1	-2.367129000	4.231603000	1.124128000
1	-2.025942000	1.850555000	1.626659000
15	0.220505000	-0.002168000	1.220077000
6	-1.369095000	-0.856381000	0.721751000
6	-1.705085000	-2.008659000	1.446433000
6	-2.202947000	-0.457057000	-0.330919000
1	-1.080017000	-2.316264000	2.277740000
1	-2.003302000	0.435746000	-0.910376000

6	1.253634000	1.623803000	0.085623000
6	2.780089000	1.692508000	-0.109972000
1	3.064931000	1.517609000	-1.151281000
1	3.308994000	0.970304000	0.515817000
1	3.139171000	2.689664000	0.169526000
6	0.456473000	-2.721454000	-0.410830000
1	0.228256000	-2.715620000	-1.480813000
1	0.948039000	-3.673750000	-0.181188000
1	-0.488285000	-2.689714000	0.134707000
6	1.656877000	-1.603709000	1.489741000
1	0.743454000	-1.500490000	2.077990000
1	2.097455000	-2.574190000	1.750281000
1	2.362586000	-0.835141000	1.809817000
6	0.917207000	1.825180000	1.572265000
1	-0.160054000	1.872760000	1.739203000
1	1.330768000	1.043028000	2.209856000
1	1.340310000	2.779098000	1.910916000
6	0.608311000	2.776211000	-0.715578000
1	0.859872000	2.719132000	-1.777646000
1	-0.480999000	2.772451000	-0.623813000
1	0.970921000	3.736755000	-0.331672000

6	-2.836660000	-2.755773000	1.121558000
6	-3.322560000	-1.215331000	-0.629682000
1	-3.083994000	-3.642804000	1.693748000
6	-3.662769000	-2.362439000	0.071215000
1	-4.552188000	-2.917377000	-0.200161000
9	-4.122913000	-0.818838000	-1.653157000
7	1.404752000	-0.568683000	0.101947000
6	2.401698000	-1.507651000	0.652701000
1	2.017594000	-1.953331000	1.576665000
1	2.528381000	-2.338382000	-0.052292000
6	3.761625000	-0.864627000	0.951778000
1	3.608925000	-0.050914000	1.668791000
1	4.154904000	-0.404100000	0.040263000
6	4.771575000	-1.871605000	1.510001000
1	4.961585000	-2.682610000	0.799284000
1	4.409765000	-2.324227000	2.438746000
1	5.729541000	-1.392522000	1.727897000
6	1.114455000	-0.716019000	-1.331398000
1	0.696872000	-1.715173000	-1.535678000
1	0.336789000	0.004290000	-1.593963000
6	2.316455000	-0.479433000	-2.254302000
1	3.115063000	-1.190793000	-2.020795000
1	2.723701000	0.519270000	-2.065529000
6	1.932890000	-0.616756000	-3.731292000
1	1.160539000	0.106603000	-4.010420000
1	1.545102000	-1.616302000	-3.950946000
1	2.795957000	-0.446979000	-4.380133000

$P(Et)_2$
E(RB3LYP) = -731.585029693

6	0.839105000	0.003839000	0.229440000
6	1.317384000	-0.266551000	-1.061021000
6	1.771903000	0.241588000	1.246803000
6	2.684844000	-0.299066000	-1.324329000
6	3.142168000	0.216431000	0.985243000
6	3.601411000	-0.055476000	-0.301054000
1	0.621524000	-0.457231000	-1.870972000
1	3.036185000	-0.513106000	-2.328063000
1	4.665824000	-0.080133000	-0.506646000
1	3.848114000	0.404069000	1.786924000
1	1.419476000	0.443904000	2.252893000
15	-0.964872000	0.070434000	0.671419000
6	-1.620769000	-1.413123000	-0.281730000
1	-1.659863000	-1.193228000	-1.354408000
1	-0.882055000	-2.208709000	-0.148188000
6	-2.988825000	-1.899394000	0.216606000
1	-3.765065000	-1.140043000	0.095128000
1	-2.949918000	-2.160952000	1.277225000
1	-3.307657000	-2.787797000	-0.336973000
6	-1.489850000	1.499489000	-0.429913000
1	-0.896350000	2.357103000	-0.098266000
1	-1.199515000	1.296708000	-1.466659000
6	-2.982773000	1.837690000	-0.345479000
1	-3.293373000	2.015777000	0.687849000
1	-3.605298000	1.034146000	-0.746921000
1	-3.206532000	2.740414000	-0.921604000

$Si(Me)_2OMe$
E(RB3LYP) = -716.317036779

6	0.598008000	-0.154674000	-0.075662000
6	1.401323000	-1.084991000	0.602889000
6	1.240276000	0.941529000	-0.678039000
6	2.786362000	-0.933718000	0.673784000
6	2.622742000	1.100763000	-0.608505000
6	3.399814000	0.160459000	0.067467000
1	0.946028000	-1.942965000	1.087444000
1	3.384711000	-1.667374000	1.203351000
1	4.476214000	0.281191000	0.122167000
1	3.094114000	1.956503000	-1.079951000
1	0.650720000	1.685974000	-1.204910000
14	-1.277835000	-0.343261000	-0.228614000
6	-1.907599000	-1.606562000	1.018082000
1	-1.626187000	-1.353485000	2.044352000
1	-2.999382000	-1.663838000	0.974022000
1	-1.518852000	-2.607193000	0.805077000
6	-1.774736000	-0.806036000	-1.974506000
1	-2.862666000	-0.875945000	-2.062855000
1	-1.427056000	-0.055678000	-2.689538000
1	-1.345237000	-1.769872000	-2.263490000
8	-1.992933000	1.149509000	0.027207000
6	-1.908544000	1.918751000	1.217045000
1	-2.388551000	1.408877000	2.061394000
1	-0.867848000	2.136969000	1.485152000
1	-2.428734000	2.863298000	1.045390000

GeH_3
E(RB3LYP) = -2310.51529419

6	-2.941802000	0.000146000	0.008472000
6	-2.242265000	-1.205390000	0.002522000
6	-2.242003000	1.205527000	0.002708000
1	-2.781172000	-2.146634000	0.002898000
1	-2.780707000	2.146887000	0.003278000
6	-0.847739000	-1.203884000	-0.007654000
6	-0.847478000	1.203663000	-0.007542000
1	-0.320250000	-2.152600000	-0.017863000
1	-0.319675000	2.152191000	-0.017591000
6	-0.130535000	-0.000214000	-0.010342000
1	-4.026117000	0.000253000	0.014306000
1	2.372561000	-0.013829000	1.443282000
1	2.351846000	-1.252198000	-0.722711000

OCH_2F
E(RB3LYP) = -446.142314962

6	2.598713000	0.529568000	0.020521000
6	1.533148000	1.422463000	0.085139000
6	2.342048000	-0.839270000	-0.074548000
1	1.720068000	2.488747000	0.144224000
1	3.163667000	-1.544468000	-0.128902000
6	0.214034000	0.965831000	0.055287000
6	1.034176000	-1.310470000	-0.094318000
1	-0.605941000	1.671489000	0.061943000
1	0.814746000	-2.369125000	-0.160904000
6	-0.024772000	-0.405651000	-0.021886000
1	3.618907000	0.894215000	0.037499000
8	-1.292951000	-0.963717000	-0.055596000
6	-2.355350000	-0.246647000	0.455320000

1	2.350338000	1.264892000	-0.702536000
32	1.833253000	0.000061000	0.002123000

1	-3.175906000	-0.948787000	0.593646000
1	-2.090542000	0.277939000	1.377926000
9	-2.794820000	0.727198000	-0.448195000

OCOMe

E(RB3LYP) = -460.248599472

6	0.195214000	0.000094000	-0.449611000
6	0.859114000	-1.211785000	-0.283246000
6	0.859220000	1.211866000	-0.283093000
6	2.204568000	-1.206527000	0.080334000
6	2.204700000	1.206422000	0.080494000
6	2.878411000	-0.000087000	0.267039000
1	0.325671000	-2.140060000	-0.450975000
1	2.727141000	-2.147295000	0.210420000
1	3.925320000	-0.000168000	0.546875000
1	2.727342000	2.147137000	0.210689000
1	0.325917000	2.140247000	-0.450666000
8	-1.128555000	0.000168000	-0.883522000
6	-2.193761000	0.000018000	-0.008061000
8	-3.299724000	-0.000017000	-0.466939000
6	-1.876312000	-0.000102000	1.468834000
1	-1.288079000	0.878587000	1.742086000
1	-2.815515000	0.000059000	2.017118000
1	-1.288489000	-0.879095000	1.741999000

C=CMe

E(RB3LYP) = -347.812391216

6	-0.034022000	-0.000042000	-0.000499000
6	-0.751107000	-1.209502000	-0.000208000
6	-0.751035000	1.209468000	-0.000086000
6	-2.141977000	-1.205675000	0.000476000
6	-2.141899000	1.205728000	0.000598000
6	-2.843067000	0.000046000	0.000908000
1	-0.206128000	-2.145890000	-0.000397000
1	-2.680401000	-2.146867000	0.000774000
1	-3.927131000	0.000083000	0.001509000
1	-2.680270000	2.146950000	0.000996000
1	-0.205992000	2.145820000	-0.000179000
6	1.394305000	-0.000061000	-0.001295000
6	2.601472000	-0.000025000	-0.001387000
6	4.058059000	0.000026000	0.000382000
1	4.451135000	-0.008509000	1.021797000
1	4.452278000	-0.879911000	-0.516330000
1	4.452136000	0.888548000	-0.501507000

$CH=CH_2$

E(RB3LYP) = -309.730778836

6	-0.514207000	-0.220563000	-0.000271000
6	-0.009021000	1.090529000	-0.000348000
6	0.406180000	-1.279737000	-0.000082000
6	1.359984000	1.327628000	-0.000049000
6	1.779084000	-1.044346000	0.000183000
6	2.262401000	0.261551000	0.000270000
1	-0.691230000	1.932597000	-0.000824000
1	1.727885000	2.347766000	-0.000091000
1	3.329927000	0.450228000	0.000500000
1	2.469235000	-1.880689000	0.000296000
1	0.036460000	-2.300170000	-0.000177000
6	-1.953511000	-0.528934000	-0.000264000
6	-2.973340000	0.335198000	0.000448000
1	-2.833428000	1.410452000	0.001027000
1	-3.997861000	-0.016491000	0.000546000
1	-2.186405000	-1.591643000	-0.000601000

$OCH=CH_2$

E(RB3LYP) = -384.962058853

6	-0.035805000	-0.270562000	-0.062906000
6	0.368929000	1.063246000	-0.118334000
6	0.907142000	-1.295765000	0.023130000
6	1.730348000	1.364933000	-0.064818000
6	2.260717000	-0.980453000	0.066285000
6	2.679646000	0.350815000	0.027988000
1	-0.363087000	1.854204000	-0.224728000
1	2.044940000	2.401591000	-0.109182000
1	3.735223000	0.592552000	0.064942000
1	2.991575000	-1.778303000	0.134873000
1	0.562930000	-2.322285000	0.057061000
8	-1.356988000	-0.656298000	-0.136680000
6	-2.325538000	0.187937000	0.342027000
1	-2.005497000	0.841905000	1.148145000
6	-3.572515000	0.146865000	-0.112924000
1	-4.328299000	0.773756000	0.339734000
1	-3.859432000	-0.515125000	-0.920091000

OC_6H_4-4F

E(RB3LYP) = -637.920464911

6	-1.643798000	0.483589000	-0.019958000
6	-1.690718000	-0.711172000	0.698535000
6	-2.794940000	1.000335000	-0.614292000
6	-2.902949000	-1.391538000	0.808502000
6	-3.998801000	0.313107000	-0.491220000
6	-4.059311000	-0.887311000	0.217013000
1	-0.797153000	-1.101812000	1.168669000
1	-2.939528000	-2.319318000	1.368510000
1	-4.997338000	-1.421896000	0.308307000
1	-4.892001000	0.716878000	-0.954504000
1	-2.728984000	1.933511000	-1.160436000
8	-0.501329000	1.253598000	-0.130616000
6	0.749384000	0.664927000	-0.087658000
6	1.693872000	1.220497000	0.771641000
6	1.095277000	-0.385345000	-0.938513000
1	1.403319000	2.041925000	1.414703000
1	0.356492000	-0.801128000	-1.612412000
6	2.995722000	0.723266000	0.789318000
6	2.392055000	-0.892013000	-0.918167000
1	3.749291000	1.138630000	1.446539000
1	2.688755000	-1.705311000	-1.568607000
6	3.318138000	-0.327436000	-0.053941000
9	4.582688000	-0.819523000	-0.037045000

$CH=CHC_6H_5$

E(RB3LYP) = -540.846679662

6	1.938430000	0.186166000	0.000072000
6	2.491356000	-1.107828000	0.000240000
6	2.826573000	1.275555000	-0.000140000
6	3.867307000	-1.297377000	0.000171000
6	4.205710000	1.086590000	-0.000211000
6	4.734154000	-0.202102000	-0.000060000
1	1.841702000	-1.975074000	0.000452000
1	4.268848000	-2.304778000	0.000317000
1	5.807366000	-0.354523000	-0.000104000
1	4.866765000	1.946162000	-0.000370000
1	2.424134000	2.283485000	-0.000256000
6	0.497157000	0.453197000	0.000109000
6	-0.497176000	-0.453240000	-0.000112000
1	-0.241235000	-1.509578000	-0.000389000
1	0.241231000	1.509536000	0.000310000
6	-1.938452000	-0.186193000	-0.000052000
6	-2.491333000	1.107826000	0.000116000
6	-2.826596000	-1.275573000	-0.000171000
1	-1.841630000	1.975034000	0.000248000
1	-2.424163000	-2.283506000	-0.000276000
6	-3.867274000	1.297408000	0.000154000
6	-4.205726000	-1.086570000	-0.000136000
1	-4.268804000	2.304814000	0.000290000
1	-4.866839000	-1.946100000	-0.000214000
6	-4.734134000	0.202139000	0.000015000
1	-5.807350000	0.354546000	0.000031000

Si(C6H5)3
E(RB3LYP) = -1216.37888624

6	-2.795875000	-1.736566000	-3.381361000
6	-3.093020000	-0.515981000	-2.776511000
6	-1.675209000	-2.454695000	-2.969503000
1	-3.967790000	0.045692000	-3.086387000
1	-1.441894000	-3.408804000	-3.429826000
6	-2.269826000	-0.018805000	-1.767657000
6	-0.853270000	-1.951409000	-1.961248000
1	-2.529258000	0.925592000	-1.299227000
1	0.009246000	-2.530797000	-1.649638000
6	-1.129153000	-0.722089000	-1.341415000
1	-3.436498000	-2.127020000	-4.164553000
14	0.000223000	-0.000110000	-0.000787000
6	1.109167000	-1.358901000	0.719164000
6	0.824083000	-1.976179000	1.947675000
6	2.243401000	-1.801169000	0.015348000
6	1.630973000	-2.997177000	2.449713000
6	3.051651000	-2.822555000	0.511385000
6	2.745669000	-3.424390000	1.731303000
1	-0.033820000	-1.652770000	2.527419000
1	2.509679000	-1.335732000	-0.928628000
1	1.390705000	-3.455341000	3.403142000
1	3.921802000	-3.144551000	-0.050648000
1	3.374889000	-4.217192000	2.120886000
6	-1.094228000	0.737262000	1.360514000
6	-2.239495000	0.051709000	1.803085000
6	-0.788071000	1.959775000	1.979349000
6	-3.037770000	0.559066000	2.826734000
6	-1.585039000	2.473395000	3.002351000
6	-2.710643000	1.772652000	3.430300000
1	-2.522035000	-0.886905000	1.336431000
1	0.078756000	2.525997000	1.655505000
1	-3.916580000	0.010896000	3.149115000
1	-1.328365000	3.421995000	3.461643000
1	-3.332038000	2.171239000	4.224809000
6	1.114746000	1.343410000	-0.740155000
6	0.817605000	1.964896000	-1.963614000
6	2.265924000	1.770696000	-0.054893000
1	-0.053531000	1.652517000	-2.529518000
1	2.541574000	1.301230000	0.884372000
6	1.629047000	2.975918000	-2.478330000
6	3.078741000	2.782265000	-0.563460000
1	1.379056000	3.437672000	-3.427506000
1	3.961854000	3.092997000	-0.015481000
6	2.760313000	3.388958000	-1.777747000
1	3.392805000	4.174294000	-2.177050000

SiMe(C6H5)2
E(RB3LYP) = -1024.60262850

6	2.865628000	-3.403359000	-0.748632000
6	3.280336000	-2.546408000	0.270526000
6	1.594614000	-3.254872000	-1.299119000
1	4.268242000	-2.656526000	0.704827000
1	1.264606000	-3.918644000	-2.091078000
6	2.425172000	-1.547763000	0.732059000
6	0.742405000	-2.253967000	-0.831614000
1	2.772570000	-0.890870000	1.523855000
1	-0.245828000	-2.157210000	-1.268802000
6	1.138069000	-1.378595000	0.192263000
1	3.529112000	-4.181742000	-1.109408000
14	0.000340000	-0.000642000	0.824248000
6	0.000466000	-0.001041000	2.713446000
1	-0.649842000	0.784331000	3.108396000
1	-0.354329000	-0.957226000	3.107962000
1	1.006101000	0.169330000	3.107791000
6	-1.761960000	-0.295715000	0.191889000
6	-2.311817000	0.468741000	-0.849432000
6	-2.561707000	-1.309977000	0.747251000
6	-3.604022000	0.231336000	-1.318728000
6	-3.853565000	-1.551164000	0.283906000
6	-4.378008000	-0.779128000	-0.752359000
1	-1.726018000	1.263681000	-1.298733000
1	-2.174789000	-1.926400000	1.553174000
1	-4.005733000	0.836490000	-2.124403000
1	-4.450573000	-2.339157000	0.730389000
1	-5.383507000	-0.964145000	-1.114322000
6	0.624254000	1.673919000	0.191829000
6	1.573808000	1.770333000	-0.837905000
6	0.132163000	2.872744000	0.737359000
6	2.013367000	3.009349000	-1.305026000
6	0.568149000	4.113157000	0.276079000
6	1.511803000	4.183734000	-0.748362000
1	1.980357000	0.867069000	-1.280437000
1	-0.605353000	2.844628000	1.533886000
1	2.748288000	3.056272000	-2.101511000
1	0.173513000	5.023243000	0.715060000
1	1.853490000	5.147924000	-1.108700000

$NHCSNH_2$
E(RB3LYP) = -779.398995865

6	-3.238749000	0.408663000	0.045862000
6	-2.876554000	-0.875609000	0.446245000
6	-2.262577000	1.269103000	-0.454376000
1	-3.622361000	-1.557654000	0.838258000
1	-2.533996000	2.268527000	-0.774993000
6	-1.550060000	-1.287286000	0.357499000
6	-0.935210000	0.862957000	-0.559841000
1	-1.268331000	-2.282537000	0.687341000
1	-0.185691000	1.534664000	-0.950940000
6	-0.572546000	-0.420727000	-0.143451000
1	-4.269375000	0.734918000	0.121523000
7	0.747426000	-0.923504000	-0.271490000
1	0.794196000	-1.931984000	-0.328312000
6	1.948752000	-0.296680000	-0.061301000
16	2.174985000	1.259343000	0.497158000
7	3.018028000	-1.124249000	-0.310988000
1	3.920603000	-0.678546000	-0.260886000
1	2.928684000	-1.865143000	-0.992991000

CH(OH)Me
E(RB3LYP) = -386.205298708

6	-0.148829000	-0.163711000	0.117527000
6	0.719921000	-1.247065000	0.273722000
6	0.390978000	1.099944000	-0.148942000
6	2.099466000	-1.078723000	0.157509000
6	1.768585000	1.271827000	-0.260404000
6	2.627300000	0.182517000	-0.109980000
1	0.314538000	-2.230846000	0.490754000
1	2.759945000	-1.929594000	0.283074000
1	3.699633000	0.317761000	-0.195777000
1	2.173654000	2.256910000	-0.464733000
1	-0.274743000	1.948542000	-0.259585000
6	-1.653357000	-0.363641000	0.208459000
1	-1.838705000	-1.327649000	0.702336000
8	-2.290863000	0.681246000	0.956766000
1	-1.868257000	0.739560000	1.820419000
6	-2.328589000	-0.380643000	-1.160282000
1	-2.170125000	0.571358000	-1.672700000
1	-1.918591000	-1.181098000	-1.780174000
1	-3.403288000	-0.537941000	-1.043401000

SH
E(RB3LYP) = -630.525260845

NHCHO
E(RB3LYP) = -401.057990644

6	2.295469000	0.004407000	0.000026000
6	1.593327000	-1.199959000	0.000018000
6	1.589382000	1.205759000	0.000018000
1	2.129201000	-2.142568000	0.000024000
1	2.122149000	2.150253000	0.000023000
6	0.201212000	-1.207270000	0.000004000
6	0.196411000	1.209170000	0.000003000
1	-0.334435000	-2.150053000	-0.000002000
1	-0.337998000	2.152545000	-0.000004000
6	-0.506115000	0.000005000	-0.000003000
1	3.379017000	0.006715000	0.000037000
1	-2.512755000	1.245580000	-0.000044000
16	-2.291456000	-0.083446000	-0.000026000

6	-0.098247000	-0.389156000	0.000000000
6	0.961711000	-1.306311000	0.000131000
6	0.175268000	0.984375000	-0.000005000
6	2.277739000	-0.860320000	0.000253000
6	1.500755000	1.415024000	0.000120000
6	2.556055000	0.506097000	0.000246000
1	0.752649000	-2.371975000	0.000138000
1	3.085712000	-1.583071000	0.000353000
1	3.581706000	0.855624000	0.000341000
1	1.703976000	2.480043000	0.000115000
1	-0.639437000	1.692295000	-0.000102000
7	-1.411460000	-0.911298000	-0.000120000
1	-1.478693000	-1.919168000	-0.000114000
6	-2.612103000	-0.250726000	-0.000226000
8	-2.779844000	0.949875000	-0.000324000
1	-3.454010000	-0.967557000	-0.000411000

$S(NMe_2)_3$

E(RB3LYP) = -1033.58762649

6	4.254503000	-0.254606000	-0.405519000
6	3.690324000	0.766776000	0.360259000
6	3.426230000	-1.153478000	-1.075073000
1	4.332225000	1.474886000	0.874422000
1	3.856457000	-1.942613000	-1.682527000
6	2.304276000	0.881038000	0.469980000
6	2.039977000	-1.023777000	-0.977869000
1	1.866927000	1.675621000	1.063833000
1	1.396900000	-1.702762000	-1.533817000
6	1.470067000	-0.020632000	-0.193201000
1	5.332222000	-0.341934000	-0.487250000
16	-0.475874000	-0.034040000	-0.303248000
7	-0.740766000	-0.913730000	1.165184000
1	0.340107000	0.342466000	2.457836000
6	0.162952000	-0.719093000	2.297701000
1	1.127054000	-1.230196000	2.184186000
1	-0.346093000	-1.119158000	3.180008000
1	-1.573432000	-2.725558000	1.772298000
6	-1.049524000	-2.321570000	0.901911000
1	-0.146676000	-2.923879000	0.727261000
1	-1.709682000	-2.394704000	0.039399000
7	-0.570770000	1.618994000	0.287358000
1	-1.960359000	1.260072000	1.824534000
6	-1.782258000	1.978469000	1.027269000
1	-2.666550000	2.032391000	0.385548000
1	-1.584544000	2.955832000	1.478190000
1	-0.216355000	3.536815000	-0.439081000
6	-0.354007000	2.531597000	-0.845857000
1	-1.205280000	2.538994000	-1.538792000
1	0.553590000	2.259427000	-1.386351000
7	-2.533135000	-0.131674000	-0.743329000
1	-3.453451000	-0.273599000	1.139962000
6	-3.648167000	-0.511935000	0.091542000
1	-3.877321000	-1.596615000	0.042556000
1	-4.581004000	0.006825000	-0.195587000
1	-3.436752000	-0.116474000	-2.665571000
6	-2.661422000	-0.644041000	-2.083973000
1	-2.921406000	-1.723637000	-2.125715000
1	-1.717608000	-0.515182000	-2.630881000

C(OMe)3

E(RB3LYP) = -615.307755645

6	0.631155000	0.118389000	-0.019328000
6	1.289977000	1.319230000	0.259635000
6	1.387081000	-1.017712000	-0.320246000
6	2.680818000	1.382303000	0.231185000
6	2.780138000	-0.954275000	-0.346910000
6	3.430719000	0.246075000	-0.071724000
1	0.705764000	2.200090000	0.490594000
1	3.180239000	2.320894000	0.444788000
1	4.513624000	0.296929000	-0.094073000
1	3.354371000	-1.843050000	-0.584159000
1	0.884217000	-1.951651000	-0.540727000
6	-0.894905000	0.036020000	0.089214000
8	-1.311619000	-0.235746000	1.404527000
6	-0.999820000	-1.513093000	1.956843000
1	-1.430190000	-2.318767000	1.358190000
1	0.081823000	-1.654717000	2.048032000
1	-1.444896000	-1.517770000	2.951597000
8	-1.440004000	-0.994996000	-0.717862000
6	-1.345203000	-0.807166000	-2.130063000
1	-1.915509000	0.067250000	-2.454309000
1	-0.307149000	-0.692944000	-2.456221000
1	-1.769062000	-1.705495000	-2.579006000
8	-1.408807000	1.284684000	-0.251086000
6	-2.808860000	1.478954000	-0.012047000
1	-3.401351000	0.666599000	-0.440677000
1	-3.015129000	1.550773000	1.056711000
1	-3.059918000	2.417976000	-0.504718000

SiH(Me)2

E(RB3LYP) = -601.709533760

6	-0.227981000	-0.169738000	-0.000436000
6	-0.780723000	1.122559000	0.001914000
6	-1.116515000	-1.256567000	-0.002312000
6	-2.159617000	1.322095000	0.002402000
6	-2.498275000	-1.064134000	-0.001846000
6	-3.022621000	0.226488000	0.000521000
1	-0.130125000	1.992860000	0.003376000
1	-2.561095000	2.329800000	0.004236000
1	-4.096321000	0.378976000	0.000885000
1	-3.163753000	-1.920776000	-0.003342000
1	-0.726286000	-2.269602000	-0.004180000

CH_2OMe

E(RB3LYP) = -386.185992263

6	0.036018000	0.222268000	0.429676000
6	-0.469073000	-1.082151000	0.380957000
6	-0.803312000	1.282668000	0.082141000
6	-1.785258000	-1.317256000	-0.006423000
6	-2.125680000	1.051287000	-0.298743000
6	-2.619113000	-0.250126000	-0.344761000
1	0.180889000	-1.910917000	0.639731000
1	-2.163956000	-2.332919000	-0.041582000
1	-3.644750000	-0.434080000	-0.644471000
1	-2.764970000	1.885638000	-0.565478000
1	-0.421131000	2.298659000	0.107520000

14	1.643111000	-0.438232000	-0.001020000
6	2.425549000	0.303027000	1.548656000
1	2.002086000	-0.142014000	2.453110000
1	3.506167000	0.130974000	1.562360000
1	2.259862000	1.383385000	1.600146000
6	2.425590000	0.310505000	-1.547081000
1	3.506219000	0.138582000	-1.561542000
1	2.002213000	-0.130234000	-2.453679000
1	2.259855000	1.391092000	-1.593435000
1	1.865185000	-1.913209000	-0.004559000

CH2CH(OH)Me
E(RB3LYP) = -425.529943966

6	-0.372818000	-0.133287000	-0.476350000
6	-1.026095000	-1.243894000	0.073102000
6	-1.094939000	1.057020000	-0.613282000
6	-2.356217000	-1.166331000	0.479601000
6	-2.427106000	1.139527000	-0.209969000
6	-3.062059000	0.028091000	0.340276000
1	-0.490604000	-2.182879000	0.176000000
1	-2.843316000	-2.039457000	0.899745000
1	-4.098369000	0.089607000	0.652730000
1	-2.968858000	2.071463000	-0.328711000
1	-0.609919000	1.927115000	-1.043782000
6	1.078385000	-0.221399000	-0.892204000
1	1.233333000	-1.148286000	-1.458676000
1	1.334697000	0.604874000	-1.562047000
6	2.079551000	-0.213893000	0.284112000
1	1.813139000	-1.027667000	0.973703000
6	2.102959000	1.097730000	1.052784000
1	2.840152000	1.045848000	1.856489000
1	2.380016000	1.920670000	0.387562000
1	1.124993000	1.311946000	1.488262000
8	3.413483000	-0.421614000	-0.200064000
1	3.446895000	-1.261700000	-0.669188000

Si(Me)2OSiMe3
E(RB3LYP) = -1085.79446118

6	1.632162000	0.237244000	0.060291000
6	2.559961000	0.365862000	-0.985196000
6	1.865626000	-0.770075000	1.013097000
6	3.671740000	-0.472328000	-1.078630000
6	2.972013000	-1.611982000	0.925991000
6	3.879763000	-1.463778000	-0.122616000
1	2.418757000	1.128573000	-1.744353000
1	4.372817000	-0.351745000	-1.897618000
1	4.742784000	-2.116816000	-0.192940000
1	3.127834000	-2.381813000	1.674275000
1	1.170913000	-0.905765000	1.836888000
14	0.123417000	1.367575000	0.225962000
6	0.013387000	2.541449000	-1.239409000
1	-0.043727000	2.003576000	-2.190078000
1	-0.886817000	3.157506000	-1.152426000
1	0.871863000	3.218579000	-1.284715000
6	0.220166000	2.333111000	1.834380000
1	-0.658679000	2.973325000	1.957126000
1	0.266545000	1.661623000	2.696474000
1	1.110211000	2.969265000	1.859719000
8	-1.243946000	0.437127000	0.288526000
14	-2.370710000	-0.709162000	-0.129045000
6	-4.070242000	-0.012436000	0.274072000
1	-4.270535000	0.896411000	-0.301237000
1	-4.860844000	-0.733939000	0.043506000
1	-4.148603000	0.241029000	1.335465000
6	-2.237585000	-1.081949000	-1.970293000
1	-1.246295000	-1.467795000	-2.226719000
1	-2.974213000	-1.832796000	-2.274525000
1	-2.413979000	-0.184217000	-2.570767000
6	-2.045457000	-2.266754000	0.873947000
1	-2.780650000	-3.045351000	0.645705000

6	1.462523000	0.471598000	0.882723000
1	1.723479000	1.527502000	0.719049000
1	1.556314000	0.269170000	1.953329000
8	2.423339000	-0.374092000	0.265261000
6	2.639555000	-0.086595000	-1.106805000
1	1.732662000	-0.237218000	-1.704765000
1	2.986555000	0.947337000	-1.244023000
1	3.414235000	-0.770592000	-1.454004000

C6H5
E(RB3LYP) = -463.422745775

6	0.742819000	-0.000004000	0.000002000
6	1.463809000	-1.126924000	0.422225000
6	1.463809000	1.126924000	-0.422227000
6	2.856251000	-1.127246000	0.422499000
6	2.856244000	1.127250000	-0.422501000
6	3.559096000	0.000001000	0.000000000
1	0.928293000	-2.000763000	0.775917000
1	3.392854000	-2.006441000	0.761779000
1	4.643195000	0.000006000	-0.000001000
1	3.392852000	2.006442000	-0.761780000
1	0.928283000	2.000757000	-0.775919000
6	-0.742820000	-0.000001000	0.000001000
6	-1.463809000	-1.126931000	-0.422221000
6	-1.463807000	1.126929000	0.422222000
1	-0.928286000	-2.000768000	-0.775912000
1	-0.928283000	2.000765000	0.775915000
6	-2.856249000	-1.127252000	-0.422500000
6	-2.856247000	1.127253000	0.422499000
1	-3.392858000	-2.006446000	-0.761782000
1	-3.392855000	2.006448000	0.761782000
6	-3.559095000	0.000001000	0.000000000
1	-4.643198000	0.000002000	-0.000001000

$Si(OEt)_3$
E(RB3LYP) = -984.850103219

6	-1.381915000	0.234086000	0.090565000
6	-2.221500000	-0.886713000	-0.026161000
6	-1.980962000	1.488769000	0.287824000
6	-3.607222000	-0.762102000	0.059450000
6	-3.366227000	1.617720000	0.370403000
6	-4.181567000	0.492278000	0.258441000
1	-1.790377000	-1.869583000	-0.190741000
1	-4.237266000	-1.640216000	-0.032486000
1	-5.259589000	0.592574000	0.322975000
1	-3.810169000	2.595938000	0.520616000
1	-1.354147000	2.369528000	0.369603000
14	0.473540000	0.034442000	0.031420000
8	1.094448000	1.528766000	-0.273029000
6	2.464640000	1.928225000	-0.143071000
1	3.074811000	1.376731000	-0.868500000
1	2.822939000	1.671134000	0.858956000
6	2.571163000	3.422872000	-0.387541000
1	1.977176000	3.975716000	0.344207000
1	2.210274000	3.677869000	-1.386924000
1	3.612916000	3.746410000	-0.302228000
8	1.141863000	-0.489096000	1.444836000
6	1.090627000	-1.803255000	2.005545000
1	1.427404000	-2.531212000	1.259360000
1	0.053837000	-2.045333000	2.271148000
6	1.973658000	-1.851540000	3.240175000
1	1.637369000	-1.123204000	3.981892000
1	3.010565000	-1.625144000	2.980210000
1	1.939290000	-2.847758000	3.691458000
8	0.900620000	-1.103965000	-1.096394000
6	0.610736000	-1.066766000	-2.497261000
1	1.089141000	-0.187939000	-2.945838000
1	-0.470874000	-0.967867000	-2.649817000
6	1.125052000	-2.339427000	-3.146892000
1	0.640862000	-3.217211000	-2.711901000

	1 2.203822000 -2.435963000 -3.002820000 1 0.918117000 -2.327180000 -4.221210000
$SeCH=CH_2$ E(RB3LYP) = -2711.26783386 6 0.616291000 -0.169350000 -0.064969000 6 1.010582000 1.138916000 -0.358857000 6 1.574234000 -1.120990000 0.295369000 6 2.356048000 1.492950000 -0.273742000 6 2.920577000 -0.764459000 0.355040000 6 3.314717000 0.543356000 0.077482000 1 0.274930000 1.875417000 -0.659460000 1 2.655202000 2.511231000 -0.496695000 1 4.360994000 0.820849000 0.134051000 1 3.658818000 -1.508262000 0.633580000 1 1.269564000 -2.132154000 0.539642000 6 -2.066866000 0.798917000 0.603219000 1 -1.514757000 1.221419000 1.436161000 6 -3.262742000 1.256048000 0.239385000 1 -3.733658000 2.063414000 0.790370000 1 -3.812593000 0.844116000 -0.599605000 34 -1.233399000 -0.727893000 -0.206341000	PMe_2 E(RB3LYP) = -652.941730810 6 -0.159491000 -0.088284000 -0.204377000 6 -0.714811000 1.126541000 0.217149000 6 -1.026383000 -1.164562000 -0.446193000 6 -2.091445000 1.258070000 0.400642000 6 -2.399531000 -1.040420000 -0.248708000 6 -2.937266000 0.174557000 0.174135000 1 -0.079598000 1.984142000 0.404115000 1 -2.501564000 2.209230000 0.722819000 1 -4.006939000 0.277610000 0.318341000 1 -3.050202000 -1.887426000 -0.436988000 1 -0.621196000 -2.106964000 -0.802137000 15 1.649427000 -0.383481000 -0.498518000 6 2.363860000 1.331592000 -0.425029000 1 3.449340000 1.244850000 -0.516491000 1 2.005762000 1.920455000 -1.272194000 1 2.138887000 1.862112000 0.504345000 6 2.153788000 -0.991314000 1.193960000 1 1.690205000 -1.961540000 1.383145000 1 3.238309000 -1.127984000 1.214150000 1 1.863266000 -0.299343000 1.989197000
$C(Me)=CH_2$ E(RB3LYP) = -349.056608095 6 -0.206253712 0.051524401 -0.012868532 6 0.567793430 1.195833160 0.241394786 6 0.469777103 -1.157759386 -0.237743463 6 1.957743092 1.139144518 0.243823180 6 1.861790027 -1.215549775 -0.238939403 6 2.613304802 -0.067387018 -0.000262472 1 0.071796123 2.133630497 0.462144250 1 2.530761618 2.036772539 0.449037588 1 3.696449137 -0.112913196 0.005126140 1 2.358708631 -2.161096913 -0.426341705 1 -0.092673753 -2.063354171 -0.430174536 6 -1.693333859 0.119100336 -0.035267018 6 -2.339369849 1.213076930 -0.459926468 1 -3.422477671 1.261696148 -0.455089259 6 -2.458255339 -1.097975586 0.430744989 1 -3.529155571 -0.892095473 0.466276066 1 -2.307648848 -1.949140258 -0.241187877 1 -2.130431091 -1.414336267 1.425839522 1 -1.814504336 2.080789503 -0.841370130	CH_2CH_2COOH E(RB3LYP) = -499.593122219 6 0.637792000 0.457721000 0.571952000 6 1.508864000 1.250006000 -0.185615000 6 0.976151000 -0.882049000 0.788203000 6 2.681840000 0.718822000 -0.716116000 6 2.150026000 -1.417926000 0.259362000 6 3.005981000 -0.619452000 -0.495639000 1 1.270137000 2.295439000 -0.357148000 1 3.344851000 1.349847000 -1.297672000 1 3.919917000 -1.033958000 -0.905836000 1 2.396273000 -2.458420000 0.440476000 1 0.315039000 -1.508652000 1.377423000 6 -0.644113000 1.039117000 1.130695000 1 -0.987799000 0.439113000 1.975653000 1 -0.449845000 2.045832000 1.513153000 6 -1.782286000 1.150652000 0.092243000 1 -2.640383000 1.650819000 0.556713000 1 -1.476361000 1.749590000 -0.766131000 6 -2.289785000 -0.165610000 -0.451118000 8 -2.495094000 -0.414105000 -1.611828000 8 -2.539799000 -1.067212000 0.535959000 1 -2.879505000 -1.866761000 0.106509000
$Si(Me)(OSiMe_3)_2$ E(RB3LYP) = -1530.54439919 6 -1.509851000 -1.262293000 0.263811000 6 -2.824365000 -0.986713000 0.677632000 6 -1.317804000 -2.321863000 -0.635771000 6 -3.903339000 -1.734863000 0.210671000 6 -2.393227000 -3.074754000 -1.107132000 6 -3.688565000 -2.782192000 -0.684848000 1 -3.015162000 -0.174928000 1.373929000 1 -4.909160000 -1.503041000 0.544334000 1 -4.526159000 -3.366624000 -1.049858000 1 -2.220552000 -3.888841000 -1.803091000 1 -0.313480000 -2.557267000 -0.970338000 14 -0.065865000 -0.251781000 0.923721000 8 1.291837000 -0.810327000 0.179833000 8 -0.298678000 1.342504000 0.582567000 6 0.108294000 -0.410830000 2.779082000 1 0.282302000 -1.451249000 3.067790000 1 0.946568000 0.190977000 3.142170000 1 -0.795113000 -0.067081000 3.290893000 14 2.904072000 -0.859920000 -0.228711000 6 3.413811000 -2.667279000 -0.312325000 1 2.824709000 -3.209867000 -1.057702000	$OPO(C_3H_7)_2$ E(RB3LYP) = -960.782475784 6 1.854552000 -0.647659000 -0.214861000 6 2.370045000 -0.410288000 1.059640000 6 2.677345000 -0.607287000 -1.339289000 6 3.727375000 -0.119293000 1.193778000 6 4.032406000 -0.324315000 -1.187304000 6 4.562276000 -0.076127000 0.078623000 1 1.714712000 -0.455257000 1.920032000 1 4.132042000 0.066967000 2.182297000 1 5.616803000 0.145334000 0.194602000 1 4.673474000 -0.297405000 -2.061328000 1 2.248476000 -0.806458000 -2.314039000 8 0.523736000 -0.986921000 -0.421465000 15 -0.773246000 -0.250726000 0.296724000 8 -0.761365000 -0.224719000 1.788594000 6 -0.762658000 1.419222000 -0.459337000 1 0.260856000 1.788883000 -0.329105000 1 -0.925588000 1.313472000 -1.537403000 6 -1.757096000 2.409794000 0.166256000 1 -1.603163000 2.427867000 1.248351000 1 -2.782270000 2.060173000 0.007244000 6 -1.607181000 3.821256000 -0.410068000

1	4.469201000	-2.768210000	-0.585546000
1	3.269896000	-3.163763000	0.651863000
6	3.121502000	-0.041098000	-1.907779000
1	2.823835000	1.011244000	-1.877839000
1	4.165856000	-0.081740000	-2.233933000
1	2.514809000	-0.538240000	-2.670425000
6	3.913228000	0.048946000	1.074842000
1	4.978767000	0.039336000	0.823079000
1	3.602819000	1.094796000	1.159814000
1	3.802549000	-0.414376000	2.059895000
14	-0.745289000	2.672216000	-0.314273000
6	-0.966445000	2.174843000	-2.114908000
1	-1.731470000	1.399731000	-2.218186000
1	-1.272591000	3.030373000	-2.725840000
1	-0.035730000	1.782127000	-2.535148000
6	-2.358698000	3.337480000	0.386849000
1	-2.253080000	3.588460000	1.446585000
1	-2.676564000	4.243171000	-0.139849000
1	-3.162187000	2.600759000	0.294208000
6	0.617602000	3.956925000	-0.145078000
1	0.367279000	4.874254000	-0.687824000
1	0.777269000	4.222929000	0.904047000
1	1.566424000	3.584582000	-0.542826000

1	-1.780646000	3.832840000	-1.490699000
1	-0.602162000	4.214936000	-0.230458000
1	-2.321408000	4.509738000	0.049407000
6	-2.077006000	-1.295478000	-0.439423000
1	-2.059282000	-1.166592000	-1.526367000
1	-1.756712000	-2.322741000	-0.235786000
6	-3.481050000	-1.053271000	0.135959000
1	-3.818783000	-0.042109000	-0.113625000
1	-3.430898000	-1.101805000	1.227180000
6	-4.501135000	-2.069501000	-0.386907000
1	-4.215093000	-3.089841000	-0.114468000
1	-4.584804000	-2.027352000	-1.477372000
1	-5.493083000	-1.878950000	0.031243000

$Si(C_6H_5)Me_2$
E(RB3LYP) = -832.825415420

6	1.543461000	0.075288000	-0.034585000
6	2.768160000	0.468638000	0.530388000
6	1.498917000	-1.171206000	-0.681490000
6	3.900046000	-0.341925000	0.450570000
6	2.626693000	-1.986366000	-0.765746000
6	3.831462000	-1.572704000	-0.199588000
1	2.847425000	1.420728000	1.045787000
1	4.832751000	-0.014331000	0.897263000
1	4.709592000	-2.206108000	-0.262225000
1	2.564516000	-2.944991000	-1.269697000
1	0.567855000	-1.517037000	-1.119506000
14	0.026019000	1.212671000	0.008163000
6	0.018024000	2.307063000	-1.531802000
1	-0.021175000	1.712448000	-2.448813000
1	-0.830716000	2.997919000	-1.535894000
1	0.932772000	2.906188000	-1.568955000
6	0.089104000	2.304255000	1.549132000
1	-0.794317000	2.948374000	1.590568000
1	0.108350000	1.707296000	2.465135000
1	0.970379000	2.952847000	1.552578000
6	-1.543580000	0.150698000	0.048867000
6	-2.569141000	0.303648000	-0.897304000
6	-1.730999000	-0.809642000	1.058449000
6	-3.732418000	-0.465150000	-0.840180000
6	-2.890059000	-1.579693000	1.122978000
6	-3.895308000	-1.408735000	0.171150000
1	-2.464671000	1.031339000	-1.695490000
1	-0.957667000	-0.967428000	1.804598000
1	-4.508701000	-0.327518000	-1.585304000
1	-3.008964000	-2.313914000	1.912601000
1	-4.797859000	-2.008233000	0.218039000

C_6H_4-4$CHMe_2$
E(RB3LYP) = -581.397825800

6	2.018951000	-0.003320000	-0.002509000
6	2.788183000	-1.147188000	0.259227000
6	2.691547000	1.206387000	-0.232385000
6	4.178889000	-1.084337000	0.289177000
6	4.082180000	1.270397000	-0.201582000
6	4.832798000	0.125042000	0.059045000
1	2.290589000	-2.088399000	0.464150000
1	4.752259000	-1.980062000	0.501492000
1	5.915541000	0.174359000	0.082338000
1	4.580484000	2.214869000	-0.390842000
1	2.120068000	2.099055000	-0.460556000
6	0.535952000	-0.071231000	-0.037176000
6	-0.127902000	-1.154957000	-0.625846000
6	-0.251643000	0.948888000	0.517199000
1	0.448510000	-1.950345000	-1.085276000
1	0.229881000	1.790509000	1.002749000
6	-1.519024000	-1.212417000	-0.659114000
6	-1.640393000	0.885887000	0.482500000
1	-2.002944000	-2.061456000	-1.132243000
1	-2.211553000	1.691899000	0.931487000
6	-2.304952000	-0.196434000	-0.107882000
6	-3.823594000	-0.275369000	-0.151525000
1	-4.076930000	-1.204567000	-0.674838000
6	-4.438219000	0.886871000	-0.952516000
1	-5.523978000	0.772431000	-1.025459000
1	-4.237338000	1.849621000	-0.473099000
1	-4.030907000	0.927396000	-1.965937000
6	-4.435026000	-0.360489000	1.259003000
1	-4.023850000	-1.205016000	1.817734000
1	-4.235812000	0.548906000	1.833732000
1	-5.520505000	-0.485577000	1.200886000

$CH(OH)C_6H_5$
E(RB3LYP) = -577.981408665

6	-1.284997000	-0.338245000	-0.107676000
6	-1.290037000	0.865269000	0.600638000
6	-2.473649000	-0.775745000	-0.701138000
6	-2.461152000	1.612985000	0.717473000
6	-3.644276000	-0.030648000	-0.588287000
6	-3.640372000	1.168314000	0.123743000
1	-0.376925000	1.225647000	1.058642000
1	-2.449864000	2.545742000	1.270472000
1	-4.549406000	1.752812000	0.211898000
1	-4.557010000	-0.383638000	-1.055386000
1	-2.481199000	-1.711825000	-1.250214000
6	-0.047580000	-1.218657000	-0.218059000

C_6H_4-4Et
E(RB3LYP) = -542.074306072

6	-1.651131000	-0.003257000	-0.014682000
6	-2.308150000	1.176350000	0.366816000
6	-2.433710000	-1.131954000	-0.301398000
6	-3.696727000	1.226138000	0.457772000
6	-3.822303000	-1.083387000	-0.209612000
6	-4.460753000	0.096207000	0.170127000
1	-1.723804000	2.054678000	0.617036000
1	-4.182044000	2.146799000	0.762711000
1	-5.541875000	0.134448000	0.240977000
1	-4.407016000	-1.966116000	-0.444285000
1	-1.950381000	-2.048011000	-0.621907000
6	-0.170228000	-0.054820000	-0.111792000

1	-0.097576000	-1.723508000	-1.192401000
8	-0.157312000	-2.205610000	0.820624000
1	0.568438000	-2.832078000	0.715923000
6	1.274468000	-0.466586000	-0.161298000
6	1.967063000	-0.299264000	1.041319000
6	1.813573000	0.077297000	-1.331738000
1	1.558175000	-0.722768000	1.951204000
1	1.287969000	-0.050405000	-2.273188000
6	3.172541000	0.402059000	1.071881000
6	3.015104000	0.780688000	-1.302408000
1	3.700099000	0.523053000	2.011717000
1	3.420481000	1.194407000	-2.219148000
6	3.699030000	0.945638000	-0.097961000
1	4.637021000	1.488815000	-0.073442000

C_6H_4-4CMe_3

E(RB3LYP) = -620.718604789

6	-2.330650000	-0.004657000	0.002000000
6	-3.047028000	1.133052000	0.403587000
6	-3.058292000	-1.134000000	-0.402901000
6	-4.439420000	1.141711000	0.400296000
6	-4.450680000	-1.126704000	-0.405272000
6	-5.148286000	0.011511000	-0.003897000
1	-2.507805000	2.009927000	0.743853000
1	-4.971458000	2.029987000	0.722883000
1	-6.232384000	0.017740000	-0.006258000
1	-4.991518000	-2.008755000	-0.730300000
1	-2.527500000	-2.016756000	-0.741168000
6	-0.846126000	-0.013148000	0.005703000
6	-0.109458000	1.107189000	-0.406422000
6	-0.123877000	-1.136992000	0.420205000
1	-0.630872000	1.990557000	-0.758305000
1	-0.654984000	-2.015272000	0.770421000
6	1.279700000	1.095998000	-0.401814000
6	1.270336000	-1.142911000	0.423457000
1	1.801010000	1.984959000	-0.738974000
1	1.775445000	-2.037674000	0.763525000
6	2.009763000	-0.028525000	0.013130000
6	3.547837000	0.000051000	-0.000464000
6	4.051979000	1.148644000	0.904313000
1	3.692034000	2.122260000	0.564089000
1	3.715638000	1.009486000	1.935417000
1	5.146068000	1.179230000	0.904203000
6	4.044052000	0.233039000	-1.446968000
1	5.137994000	0.258988000	-1.474127000
1	3.706552000	-0.569514000	-2.108651000
1	3.678136000	1.178070000	-1.854891000
6	4.161677000	-1.316098000	0.510292000
1	5.252472000	-1.245967000	0.483523000
1	3.870494000	-1.527441000	1.542926000
1	3.871521000	-2.168779000	-0.109632000

C_6H_4-4Me

E(RB3LYP) = -502.750297008

6	-1.216359000	-0.000191000	-0.000068000
6	-1.936588000	1.129840000	0.415856000
6	-1.939753000	-1.129005000	-0.413739000
6	-3.329014000	1.131638000	0.417687000
6	-3.332200000	-1.128492000	-0.411080000
6	-4.033793000	0.002144000	0.004427000
1	-1.399991000	2.005556000	0.763276000
1	-3.864255000	2.013790000	0.751569000
1	-5.117908000	0.003041000	0.006136000
1	-3.869960000	-2.009736000	-0.743306000
1	-1.405823000	-2.005585000	-0.763046000
6	0.268558000	-0.000988000	-0.001977000
6	0.994705000	1.122485000	-0.421229000
6	0.995027000	-1.126743000	0.410837000
1	0.464632000	1.999841000	-0.774889000
6	0.558991000	1.013523000	-0.653178000
6	0.547758000	-1.175014000	0.329727000
1	0.032016000	1.882088000	-1.032334000
1	0.015655000	-2.011306000	0.769498000
6	1.946379000	0.962050000	-0.745594000
6	1.935583000	-1.221080000	0.236281000
1	2.480455000	1.799457000	-1.184577000
1	2.462594000	-2.101544000	0.591435000
6	2.663185000	-0.154124000	-0.300851000
6	4.173961000	-0.189471000	-0.364544000
1	4.507952000	-1.225015000	-0.485011000
1	4.512418000	0.351888000	-1.254055000
6	4.843255000	0.416917000	0.881576000
1	4.549798000	-0.122907000	1.785981000
1	5.933114000	0.373656000	0.798924000
1	4.554461000	1.463412000	1.011737000

$CH(C_6H_5)_2$

E(RB3LYP) = -733.844772144

6	-1.297388000	0.699530000	-0.323896000
6	-1.388766000	1.512848000	0.808825000
6	-2.449545000	0.501351000	-1.094916000
6	-2.600813000	2.104882000	1.166625000
6	-3.659768000	1.092378000	-0.743040000
6	-3.740315000	1.896864000	0.393684000
1	-0.506847000	1.694083000	1.411916000
1	-2.649984000	2.733830000	2.048839000
1	-4.680699000	2.360857000	0.669280000
1	-4.538670000	0.928014000	-1.356833000
1	-2.397482000	-0.127991000	-1.977883000
6	0.000196000	0.000752000	-0.738865000
1	0.000679000	0.000965000	-1.834399000
6	1.253755000	0.775109000	-0.322091000
6	2.000858000	0.446818000	0.812316000
6	1.661397000	1.871452000	-1.092295000
1	1.716076000	-0.407357000	1.415414000
1	1.093530000	2.141263000	-1.977411000
6	3.119893000	1.199082000	1.172274000
6	2.780065000	2.621044000	-0.739372000
1	3.686459000	0.927160000	2.056215000
1	3.080287000	3.462820000	-1.353769000
6	3.513746000	2.288097000	0.399036000
1	4.386757000	2.868607000	0.675509000
6	0.043765000	-1.472489000	-0.323832000
6	-0.634861000	-1.963067000	0.794767000
6	0.810512000	-2.367064000	-1.081336000
1	-1.248241000	-1.294691000	1.387444000
1	1.343887000	-2.004605000	-1.954764000
6	-0.541763000	-3.308636000	1.153023000
6	0.902209000	-3.710748000	-0.729785000
1	-1.076767000	-3.668889000	2.024928000
1	1.499030000	-4.386110000	-1.333070000
6	0.226337000	-4.187276000	0.393686000
1	0.294898000	-5.233509000	0.669746000

$N{=}CHC_6H_5$

E(RB3LYP) = -556.893472536

6	4.602307000	-0.221880000	-0.039820000
6	3.755193000	-1.204045000	0.470962000
6	4.064728000	0.988990000	-0.479422000
1	4.166657000	-2.137955000	0.838110000
1	4.717606000	1.763242000	-0.866944000
6	2.380150000	-0.990381000	0.526670000
6	2.694929000	1.216389000	-0.409708000
1	1.730990000	-1.745069000	0.955963000
1	2.267483000	2.158243000	-0.732910000
6	1.832933000	0.219238000	0.069875000
1	5.672129000	-0.391240000	-0.080070000
7	0.457791000	0.506871000	0.122001000
6	-0.399167000	-0.390992000	-0.175065000
1	-0.091106000	-1.382876000	-0.534124000
6	-1.848591000	-0.173760000	-0.084536000

1	0.465271000	-2.006315000	0.759444000
6	2.386350000	1.118583000	-0.425099000
6	2.386529000	-1.125715000	0.406242000
1	2.918478000	2.000169000	-0.768952000
1	2.918912000	-2.011797000	0.737978000
6	3.110503000	-0.003245000	-0.008878000
6	4.619599000	0.006201000	0.017393000
1	4.993701000	0.346188000	0.989595000
1	5.028133000	-0.991892000	-0.158160000
1	5.027426000	0.677671000	-0.741871000

6	-2.719814000	-1.206728000	-0.455333000
6	-2.384722000	1.043491000	0.364901000
1	-2.311453000	-2.150099000	-0.804177000
1	-1.704684000	1.836824000	0.649865000
6	-4.099613000	-1.032342000	-0.379987000
6	-3.760343000	1.216045000	0.437910000
1	-4.764202000	-1.838475000	-0.669181000
1	-4.168032000	2.158708000	0.785597000
6	-4.622036000	0.179567000	0.066535000
1	-5.695646000	0.319050000	0.125971000

$SiMe_3$

E(RB3LYP) = -641.048503487

6	0.428723000	0.016961000	-0.000007000
6	1.150581000	-1.189660000	0.000171000
6	1.168986000	1.209973000	-0.000143000
6	2.543742000	-1.206201000	0.000210000
6	2.564314000	1.202276000	-0.000108000
6	3.255468000	-0.006936000	0.000087000
1	0.621865000	-2.138877000	0.000269000
1	3.074178000	-2.152490000	0.000331000
1	4.339923000	-0.016213000	0.000105000
1	3.109991000	2.139890000	-0.000244000
1	0.654934000	2.165676000	-0.000318000
14	-1.468488000	0.004082000	-0.000074000
6	-2.087302000	-0.897912000	1.541527000
1	-1.751840000	-0.395838000	2.453705000
1	-3.181288000	-0.935681000	1.561552000
1	-1.720670000	-1.928085000	1.578192000
6	-2.086903000	-0.898140000	-1.541699000
1	-3.180901000	-0.934527000	-1.563040000
1	-1.749658000	-0.397137000	-2.453813000
1	-1.721512000	-1.928795000	-1.577190000
6	-2.124210000	1.775189000	0.000095000
1	-1.798826000	2.330223000	0.884994000
1	-1.799050000	2.330739000	-0.884553000
1	-3.218717000	1.770670000	0.000255000

$GeMe_3$

E(RB3LYP) = -2428.52085057

6	-3.568315000	-0.004693000	0.000016000
6	-2.873858000	1.202985000	-0.000020000
6	-2.860602000	-1.206254000	0.000060000
1	-3.417074000	2.142072000	-0.000055000
1	-3.394219000	-2.150803000	0.000092000
6	-1.478153000	1.206978000	-0.000015000
6	-1.466585000	-1.194837000	0.000058000
1	-0.958040000	2.159487000	-0.000045000
1	-0.938180000	-2.144003000	0.000089000
6	-0.748621000	0.010461000	0.000026000
1	-4.652752000	-0.010721000	0.000010000
32	1.228347000	0.002539000	-0.000013000
6	1.897445000	1.859214000	-0.000334000
1	1.559460000	2.399672000	-0.887502000
1	1.559471000	2.399941000	0.886674000
1	2.990132000	1.855334000	-0.000338000
6	1.876537000	-0.938172000	-1.611563000
1	1.497654000	-1.962356000	-1.640938000
1	1.541540000	-0.423140000	-2.514514000
1	2.968764000	-0.976305000	-1.617478000
6	1.876732000	-0.937519000	1.611845000
1	2.968964000	-0.975519000	1.617701000
1	1.541743000	-0.422164000	2.514617000
1	1.497962000	-1.961732000	1.641667000

NHCOMe

E(RB3LYP) = -440.391353964

6	0.305512000	-0.286726000	-0.000021000
6	1.242064000	-1.330886000	-0.000002000
6	0.754565000	1.040007000	-0.000020000
6	2.604515000	-1.057894000	0.000016000
6	2.124686000	1.296809000	0.000005000
6	3.056014000	0.261397000	0.000018000
1	0.898852000	-2.361456000	-0.000005000
1	3.312754000	-1.878749000	0.000027000
1	4.117999000	0.476857000	0.000034000
1	2.462214000	2.327301000	0.000007000
1	0.037394000	1.845879000	-0.000037000
7	-1.060864000	-0.646492000	-0.000039000
1	-1.235772000	-1.639477000	-0.000045000
6	-2.177210000	0.161399000	-0.000006000
8	-2.136909000	1.378547000	0.000009000
6	-3.499391000	-0.588669000	0.000026000
1	-4.069542000	-0.284856000	-0.880248000
1	-3.397760000	-1.675950000	-0.000133000
1	-4.069349000	-0.285105000	0.880514000

$CH_2CH{=}CH_2$

E(RB3LYP) = -349.050340666

6	-0.129351000	-0.000440000	0.550118000
6	0.544916000	1.201165000	0.308092000
6	0.545182000	-1.201649000	0.307072000
6	1.856013000	1.204464000	-0.164730000
6	1.856247000	-1.204147000	-0.165771000
6	2.516288000	0.000344000	-0.403992000
1	0.037701000	2.143024000	0.492103000
1	2.362465000	2.146763000	-0.342870000
1	3.537266000	0.000570000	-0.768864000
1	2.362901000	-2.146146000	-0.344910000
1	0.038130000	-2.143780000	0.490189000
6	-1.558871000	-0.000642000	1.042807000
1	-1.724774000	-0.872811000	1.687790000
1	-1.724637000	0.870694000	1.688960000
6	-2.624409000	-0.000034000	-0.031519000
1	-3.644671000	-0.000641000	0.348985000
6	-2.429489000	0.000890000	-1.347782000
1	-1.435861000	0.001877000	-1.781784000
1	-3.267676000	0.000745000	-2.035364000

$NHCOC_6H_5$

E(RB3LYP) = -632.172790635

6	-1.879799000	0.192535000	0.049121000
6	-2.619351000	1.353086000	0.322711000
6	-2.555103000	-1.000853000	-0.238279000
6	-4.008321000	1.325675000	0.308482000
6	-3.948800000	-1.011136000	-0.249208000
6	-4.684227000	0.140189000	0.021382000
1	-2.100882000	2.280804000	0.546987000
1	-4.561688000	2.233086000	0.522456000
1	-5.767510000	0.116127000	0.010164000
1	-4.461717000	-1.940050000	-0.472541000
1	-1.990898000	-1.897503000	-0.441244000

$CH_2C_6H_5$

E(RB3LYP) = -502.743462648

6	1.277826000	0.303953000	0.553248000
6	1.504374000	0.896876000	-0.695316000
6	2.265241000	-0.532968000	1.079759000
6	2.685165000	0.661506000	-1.393411000
6	3.449973000	-0.773896000	0.382337000
6	3.663641000	-0.176729000	-0.856912000
1	0.745426000	1.542290000	-1.125494000
1	2.842954000	1.131024000	-2.358265000
1	4.582681000	-0.361401000	-1.401659000
1	4.202808000	-1.427722000	0.808866000
1	2.107982000	-1.000622000	2.046760000

7	-0.473307000	0.306955000	0.070113000
1	-0.128097000	1.227435000	0.294485000
6	0.481710000	-0.674940000	-0.074519000
8	0.221497000	-1.859909000	-0.209925000
6	1.904355000	-0.183355000	-0.037432000
6	2.289508000	1.102642000	-0.435740000
6	2.885375000	-1.089043000	0.381746000
1	1.557933000	1.806661000	-0.817792000
1	2.579648000	-2.089532000	0.661519000
6	3.629989000	1.481006000	-0.396790000
6	4.221501000	-0.706494000	0.431383000
1	3.918367000	2.474586000	-0.720464000
1	4.971917000	-1.412859000	0.767786000
6	4.597223000	0.580038000	0.043934000
1	5.639744000	0.875723000	0.076507000

6	-0.003932000	0.579271000	1.320225000
1	0.034878000	0.041711000	2.273819000
1	-0.050101000	1.643528000	1.574381000
6	-1.279420000	0.198693000	0.586682000
6	-1.466879000	-1.102637000	0.104166000
6	-2.303091000	1.130919000	0.397057000
1	-0.679297000	-1.838074000	0.231635000
1	-2.175839000	2.144862000	0.763504000
6	-2.645435000	-1.460778000	-0.543998000
6	-3.485699000	0.776941000	-0.254091000
1	-2.772154000	-2.474058000	-0.909355000
1	-4.266851000	1.516575000	-0.391850000
6	-3.660842000	-0.520941000	-0.726302000
1	-4.578017000	-0.799371000	-1.233006000

NHCOCH(Me)$_2$
E(RB3LYP) = -519.040362523

6	-1.100352000	0.274089000	-0.000093000
6	-2.012995000	1.339308000	-0.000252000
6	-1.579878000	-1.042089000	0.000152000
6	-3.381315000	1.097315000	-0.000167000
6	-2.955437000	-1.267756000	0.000239000
6	-3.862922000	-0.211323000	0.000087000
1	-1.646561000	2.361806000	-0.000444000
1	-4.070739000	1.934073000	-0.000292000
1	-4.929572000	-0.402412000	0.000156000
1	-3.316380000	-2.290303000	0.000433000
1	-0.880790000	-1.863764000	0.000265000
7	0.273975000	0.601399000	-0.000189000
1	0.474476000	1.589860000	-0.000326000
6	1.372514000	-0.229561000	-0.000117000
8	1.302986000	-1.446731000	0.000012000
6	2.722130000	0.498226000	-0.000128000
1	2.550646000	1.581769000	-0.000540000
6	3.504267000	0.125996000	-1.269942000
1	3.664431000	-0.953525000	-1.308992000
1	2.967624000	0.422667000	-2.175299000
1	4.478314000	0.622424000	-1.274192000
6	3.503732000	0.126887000	1.270300000
1	2.966670000	0.424117000	2.175224000
1	3.663965000	-0.952596000	1.310114000
1	4.477743000	0.623390000	1.274655000

NHCSNHEt
E(RB3LYP) = -858.041293840

6	1.351812000	-0.416321000	0.114079000
6	1.891127000	0.756315000	0.651257000
6	2.206069000	-1.376185000	-0.440144000
6	3.267048000	0.961841000	0.611847000
6	3.582300000	-1.168072000	-0.460745000
6	4.120051000	0.006697000	0.059803000
1	1.238713000	1.499083000	1.085648000
1	3.674832000	1.877065000	1.026098000
1	5.190243000	0.175880000	0.037398000
1	4.230046000	-1.921643000	-0.894153000
1	1.788888000	-2.284353000	-0.864518000
7	-0.030700000	-0.719020000	0.175207000
1	-0.229031000	-1.710000000	0.147117000
6	-1.119837000	0.102204000	-0.045332000
7	-2.299989000	-0.544066000	0.182256000
1	-2.268293000	-1.392095000	0.731745000
6	-3.615938000	0.073826000	0.035971000
1	-3.722308000	0.898640000	0.749105000
1	-3.679018000	0.513165000	-0.961026000
6	-4.711612000	-0.967034000	0.241954000
1	-4.666796000	-1.407424000	1.243568000
1	-4.639192000	-1.772632000	-0.493819000
1	-5.692560000	-0.499537000	0.134383000
16	-1.046051000	1.689113000	-0.565996000

Ge(Et)$_3$
E(RB3LYP) = -2546.48122580

6	3.971832000	-0.000729000	0.381495000
6	3.409022000	-0.000642000	-0.894350000
6	3.140827000	-0.000557000	1.499642000
1	4.049071000	-0.000778000	-1.770352000
1	3.570606000	-0.000633000	2.495795000
6	2.023065000	-0.000376000	-1.044977000
6	1.754039000	-0.000290000	1.341029000
1	1.608459000	-0.000319000	-2.049068000
1	1.128790000	-0.000175000	2.227987000
6	1.167932000	-0.000199000	0.067563000
1	5.049579000	-0.000935000	0.502158000
32	-0.795368000	0.000218000	-0.191699000
6	-1.307691000	1.614994000	-1.231510000
1	-0.785188000	1.564060000	-2.192772000
1	-2.375526000	1.537461000	-1.462139000
6	-1.692853000	0.000195000	1.581288000
1	-1.344776000	-0.875288000	2.138662000
1	-1.345644000	0.876450000	2.138010000
6	-1.308503000	-1.613890000	-1.232114000
1	-2.376166000	-1.535412000	-1.463208000
1	-0.785516000	-1.563269000	-2.193121000
6	-1.004712000	2.948399000	-0.534311000
1	-1.550074000	3.043182000	0.409465000
1	0.060502000	3.048802000	-0.307718000
1	-1.288859000	3.801037000	-1.159825000
6	-3.227150000	-0.000561000	1.504492000

$N(C_6H_5)_2$
E(RB3LYP) = -749.885371791

6	1.397795000	-0.261243000	0.001696000
6	2.263688000	0.496596000	-0.799409000
6	1.933589000	-1.281095000	0.800925000
6	3.632090000	0.242873000	-0.791969000
6	3.301250000	-1.538599000	0.789702000
6	4.160611000	-0.777586000	-0.002119000
1	1.859548000	1.283902000	-1.424083000
1	4.286130000	0.838861000	-1.418972000
1	5.225869000	-0.976691000	-0.003596000
1	3.697664000	-2.330873000	1.415212000
1	1.274210000	-1.869623000	1.427242000
7	0.000829000	-0.000380000	0.003442000
6	-0.924370000	-1.079229000	0.001845000
6	-2.069393000	-1.036901000	0.809727000
6	-0.707804000	-2.203350000	-0.807634000
1	-2.243701000	-0.174861000	1.442138000
1	0.171494000	-2.244030000	-1.438998000
6	-2.977392000	-2.091577000	0.798963000
6	-1.612557000	-3.260707000	-0.799849000
1	-3.857065000	-2.041569000	1.431221000
1	-1.429024000	-4.121669000	-1.433229000
6	-2.754639000	-3.211750000	-0.001160000
1	-3.460364000	-4.034179000	-0.002259000
6	-0.472238000	1.340009000	0.001776000
6	0.134308000	2.311073000	0.810826000
6	-1.553099000	1.712998000	-0.809474000

1	-3.606410000	-0.882282000	0.979258000
1	-3.676952000	-0.000473000	2.502709000
1	-3.607232000	0.880494000	0.978734000
6	-1.006929000	-2.947652000	-0.534947000
1	-1.552524000	-3.041979000	0.408737000
1	-1.291776000	-3.799981000	-1.160560000
1	0.058151000	-3.049081000	-0.308173000

1	0.967320000	2.032034000	1.444619000
1	-2.025590000	0.971053000	-1.441697000
6	-0.326824000	3.624111000	0.799312000
6	-2.018270000	3.024670000	-0.802483000
1	0.154191000	4.361661000	1.432372000
1	-2.854895000	3.295126000	-1.437320000
6	-1.407362000	3.989969000	-0.002723000
1	-1.767893000	5.011951000	-0.004444000

NMeCOMe

E(RB3LYP) = -479.697490133

6	0.405029000	0.167858000	-0.096305000
6	0.974249000	-1.018541000	-0.570624000
6	1.231671000	1.146808000	0.464059000
6	2.348642000	-1.214959000	-0.480034000
6	2.608614000	0.946189000	0.543433000
6	3.173504000	-0.236328000	0.073995000
1	0.340653000	-1.783936000	-0.994939000
1	2.777044000	-2.139690000	-0.850098000
1	4.243717000	-0.395173000	0.138878000
1	3.235284000	1.714818000	0.981700000
1	0.802917000	2.064217000	0.849657000
7	-1.003325000	0.405753000	-0.208087000
6	-1.430401000	1.752867000	-0.597832000
1	-0.657974000	2.197133000	-1.224201000
1	-2.348219000	1.708013000	-1.181751000
1	-1.599449000	2.408501000	0.264265000
6	-1.914301000	-0.553260000	0.213245000
8	-1.569901000	-1.648773000	0.621692000
6	-3.386975000	-0.178385000	0.139194000
1	-3.710800000	-0.037037000	-0.896023000
1	-3.951090000	-1.000875000	0.573471000
1	-3.609791000	0.740443000	0.687324000

$P(N(Me)_2)_2$

E(RB3LYP) = -842.310107595

6	-0.961975000	-0.000044000	0.311648000
6	-1.676169000	-1.203776000	0.224735000
6	-1.676593000	1.203560000	0.226222000
6	-3.055969000	-1.204087000	0.029380000
6	-3.056388000	1.203632000	0.030889000
6	-3.751649000	-0.000284000	-0.071100000
1	-1.144073000	-2.144076000	0.311915000
1	-3.588111000	-2.146660000	-0.041647000
1	-4.825479000	-0.000393000	-0.221565000
1	-3.588846000	2.146119000	-0.038920000
1	-1.144809000	2.143937000	0.314480000
15	0.823243000	0.000062000	0.799266000
7	1.359157000	-1.431086000	-0.005504000
7	1.358952000	1.431360000	-0.005782000
6	1.185734000	-1.710020000	-1.427526000
1	0.275409000	-1.243882000	-1.803599000
1	2.034853000	-1.353036000	-2.029340000
1	1.097802000	-2.791674000	-1.587911000
6	2.508058000	-2.123066000	0.571766000
1	3.458423000	-1.837163000	0.094694000
1	2.578988000	-1.899880000	1.637434000
1	2.390985000	-3.207506000	0.455597000
6	1.184308000	1.710651000	-1.427557000
1	1.097098000	2.792409000	-1.587647000
1	2.032466000	1.353100000	-2.030386000
1	0.273154000	1.245386000	-1.802710000
6	2.508422000	2.122894000	0.570768000
1	3.458373000	1.836983000	0.092872000
1	2.391511000	3.207415000	0.455099000
1	2.580156000	1.899312000	1.636307000

NHCOOMe

E(RB3LYP) = -515.640406351

6	-0.755830000	-0.302363000	0.000020000
6	-1.717255000	-1.322992000	0.000154000
6	-1.171246000	1.034653000	-0.000150000
6	-3.072410000	-1.014580000	0.000080000
6	-2.533979000	1.326684000	-0.000206000
6	-3.491431000	0.315196000	-0.000093000
1	-1.399056000	-2.361219000	0.000321000
1	-3.800745000	-1.817649000	0.000184000
1	-4.547564000	0.557399000	-0.000145000
1	-2.844888000	2.365541000	-0.000344000
1	-0.435649000	1.824491000	-0.000174000
7	0.598439000	-0.694035000	-0.000015000
1	0.782580000	-1.686118000	-0.000375000
6	1.715402000	0.098008000	0.000152000
8	1.756330000	1.307499000	0.000513000
8	2.815542000	-0.702760000	-0.000117000
6	4.076991000	-0.014804000	-0.000238000
1	4.174096000	0.608934000	-0.889844000
1	4.174347000	0.608821000	0.889413000
1	4.831381000	-0.798680000	-0.000405000

cyclopropyl

E(RB3LYP) = -349.039138099

6	-0.141799000	-0.000029000	0.263046000
6	0.566085000	-1.202033000	0.148656000
6	0.566023000	1.202008000	0.148631000
6	1.941932000	-1.204335000	-0.074892000
6	1.941871000	1.204376000	-0.074919000
6	2.634950000	0.000037000	-0.187228000
1	0.031144000	-2.142162000	0.233182000
1	2.472167000	-2.146357000	-0.163327000
1	3.704716000	0.000063000	-0.363977000
1	2.472057000	2.146423000	-0.163375000
1	0.031036000	2.142113000	0.233139000
6	-1.614470000	-0.000069000	0.549350000
6	-2.585455000	0.755501000	-0.325831000
6	-2.585420000	-0.755471000	-0.326002000
1	-1.854366000	-0.000172000	1.610179000
1	-2.188081000	-1.252744000	-1.203270000
1	-2.188188000	1.252978000	-1.203013000
1	-3.411371000	1.272594000	0.147992000
1	-3.411407000	-1.272647000	0.147604000

C_6H_4-4OMe

E(RB3LYP) = -577.978972944

6	1.632351000	0.000402000	0.004684000
6	2.409159000	1.076102000	-0.452569000
6	2.298985000	-1.156427000	0.436945000
6	3.799216000	0.998526000	-0.476173000
6	3.688860000	-1.236374000	0.410041000
6	4.446464000	-0.158769000	-0.046054000

$CH_2PO(OEt)_2$

E(RB3LYP) = -996.721740740

6	-1.776528000	-0.714838000	-0.485380000
6	-2.337884000	-1.338228000	0.634810000
6	-2.562929000	0.171137000	-1.227516000
6	-3.658169000	-1.085421000	0.998179000
6	-3.884692000	0.424336000	-0.865205000
6	-4.437021000	-0.204532000	0.248710000

1	1.918036000	1.972199000	-0.815101000
1	4.377395000	1.840358000	-0.841207000
1	5.528671000	-0.219817000	-0.065289000
1	4.181290000	-2.138328000	0.756790000
1	1.723163000	-1.991154000	0.820703000
6	0.150837000	0.084317000	0.029694000
6	-0.506089000	1.265511000	0.417502000
6	-0.646383000	-1.005545000	-0.332536000
1	0.078421000	2.124067000	0.728290000
1	-0.176169000	-1.925572000	-0.661268000
6	-1.888755000	1.350335000	0.442301000
6	-2.040027000	-0.936932000	-0.314419000
1	-2.388976000	2.259769000	0.753126000
1	-2.614473000	-1.802880000	-0.615026000
6	-2.669170000	0.247452000	0.075201000
8	-4.020971000	0.428101000	0.130508000
6	-4.867140000	-0.657216000	-0.223519000
1	-4.712749000	-0.962009000	-1.264338000
1	-4.711051000	-1.518085000	0.435780000
1	-5.885628000	-0.291647000	-0.103103000

1	-1.732637000	-2.010979000	1.232041000
1	-4.078170000	-1.576210000	1.869087000
1	-5.465560000	-0.009951000	0.531116000
1	-4.481708000	1.111765000	-1.454248000
1	-2.137960000	0.666747000	-2.093931000
6	-0.346409000	-0.993312000	-0.888876000
1	-0.131523000	-2.065947000	-0.846464000
1	-0.149665000	-0.660221000	-1.910038000
15	0.909495000	-0.211772000	0.178393000
8	0.872998000	-0.574161000	1.618764000
8	2.330462000	-0.548226000	-0.536803000
6	3.201437000	-1.600518000	-0.048847000
1	2.897201000	-2.541364000	-0.519486000
1	3.073081000	-1.693741000	1.031485000
6	4.629176000	-1.249288000	-0.417461000
1	4.936774000	-0.320095000	0.067284000
1	4.734788000	-1.128928000	-1.497955000
1	5.302312000	-2.047492000	-0.091313000
8	0.713829000	1.341503000	-0.187798000
6	1.415388000	2.379014000	0.545751000
1	2.478692000	2.319156000	0.295049000
1	1.294955000	2.193304000	1.615907000
6	0.828490000	3.715537000	0.141242000
1	-0.234214000	3.761277000	0.388065000
1	0.944843000	3.882418000	-0.931914000
1	1.342898000	4.520595000	0.673695000

OH

E(RB3LYP) = -307.558629826

6	-1.854961000	0.026899000	-0.000016000
6	-1.169892000	-1.188807000	0.000001000
6	-1.131235000	1.217365000	-0.000008000
1	-1.722146000	-2.122030000	0.000030000
1	-1.649547000	2.169772000	-0.000012000
6	0.221429000	-1.221530000	0.000025000
6	0.262698000	1.197921000	0.000020000
1	0.763980000	-2.159071000	0.000006000
1	0.822994000	2.128555000	0.000074000
6	0.937822000	-0.024148000	0.000021000
1	-2.938239000	0.045526000	-0.000074000
8	2.305091000	-0.110294000	-0.000040000
1	2.687072000	0.773396000	0.000030000

Me

E(RB3LYP) = -271.638813296

6	-1.902625000	-0.000095000	0.008474000
6	-1.199389000	-1.203615000	0.002198000
6	-1.199786000	1.203384000	0.002202000
1	-1.735944000	-2.146151000	0.002102000
1	-1.736368000	2.145904000	0.002113000
6	0.194216000	-1.200440000	-0.009078000
6	0.194056000	1.200564000	-0.009077000
1	0.732059000	-2.143470000	-0.017974000
1	0.731571000	2.143761000	-0.017984000
6	0.913158000	0.000265000	-0.012157000
1	-2.986805000	-0.000341000	0.014213000
6	2.423192000	0.000051000	0.009647000
1	2.800342000	-0.009611000	1.038249000
1	2.829095000	-0.879752000	-0.495173000
1	2.829122000	0.888985000	-0.478800000

$(CH_2)_4NMe_2$

E(RB3LYP) = -523.604373433

6	-1.910945000	0.706615000	-0.311000000
6	-2.642202000	0.632238000	0.881606000
6	-2.072127000	-0.320078000	-1.247204000
6	-3.500737000	-0.435109000	1.133711000
6	-2.930805000	-1.391339000	-1.000764000
6	-3.647108000	-1.453826000	0.192249000
1	-2.543261000	1.423389000	1.618867000
1	-4.060197000	-0.469380000	2.062272000
1	-4.316970000	-2.284213000	0.385180000
1	-3.041234000	-2.174818000	-1.742638000
1	-1.522498000	-0.278846000	-2.182351000
6	-0.966786000	1.863312000	-0.562996000
1	-1.474153000	2.799869000	-0.306511000
6	0.354406000	1.789730000	0.232271000
1	0.124085000	1.736373000	1.303385000
1	0.896700000	2.731572000	0.083014000
1	-0.738142000	1.918373000	-1.632694000
6	1.262557000	0.617299000	-0.152642000
1	0.724485000	-0.324653000	-0.007010000
1	1.499262000	0.681785000	-1.221445000
6	2.565248000	0.611559000	0.671883000
1	2.309242000	0.551360000	1.736527000
1	3.079351000	1.570217000	0.531769000
7	3.538624000	-0.445810000	0.398837000
6	3.079180000	-1.784993000	0.732527000

$CH_2CH_2Si(Me)_3$

E(RB3LYP) = -719.695646458

6	-1.330338000	-0.464555000	-0.710956000
6	-1.817816000	0.828937000	-0.923474000
6	-1.993384000	-1.272736000	0.221885000
6	-2.925009000	1.307600000	-0.222219000
6	-3.098992000	-0.801165000	0.924787000
6	-3.568673000	0.494442000	0.707169000
1	-1.327779000	1.469732000	-1.649916000
1	-3.284248000	2.314529000	-0.405082000
1	-4.429767000	0.862694000	1.253354000
1	-3.597599000	-1.445910000	1.640430000
1	-1.643647000	-2.285624000	0.396074000
6	-0.132772000	-0.989728000	-1.476682000
1	0.136729000	-0.266656000	-2.252411000
6	1.111921000	-1.312063000	-0.613048000
1	0.841839000	-2.036582000	0.165329000
1	1.840774000	-1.831510000	-1.249333000
1	-0.435275000	-1.900847000	-2.007247000
14	2.055468000	0.122806000	0.214263000
6	1.122698000	0.835853000	1.694033000
1	0.938342000	0.067786000	2.451579000
1	1.705720000	1.633025000	2.167066000
1	0.154856000	1.253006000	1.405028000
6	3.709587000	-0.574928000	0.814696000
1	4.305294000	-0.966702000	-0.015844000

1	2.679129000	-1.794518000	1.749961000
1	2.298715000	-2.175474000	0.055092000
1	3.924202000	-2.478814000	0.697494000
6	4.145174000	-0.376112000	-0.920826000
1	3.459470000	-0.638502000	-1.746839000
1	4.521428000	0.634660000	-1.100967000
1	4.994881000	-1.063485000	-0.967855000

1	3.562383000	-1.390642000	1.529820000
6	2.385243000	1.491789000	-1.050240000
1	2.999118000	2.284958000	-0.611610000
1	2.918768000	1.109350000	-1.926340000
1	1.457659000	1.954019000	-1.400618000

$CH_2PO(C_6H_5)_2$

E(RB3LYP) = -1151.10271892

6	-1.959352000	-1.370424000	-0.503859000
6	-2.564643000	-1.974247000	0.605736000
6	-2.768433000	-0.708582000	-1.433170000
6	-3.945989000	-1.920922000	0.773121000
6	-4.151181000	-0.655480000	-1.266110000
6	-4.744667000	-1.263390000	-0.162119000
1	-1.946559000	-2.468799000	1.345986000
1	-4.399101000	-2.392820000	1.637922000
1	-5.820262000	-1.225347000	-0.030937000
1	-4.762495000	-0.141060000	-1.999323000
1	-2.314966000	-0.233426000	-2.297165000
6	-0.462557000	-1.433301000	-0.693039000
1	-0.091109000	-2.455507000	-0.569314000
1	-0.188566000	-1.104357000	-1.698350000
15	0.486039000	-0.434412000	0.545668000
8	0.250809000	-0.856181000	1.968257000
6	2.245825000	-0.616954000	0.058695000
6	2.703451000	-0.629154000	-1.265067000
6	3.167347000	-0.763254000	1.102490000
1	2.010180000	-0.539534000	-2.093852000
1	2.804039000	-0.778604000	2.123625000
6	4.062511000	-0.769547000	-1.538536000
6	4.525979000	-0.900403000	0.826074000
1	4.407127000	-0.780370000	-2.566519000
1	5.232085000	-1.012285000	1.641244000
6	4.975422000	-0.901871000	-0.493157000
1	6.032558000	-1.011676000	-0.707670000
6	0.014368000	1.315681000	0.271466000
6	-0.656456000	1.958704000	1.316658000
6	0.279418000	2.015486000	-0.911446000
1	-0.849291000	1.409679000	2.230935000
1	0.814314000	1.540674000	-1.726202000
6	-1.062293000	3.284872000	1.176548000
6	-0.127584000	3.339972000	-1.048691000
1	-1.582255000	3.777352000	1.990605000
1	0.084170000	3.877466000	-1.966304000
6	-0.799881000	3.975580000	-0.004516000
1	-1.114629000	5.007636000	-0.112233000

NHPO(C3H7)2

E(RB3LYP) = -940.900924636

6	-1.559780000	-0.607887000	-0.308597000
6	-2.151829000	-0.712574000	0.958568000
6	-2.382435000	-0.558206000	-1.443166000
6	-3.539363000	-0.745841000	1.072369000
6	-3.766897000	-0.610939000	-1.315497000
6	-4.357062000	-0.698262000	-0.055712000
1	-1.522180000	-0.786838000	1.836426000
1	-3.982641000	-0.826716000	2.058886000
1	-5.435426000	-0.733908000	0.044161000
1	-4.384674000	-0.576706000	-2.206188000
1	-1.933152000	-0.478949000	-2.428847000
7	-0.157704000	-0.577030000	-0.469747000
1	0.148831000	-0.633174000	-1.430809000
15	0.992780000	-0.003516000	0.657119000
8	0.878797000	-0.621065000	2.014728000
6	0.803417000	1.822237000	0.738617000
1	-0.164031000	1.984684000	1.226515000
1	1.563013000	2.171973000	1.446461000
6	0.878037000	2.601472000	-0.581462000
1	0.129832000	2.209905000	-1.278642000
1	1.855530000	2.447782000	-1.051989000
6	0.647805000	4.104146000	-0.385045000
1	1.395451000	4.534563000	0.287900000
1	-0.338500000	4.297753000	0.046507000
1	0.707068000	4.639557000	-1.336533000
6	2.564874000	-0.357664000	-0.217959000
1	2.532617000	0.061399000	-1.230386000
1	3.331365000	0.204079000	0.328273000
6	2.928540000	-1.851034000	-0.245178000
1	2.166096000	-2.405541000	-0.801364000
1	2.900648000	-2.237748000	0.776902000
6	4.305681000	-2.102770000	-0.866388000
1	5.093228000	-1.592679000	-0.303153000
1	4.351233000	-1.744843000	-1.900044000
1	4.541625000	-3.170189000	-0.873762000

SMe

E(RB3LYP) = -669.848424146

6	-2.638120000	-0.346478000	-0.000035000
6	-1.701608000	-1.375442000	0.000056000
6	-2.195070000	0.977429000	-0.000090000
1	-2.029579000	-2.409249000	0.000110000
1	-2.911850000	1.791166000	-0.000150000
6	-0.334161000	-1.095909000	0.000102000
6	-0.835904000	1.266589000	-0.000055000
1	0.370253000	-1.917059000	0.000226000
1	-0.502551000	2.298809000	-0.000097000
6	0.109879000	0.230043000	0.000023000
1	-3.698540000	-0.569549000	-0.000067000
16	1.824272000	0.720014000	0.000122000
6	2.725011000	-0.861608000	-0.000201000
1	2.511239000	-1.445861000	0.895736000
1	2.511279000	-1.445492000	-0.896387000
1	3.781232000	-0.590732000	-0.000115000

CH_2OH

E(RB3LYP) = -346.874092749

6	-2.304942000	0.329558000	-0.000035000
6	-1.880340000	-0.999774000	-0.000026000
6	-1.359339000	1.351428000	-0.000024000
1	-2.608042000	-1.803790000	-0.000034000
1	-1.680723000	2.387307000	-0.000031000
6	-0.520752000	-1.296875000	-0.000005000
6	0.004477000	1.053728000	-0.000003000
1	-0.198676000	-2.334479000	0.000003000
1	0.741163000	1.846225000	0.000006000
6	0.433668000	-0.273520000	0.000007000
1	-3.363610000	0.563569000	-0.000051000
6	1.901761000	-0.634894000	0.000029000
1	2.121997000	-1.246649000	0.886190000
1	2.122025000	-1.246650000	-0.886124000
8	2.699092000	0.545644000	0.000041000
1	3.625922000	0.291415000	0.000052000

SEt

E(RB3LYP) = -709.173356431

6	0.386439000	0.265985000	0.000101000
6	0.758460000	-1.082501000	0.000199000
6	1.388210000	1.248907000	-0.000111000

isopropyl

E(RB3LYP) = -350.286302909

6	0.137063000	-0.193508000	-0.000059000
6	-0.750138000	-1.274668000	-0.000211000
6	-0.402906000	1.099403000	0.000176000

6	2.108733000	-1.435682000	0.000082000
6	2.729699000	0.886599000	-0.000223000
6	3.100117000	-0.459405000	-0.000129000
1	0.011109000	-1.864368000	0.000378000
1	2.379919000	-2.485859000	0.000160000
1	4.146796000	-0.740075000	-0.000221000
1	3.489555000	1.660287000	-0.000393000
1	1.111689000	2.297756000	-0.000204000
16	-1.297672000	0.851926000	0.000295000
6	-2.308224000	-0.679317000	-0.000133000
1	-2.063350000	-1.266081000	-0.888075000
1	-2.063645000	-1.266413000	0.887672000
6	-3.788123000	-0.299728000	-0.000292000
1	-4.049797000	0.284963000	-0.885336000
1	-4.050073000	0.284636000	0.884886000
1	-4.401314000	-1.204814000	-0.000554000

6	-2.131061000	-1.077422000	-0.000157000
6	-1.780768000	1.302997000	0.000214000
6	-2.652171000	0.213955000	0.000025000
1	-0.354663000	-2.285796000	-0.000341000
1	-2.797463000	-1.933199000	-0.000275000
1	-3.724835000	0.371712000	0.000038000
1	-2.175233000	2.313388000	0.000395000
1	0.257225000	1.960428000	0.000369000
6	1.641426000	-0.426598000	-0.000120000
1	1.792949000	-1.512091000	-0.000418000
6	2.310742000	0.131676000	-1.269345000
1	1.861885000	-0.290974000	-2.171826000
1	2.211357000	1.219805000	-1.325193000
1	3.379046000	-0.104923000	-1.276568000
6	2.310722000	0.130925000	1.269415000
1	3.379022000	-0.105738000	1.276586000
1	2.211411000	1.219037000	1.325933000
1	1.861844000	-0.292209000	2.171670000

CH_2NMe_2

E(RB3LYP) = -405.634834628

6	-0.369825000	0.224431000	-0.371182000
6	-1.270350000	1.269991000	-0.155994000
6	-0.837989000	-1.092254000	-0.289575000
6	-2.612375000	1.012202000	0.127033000
6	-2.175250000	-1.353359000	-0.003695000
6	-3.068606000	-0.301205000	0.204148000
1	-0.919532000	2.296077000	-0.207703000
1	-3.296827000	1.836966000	0.292699000
1	-4.109887000	-0.505479000	0.427194000
1	-2.522932000	-2.379032000	0.056656000
1	-0.139759000	-1.907850000	-0.440234000
6	1.077779000	0.506210000	-0.724502000
1	1.237290000	0.259177000	-1.780104000
1	1.269979000	1.591770000	-0.625687000
7	2.033875000	-0.281271000	0.053604000
6	2.039206000	0.091674000	1.463517000
1	1.037447000	-0.013153000	1.883086000
1	2.710913000	-0.570575000	2.014905000
1	2.373924000	1.134026000	1.624802000
6	3.372013000	-0.215809000	-0.517775000
1	4.045400000	-0.863968000	0.048376000
1	3.353114000	-0.566680000	-1.552579000
1	3.796129000	0.806327000	-0.508497000

NHCOOEt

E(RB3LYP) = -554.969842580

6	1.222266000	-0.281820000	0.000113000
6	2.106836000	-1.369930000	-0.000070000
6	1.735452000	1.021207000	0.000178000
6	3.480889000	-1.161790000	-0.000177000
6	3.115869000	1.212397000	0.000057000
6	3.996696000	0.133511000	-0.000117000
1	1.714097000	-2.382288000	-0.000131000
1	4.148354000	-2.016197000	-0.000316000
1	5.067807000	0.297252000	-0.000205000
1	3.501858000	2.225765000	0.000105000
1	1.059572000	1.862657000	0.000303000
7	-0.156819000	-0.574404000	0.000269000
1	-0.412942000	-1.550188000	0.000415000
6	-1.214821000	0.297185000	0.000091000
8	-1.162511000	1.506546000	-0.000220000
8	-2.368853000	-0.420041000	0.000134000
6	-3.592183000	0.354307000	-0.000127000
1	-3.599608000	0.997014000	0.882960000
1	-3.599432000	0.996698000	-0.883446000
6	-4.749039000	-0.623159000	-0.000068000
1	-4.724892000	-1.260478000	0.886782000
1	-4.724707000	-1.260805000	-0.886678000
1	-5.693259000	-0.072099000	-0.000268000

$CH_2C(Me)_3$

E(RB3LYP) = -428.934512666

6	-0.604884000	0.000215000	-0.545999000
6	-1.294793000	1.199835000	-0.328483000
6	-1.294424000	-1.199627000	-0.328614000
6	-2.618658000	1.203040000	0.107029000
6	-2.618293000	-1.203287000	0.106907000
6	-3.285525000	-0.000242000	0.330451000
1	-0.791677000	2.143978000	-0.510203000
1	-3.131019000	2.145790000	0.265543000
1	-4.316519000	-0.000405000	0.665963000
1	-3.130335000	-2.146226000	0.265328000
1	-0.791017000	-2.143600000	-0.510422000
6	0.834844000	0.000364000	-1.014114000
1	0.999853000	-0.876508000	-1.649947000
1	0.999851000	0.877616000	-1.649374000
6	1.942538000	0.000014000	0.087894000
6	1.839669000	1.255908000	0.970962000
1	2.647499000	1.269435000	1.709148000
1	1.921743000	2.169359000	0.372796000
1	0.891681000	1.290993000	1.512981000
6	3.305944000	-0.000384000	-0.629350000
1	3.420162000	-0.885323000	-1.263549000
1	3.420552000	0.884018000	-1.264178000
1	4.126673000	-0.000337000	0.094526000
6	1.839154000	-1.255717000	0.971015000
1	0.891264000	-1.290608000	1.513223000

$CH_2CH(Me)_2$

E(RB3LYP) = -389.611735092

6	-0.388436000	0.111293000	0.477837000
6	-1.024124000	1.238897000	-0.058187000
6	-1.133724000	-1.065423000	0.605593000
6	-2.357070000	1.190781000	-0.459051000
6	-2.469311000	-1.119745000	0.206908000
6	-3.085769000	0.008589000	-0.328933000
1	-0.470128000	2.167575000	-0.156490000
1	-2.829318000	2.077353000	-0.868213000
1	-4.124275000	-0.030031000	-0.637981000
1	-3.027295000	-2.043233000	0.317271000
1	-0.663613000	-1.949284000	1.025006000
6	1.064828000	0.173612000	0.894886000
1	1.219998000	1.064530000	1.514234000
1	1.299546000	-0.689084000	1.529132000
6	2.075749000	0.215665000	-0.277595000
1	1.803304000	1.065585000	-0.916551000
6	2.018858000	-1.055657000	-1.133587000
1	2.719527000	-0.992098000	-1.971218000
1	2.290796000	-1.936308000	-0.540375000
1	1.020060000	-1.223282000	-1.543351000
6	3.495120000	0.458230000	0.252381000
1	4.216805000	0.518559000	-0.567490000
1	3.556824000	1.390003000	0.822658000
1	3.811058000	-0.357723000	0.911868000

1	1.920783000	-2.169256000	0.372851000
1	2.647064000	-1.269641000	1.709116000

$CH_2CH_2C_6H_5$			
E(RB3LYP) = -542.067994851			
6	1.554128000	0.728706000	0.361199000
6	2.588027000	0.800294000	-0.580687000
6	1.442452000	-0.431897000	1.133951000
6	3.481738000	-0.255147000	-0.748723000
6	2.334989000	-1.490643000	0.970845000
6	3.357189000	-1.406811000	0.027735000
1	2.699195000	1.696589000	-1.183880000
1	4.279058000	-0.176011000	-1.479761000
1	4.053756000	-2.228168000	-0.097845000
1	2.231341000	-2.380519000	1.582085000
1	0.647971000	-0.507803000	1.868783000
6	0.579183000	1.874372000	0.517631000
1	0.152690000	1.860324000	1.525142000
1	1.118894000	2.821928000	0.417377000
6	-0.579215000	1.874402000	-0.517611000
1	-1.118912000	2.821960000	-0.417307000
1	-0.152716000	1.860411000	-1.525121000
6	-1.554146000	0.728731000	-0.361205000
6	-1.442511000	-0.431816000	-1.134035000
6	-2.587994000	0.800268000	0.580752000
1	-0.648073000	-0.507671000	-1.868920000
1	-2.699126000	1.696544000	1.183979000
6	-2.335029000	-1.490587000	-0.970925000
6	-3.481667000	-0.255193000	0.748797000
1	-2.231421000	-2.380417000	-1.582239000
1	-4.278934000	-0.176128000	1.479901000
6	-3.357148000	-1.406822000	-0.027734000
1	-4.053706000	-2.228184000	0.097860000

$NHCOO(CH_2)_3CH_3$			
E(RB3LYP) = -633.618202712			
6	-2.269483000	-0.296546000	-0.000025000
6	-3.115474000	-1.414967000	0.000126000
6	-2.827655000	0.987782000	-0.000276000
6	-4.495920000	-1.254809000	0.000026000
6	-4.213915000	1.130800000	-0.000360000
6	-5.056571000	0.021802000	-0.000214000
1	-2.687611000	-2.412947000	0.000325000
1	-5.133187000	-2.131965000	0.000144000
1	-6.132717000	0.148297000	-0.000283000
1	-4.635112000	2.130053000	-0.000546000
1	-2.181307000	1.852236000	-0.000391000
7	-0.881342000	-0.539817000	0.000067000
1	-0.591061000	-1.506200000	0.000131000
6	0.145942000	0.368053000	0.000212000
8	0.052214000	1.574952000	0.000144000
8	1.323668000	-0.309727000	0.000445000
6	2.520277000	0.502954000	0.000571000
1	2.509406000	1.146772000	-0.882642000
1	2.509780000	1.145889000	0.884444000
6	3.715456000	-0.433891000	-0.000125000
1	3.659662000	-1.084428000	-0.879952000
1	3.659954000	-1.085368000	0.879023000
6	5.046771000	0.327812000	0.000071000
1	5.090498000	0.985448000	-0.876157000
1	5.090786000	0.984457000	0.877028000
6	6.262867000	-0.602756000	-0.000643000
1	6.266481000	-1.249353000	0.882235000
1	6.266077000	-1.248513000	-0.884134000
1	7.196923000	-0.034868000	-0.000581000

$(CH_2)_3CH_3$			
E(RB3LYP) = -389.610795719			
6	-0.559075000	0.426484000	-0.550209000
6	-1.224956000	1.166367000	0.435683000
6	-1.113589000	-0.796266000	-0.942138000
6	-2.401768000	0.697786000	1.014900000
6	-2.292097000	-1.270835000	-0.366109000
6	-2.939935000	-0.525791000	0.616445000
1	-0.819976000	2.124167000	0.748446000
1	-2.902122000	1.289790000	1.773597000
1	-3.857165000	-0.891082000	1.064513000
1	-2.704194000	-2.221230000	-0.687521000
1	-0.618984000	-1.382959000	-1.709819000
6	0.729219000	0.940260000	-1.157799000
1	0.602481000	1.996081000	-1.420962000
6	1.961817000	0.809949000	-0.237541000
1	1.763917000	1.335548000	0.704678000
1	2.801672000	1.334081000	-0.710081000
1	0.925373000	0.409392000	-2.095672000
6	2.377692000	-0.633577000	0.064530000
1	1.542975000	-1.164401000	0.534183000
1	2.579043000	-1.154281000	-0.880237000
6	3.611642000	-0.721886000	0.967543000
1	3.428169000	-0.242667000	1.934428000
1	3.890429000	-1.761467000	1.161014000
1	4.474678000	-0.225923000	0.511600000

CH(Me)(Et)			
E(RB3LYP) = -389.610149329			
6	-0.108894000	0.201236000	-0.228969000
6	-0.695796000	0.577369000	0.986635000
6	-0.931726000	-0.370581000	-1.204581000
6	-2.056134000	0.387661000	1.217622000
6	-2.295032000	-0.562987000	-0.979744000
6	-2.862996000	-0.184145000	0.233972000
1	-0.085698000	1.024480000	1.764578000
1	-2.487712000	0.687268000	2.166581000
1	-3.922098000	-0.331616000	0.413040000
1	-2.910921000	-1.009070000	-1.753102000
1	-0.498916000	-0.669972000	-2.154112000
6	1.376106000	0.414317000	-0.490307000
1	1.578406000	0.040528000	-1.501711000
6	1.744242000	1.909431000	-0.468260000
1	1.589342000	2.342550000	0.524410000
1	1.134780000	2.476128000	-1.176719000
1	2.796256000	2.051526000	-0.733287000
6	2.272558000	-0.388039000	0.479016000
1	3.316809000	-0.129067000	0.268436000
1	2.079757000	-0.056162000	1.506079000
6	2.098050000	-1.906109000	0.386620000
1	2.320246000	-2.267290000	-0.622839000
1	1.075843000	-2.207762000	0.628974000
1	2.771642000	-2.420462000	1.077645000

$(CH_2)_6CH_3$			
E(RB3LYP) = -507.583772747			
6	-2.280497000	0.590367000	-0.263183000
6	-2.889156000	0.454250000	0.991291000
6	-2.462019000	-0.434836000	-1.197374000
6	-3.649148000	-0.670060000	1.304287000
6	-3.221572000	-1.563621000	-0.889696000
6	-3.817288000	-1.686034000	0.363492000
1	-2.771570000	1.241945000	1.729452000
1	-4.114778000	-0.751436000	2.280511000
1	-4.410692000	-2.560970000	0.604071000

$NHCOC_6H_4$-4OMe			
E(RB3LYP) = -746.730635322			
6	-2.749872000	-0.205189000	-0.053515000
6	-3.455745000	-1.388750000	-0.318755000
6	-3.461287000	0.973916000	0.206063000
6	-4.845047000	-1.398153000	-0.323955000
6	-4.854728000	0.947232000	0.197855000
6	-5.556211000	-0.227017000	-0.064656000
1	-2.910249000	-2.305961000	-0.521281000
1	-5.371009000	-2.323279000	-0.531333000
1	-5.394928000	1.865631000	0.399638000

1	-3.349677000	-2.345031000	-1.630922000
1	-2.006145000	-0.347556000	-2.178615000
6	-1.442028000	1.810648000	-0.581543000
1	-1.988333000	2.708201000	-0.271330000
6	-0.055327000	1.822549000	0.096920000
1	-0.186606000	1.731221000	1.181894000
1	0.403757000	2.803843000	-0.074501000
1	-1.311169000	1.887966000	-1.666281000
6	0.897864000	0.728284000	-0.394563000
1	0.437981000	-0.254664000	-0.241739000
1	1.038661000	0.834659000	-1.478533000
6	2.265256000	0.760026000	0.297888000
1	2.123933000	0.645545000	1.380465000
1	2.723098000	1.747679000	0.154592000
6	3.230632000	-0.320769000	-0.201379000
1	2.771680000	-1.308310000	-0.062202000
1	3.376183000	-0.204395000	-1.283438000
6	4.595898000	-0.297542000	0.495277000
1	5.054597000	0.689338000	0.357495000
1	4.451115000	-0.416265000	1.576070000
6	5.553547000	-1.379694000	-0.011874000
1	5.138641000	-2.380378000	0.145722000
1	5.745362000	-1.267507000	-1.083782000
1	6.516988000	-1.335293000	0.503805000

1	-2.923534000	1.888197000	0.401979000
7	-1.341631000	-0.283603000	-0.052747000
1	-0.971698000	-1.198862000	-0.256845000
6	-0.412421000	0.726481000	0.085262000
8	-0.712268000	1.906630000	0.187929000
6	1.018578000	0.277024000	0.083694000
6	1.443890000	-1.012863000	0.440013000
6	1.988773000	1.220416000	-0.260708000
1	0.732039000	-1.762542000	0.768736000
1	1.665473000	2.223266000	-0.511079000
6	2.787727000	-1.349405000	0.430822000
6	3.341438000	0.895275000	-0.284193000
1	3.120951000	-2.338962000	0.718701000
1	4.062490000	1.650774000	-0.565417000
6	3.747970000	-0.398721000	0.059992000
1	-6.639823000	-0.231419000	-0.068651000
8	5.038790000	-0.824726000	0.073904000
6	6.068413000	0.094042000	-0.276543000
1	5.948002000	0.453601000	-1.303642000
1	6.092156000	0.945908000	0.410760000
1	7.000493000	-0.462094000	-0.195274000

CH_2NH_2

E(RB3LYP) = -327.002665593

6	2.319869000	0.275902000	-0.105421000
6	1.845511000	-1.033416000	-0.139460000
6	1.419265000	1.329295000	0.055045000
1	2.535841000	-1.859480000	-0.270941000
1	1.780681000	2.351719000	0.079489000
6	0.479228000	-1.284408000	-0.013643000
6	0.055739000	1.075679000	0.184377000
1	0.115741000	-2.307040000	-0.049000000
1	-0.647654000	1.891794000	0.299561000
6	-0.430091000	-0.236458000	0.155070000
1	3.380870000	0.474984000	-0.207374000
6	-1.908422000	-0.524079000	0.334599000
1	-2.099019000	-1.566620000	0.039240000
1	-2.158121000	-0.453535000	1.400004000
7	-2.747382000	0.453466000	-0.369143000
1	-3.728289000	0.309383000	-0.155713000
1	-2.634975000	0.369442000	-1.374670000

$NHCONH_2$

E(RB3LYP) = -456.450860644

6	-0.288319000	-0.295253000	-0.007670000
6	-1.239410000	-1.325430000	0.034233000
6	-0.721385000	1.036082000	-0.049003000
6	-2.598426000	-1.034393000	0.034880000
6	-2.087781000	1.310709000	-0.049148000
6	-3.033744000	0.289270000	-0.007449000
1	-0.910492000	-2.360288000	0.065616000
1	-3.316490000	-1.846041000	0.068654000
1	-4.092679000	0.518994000	-0.006739000
1	-2.410861000	2.345432000	-0.080237000
1	0.005024000	1.833423000	-0.072498000
7	1.070524000	-0.675512000	-0.018903000
1	1.230799000	-1.667379000	0.069548000
6	2.191979000	0.134322000	0.020448000
8	2.171785000	1.348148000	0.101625000
7	3.382372000	-0.586542000	0.004477000
1	4.193818000	-0.000864000	-0.124493000
1	3.418835000	-1.465930000	-0.489611000

$(CH_2)_4CH_3$

E(RB3LYP) = -428.935185218

6	-1.112698000	0.661222000	-0.356656000
6	-1.767058000	0.815313000	0.872570000
6	-1.514581000	-0.388624000	-1.188844000
6	-2.784443000	-0.053271000	1.259843000
6	-2.533145000	-1.261879000	-0.806683000
6	-3.171099000	-1.098248000	0.420606000
1	-1.481001000	1.629658000	1.531473000
1	-3.279951000	0.088038000	2.214282000
1	-3.964560000	-1.774083000	0.719228000
1	-2.828332000	-2.067932000	-1.469672000
1	-1.026858000	-0.522943000	-2.149271000
6	0.002300000	1.604337000	-0.757878000
1	-0.329745000	2.636401000	-0.599704000
6	1.323387000	1.391911000	0.011950000
1	1.133249000	1.497306000	1.086886000
1	2.012863000	2.201127000	-0.257730000
1	0.192914000	1.502165000	-1.831608000
6	1.999041000	0.043333000	-0.255078000
1	1.311767000	-0.769347000	0.006603000
1	2.193469000	-0.055917000	-1.331544000
6	3.313352000	-0.140215000	0.512990000
1	3.118807000	-0.039782000	1.587797000
1	4.002724000	0.672266000	0.251938000
6	3.988282000	-1.487923000	0.242115000

cyclopentyl

E(RB3LYP) = -427.718402154

6	-0.603201000	-0.209350000	0.003034000
6	-1.508725000	-1.275772000	0.024485000
6	-1.123645000	1.091918000	-0.022343000
6	-2.886189000	-1.056620000	0.020872000
6	-2.497752000	1.317257000	-0.026278000
6	-3.386747000	0.242548000	-0.004574000
1	-1.129078000	-2.292705000	0.044180000
1	-3.566046000	-1.901562000	0.037944000
1	-4.456724000	0.417544000	-0.007452000
1	-2.875948000	2.333657000	-0.046275000
1	-0.449800000	1.942105000	-0.039352000
6	0.888693000	-0.467298000	0.007470000
6	1.669578000	0.091493000	-1.202532000
6	1.665638000	0.132450000	1.202158000
6	3.149216000	-0.011035000	-0.779857000
6	3.152056000	0.082669000	0.776172000
1	1.036659000	-1.554516000	0.023761000
1	1.347608000	1.168739000	1.355080000
1	1.389415000	1.138035000	-1.363465000
1	3.760731000	0.766107000	-1.244231000
1	1.449095000	-0.446204000	-2.128063000
1	3.565130000	-0.970476000	-1.100265000
1	3.696523000	0.960509000	1.131950000
1	3.649312000	-0.789023000	1.209549000

1	3.336226000	-2.320137000	0.525395000
1	4.228475000	-1.603641000	-0.819606000
1	4.919923000	-1.588920000	0.805912000

cyclohexyl
E(RB3LYP) = -467.050876679

6	0.919984000	0.184534000	-0.054422000
6	1.817904000	1.229564000	-0.297819000
6	1.448961000	-1.077577000	0.248484000
6	3.196761000	1.027646000	-0.240871000
6	2.825010000	-1.285508000	0.306912000
6	3.706198000	-0.232509000	0.062648000
1	1.431493000	2.216182000	-0.534597000
1	3.870920000	1.855253000	-0.433252000
1	4.777350000	-0.393965000	0.108565000
1	3.210449000	-2.271290000	0.544085000
1	0.780904000	-1.910040000	0.442388000
6	-0.578328000	0.425361000	-0.111925000
6	-1.262357000	0.198639000	1.254854000
6	-2.770940000	0.477041000	1.192373000
6	-3.454942000	-0.351276000	0.096355000
6	-2.783675000	-0.134900000	-1.266605000
6	-1.274691000	-0.413537000	-1.206619000
1	-0.723765000	1.481810000	-0.374065000
1	-0.788509000	0.832781000	2.011010000
1	-1.097891000	-0.838558000	1.572588000
1	-3.228827000	0.272115000	2.165717000
1	-2.932831000	1.544390000	0.991928000
1	-4.519105000	-0.099708000	0.038988000
1	-3.400165000	-1.415585000	0.360771000
1	-3.249973000	-0.771897000	-2.025494000
1	-2.947285000	0.901757000	-1.589337000
1	-0.809826000	-0.208846000	-2.176381000
1	-1.112246000	-1.479263000	-1.003106000

$CH_2CH_2CH_3$
E(RB3LYP) = -350.286475300

6	-0.011077000	-0.152866000	-0.528154000
6	0.702829000	-1.247731000	-0.023689000
6	0.623900000	1.093144000	-0.550430000
6	2.005181000	-1.101936000	0.447773000
6	1.928187000	1.245578000	-0.079771000
6	2.623335000	0.148223000	0.422922000
1	0.234917000	-2.227477000	-0.006363000
1	2.540091000	-1.964715000	0.829727000
1	3.638006000	0.263448000	0.787165000
1	2.400635000	2.221461000	-0.108417000
1	0.092688000	1.954096000	-0.943827000
6	-1.433305000	-0.322527000	-1.019326000
1	-1.710874000	0.542722000	-1.631163000
1	-1.481706000	-1.196480000	-1.678338000
6	-2.475380000	-0.498167000	0.106175000
1	-2.199289000	-1.365428000	0.716518000
1	-3.439551000	-0.741576000	-0.354316000
6	-2.636024000	0.730865000	1.004700000
1	-1.698559000	0.986034000	1.505588000
1	-2.952148000	1.604540000	0.425146000
1	-3.390079000	0.555867000	1.777083000

$C(Et)_3$
E(RB3LYP) = -507.570980677

6	0.638940000	-0.000007000	-0.011512000
6	1.505136000	0.000058000	1.094523000
6	1.231343000	-0.000029000	-1.280291000
6	2.888278000	0.000045000	0.943408000
6	2.618969000	-0.000050000	-1.439706000
6	3.456500000	-0.000029000	-0.329984000
1	1.097643000	0.000115000	2.098797000
1	3.523546000	0.000089000	1.822699000
1	4.533796000	-0.000055000	-0.451958000
1	3.040014000	-0.000083000	-2.439409000
1	0.617153000	-0.000012000	-2.170503000
1	1.469589000	-0.401770000	2.134994000

$C(Me)_3$
E(RB3LYP) = -389.607025573

6	0.078226000	0.028420000	0.000058000
6	0.819295000	1.215621000	0.000073000
6	0.796603000	-1.178021000	0.000097000
6	2.215642000	1.201838000	0.000036000
6	2.187910000	-1.198276000	0.000074000
6	2.908134000	-0.004135000	0.000032000
1	0.314106000	2.172553000	0.000098000
1	2.758501000	2.140939000	0.000030000
1	3.992227000	-0.016516000	0.000035000
1	2.710630000	-2.148718000	0.000072000
1	0.265078000	-2.122960000	0.000120000
6	-1.461395000	0.005609000	0.000040000
6	-2.069679000	1.420169000	-0.000199000
1	-1.777187000	1.990011000	-0.886424000
1	-1.777591000	1.990161000	0.886106000
1	-3.160683000	1.347840000	-0.000409000
6	-1.965209000	-0.733190000	-1.261920000
1	-1.626030000	-0.228284000	-2.170680000
1	-1.606729000	-1.764349000	-1.299566000
1	-3.059375000	-0.759597000	-1.275445000
6	-1.965865000	-0.732953000	1.261837000
1	-1.607936000	-1.764303000	1.299556000
1	-1.626934000	-0.228392000	2.170814000
1	-3.060033000	-0.758868000	1.274925000

cyclobutyl
E(RB3LYP) = -388.365690757

6	0.253045000	0.000008000	-0.243492000
6	0.962832000	1.201153000	-0.128712000
6	0.962800000	-1.201151000	-0.128655000
6	2.339375000	1.203435000	0.090770000
6	2.339339000	-1.203458000	0.090834000
6	3.033886000	-0.000017000	0.201390000
1	0.433653000	2.144914000	-0.210029000
1	2.868911000	2.146029000	0.178155000
1	4.104036000	-0.000032000	0.375334000
1	2.868852000	-2.146059000	0.178276000
1	0.433594000	-2.144902000	-0.209934000
6	-1.230169000	0.000037000	-0.516367000
6	-2.147284000	-1.084779000	0.123631000
6	-2.147255000	1.084773000	0.123807000
6	-3.245182000	-0.000004000	0.285725000
1	-1.389593000	0.000123000	-1.601913000
1	-1.756699000	1.408536000	1.092245000
1	-1.756744000	-1.408697000	1.092021000
1	-3.819320000	-0.000075000	1.213786000
1	-2.386261000	-1.967365000	-0.473156000
1	-3.942533000	0.000079000	-0.555535000
1	-2.386216000	1.967461000	-0.472837000

$CH_2OSi(CH_3)_3$
E(RB3LYP) = -755.649473620

6	-1.588421000	-0.354597000	0.000217000
6	-1.887736000	1.007130000	0.000250000
6	-2.637433000	-1.280810000	0.000012000
6	-3.216115000	1.436226000	0.000073000
6	-3.962048000	-0.853781000	-0.000175000
6	-4.256310000	0.510518000	-0.000140000
1	-1.074379000	1.721029000	0.000397000
1	-3.436041000	2.498391000	0.000101000
1	-5.287413000	0.845844000	-0.000283000
1	-4.764349000	-1.583481000	-0.000337000
1	-2.417321000	-2.344857000	-0.000003000

6	-0.889712000	0.000025000	0.214230000
6	-1.279240000	1.254797000	1.054689000
1	-0.754367000	1.202193000	2.013550000
1	-2.343700000	1.187019000	1.301649000
6	-1.654774000	-0.000110000	-1.137174000
1	-1.343101000	0.871375000	-1.720170000
1	-1.343090000	-0.871752000	-1.719937000
6	-1.279234000	-1.254665000	1.054781000
1	-0.754437000	-1.201951000	2.013680000
1	-2.343713000	-1.186908000	1.301651000
6	-0.994195000	-2.615202000	0.410466000
1	-1.234898000	-3.422655000	1.107762000
1	-1.591250000	-2.777031000	-0.490967000
1	0.059027000	-2.716129000	0.135913000
6	-0.994290000	2.615298000	0.410254000
1	0.058879000	2.716188000	0.135475000
1	-1.591547000	2.777114000	-0.491040000
1	-1.234811000	3.422785000	1.107576000
6	-3.186564000	-0.000121000	-1.053276000
1	-3.612682000	-0.000336000	-2.060504000
1	-3.574690000	-0.882481000	-0.538169000
1	-3.574716000	0.882445000	-0.538541000

6	-0.159292000	-0.858186000	0.000354000
1	-0.008996000	-1.494966000	0.884258000
1	-0.008807000	-1.494881000	-0.883572000
8	0.767135000	0.209816000	0.000511000
14	2.442967000	0.077502000	-0.000049000
6	3.014371000	-0.843270000	-1.541214000
1	2.669225000	-0.341974000	-2.450336000
1	4.107532000	-0.890775000	-1.582250000
1	2.644425000	-1.872922000	-1.565896000
6	3.054773000	1.848404000	-0.002166000
1	2.696769000	2.387362000	0.879431000
1	4.148549000	1.888166000	0.000960000
1	2.702003000	2.383529000	-0.888205000
6	3.015623000	-0.839991000	1.542597000
1	4.108811000	-0.887805000	1.582601000
1	2.671568000	-0.336617000	2.450978000
1	2.645336000	-1.869460000	1.569896000

$C(Et)(Me)_2$

E(RB3LYP) = -428.927780827

6	-0.446883000	0.086199000	-0.100535000
6	-1.266530000	1.185703000	0.181175000
6	-1.070261000	-1.168103000	-0.203474000
6	-2.645132000	1.042713000	0.350318000
6	-2.443843000	-1.317107000	-0.036071000
6	-3.242350000	-0.208598000	0.242552000
1	-0.838736000	2.175390000	0.271536000
1	-3.249447000	1.917222000	0.566408000
1	-4.312831000	-0.320994000	0.372507000
1	-2.891005000	-2.301408000	-0.124318000
1	-0.477799000	-2.050093000	-0.418585000
6	1.079750000	0.206249000	-0.276375000
6	1.541437000	1.675588000	-0.273996000
1	1.352497000	2.163964000	0.686165000
1	1.038278000	2.251778000	-1.055218000
1	2.614004000	1.735577000	-0.468155000
6	1.487819000	-0.416323000	-1.632965000
1	2.557763000	-0.287208000	-1.815298000
1	1.270293000	-1.485918000	-1.676862000
1	0.949126000	0.067359000	-2.452282000
6	1.750550000	-0.557496000	0.907555000
1	1.388099000	-0.110821000	1.840479000
1	1.381112000	-1.587790000	0.906458000
6	3.283825000	-0.587851000	0.929516000
1	3.717877000	0.412012000	1.009092000
1	3.699152000	-1.064443000	0.037728000
1	3.631327000	-1.160470000	1.794135000

$OSiMe_3$

E(RB3LYP) = -716.331512497

6	-0.873257000	-0.000266000	-0.468586000
6	-1.552583000	1.208792000	-0.294342000
6	-1.553142000	-1.209071000	-0.294205000
6	-2.899773000	1.203942000	0.060983000
6	-2.900261000	-1.203647000	0.061107000
6	-3.579892000	0.000332000	0.242737000
1	-1.020131000	2.139622000	-0.450266000
1	-3.419983000	2.146580000	0.191583000
1	-4.628284000	0.000552000	0.517199000
1	-3.420921000	-2.146017000	0.191836000
1	-1.020910000	-2.140043000	-0.450052000
8	0.436251000	-0.000722000	-0.863682000
14	1.850904000	0.000000000	0.063386000
6	1.905634000	1.541226000	1.139181000
1	1.056737000	1.582414000	1.827866000
1	2.819823000	1.556987000	1.741709000
1	1.892039000	2.451626000	0.533021000
6	1.905811000	-1.540502000	1.140188000
1	1.891952000	-2.451403000	0.534766000
1	2.819829000	-1.556009000	1.742933000
1	1.056788000	-1.580944000	1.828804000
6	3.221772000	-0.000242000	-1.211764000
1	4.206096000	0.000503000	-0.733214000
1	3.159621000	-0.884248000	-1.852324000
1	3.158831000	0.882767000	-1.853610000

NHC_6H_5

E(RB3LYP) = -518.788431465

6	1.266078000	-0.441989000	-0.018403000
6	2.363184000	-1.185401000	0.448564000
6	1.496868000	0.843094000	-0.533145000
6	3.649070000	-0.659908000	0.402204000
6	2.787289000	1.365246000	-0.558532000
6	3.872400000	0.624480000	-0.093329000
1	2.197565000	-2.178973000	0.853497000
1	4.479266000	-1.254944000	0.766522000
1	4.873392000	1.038045000	-0.120062000
1	2.944143000	2.359653000	-0.962206000
1	0.675047000	1.421253000	-0.933948000
7	0.000040000	-1.038209000	0.000501000
1	0.000056000	-2.045941000	-0.000502000
6	-1.266035000	-0.442047000	0.018767000
6	-1.497093000	0.843046000	0.533531000
6	-2.362956000	-1.185412000	-0.448655000
1	-0.675373000	1.421145000	0.934654000

$CH_2Si(Me)_3$

E(RB3LYP) = -680.376703236

6	0.928814000	-0.000544000	0.677413000
6	1.598034000	1.200076000	0.401215000
6	1.598869000	-1.200613000	0.400822000
6	2.883595000	1.202713000	-0.136138000
6	2.884417000	-1.202197000	-0.136550000
6	3.533775000	0.000528000	-0.410062000
1	1.107318000	2.144148000	0.616104000
1	3.379782000	2.146303000	-0.336321000
1	4.535242000	0.000949000	-0.825096000
1	3.381241000	-2.145382000	-0.337063000
1	1.108790000	-2.145085000	0.615413000
6	-0.474841000	-0.001152000	1.227486000
1	-0.630406000	-0.878740000	1.865165000
1	-0.630537000	0.875144000	1.866907000
14	-1.866627000	-0.000006000	-0.088955000
6	-1.736409000	1.546186000	-1.164580000
1	-0.775407000	1.591766000	-1.684374000

1	-2.197227000	-2.178964000	-0.853622000
6	-2.787494000	1.365133000	0.558513000
6	-3.648895000	-0.659954000	-0.402709000
1	-2.944571000	2.359503000	0.962196000
1	-4.478918000	-1.255019000	-0.767379000
6	-3.872450000	0.624346000	0.092867000
1	-4.873453000	1.037906000	0.119311000

1	-2.525838000	1.558201000	-1.922846000
1	-1.837899000	2.459039000	-0.569279000
6	-1.734201000	-1.542607000	-1.169405000
1	-1.834533000	-2.457476000	-0.577013000
1	-2.523542000	-1.553312000	-1.927785000
1	-0.773071000	-1.585258000	-1.689200000
6	-3.521374000	-0.002550000	0.826301000
1	-4.360719000	-0.001376000	0.123729000
1	-3.625538000	-0.887299000	1.462135000
1	-3.626180000	0.879423000	1.465877000

OMe

E(RB3LYP) = -346.867565044

6	-2.281900000	0.331482000	-0.000034000
6	-1.851199000	-0.998233000	-0.000025000
6	-1.335624000	1.349919000	-0.000023000
1	-2.576619000	-1.804243000	-0.000033000
1	-1.654020000	2.386642000	-0.000030000
6	-0.496935000	-1.301930000	-0.000004000
6	0.031610000	1.060759000	-0.000002000
1	-0.147884000	-2.327632000	0.000003000
1	0.746946000	1.872230000	0.000006000
6	0.452349000	-0.271899000	0.000007000
1	-3.339748000	0.565775000	-0.000050000
8	1.759067000	-0.669659000	0.000027000
6	2.772908000	0.324726000	0.000040000
1	2.716496000	0.955277000	-0.894217000
1	2.716469000	0.955281000	0.894294000
1	3.718560000	-0.215003000	0.000056000

NHOH

E(RB3LYP) = -362.873334973

6	0.458348000	-0.258767000	-0.066556000
6	-0.482456000	-1.295987000	-0.004399000
6	0.022988000	1.068516000	-0.067541000
6	-1.840562000	-1.003686000	0.044818000
6	-1.341764000	1.347238000	-0.013000000
6	-2.281328000	0.320384000	0.040121000
1	-0.147783000	-2.328813000	-0.003722000
1	-2.557507000	-1.815849000	0.092214000
1	-3.340354000	0.545562000	0.081610000
1	-1.669088000	2.381182000	-0.008339000
1	0.750078000	1.868370000	-0.093999000
7	1.824550000	-0.604599000	-0.207893000
1	2.051839000	-1.432068000	0.334684000
8	2.710390000	0.417002000	0.247699000
1	3.246489000	0.611600000	-0.529456000

N=CHC6H4-4-OMe

E(RB3LYP) = -671.451399432

6	5.536040000	-0.269429000	-0.048023000
6	4.677484000	-1.227454000	0.488590000
6	5.012338000	0.937973000	-0.513633000
1	5.077553000	-2.158372000	0.875669000
1	5.673782000	1.694223000	-0.921875000
6	3.305612000	-0.993370000	0.545319000
6	3.646021000	1.185188000	-0.444677000
1	2.648364000	-1.728894000	0.995180000
1	3.230030000	2.124751000	-0.788990000
6	2.771460000	0.212248000	0.062397000
1	6.603323000	-0.454206000	-0.088547000
7	1.401402000	0.519292000	0.114620000
6	0.531238000	-0.374836000	-0.161706000
1	0.828622000	-1.375932000	-0.505034000
6	-0.910283000	-0.144145000	-0.070515000
6	-1.798835000	-1.163915000	-0.421910000
6	-1.442144000	1.085890000	0.363045000
1	-1.408515000	-2.119183000	-0.758940000
1	-0.757677000	1.879464000	0.636626000
6	-3.179661000	-0.985072000	-0.351016000
6	-2.806768000	1.277854000	0.437042000
1	-3.837295000	-1.796722000	-0.630604000
1	-3.226394000	2.220044000	0.768721000
6	-3.688605000	0.242919000	0.080104000
8	-5.012352000	0.534345000	0.188543000
6	-5.965074000	-0.463865000	-0.159051000
1	-5.869701000	-0.755859000	-1.210083000
1	-5.864781000	-1.348593000	0.478334000
1	-6.941234000	-0.010450000	0.003068000

N=C(Me)NHC6H5

E(RB3LYP) = -651.597419899

6	2.006115000	-0.197378000	0.031975000
6	2.673573000	-0.868838000	1.068323000
6	2.738146000	0.177726000	-1.105499000
6	4.038724000	-1.124376000	0.981475000
6	4.102862000	-0.090014000	-1.189813000
6	4.762969000	-0.737261000	-0.146736000
1	2.105163000	-1.183367000	1.936119000
1	4.538424000	-1.636107000	1.796983000
1	5.824291000	-0.945948000	-0.215187000
1	4.650323000	0.205176000	-2.078589000
1	2.224775000	0.661975000	-1.928998000
7	0.617911000	-0.012985000	0.115290000
6	0.079647000	1.146078000	0.184322000
6	0.814105000	2.471204000	0.282257000
1	0.798559000	2.993482000	-0.678921000
1	0.341198000	3.119950000	1.024819000
1	1.852642000	2.315287000	0.566572000
7	-1.293424000	1.301478000	0.190427000
6	-2.338467000	0.367822000	0.053934000
6	-2.146764000	-1.008580000	-0.127031000
6	-3.648464000	0.874290000	0.101141000
1	-1.143461000	-1.402788000	-0.156708000
1	-3.806783000	1.939885000	0.242261000
6	-3.255649000	-1.843712000	-0.260311000
6	-4.741781000	0.028911000	-0.031790000
1	-3.092713000	-2.906739000	-0.400624000
1	-5.743165000	0.442908000	0.007359000
6	-4.553204000	-1.341332000	-0.214827000
1	-5.404726000	-2.003343000	-0.319083000
1	-1.606808000	2.252945000	0.299460000

Et

E(RB3LYP) = -310.961136615

6	0.408210000	-0.287901000	-0.012936000
6	-0.018922000	1.042524000	-0.017138000
6	-0.571095000	-1.292120000	0.003692000
6	-1.379196000	1.361170000	-0.006461000
6	-1.926329000	-0.980073000	0.013838000
6	-2.338048000	0.353713000	0.008861000
1	0.706339000	1.846759000	-0.027767000
1	-1.684199000	2.402117000	-0.009397000

OCH2CH3

E(RB3LYP) = -386.197253407

6	-0.056283000	-0.215791000	0.000002000
6	-0.948032000	-1.296529000	0.000005000
6	-0.552368000	1.091435000	-0.000016000
6	-2.317167000	-1.069004000	-0.000008000
6	-1.933461000	1.303793000	-0.000030000
6	-2.821803000	0.234365000	-0.000026000
1	-0.543006000	-2.301507000	0.000018000
1	-2.996337000	-1.914416000	-0.000005000

1	-3.393753000	0.600223000	0.017287000
1	-2.663155000	-1.775985000	0.026341000
1	-0.261788000	-2.333274000	0.008236000
6	1.874021000	-0.689339000	-0.029458000
1	2.049539000	-1.373862000	0.808963000
1	2.056403000	-1.284124000	-0.932948000
6	2.898197000	0.445342000	0.033130000
1	2.785563000	1.041426000	0.943097000
1	2.811749000	1.119058000	-0.823859000
1	3.912265000	0.037767000	0.028884000

$CH_2C(OH)(Me)_2$
E(RB3LYP) = -464.855385785

6	-0.597030000	0.107413000	0.531507000
6	-1.177810000	-1.146400000	0.302857000
6	-1.387143000	1.245683000	0.333854000
6	-2.501531000	-1.256669000	-0.116704000
6	-2.712476000	1.140767000	-0.085939000
6	-3.274665000	-0.113128000	-0.314253000
1	-0.585467000	-2.042301000	0.444908000
1	-2.930509000	-2.237839000	-0.288669000
1	-4.305698000	-0.199284000	-0.638547000
1	-3.304942000	2.037662000	-0.230341000
1	-0.961153000	2.227721000	0.514715000
6	0.839952000	0.241019000	0.984677000
1	0.990196000	1.243560000	1.397911000
1	1.032529000	-0.459779000	1.806597000
6	1.933178000	-0.000910000	-0.095394000
8	1.898048000	-1.372795000	-0.536837000
1	2.209316000	-1.932698000	0.182907000
6	1.694052000	0.830065000	-1.354445000
1	1.670284000	1.896876000	-1.116809000
1	2.495268000	0.650699000	-2.074753000
1	0.745635000	0.557647000	-1.819277000
6	3.312468000	0.303439000	0.504845000
1	4.095795000	0.076303000	-0.222071000
1	3.399152000	1.355503000	0.789615000
1	3.491228000	-0.299380000	1.402476000

$OCH_2CH=CH_2$
E(RB3LYP) = -424.282651284

6	-0.472127000	-0.235025000	0.027085000
6	-1.381867000	-1.297116000	-0.055709000
6	-0.941998000	1.080920000	0.054873000
6	-2.744986000	-1.041534000	-0.108010000
6	-2.317839000	1.321433000	0.002078000
6	-3.224638000	0.271053000	-0.078802000
1	-0.995700000	-2.309138000	-0.077392000
1	-3.439424000	-1.872036000	-0.171290000
1	-4.289479000	0.466980000	-0.119200000
1	-2.673441000	2.345717000	0.024385000
1	-0.259107000	1.917575000	0.114371000
8	0.847321000	-0.588529000	0.071691000
6	1.831944000	0.441142000	0.202645000
6	3.172760000	-0.212893000	0.324869000
1	3.257060000	-0.963909000	1.106084000
1	1.803549000	1.110953000	-0.664879000
1	1.616706000	1.032872000	1.103226000
6	4.221919000	0.093431000	-0.432117000
1	4.157033000	0.831695000	-1.225755000
1	5.185229000	-0.380948000	-0.284551000

NHCONHEt
E(RB3LYP) = -535.093463927

6	-1.255296000	-0.288643000	-0.022434000
6	-1.750676000	1.022147000	-0.028277000
6	-2.159805000	-1.361122000	0.013976000
6	-3.127784000	1.234132000	0.000186000
6	-3.530290000	-1.132333000	0.042846000
6	-4.026450000	0.170478000	0.035802000

1	-3.891083000	0.409302000	-0.000037000
1	-2.308887000	2.321285000	-0.000044000
1	0.115750000	1.941907000	-0.000019000
8	1.269653000	-0.540777000	0.000016000
6	2.241959000	0.505866000	0.000013000
1	2.106682000	1.135579000	0.888192000
1	2.106698000	1.135559000	-0.888182000
6	3.614857000	-0.138939000	0.000033000
1	3.749077000	-0.763049000	-0.886123000
1	3.749061000	-0.763029000	0.886205000
1	4.388602000	0.633420000	0.000031000

$O(CH_2)_3CH_3$
E(RB3LYP) = -464.845767459

6	-1.005093000	0.089756000	-0.143411000
6	-1.690518000	-1.095835000	0.138200000
6	-1.713088000	1.295309000	-0.238011000
6	-3.075425000	-1.063279000	0.322588000
6	-3.088376000	1.310966000	-0.052151000
6	-3.781712000	0.130584000	0.230182000
1	-1.165443000	-2.038236000	0.214875000
1	-3.598417000	-1.988094000	0.540389000
1	-4.855443000	0.145927000	0.374460000
1	-3.624571000	2.250530000	-0.128190000
1	-1.163357000	2.202708000	-0.458002000
8	0.342236000	0.176286000	-0.342134000
6	1.135739000	-1.010820000	-0.268767000
1	1.021374000	-1.469760000	0.722239000
6	2.586686000	-0.629505000	-0.518863000
1	2.657076000	-0.145914000	-1.499793000
1	3.165987000	-1.558838000	-0.585312000
1	0.790762000	-1.729791000	-1.022013000
6	3.190049000	0.279562000	0.557754000
1	3.120722000	-0.222468000	1.530825000
1	2.587630000	1.189109000	0.636389000
6	4.649119000	0.647415000	0.274481000
1	5.281355000	-0.244494000	0.214066000
1	4.743813000	1.184244000	-0.674694000
1	5.056345000	1.289864000	1.059830000

$N=NNMe_2$
E(RB3LYP) = -475.800878933

6	0.817527000	0.203201000	0.036646000
6	1.721989000	1.261801000	-0.108174000
6	1.308527000	-1.106722000	0.152651000
6	3.092077000	1.019340000	-0.153812000
6	2.678277000	-1.340571000	0.107726000
6	3.577387000	-0.282949000	-0.047233000
1	1.329133000	2.268866000	-0.186870000
1	3.780958000	1.848774000	-0.269960000
1	4.644113000	-0.473662000	-0.078013000
1	3.049683000	-2.355628000	0.200041000
1	0.613382000	-1.926106000	0.280683000
7	-0.553016000	0.564022000	0.073780000
7	-1.349207000	-0.412192000	0.007097000
7	-2.636916000	-0.093915000	0.119735000
6	-3.070875000	1.295644000	0.162570000
1	-2.543479000	1.823659000	0.957241000
1	-2.855062000	1.810742000	-0.781573000
1	-4.143933000	1.310709000	0.352493000
6	-3.571446000	-1.132410000	-0.276591000
1	-3.913637000	-0.999677000	-1.311531000
1	-3.066644000	-2.093542000	-0.194037000
1	-4.441317000	-1.123547000	0.384543000

$O(CH2)_4CH_3$
E(RB3LYP) = -504.165042859

6	-1.488356000	-0.387094000	0.011408000
6	-2.625360000	-1.174237000	0.238170000
6	-1.630193000	0.985236000	-0.215327000
6	-3.885753000	-0.593168000	0.236498000
6	-2.906248000	1.555116000	-0.213932000
6	-4.036879000	0.777857000	0.010127000

1	-1.061451000	1.851874000	-0.047395000
1	-3.497390000	2.253715000	-0.003917000
1	-5.094545000	0.351535000	0.058738000
1	-4.210035000	-1.976661000	0.071328000
1	-1.784849000	-2.380718000	0.018586000
7	0.116858000	-0.606774000	-0.068027000
1	0.319702000	-1.593678000	-0.021578000
6	1.207209000	0.253108000	-0.011968000
8	1.121408000	1.462526000	0.116558000
7	2.420089000	-0.407350000	-0.086334000
1	2.429311000	-1.327802000	-0.501528000
6	3.665602000	0.351612000	-0.184535000
1	3.801543000	0.745601000	-1.200142000
1	3.568036000	1.212702000	0.476302000
6	4.859514000	-0.509516000	0.214187000
1	4.962429000	-1.382332000	-0.439360000
1	4.761679000	-0.863104000	1.243497000
1	5.783528000	0.068350000	0.134844000

1	-2.493329000	-2.235507000	0.412069000
1	-4.757486000	-1.213565000	0.413281000
1	-5.022105000	1.228730000	0.009536000
1	-3.006254000	2.620396000	-0.391308000
1	-0.767783000	1.613132000	-0.393709000
8	-0.295604000	-1.050233000	0.027736000
6	0.913479000	-0.312591000	-0.170855000
6	2.064380000	-1.306594000	-0.095011000
1	1.816831000	-2.139545000	-0.761117000
1	2.105739000	-1.721732000	0.918018000
1	0.891094000	0.179247000	-1.152232000
1	0.994114000	0.461571000	0.599680000
6	3.446417000	-0.755667000	-0.487224000
1	3.405673000	-0.349084000	-1.506234000
1	4.122148000	-1.615585000	-0.539354000
6	4.072681000	0.291320000	0.455949000
1	3.861122000	0.012783000	1.495710000
1	5.161665000	0.237966000	0.349834000
6	3.646435000	1.744424000	0.210953000
1	2.577636000	1.901344000	0.373775000
1	4.179668000	2.424452000	0.881366000
1	3.872482000	2.049643000	-0.815733000

$OCH_2CH_2CH_3$

E(RB3LYP) = -425.521428124

6	0.610597000	-0.278280000	0.000151000
6	1.590688000	-1.279642000	-0.000115000
6	0.993313000	1.066365000	0.000258000
6	2.935578000	-0.936802000	-0.000328000
6	2.351623000	1.395010000	0.000035000
6	3.327508000	0.404868000	-0.000276000
1	1.272080000	-2.315240000	-0.000143000
1	3.684351000	-1.721251000	-0.000537000
1	4.378173000	0.669605000	-0.000449000
1	2.639356000	2.440713000	0.000113000
1	0.254536000	1.856419000	0.000570000
8	-0.682897000	-0.714505000	0.000397000
6	-1.739822000	0.245537000	0.000359000
6	-3.060615000	-0.508250000	0.000296000
1	-3.091861000	-1.159564000	0.879148000
1	-3.091097000	-1.160753000	-0.877692000
1	-1.660602000	0.885284000	0.889097000
1	-1.660644000	0.885529000	-0.888216000
6	-4.263690000	0.439204000	-0.000726000
1	-4.266101000	1.085103000	0.882766000
1	-4.265251000	1.084319000	-0.884805000
1	-5.200841000	-0.122181000	-0.000946000

$OCHMe_2$

E(RB3LYP) = -425.523837059

6	-0.345060000	-0.307646000	-0.019370000
6	-0.770659000	0.982382000	-0.353228000
6	-1.297378000	-1.287227000	0.294440000
6	-2.136605000	1.274891000	-0.375590000
6	-2.650975000	-0.981063000	0.269143000
6	-3.083301000	0.304387000	-0.067089000
1	-0.061058000	1.762245000	-0.593503000
1	-2.453664000	2.278783000	-0.636481000
1	-4.140239000	0.541944000	-0.085457000
1	-3.374586000	-1.751147000	0.513100000
1	-0.949157000	-2.280725000	0.550590000
8	0.954670000	-0.725206000	0.015248000
6	2.037325000	0.196446000	-0.225908000
1	1.763105000	0.848962000	-1.062706000
6	2.322795000	1.031376000	1.021060000
1	2.626005000	0.380686000	1.845572000
1	3.132626000	1.739782000	0.824862000
1	1.445069000	1.597378000	1.338313000
6	3.224776000	-0.661561000	-0.641134000
1	3.490261000	-1.356594000	0.159593000
1	2.987029000	-1.240693000	-1.535567000
1	4.091751000	-0.030883000	-0.854249000

NHMe

E(RB3LYP) = -327.001960322

6	2.313677000	0.334726000	-0.033966000
6	1.362743000	1.349843000	0.009656000
6	1.879134000	-0.993268000	-0.037881000
1	1.678534000	2.387686000	0.010056000
1	2.602525000	-1.800783000	-0.073571000
6	-0.000661000	1.059238000	0.048060000
6	0.525979000	-1.296995000	0.004717000
1	-0.715853000	1.871257000	0.077811000
1	0.202788000	-2.333818000	0.009578000
6	-0.441883000	-0.274550000	0.051090000
1	3.370921000	0.568779000	-0.066420000
7	-1.788549000	-0.608207000	0.131901000
1	-2.004825000	-1.549119000	-0.156751000
6	-2.841044000	0.364438000	-0.092302000
1	-2.839635000	1.125377000	0.693574000
1	-2.758848000	0.874524000	-1.063099000
1	-3.803434000	-0.147044000	-0.050732000

$NHNH_2$

E(RB3LYP) = -343.019195914

6	-0.447690000	0.247270000	-0.071301000
6	0.490190000	1.289650000	-0.001843000
6	0.006884000	-1.077463000	-0.075126000
6	1.850834000	1.010094000	0.054688000
6	1.373167000	-1.342580000	-0.016086000
6	2.305938000	-0.308883000	0.047974000
1	0.148230000	2.320627000	0.000639000
1	2.559237000	1.829774000	0.107201000
1	3.366689000	-0.524855000	0.094506000
1	1.709446000	-2.373995000	-0.020240000
1	-0.716173000	-1.879998000	-0.124723000
7	-1.809340000	0.568950000	-0.191563000
1	-2.034669000	1.498297000	0.143470000
7	-2.748270000	-0.432700000	0.129854000
1	-3.542193000	-0.361720000	-0.494395000
1	-3.063240000	-0.370414000	1.095674000

$NH(CH_2)_3CH_3$

E(RB3LYP) = -444.976683365

6	-1.053154000	0.145891000	-0.117680000
6	-1.857200000	1.299236000	-0.209588000
6	-1.681608000	-1.079541000	0.161927000

$N(C_3H_7)_2$

E(RB3LYP) = -523.611144034

6	-0.866424000	-0.082993000	0.236447000
6	-1.896233000	0.868753000	0.404903000
6	-1.244238000	-1.355306000	-0.249492000

6	-3.230241000	1.227037000	-0.023270000
6	-3.061938000	-1.136705000	0.352555000
6	-3.849034000	0.007442000	0.262893000
1	-1.389121000	2.255873000	-0.422294000
1	-3.823747000	2.131734000	-0.100726000
1	-4.921138000	-0.046166000	0.409008000
1	-3.522477000	-2.094817000	0.568955000
1	-1.098886000	-1.988932000	0.231831000
7	0.324760000	0.259741000	-0.270238000
1	0.615038000	1.088264000	-0.769847000
6	1.185152000	-0.895364000	-0.483691000
6	2.648505000	-0.476961000	-0.643117000
1	3.222052000	-1.364285000	-0.934250000
1	2.734258000	0.223454000	-1.485780000
1	1.097403000	-1.563829000	0.380160000
1	0.868523000	-1.473123000	-1.366598000
6	3.274509000	0.143813000	0.611974000
1	2.693463000	1.019273000	0.917649000
1	3.196552000	-0.573034000	1.438149000
6	4.740392000	0.538925000	0.412446000
1	5.353010000	-0.327228000	0.142288000
1	4.846787000	1.279753000	-0.386636000
1	5.162662000	0.972245000	1.323067000

6	-3.220810000	0.554919000	0.115320000
6	-2.572490000	-1.654523000	-0.530511000
6	-3.578735000	-0.706676000	-0.353020000
1	-1.672836000	1.859692000	0.773290000
1	-3.981547000	1.313997000	0.264712000
1	-4.611425000	-0.943646000	-0.578741000
1	-2.818421000	-2.643707000	-0.902243000
1	-0.495010000	-2.114741000	-0.427167000
7	0.464874000	0.210010000	0.531652000
6	1.404790000	-0.880700000	0.798627000
1	2.056246000	-0.570569000	1.623155000
1	0.847895000	-1.747519000	1.169285000
6	2.280854000	-1.305588000	-0.389580000
1	2.881101000	-0.450846000	-0.715524000
1	1.640535000	-1.571922000	-1.236493000
6	0.842983000	1.554293000	0.968900000
1	0.179478000	1.891276000	1.778036000
1	1.840716000	1.478197000	1.407981000
6	0.881451000	2.625861000	-0.135193000
1	-0.103370000	2.713535000	-0.601824000
1	1.075269000	3.586916000	0.356680000
6	1.934348000	2.381038000	-1.217539000
1	2.940207000	2.316539000	-0.788914000
1	1.737444000	1.452463000	-1.757767000
1	1.937736000	3.195177000	-1.947284000
6	3.198139000	-2.479497000	-0.034509000
1	3.866444000	-2.225664000	0.794843000
1	2.621629000	-3.360615000	0.265120000
1	3.821982000	-2.766120000	-0.884831000

$N(Et)_2$

E(RB3LYP) = -444.961827618

6	-0.484346000	-0.093501000	0.041472000
6	-1.164678000	1.135598000	-0.104695000
6	-1.274967000	-1.259038000	0.115279000
6	-2.551153000	1.188495000	-0.179205000
6	-2.663711000	-1.192336000	0.028025000
6	-3.319448000	0.026326000	-0.119267000
1	-0.603990000	2.057138000	-0.187289000
1	-3.033939000	2.152766000	-0.298156000
1	-4.400010000	0.071542000	-0.182692000
1	-3.235814000	-2.111912000	0.092835000
1	-0.817270000	-2.226537000	0.266183000
7	0.914902000	-0.123124000	0.095937000
6	1.606513000	-1.410539000	0.137413000
1	1.643265000	-1.806665000	1.166991000
1	1.027569000	-2.119355000	-0.454026000
6	3.021254000	-1.372838000	-0.444197000
1	3.692370000	-0.721611000	0.120006000
1	3.006502000	-1.034509000	-1.483121000
1	3.447442000	-2.379694000	-0.418479000
6	1.612567000	1.010734000	0.716154000
1	0.906403000	1.551219000	1.352621000
1	2.377755000	0.612645000	1.391820000
6	2.265651000	1.985123000	-0.271076000
1	1.527540000	2.416493000	-0.951045000
1	3.023793000	1.488039000	-0.879122000
1	2.747965000	2.804171000	0.272487000

$N(Me)_2$

E(RB3LYP) = -366.314051280

6	0.181533000	-0.000045000	-0.070596000
6	-0.552329000	-1.206013000	-0.031001000
6	-0.552351000	1.206001000	-0.031070000
6	-1.942475000	-1.196584000	0.016800000
6	-1.942430000	1.196633000	0.016756000
6	-2.655747000	0.000000000	0.037925000
1	-0.040818000	-2.158361000	-0.038547000
1	-2.471120000	-2.143626000	0.042786000
1	-3.738339000	0.000025000	0.077519000
1	-2.471108000	2.143657000	0.042696000
1	-0.040715000	2.158285000	-0.038683000
7	1.570816000	0.000034000	-0.160219000
6	2.295443000	1.240629000	0.061707000
1	2.149391000	1.646831000	1.074296000
1	3.360110000	1.060099000	-0.084068000
1	1.992580000	2.005179000	-0.658537000
6	2.295424000	-1.240661000	0.061616000
1	1.992443000	-2.005137000	-0.658647000
1	3.360080000	-1.060167000	-0.084308000
1	2.149384000	-1.646790000	1.074212000

NH_2

E(RB3LYP) = -287.687627634

6	1.879787000	-0.000010000	0.007521000
6	1.170680000	-1.200835000	0.003284000
6	1.170683000	1.200848000	0.003284000
1	1.703652000	-2.145499000	0.006669000
1	1.703697000	2.145488000	0.006673000
6	-0.220529000	-1.206189000	-0.004618000
6	-0.220490000	1.206183000	-0.004618000
1	-0.759695000	-2.148449000	-0.013431000
1	-0.759751000	2.148401000	-0.013421000
6	-0.937030000	-0.000019000	-0.007208000
1	2.963082000	0.000009000	0.014142000

COCl

E(RB3LYP) = -805.307681315

6	2.863050000	-0.375538000	0.000048000
6	1.930805000	-1.411770000	0.000066000
6	2.433580000	0.952601000	0.000006000
1	2.263698000	-2.442953000	0.000099000
1	3.157303000	1.759202000	-0.000008000
6	0.568631000	-1.128296000	0.000043000
6	1.075884000	1.243314000	-0.000018000
1	-0.153635000	-1.932607000	0.000057000
1	0.726846000	2.268138000	-0.000051000
6	0.133406000	0.201829000	0.000000000
1	3.923401000	-0.601523000	0.000067000

7	-2.333645000	0.000015000	-0.072815000
1	-2.787017000	0.837517000	0.261581000
1	-2.787063000	-0.837444000	0.261629000
6	-1.294689000	0.602404000	-0.000030000
8	-1.714559000	1.712747000	-0.000057000
17	-2.497949000	-0.779970000	-0.000024000

$N{=}N^+$			
E(RB3LYP) = -340.929675970			
6	-0.562714000	0.000141000	-0.000071000
6	0.096748000	-1.242973000	0.000111000
6	0.096995000	1.243137000	-0.000084000
6	1.480522000	-1.220944000	0.000284000
6	1.480745000	1.220780000	0.000092000

NH_3+			
E(RB3LYP) = -288.034437056			
6	1.917620000	0.000000000	0.006502000
6	1.226013000	1.210460000	0.001654000
6	1.226013000	-1.210460000	0.001654000
1	1.765701000	2.149131000	0.001415000
1	1.765701000	-2.149131000	0.001415000

6	2.165661000	-0.000162000	0.000275000
1	-0.461994000	-2.170434000	0.000113000
1	2.028545000	-2.154673000	0.000427000
1	3.249329000	-0.000286000	0.000411000
1	2.028971000	2.154391000	0.000088000
1	-0.461503000	2.170741000	-0.000229000
7	-1.941730000	0.000167000	-0.000247000
7	-3.048427000	-0.000113000	-0.000390000

6	-0.167791000	1.220951000	-0.006445000
6	-0.167791000	-1.220951000	-0.006445000
1	-0.709818000	2.160884000	-0.010241000
1	-0.709817000	-2.160884000	-0.010241000
6	-0.825944000	0.000000000	-0.010929000
1	3.000666000	0.000000000	0.010649000
7	-2.323729000	0.000000000	0.008904000
1	-2.699947000	-0.825326000	-0.468630000
1	-2.699948000	0.825300000	-0.468673000
1	-2.695157000	0.000025000	0.966034000

$N+(Me)_3$

E(RB3LYP) = -405.998262481

6	0.103045000	-0.027853000	0.000021000
6	0.802002000	-1.230245000	-0.000003000
6	0.780452000	1.191672000	-0.000029000
6	2.198051000	-1.205310000	0.000007000
6	2.171637000	1.201154000	-0.000060000
6	2.884158000	0.003354000	-0.000002000
1	0.304643000	-2.188617000	-0.000156000
1	2.740436000	-2.142726000	0.000018000
1	3.967095000	0.014971000	0.000030000
1	2.694938000	2.149360000	-0.000149000
1	0.254521000	2.137881000	-0.000039000
7	-1.411414000	-0.002509000	0.000031000
6	-1.910224000	0.714167000	-1.238836000
1	-1.531612000	0.190220000	-2.114026000
1	-2.999291000	0.705277000	-1.229239000
1	-1.547284000	1.737629000	-1.235125000
6	-2.020174000	-1.383065000	0.000705000
1	-1.708933000	-1.916349000	0.895642000
1	-3.101903000	-1.266390000	0.001000000
1	-1.709433000	-1.917055000	-0.893962000
6	-1.909949000	0.715384000	1.238141000
1	-2.999013000	0.705235000	1.229616000
1	-1.529973000	0.193272000	2.113851000
1	-1.548274000	1.739301000	1.232659000

$P+Me_3$

E(RB3LYP) = -692.662125777

6	-0.413165000	0.020987000	-0.000002000
6	-1.103580000	-1.202005000	-0.000001000
6	-1.126916000	1.227125000	-0.000001000
6	-2.493570000	-1.211368000	0.000000000
6	-2.519479000	1.205761000	0.000000000
6	-3.201015000	-0.008828000	0.000000000
1	-0.572045000	-2.147793000	-0.000002000
1	-3.023878000	-2.155844000	0.000000000
1	-4.284395000	-0.020423000	0.000001000
1	-3.068695000	2.139361000	0.000001000
1	-0.616508000	2.182257000	-0.000002000
15	1.390663000	0.003680000	0.000000000
6	2.009485000	-0.857259000	-1.474787000
1	3.101257000	-0.877836000	-1.463425000
1	1.634293000	-1.881614000	-1.494176000
6	2.055540000	1.690833000	-0.000027000
1	1.729784000	2.229097000	0.891266000
1	1.729788000	2.229064000	-0.891342000
6	2.009482000	-0.857211000	1.474817000
1	1.634279000	-1.881562000	1.494244000
1	3.101254000	-0.877800000	1.463451000
1	1.664014000	-0.338787000	-2.370785000
1	1.664020000	-0.338703000	2.370796000
1	3.146189000	1.637183000	-0.000023000

$S+Me_2$

E(RB3LYP) = -709.516359414

6	2.922102000	-0.253589000	0.000168000
6	2.431853000	1.049935000	-0.000393000
6	2.045826000	-1.341193000	0.000620000
1	3.113768000	1.891277000	-0.000744000
1	2.432602000	-2.352884000	0.001076000
6	1.057147000	1.279649000	-0.000558000
6	0.670877000	-1.132753000	0.000498000
1	0.668660000	2.291132000	-0.000954000
1	0.000524000	-1.983981000	0.000857000
6	0.196321000	0.180865000	-0.000040000
1	3.991550000	-0.426584000	0.000215000
16	-1.557960000	0.567853000	-0.000411000
6	-2.245705000	-0.348006000	1.420254000
1	-2.017003000	-1.408961000	1.340035000
1	-1.800286000	0.081946000	2.316198000
1	-3.322218000	-0.176229000	1.419699000
6	-2.245397000	-0.350045000	-1.419808000
1	-2.016455000	-1.410883000	-1.338385000
1	-3.321934000	-0.178466000	-1.419561000
1	-1.799999000	0.078812000	-2.316311000

$CH2NH_3+$

E(RB3LYP) = -327.368187889

6	2.337236000	-0.000090000	-0.255507000
6	1.660075000	-1.209451000	-0.100871000
6	1.660191000	1.209359000	-0.101010000
1	2.191487000	-2.147757000	-0.203154000
1	2.191692000	2.147600000	-0.203413000
6	0.301552000	-1.211659000	0.202329000
6	0.301670000	1.211735000	0.202197000
1	-0.213736000	-2.156439000	0.348534000
1	-0.213505000	2.156584000	0.348354000
6	-0.386270000	0.000083000	0.348981000
1	3.396396000	-0.000158000	-0.483636000
6	-1.854447000	0.000206000	0.641792000
1	-2.183461000	-0.888916000	1.179278000
1	-2.183400000	0.889637000	1.178805000
7	-2.657433000	-0.000138000	-0.682769000
1	-3.670779000	0.001088000	-0.527709000
1	-2.417233000	-0.824343000	-1.241825000
1	-2.415470000	0.822563000	-1.243314000

$P+(Me)C_6H_5$-C_6H_4-4Me

E(RB3LYP) = -1115.55301966

6	1.191088000	1.479994000	0.163302000
6	0.966610000	2.722582000	0.776348000
6	2.028646000	1.392856000	-0.956292000
6	1.582480000	3.863149000	0.272376000
6	2.637808000	2.542083000	-1.455013000
6	2.417330000	3.773332000	-0.841934000
1	0.314037000	2.811384000	1.637249000
1	1.411005000	4.820743000	0.749066000
1	2.896109000	4.664394000	-1.230477000
1	3.286454000	2.472147000	-2.319872000

$P+(Me)(C_6H_4$-4Me$)_2$

E(RB3LYP) = -1154.88353170

6	0.005211000	2.031916000	0.137100000
6	0.890297000	3.001229000	0.634305000
6	-0.850549000	2.345587000	-0.926400000
6	0.909768000	4.273007000	0.071961000
6	-0.820857000	3.621672000	-1.484721000
6	0.055159000	4.583269000	-0.986494000
1	1.567986000	2.773480000	1.449087000
1	1.591158000	5.020922000	0.459250000
1	0.072976000	5.575749000	-1.421082000
1	-1.484773000	3.862568000	-2.306201000

1	2.210693000	0.438284000	-1.434545000
15	0.365362000	-0.000377000	0.803696000
6	1.179140000	-1.489127000	0.166555000
6	2.446388000	-1.850818000	0.650462000
6	0.560241000	-2.264008000	-0.822647000
1	2.946112000	-1.257806000	1.407914000
1	-0.418173000	-1.993494000	-1.200178000
6	3.080259000	-2.982454000	0.149260000
6	1.205516000	-3.394197000	-1.320029000
1	4.056681000	-3.261915000	0.526262000
1	0.724406000	-3.993034000	-2.083932000
6	2.460585000	-3.753908000	-0.834685000
1	2.957769000	-4.635681000	-1.221276000
6	-1.382510000	0.008694000	0.346849000
6	-1.865985000	0.898057000	-0.620690000
6	-2.267678000	-0.898471000	0.951996000
1	-1.200618000	1.605227000	-1.100868000
1	-1.919652000	-1.608358000	1.694127000
6	-3.212836000	0.879299000	-0.969747000
6	-3.608369000	-0.903131000	0.593792000
1	-3.572771000	1.572987000	-1.721331000
1	-4.280397000	-1.609343000	1.068823000
6	-4.107335000	-0.013962000	-0.370103000
6	-5.569442000	-0.009467000	-0.727671000
1	-5.740435000	0.430549000	-1.711169000
1	-5.983565000	-1.019771000	-0.723919000
1	-6.137748000	0.578241000	0.001082000
6	0.493996000	-0.001147000	2.621546000
1	-0.040427000	0.858516000	3.026882000
1	0.053140000	-0.916145000	3.018590000
1	1.541348000	0.052615000	2.920092000
1	-1.538306000	1.604379000	-1.314578000
15	-0.000090000	0.366771000	0.854073000
6	1.484081000	-0.532368000	0.349512000
6	2.281465000	-0.068854000	-0.703972000
6	1.833403000	-1.724850000	1.003942000
1	2.029300000	0.847563000	-1.223530000
1	1.227369000	-2.116182000	1.813446000
6	3.409976000	-0.786573000	-1.088560000
6	2.962823000	-2.428103000	0.609276000
1	4.017263000	-0.416087000	-1.906821000
1	3.220023000	-3.347829000	1.123142000
6	3.773964000	-1.971939000	-0.440691000
6	5.012632000	-2.728475000	-0.839803000
1	5.843818000	-2.478289000	-0.172022000
1	4.858032000	-3.807511000	-0.775372000
1	5.321688000	-2.483513000	-1.857010000
6	-1.485465000	-0.531262000	0.350505000
6	-1.410674000	-1.558392000	-0.598029000
6	-2.733287000	-0.187124000	0.895544000
1	-0.457925000	-1.839042000	-1.030443000
1	-2.824334000	0.612759000	1.621892000
6	-2.565630000	-2.230123000	-0.987186000
6	-3.875448000	-0.868097000	0.498534000
1	-2.492639000	-3.023545000	-1.722561000
1	-4.832305000	-0.592291000	0.927997000
6	-3.813892000	-1.903258000	-0.446622000
6	-5.056464000	-2.653283000	-0.846136000
1	-5.307927000	-3.404671000	-0.090199000
1	-5.914244000	-1.983242000	-0.935084000
1	-4.923463000	-3.172060000	-1.796472000
6	-0.001273000	0.519197000	2.670482000
1	-0.871316000	1.092431000	2.992085000
1	-0.038494000	-0.473620000	3.119886000
1	0.906022000	1.027415000	2.998203000

$CH_2CH_2NMe_3$+

E(RB3LYP) = -484.656261085

6	1.032393000	-0.014950000	-0.755256000
6	1.645817000	-1.213455000	-0.369904000
6	1.639910000	1.194263000	-0.403216000
6	2.825433000	-1.201174000	0.370134000
6	2.822819000	1.209228000	0.337129000
6	3.414008000	0.011482000	0.730675000
1	1.216526000	-2.166487000	-0.665453000
1	3.293540000	-2.136757000	0.653065000
1	4.335054000	0.020399000	1.301115000
1	3.285242000	2.154913000	0.594464000
1	1.203418000	2.134552000	-0.726989000
6	-0.245549000	-0.026769000	-1.572178000
1	-0.485063000	0.982259000	-1.915555000
1	-0.081213000	-0.606923000	-2.488118000
6	-1.480049000	-0.683176000	-0.942809000
1	-1.260105000	-1.699056000	-0.612233000
1	-2.275882000	-0.734900000	-1.687816000
7	-2.122269000	0.005985000	0.273092000
6	-3.448305000	-0.666689000	0.525636000
1	-3.281878000	-1.732768000	0.670981000
1	-3.896644000	-0.236854000	1.419910000
1	-4.100015000	-0.505064000	-0.331260000
6	-2.365138000	1.466385000	0.005669000
1	-1.411913000	1.982218000	-0.071093000
1	-2.927669000	1.569691000	-0.921198000
1	-2.938632000	1.878998000	0.834272000
6	-1.271921000	-0.142571000	1.512141000
1	-1.128102000	-1.202813000	1.712118000
1	-0.310466000	0.335515000	1.350198000
1	-1.796821000	0.325729000	2.343827000

$(CH_2)_3N(Me)_3$+

E(RB3LYP) = -523.983435787

6	-1.687719000	0.797138000	-0.219413000
6	-2.195463000	0.586104000	1.069175000
6	-2.193016000	0.024608000	-1.270503000
6	-3.174492000	-0.377253000	1.301196000
6	-3.174111000	-0.940941000	-1.041684000
6	-3.664239000	-1.146537000	0.245544000
1	-1.844080000	1.196937000	1.895813000
1	-3.567121000	-0.516753000	2.301902000
1	-4.433087000	-1.888954000	0.424091000
1	-3.562985000	-1.520769000	-1.870828000
1	-1.835757000	0.193347000	-2.282049000
6	-0.612478000	1.837383000	-0.460950000
1	-0.903832000	2.788492000	-0.006906000
6	0.769355000	1.452993000	0.126143000
1	0.652074000	1.290721000	1.200598000
1	1.453982000	2.294311000	-0.009425000
1	-0.513108000	2.027870000	-1.533974000
6	1.308162000	0.201197000	-0.557838000
1	0.565247000	-0.597343000	-0.532572000
1	1.549569000	0.408270000	-1.602471000
7	2.582231000	-0.406205000	0.043540000
6	2.985293000	-1.577223000	-0.815949000
1	3.878146000	-2.035705000	-0.393790000
1	2.169820000	-2.298093000	-0.834832000
1	3.191345000	-1.222012000	-1.824058000
6	3.705309000	0.595759000	0.058238000
1	3.855554000	0.972397000	-0.952493000
1	3.451964000	1.414032000	0.727347000
1	4.610355000	0.101131000	0.408065000
6	2.330631000	-0.902802000	1.443516000
1	2.092001000	-0.062450000	2.089577000
1	1.499817000	-1.606103000	1.423182000
1	3.231092000	-1.398440000	1.803188000

$CH_2N(Me)_3$+

$P(Et)_3$+

E(RB3LYP) = -445.334253166

6	0.612737000	0.000021000	-0.521309000
6	1.295181000	-1.207584000	-0.320395000
6	1.295245000	1.207595000	-0.320331000
6	2.620194000	-1.207419000	0.106250000
6	2.620270000	1.207374000	0.106296000
6	3.281455000	-0.000042000	0.326688000
1	0.801048000	-2.153104000	-0.519282000
1	3.139721000	-2.146845000	0.251914000
1	4.315051000	-0.000104000	0.651670000
1	3.139834000	2.146781000	0.251948000
1	0.801143000	2.153135000	-0.519190000
6	-0.805444000	0.000165000	-1.015827000
1	-1.017034000	0.885180000	-1.616768000
1	-1.017212000	-0.884546000	-1.617157000
7	-1.904814000	0.000006000	0.084099000
6	-1.796065000	-1.225802000	0.949026000
1	-0.831260000	-1.224309000	1.449899000
1	-2.600500000	-1.204252000	1.682687000
1	-1.891495000	-2.110890000	0.321917000
6	-3.243279000	-0.000806000	-0.604784000
1	-4.029576000	0.000041000	0.148604000
1	-3.324345000	0.890005000	-1.225532000
1	-3.324323000	-0.893052000	-1.223470000
6	-1.797047000	1.226481000	0.948169000
1	-1.893707000	2.111069000	0.320530000
1	-2.601108000	1.204563000	1.682223000
1	-0.832009000	1.226390000	1.448611000

E(RB3LYP) = -810.634587660

6	0.930810000	0.000040000	0.042124000
6	1.768594000	-0.000071000	-1.084723000
6	1.492581000	0.000162000	1.325776000
6	3.149591000	-0.000073000	-0.924162000
6	2.877487000	0.000174000	1.476956000
6	3.704123000	0.000044000	0.356063000
1	1.355787000	-0.000174000	-2.087872000
1	3.791943000	-0.000166000	-1.796452000
1	4.780731000	0.000050000	0.477995000
1	3.307300000	0.000266000	2.471283000
1	0.867888000	0.000256000	2.210273000
15	-0.861384000	-0.000021000	-0.212425000
6	-1.346246000	-1.479567000	-1.179516000
1	-2.411764000	-1.375925000	-1.405533000
1	-0.816899000	-1.406953000	-2.134500000
6	-1.728881000	0.000022000	1.399391000
1	-1.380461000	0.878307000	1.949153000
1	-1.380434000	-0.878180000	1.949271000
6	-1.346278000	1.479426000	-1.179655000
1	-0.816820000	1.406791000	-2.134573000
1	-2.411762000	1.375697000	-1.405810000
6	-1.048038000	2.818347000	-0.491512000
1	0.013435000	2.926714000	-0.261130000
1	-1.617862000	2.939880000	0.431897000
1	-1.328653000	3.635643000	-1.158000000
6	-3.261436000	-0.000015000	1.288541000
1	-3.690836000	0.000026000	2.291775000
1	-3.637831000	0.885921000	0.773523000
1	-3.637799000	-0.886024000	0.773625000
6	-1.047805000	-2.818401000	-0.491293000
1	0.013738000	-2.926717000	-0.261224000
1	-1.617334000	-2.939832000	0.432316000
1	-1.328621000	-3.635788000	-1.157585000

$CH2NHMe_2$+

E(RB3LYP) = -406.016110717

6	-3.070904000	-0.009727000	-0.352793000
6	-2.461728000	1.126708000	0.176327000
6	-2.356010000	-1.202848000	-0.457174000
1	-3.021751000	2.048932000	0.273317000
1	-2.835106000	-2.091921000	-0.848991000
6	-1.132589000	1.076367000	0.590431000
6	-1.030911000	-1.257573000	-0.034882000
1	-0.668966000	1.960796000	1.015468000
1	-0.496371000	-2.202752000	-0.082186000
6	-0.405550000	-0.114197000	0.481010000
1	-4.105774000	0.029599000	-0.671159000
6	1.027439000	-0.182074000	0.923530000
1	1.311406000	0.659705000	1.555971000
1	1.242385000	-1.109462000	1.456603000
7	2.006957000	-0.163032000	-0.264903000
1	1.673146000	-0.882586000	-0.911572000
6	3.398934000	-0.534738000	0.158760000
1	4.047333000	-0.543562000	-0.715942000
1	3.752227000	0.204998000	0.875723000
1	3.379389000	-1.520774000	0.619797000
6	1.985302000	1.140647000	-1.012116000
1	0.964648000	1.353400000	-1.321297000
1	2.350178000	1.923108000	-0.347940000
1	2.634659000	1.056356000	-1.882033000

$CH_2CH_2NHMe_2$+

E(RB3LYP) = -445.343742463

6	-0.772745000	0.265086000	-0.748656000
6	-1.508910000	1.259863000	-0.089390000
6	-1.195020000	-1.066590000	-0.641289000
6	-2.634990000	0.929411000	0.659736000
6	-2.323189000	-1.398457000	0.112048000
6	-3.041761000	-0.401374000	0.765607000
1	-1.218632000	2.301963000	-0.183823000
1	-3.203646000	1.710977000	1.149727000
1	-3.922910000	-0.655414000	1.342518000
1	-2.646311000	-2.431071000	0.171618000
1	-0.669121000	-1.847503000	-1.183059000
6	0.475360000	0.621521000	-1.533397000
1	0.741814000	-0.187811000	-2.217586000
1	0.303548000	1.502624000	-2.158059000
6	1.654774000	0.965268000	-0.612473000
1	1.431378000	1.859669000	-0.030879000
1	2.585178000	1.125882000	-1.159334000
7	1.915142000	-0.140082000	0.399696000
1	0.979836000	-0.466306000	0.681797000
6	2.638153000	-1.312942000	-0.197039000
1	2.097982000	-1.661343000	-1.073626000
1	3.641613000	-0.995102000	-0.476693000
1	2.691369000	-2.108733000	0.544168000
6	2.615193000	0.367196000	1.626767000
1	3.578120000	0.783833000	1.334060000
1	1.999942000	1.135701000	2.091099000
1	2.762661000	-0.460687000	2.318707000

$CH2CH2NH_3$+

E(RB3LYP) = -366.696687911

6	0.027379000	-0.195114000	0.565848000
6	-0.675470000	-1.275366000	0.014115000
6	-0.597087000	1.058405000	0.624775000
6	-1.970509000	-1.104106000	-0.467964000
6	-1.895261000	1.229711000	0.139338000

CH2CH2CH2-

E(RB3LYP) = -349.623070721

6	-0.090522000	-0.271170000	-0.004847000
6	-0.537336000	1.055740000	-0.019642000
6	-1.056763000	-1.286608000	0.018718000
6	-1.905002000	1.353593000	-0.014844000
6	-2.423532000	-0.997570000	0.008394000

6	-2.580904000	0.149496000	-0.409754000
1	-0.221455000	-2.261308000	-0.014228000
1	-2.508565000	-1.951121000	-0.876782000
1	-3.591738000	0.278160000	-0.777660000
1	-2.372204000	2.200278000	0.207310000
1	-0.088411000	1.896489000	1.093563000
6	1.453039000	-0.368920000	1.053300000
1	1.735027000	0.454368000	1.717033000
1	1.562888000	-1.287413000	1.636182000
6	2.445971000	-0.462451000	-0.110181000
1	3.487220000	-0.467876000	0.212475000
1	2.255798000	-1.337977000	-0.730755000
7	2.267913000	0.741281000	-1.029045000
1	1.260393000	0.863283000	-1.216603000
1	2.763072000	0.631201000	-1.917396000
1	2.599635000	1.603013000	-0.586689000

6	-2.854032000	0.331830000	-0.006066000
1	0.214201000	1.835172000	-0.070821000
1	-2.229265000	2.391196000	-0.020629000
1	-3.915357000	0.565047000	-0.009073000
1	-3.150157000	-1.805689000	0.011566000
1	-0.724659000	-2.322202000	0.040898000
6	1.388792000	-0.610343000	-0.007899000
1	1.536606000	-1.303593000	0.876857000
1	1.561916000	-1.280214000	-0.868730000
6	2.353272000	0.540145000	-0.058600000
1	2.173394000	1.232486000	0.781066000
1	4.051328000	-0.504638000	-0.942323000
6	3.784119000	0.047645000	-0.026764000
1	4.027645000	-0.663116000	0.816705000
1	4.500374000	0.875979000	0.053790000

S-

E(RB3LYP) = -629.979067734

6	-0.595662000	-0.000240000	-0.000075000
6	0.164209000	-1.200920000	0.000115000
6	0.164051000	1.200771000	-0.000075000
6	1.555085000	-1.199152000	0.000285000
6	1.554794000	1.199405000	0.000097000
6	2.276541000	0.000102000	0.000278000
1	-0.375970000	-2.141884000	0.000123000
1	2.087219000	-2.148310000	0.000426000
1	3.362070000	0.000338000	0.000409000
1	2.086960000	2.148514000	0.000088000
1	-0.376865000	2.141316000	-0.000216000
16	-2.343595000	0.000014000	-0.000286000

O-

E(RB3LYP) = -306.993982233

6	-1.077858000	-0.000051000	-0.000126000
6	-0.287488000	-1.211784000	0.000055000
6	-0.287406000	1.211846000	-0.000132000
6	1.100182000	-1.200115000	0.000229000
6	1.100221000	1.200105000	0.000042000
6	1.827688000	-0.000052000	0.000230000
1	-0.831455000	-2.153367000	0.000068000
1	1.637311000	-2.148457000	0.000372000
1	2.913260000	0.000021000	0.000356000
1	1.637556000	2.148344000	0.000034000
1	-0.831427000	2.153383000	-0.000274000
8	-2.347160000	0.000048000	-0.000293000

SO_2-

E(RB3LYP) = -780.429018759

6	-0.088888000	-0.000025000	-0.108774000
6	-0.785577000	-1.205992000	-0.060358000
6	-0.785524000	1.205971000	-0.060273000
6	-2.178117000	-1.207581000	0.036987000
6	-2.178092000	1.207605000	0.037051000
6	-2.878824000	0.000026000	0.079766000
1	-0.217185000	-2.130873000	-0.066322000
1	-2.719012000	-2.149027000	0.087610000
1	-3.962198000	0.000040000	0.155632000
1	-2.718958000	2.149064000	0.087743000
1	-0.217037000	2.130793000	-0.066228000
16	1.777956000	-0.000028000	-0.353270000
8	2.172317000	1.287643000	0.369124000
8	2.172337000	-1.287590000	0.369312000

CO_2-

E(RB3LYP) = -420.396698265

6	0.278996000	0.000027000	0.000073000
6	-0.437762000	-1.201270000	0.000278000
6	-0.437864000	1.201242000	-0.000161000
6	-1.833036000	-1.205625000	0.000277000
6	-1.833123000	1.205505000	-0.000302000
6	-2.538160000	-0.000085000	-0.000056000
1	0.135597000	-2.121654000	0.000412000
1	-2.374245000	-2.148347000	0.000499000
1	-3.624554000	-0.000077000	-0.000151000
1	-2.374426000	2.148179000	-0.000570000
1	0.135372000	2.121715000	-0.000214000
6	1.833893000	0.000042000	0.000060000
8	2.368794000	1.133500000	0.000543000
8	2.369281000	-1.133354000	-0.000667000

PO_3H-

E(RB3LYP) = -799.408026958

6	0.409336000	0.038844000	0.111948000
6	1.072249000	-1.185482000	0.268664000
6	1.181498000	1.176196000	-0.148975000
6	2.461558000	-1.275007000	0.170154000
6	2.571541000	1.095908000	-0.251516000
6	3.217264000	-0.130852000	-0.090869000
1	0.490325000	-2.082342000	0.462791000
1	2.955581000	-2.235017000	0.293101000
1	4.298714000	-0.195585000	-0.167797000
1	3.153638000	1.990837000	-0.454532000
1	0.662438000	2.121738000	-0.264877000
15	-1.476556000	0.162184000	0.280846000
8	-3.131080000	-0.616895000	-0.108953000
8	-1.803372000	-1.019343000	-0.785534000
8	-1.732615000	1.640841000	0.141664000
1	-1.556508000	-0.386863000	1.584774000

OPO_3H-

E(RB3LYP) = -874.690324706

6	-0.872695000	0.375172000	0.239160000
6	-1.149870000	-0.977217000	-0.042880000
6	-1.943440000	1.291215000	0.236201000
6	-2.454417000	-1.375982000	-0.323918000
6	-3.240627000	0.875217000	-0.042909000
6	-3.511994000	-0.464581000	-0.329311000
1	-0.336416000	-1.689686000	-0.011099000
1	-2.646010000	-2.423809000	-0.537705000
1	-4.523229000	-0.790010000	-0.550031000
1	-4.046030000	1.604491000	-0.040391000
1	-1.722573000	2.330284000	0.454432000
8	0.343750000	0.858446000	0.528961000
15	1.951938000	0.077295000	0.330940000
8	3.418378000	0.003485000	-0.664905000
8	1.748827000	-1.295178000	0.891256000
8	2.061281000	0.480780000	-1.237349000
1	2.455545000	1.086093000	1.158929000

SO_3^-

E(RB3LYP) = -855.687802103

6	-0.275245000	0.000230000	-0.034605000
6	-0.973567000	1.206939000	-0.023594000

NNO_2-

E(RB3LYP) = -491.688640958

6	-0.155344000	0.304481000	-0.000020000
6	-1.149356000	1.321821000	-0.000015000

6	-0.973347000	-1.206765000	-0.023668000
6	-2.367967000	1.206090000	0.002281000
6	-2.367657000	-1.206268000	0.002187000
6	-3.069998000	-0.000108000	0.017523000
1	-0.412037000	2.133310000	-0.052118000
1	-2.908027000	2.148297000	0.006144000
1	-4.155505000	-0.000261000	0.035344000
1	-2.907627000	-2.148523000	0.005905000
1	-0.411712000	-2.133063000	-0.052224000
16	1.556671000	0.000040000	0.003002000
8	1.935953000	-1.250402000	-0.703365000
8	1.936120000	1.250559000	-0.703118000
8	1.884783000	-0.000296000	1.452505000

6	-0.627081000	-1.035588000	-0.000050000
6	-2.504619000	1.034252000	0.000001000
6	-1.995329000	-1.307144000	-0.000001000
6	-2.951322000	-0.292594000	0.000031000
1	-0.800656000	2.348664000	0.000098000
1	-3.222432000	1.850358000	0.000036000
1	-4.011665000	-0.524337000	0.000047000
1	-2.316619000	-2.345962000	-0.000001000
1	0.089580000	-1.839632000	-0.000173000
7	1.130940000	0.816818000	0.000031000
7	2.187966000	0.011079000	-0.000135000
8	2.105835000	-1.249864000	0.000101000
8	3.310134000	0.570396000	0.000030000

$OCH_2CH_2CH_2O$-

E(RB3LYP) = -500.161965224

6	-0.993853000	-0.362481000	-0.000586000
6	-2.081073000	-1.243898000	-0.153530000
6	-1.252794000	1.011051000	0.142262000
6	-3.383679000	-0.765785000	-0.161587000
6	-2.569283000	1.474584000	0.132486000
6	-3.643475000	0.601166000	-0.017482000
1	-1.867627000	-2.300892000	-0.264650000
1	-4.205967000	-1.464598000	-0.281847000
1	-4.661924000	0.973483000	-0.024427000
1	-2.749462000	2.539555000	0.242168000
1	-0.434867000	1.709331000	0.251900000
8	0.230337000	-0.917640000	-0.000712000
6	1.398438000	-0.061411000	0.190954000
6	2.664829000	-0.878649000	0.120164000
1	2.707964000	-1.385225000	-0.851686000
1	2.682097000	-1.638497000	0.916578000
1	1.434223000	0.703225000	-0.587992000
1	1.304965000	0.427452000	1.169538000
6	3.898576000	0.087548000	0.241226000
1	3.902343000	0.402269000	1.334810000
1	4.797843000	-0.597080000	0.168953000
8	3.877701000	1.099919000	-0.628885000

OCH_2CH_2O-

E(RB3LYP) = -460.836590082

6	0.520444000	-0.285015000	-0.000021000
6	1.514233000	-1.285285000	-0.000135000
6	0.925973000	1.062007000	-0.000038000
6	2.860214000	-0.949023000	-0.000255000
6	2.284096000	1.382354000	-0.000160000
6	3.262841000	0.391102000	-0.000269000
1	1.191407000	-2.320280000	-0.000123000
1	3.605474000	-1.738994000	-0.000340000
1	4.315383000	0.652345000	-0.000363000
1	2.575214000	2.428627000	-0.000168000
1	0.183155000	1.847951000	0.000049000
8	-0.751290000	-0.701849000	0.000101000
6	-1.847080000	0.276103000	0.000169000
6	-3.231607000	-0.412324000	0.000215000
1	-3.221092000	-1.109663000	0.889014000
1	-3.221182000	-1.109610000	-0.888628000
1	-1.758057000	0.903395000	0.893841000
1	-1.758135000	0.903435000	-0.893482000
8	-4.204566000	0.509759000	0.000294000

CF_2OCF_2-

E(RB3LYP) = -782.696246263

6	-3.661347000	0.773146000	0.072309000
6	-2.609950000	1.686255000	0.010489000
6	-3.384981000	-0.594921000	0.096214000
1	-2.816039000	2.751701000	-0.006639000
1	-4.197774000	-1.312551000	0.146482000
6	-1.289581000	1.237570000	-0.028204000
6	-2.066879000	-1.042976000	0.058295000
1	-0.458211000	1.929720000	-0.071094000
1	-1.846852000	-2.103490000	0.081192000
6	-1.012615000	-0.128229000	-0.003882000
1	-4.688429000	1.122867000	0.103520000
6	0.428158000	-0.626820000	-0.070681000
9	0.563654000	-1.326409000	-1.287515000
9	0.563866000	-1.656328000	0.880725000
8	1.297956000	0.338405000	0.077175000
6	2.835409000	-0.028259000	-0.012413000
9	3.245803000	0.604134000	1.186793000
9	3.203829000	0.961927000	-0.958183000

$B(OH)_3$-

E(RB3LYP) = -484.308978774

6	-0.088460000	0.019704000	-0.019815000
6	-0.814281000	-1.184140000	-0.026053000
6	-0.847093000	1.201852000	-0.001194000
6	-2.209842000	-1.214622000	-0.003297000
6	-2.244329000	1.190107000	0.019778000
6	-2.936685000	-0.021960000	0.021272000
1	-0.259169000	-2.117781000	-0.059313000
1	-2.734920000	-2.167508000	-0.007949000
1	-4.023276000	-0.037899000	0.037068000
1	-2.796778000	2.127341000	0.032977000
1	-0.314383000	2.147708000	-0.011815000
5	1.561649000	0.026177000	0.006009000
8	2.014005000	1.333226000	-0.526995000
1	2.883420000	1.488372000	-0.147316000
8	2.079003000	-0.168928000	1.386052000
1	2.530489000	-1.016760000	1.389193000
8	2.114150000	-1.118640000	-0.794873000
1	2.093250000	-0.865267000	-1.720502000

CH_2CO_2-

E(RB3LYP) = -459.717012055

6	0.222848000	0.267186000	-0.427079000
6	0.721934000	-1.045492000	-0.355670000
6	1.093246000	1.312161000	-0.084168000
6	2.035891000	-1.292889000	0.031235000
6	2.411070000	1.067097000	0.304810000
6	2.893333000	-0.239463000	0.361028000
1	0.039796000	-1.859592000	-0.569094000
1	2.394668000	-2.316983000	0.083625000
1	3.917638000	-0.436167000	0.662468000
1	3.059490000	1.898737000	0.565746000
1	0.725286000	2.333341000	-0.119389000

OCH_2O-

E(RB3LYP) = -421.552052350

6	-2.893532000	0.504721000	-0.000036000
6	-2.587665000	-0.864515000	-0.000028000
6	-1.825730000	1.410252000	-0.000032000
1	-3.397518000	-1.592615000	-0.000032000
1	-2.031562000	2.479685000	-0.000039000
6	-1.276308000	-1.316003000	-0.000016000
6	-0.504671000	0.978849000	-0.000020000
1	-1.056179000	-2.379858000	-0.000009000
1	0.300759000	1.708054000	-0.000018000
6	-0.150856000	-0.417157000	-0.000010000
1	-3.922246000	0.850069000	-0.000046000

6	-1.197544000	0.540438000	-0.832319000
1	-1.364401000	1.616201000	-0.915502000
1	-1.390987000	0.086928000	-1.811849000
6	-2.295573000	-0.075094000	0.143490000
8	-3.090125000	0.753527000	0.634882000
8	-2.246465000	-1.319293000	0.272122000
8	1.055979000	-0.840867000	0.000000000
6	3.106519000	0.510832000	0.000055000
1	2.625358000	0.849009000	-0.931752000
1	2.625317000	0.848991000	0.931846000
8	4.150212000	-0.109783000	0.000071000

Substituted pyridines

SO2CN
E(RB3LYP) = -889.215627848

6	0.463689000	0.000345000	-0.184521000
6	1.137293000	-1.209684000	-0.072136000
6	2.509968000	-1.145716000	0.169810000
7	3.185591000	-0.000615000	0.293329000
6	2.510132000	1.144971000	0.173510000
6	1.137457000	1.209906000	-0.068199000
1	0.624319000	-2.156743000	-0.178584000
1	3.088238000	-2.059221000	0.265271000
1	3.088532000	2.058085000	0.271885000
1	0.624564000	2.157352000	-0.171537000
16	-1.306107000	0.001007000	-0.496940000
8	-1.691221000	-1.273561000	-1.075047000
6	-1.944080000	-0.002197000	1.175033000
7	-2.379325000	-0.004426000	2.244517000
8	-1.691099000	1.277805000	-1.070190000

C(CN)3
E(RB3LYP) = -564.416617138

6	0.455194000	0.037178000	-0.000029000
6	1.164414000	1.230920000	-0.000028000
6	2.559597000	1.160991000	-0.000020000
7	3.244643000	0.017962000	-0.000011000
6	2.543939000	-1.119753000	-0.000011000
6	1.152592000	-1.168576000	-0.000020000
1	0.668593000	2.193192000	-0.000040000
1	3.145176000	2.075137000	-0.000022000
1	3.118705000	-2.040530000	-0.000005000
1	0.641825000	-2.124312000	-0.000025000
6	-1.101937000	0.005190000	-0.000003000
6	-1.582185000	-0.709715000	-1.206578000
7	-1.930438000	-1.271234000	-2.149032000
6	-1.582129000	-0.709258000	1.206867000
7	-1.930330000	-1.270419000	2.149554000
6	-1.680396000	1.365797000	-0.000249000
7	-2.119422000	2.429385000	-0.000437000

NO2
E(RB3LYP) = -452.909787782

6	0.000000000	0.000000000	-0.231885000
6	0.000000000	1.207444000	0.449786000
6	0.000000000	1.144073000	1.842539000
7	0.000000000	0.000000000	2.532267000
6	0.000000000	-1.144073000	1.842539000
6	0.000000000	-1.207444000	0.449786000
1	0.000000000	2.147787000	-0.083203000
1	0.000000000	2.058432000	2.427327000
1	0.000000000	-2.058432000	2.427327000
1	0.000000000	-2.147787000	-0.083203000
7	0.000000000	0.000000000	-1.719448000
8	0.000000000	-1.085494000	-2.280910000
8	0.000000000	1.085494000	-2.280910000

CN
E(RB3LYP) = -340.613930868

6	0.000000000	0.000000000	0.600891000
6	0.000000000	1.203648000	-0.112454000
6	0.000000000	1.142802000	-1.503069000
7	0.000000000	0.000000000	-2.195429000
6	0.000000000	-1.142802000	-1.503069000
6	0.000000000	-1.203648000	-0.112454000
1	0.000000000	2.155476000	0.402887000
1	0.000000000	2.057917000	-2.087356000
1	0.000000000	-2.057917000	-2.087356000
1	0.000000000	-2.155476000	0.402887000
6	0.000000000	0.000000000	2.033431000
7	0.000000000	0.000000000	3.188184000

N(CF3)2
E(RB3LYP) = -977.998755219

6	0.933397000	0.000054000	0.000026000
6	1.637016000	-0.765597000	-0.923765000
6	3.029186000	-0.736970000	-0.870646000
7	3.723546000	0.000053000	-0.000035000
6	3.029222000	0.737084000	0.870601000
6	1.637056000	0.765706000	0.923783000
1	1.121719000	-1.365262000	-1.663399000
1	3.610489000	-1.328037000	-1.571795000
1	3.610552000	1.328144000	1.571733000
1	1.121798000	1.365375000	1.663443000
7	-0.509597000	0.000032000	0.000094000
6	-1.221461000	-1.207602000	0.240408000
9	-0.468885000	-2.045393000	0.968209000
9	-2.365282000	-0.980590000	0.902484000
9	-1.548823000	-1.865591000	-0.897949000
6	-1.221604000	1.207555000	-0.240386000
9	-2.364952000	0.980478000	-0.903264000
9	-1.549879000	1.865160000	0.897937000
9	-0.468743000	2.045691000	-0.967475000

CHO
E(RB3LYP) = -361.705418932

6	0.000000000	0.563537000	0.000000000
6	-1.321983000	0.117778000	0.000000000
6	-1.563153000	-1.255403000	0.000000000
7	-0.590506000	-2.170044000	0.000000000
6	0.675650000	-1.732682000	0.000000000
6	1.024367000	-0.386705000	0.000000000
1	-2.147532000	0.821983000	0.000000000
1	-2.580033000	-1.636528000	0.000000000
1	1.444130000	-2.499834000	0.000000000
1	2.060058000	-0.069600000	0.000000000
6	0.297352000	2.021329000	0.000000000
8	1.410203000	2.491235000	0.000000000
1	-0.598102000	2.677286000	0.000000000

NHNO2
E(RB3LYP) = -508.265722476

6	0.240175000	-0.278253000	0.112019000

COCH3
E(RB3LYP) = -401.039351105

6	0.196055000	-0.056260000	-0.000010000

6	0.695210000	1.041593000	0.148648000
6	2.067703000	1.255852000	0.032988000
7	2.982466000	0.292708000	-0.097156000
6	2.528105000	-0.964130000	-0.119538000
6	1.185314000	-1.303458000	-0.023643000
1	0.017017000	1.871798000	0.256582000
1	2.445310000	2.273925000	0.052523000
1	3.274543000	-1.745782000	-0.225140000
1	0.882848000	-2.344547000	-0.055648000
7	-1.100116000	-0.681971000	0.260027000
1	-1.321390000	-1.667729000	0.213442000
7	-2.235158000	0.061492000	-0.031994000
8	-3.267403000	-0.592460000	-0.096201000
8	-2.123562000	1.267099000	-0.161393000

6	-0.451138000	1.182110000	-0.000010000
6	-1.845195000	1.212640000	0.000002000
7	-2.608270000	0.117444000	0.000007000
6	-1.982790000	-1.066045000	0.000004000
6	-0.599334000	-1.205624000	-0.000002000
1	0.101517000	2.113331000	-0.000015000
1	-2.370906000	2.163171000	0.000004000
1	-2.622699000	-1.943502000	0.000010000
1	-0.130757000	-2.181678000	0.000000000
6	1.697079000	-0.204984000	-0.000017000
8	2.198854000	-1.310618000	0.000004000
6	2.552076000	1.044994000	0.000011000
1	2.344149000	1.658165000	-0.881874000
1	2.344175000	1.658099000	0.881948000
1	3.601052000	0.754265000	-0.000012000

OCF3
E(RB3LYP) = -660.739443711

6	0.524809000	0.360647000	-0.004847000
6	1.515214000	1.335765000	-0.001961000
6	2.839886000	0.914392000	0.001830000
7	3.214126000	-0.369539000	0.002975000
6	2.241093000	-1.281161000	0.000163000
6	0.877509000	-0.982973000	-0.003938000
1	1.250280000	2.385104000	-0.002643000
1	3.639414000	1.648951000	0.004164000
1	2.555720000	-2.320575000	0.001056000
1	0.148069000	-1.779402000	-0.006459000
8	-0.777754000	0.853325000	-0.010204000
6	-1.856192000	0.036597000	0.000615000
9	-2.940964000	0.806733000	-0.000915000
9	-1.907736000	-0.771268000	-1.078103000
9	-1.898439000	-0.754743000	1.091630000

Cl
E(RB3LYP) = -707.973812530

6	0.000000000	0.000000000	0.497473000
6	0.000000000	1.202054000	-0.199175000
6	0.000000000	1.139369000	-1.591954000
7	0.000000000	0.000000000	-2.289275000
6	0.000000000	-1.139369000	-1.591954000
6	0.000000000	-1.202054000	-0.199175000
1	0.000000000	2.152906000	0.317287000
1	0.000000000	2.057920000	-2.171521000
1	0.000000000	-2.057920000	-2.171521000
1	0.000000000	-2.152906000	0.317287000
17	0.000000000	0.000000000	2.249535000

NHCN
E(RB3LYP) = -395.980088052

6	-0.121752000	-0.368829000	0.000069000
6	0.165645000	0.996298000	0.000104000
6	1.502878000	1.381120000	0.000032000
7	2.533778000	0.530700000	-0.000063000
6	2.235886000	-0.772127000	-0.000090000
6	0.940181000	-1.275857000	-0.000033000
1	-0.624286000	1.737378000	0.000191000
1	1.753887000	2.437738000	0.000054000
1	3.078215000	-1.457830000	-0.000164000
1	0.767563000	-2.346619000	-0.000072000
7	-1.444112000	-0.848618000	0.000116000
1	-1.592033000	-1.847707000	0.000109000
6	-2.525028000	-0.067452000	0.000133000
7	-3.456839000	0.620507000	-0.000253000

SiH3
E(RB3LYP) = -539.069301406

6	0.007143000	0.457133000	0.000000000
6	0.010558000	-0.280180000	1.191350000
6	0.010558000	-1.672996000	1.139364000
7	0.009942000	-2.370866000	0.000000000
6	0.010558000	-1.672996000	-1.139364000
6	0.010558000	-0.280180000	-1.191350000
1	0.017588000	0.213152000	2.157863000
1	0.013558000	-2.255180000	2.056955000
1	0.013558000	-2.255180000	-2.056955000
1	0.017588000	0.213152000	-2.157863000
14	-0.023369000	2.345275000	0.000000000
1	0.661353000	2.849370000	-1.217010000
1	-1.423694000	2.842852000	0.000000000
1	0.661353000	2.849370000	1.217010000

CH2F
E(RB3LYP) = -386.941897907

6	-0.438337000	0.273149000	0.000000000
6	0.525454000	1.283901000	0.000000000
6	1.871036000	0.930140000	0.000000000
7	2.305620000	-0.334489000	0.000000000
6	1.376161000	-1.293119000	0.000000000
6	0.003226000	-1.047550000	0.000000000
1	0.242111000	2.331643000	0.000000000
1	2.637146000	1.700355000	-0.000001000
1	1.744339000	-2.315251000	0.000000000
1	-0.704505000	-1.866010000	0.000001000
6	-1.901481000	0.630165000	0.000001000
1	-2.161241000	1.211376000	0.889832000
1	-2.161241000	1.211379000	-0.889828000
9	-2.705812000	-0.510243000	-0.000001000

CH=CH2
E(RB3LYP) = -325.771328617

6	-0.506713000	-0.223109000	-0.000062000
6	0.009079000	1.081294000	-0.000096000
6	1.385217000	1.270129000	-0.000029000
7	2.278969000	0.272650000	0.000056000
6	1.790546000	-0.969826000	0.000071000
6	0.429422000	-1.264812000	0.000005000
1	-0.645616000	1.944284000	-0.000195000
1	1.795226000	2.276225000	-0.000055000
1	2.522527000	-1.772798000	0.000130000
1	0.100327000	-2.298410000	0.000017000
6	-1.944066000	-0.537286000	-0.000095000
6	-2.956438000	0.334061000	0.000148000
1	-2.807055000	1.407968000	0.000435000
1	-3.983970000	-0.008959000	0.000032000
1	-2.176501000	-1.599559000	-0.000412000

C6H5
E(RB3LYP) = -479.463626393

6	-0.745859000	0.000000000	0.000000000
6	-1.481851000	-1.118380000	-0.411653000
6	-2.872552000	-1.067453000	-0.393412000

SiMe3
E(RB3LYP) = -657.089171782

6	0.431974000	0.016348000	0.000011000
6	1.185379000	1.197853000	0.000005000
6	2.578845000	1.136882000	-0.000001000

7	-3.574425000	0.000000000	0.000000000
6	-2.872552000	1.067453000	0.393412000
6	-1.481851000	1.118380000	0.411653000
1	-0.980969000	-2.011412000	-0.766421000
1	-3.452094000	-1.927615000	-0.717374000
1	-3.452094000	1.927615000	0.717374000
1	-0.980969000	2.011412000	0.766421000
6	0.737707000	0.000000000	0.000000000
6	1.455871000	1.140202000	-0.388523000
6	1.455871000	-1.140202000	0.388523000
1	0.920466000	2.024503000	-0.714911000
1	0.920466000	-2.024503000	0.714911000
6	2.848005000	1.139358000	-0.390847000
6	2.848005000	-1.139358000	0.390847000
1	3.385014000	2.027341000	-0.704970000
1	3.385015000	-2.027341000	0.704970000
6	3.549621000	0.000000000	0.000000000
1	4.633645000	0.000000000	0.000000000

7	3.270365000	-0.005548000	-0.000002000
6	2.560993000	-1.139148000	0.000004000
6	1.168891000	-1.177979000	0.000011000
1	0.704314000	2.170085000	0.000004000
1	3.166757000	2.051260000	-0.000005000
1	3.135584000	-2.061814000	0.000003000
1	0.674417000	-2.144710000	0.000016000
14	-1.471271000	0.003807000	-0.000001000
6	-2.072021000	-0.900147000	1.544937000
1	-1.733140000	-0.397119000	2.455162000
1	-3.165620000	-0.941043000	1.571785000
1	-1.702391000	-1.929209000	1.578219000
6	-2.071985000	-0.900170000	-1.544941000
1	-3.165597000	-0.940462000	-1.572152000
1	-1.732512000	-0.397548000	-2.455168000
1	-1.702923000	-1.929449000	-1.577850000
6	-2.114245000	1.777221000	-0.000016000
1	-1.785912000	2.330334000	0.884887000
1	-1.786028000	2.330285000	-0.884991000
1	-3.208691000	1.779761000	0.000056000

H

E(RB3LYP) = -248.351216199

6	0.000000000	0.000000000	-1.383082000
6	0.000000000	1.196436000	-0.671664000
6	0.000000000	1.141427000	0.721074000
7	0.000000000	0.000000000	1.417157000
6	0.000000000	-1.141427000	0.721074000
6	0.000000000	-1.196436000	-0.671664000
1	0.000000000	0.000000000	-2.467376000
1	0.000000000	2.153484000	-1.179805000
1	0.000000000	2.056850000	1.306228000
1	0.000000000	-2.056850000	1.306228000
1	0.000000000	-2.153484000	-1.179805000

SMe

E(RB3LYP) = -685.890620179

6	0.107471000	-0.233314000	0.000148000
6	-0.349173000	1.087673000	0.000312000
6	-1.723987000	1.319894000	0.000085000
7	-2.650755000	0.360230000	-0.000141000
6	-2.201355000	-0.901373000	-0.000157000
6	-0.857477000	-1.250378000	-0.000120000
1	0.329809000	1.929603000	0.000575000
1	-2.092847000	2.342263000	0.000240000
1	-2.959459000	-1.679557000	-0.000540000
1	-0.567035000	-2.294767000	-0.000386000
16	1.810434000	-0.723778000	0.000275000
6	2.711002000	0.859252000	-0.000497000
1	2.495722000	1.441976000	0.895647000
1	3.766979000	0.588153000	0.000048000
1	2.496284000	1.440637000	-0.897623000

OH

E(RB3LYP) = -323.601550182

6	0.000000000	0.931145000	0.000000000
6	-1.193779000	0.208223000	0.000000000
6	-1.121385000	-1.182309000	0.000000000
7	0.021476000	-1.873452000	0.000000000
6	1.153482000	-1.159443000	0.000000000
6	1.205015000	0.229875000	0.000000000
1	-2.156472000	0.709523000	0.000000000
1	-2.036573000	-1.767844000	0.000000000
1	2.077703000	-1.730353000	0.000000000
1	2.147703000	0.762098000	0.000000000
8	0.049948000	2.290215000	0.000000000
1	-0.842274000	2.654082000	0.000000000

CH2NMe2

E(RB3LYP) = -421.676034657

6	0.382146000	-0.300822000	-0.290240000
6	0.821929000	1.022725000	-0.367870000
6	2.167439000	1.303012000	-0.147422000
7	3.086891000	0.373408000	0.138080000
6	2.661286000	-0.890113000	0.212997000
6	1.335719000	-1.272759000	0.012989000
1	0.118837000	1.817376000	-0.586717000
1	2.527349000	2.326836000	-0.202985000
1	3.415010000	-1.636283000	0.449870000
1	1.055727000	-2.317751000	0.096301000
6	-1.059400000	-0.674318000	-0.572311000
1	-1.198845000	-0.690650000	-1.659206000
1	-1.240865000	-1.707267000	-0.219690000
7	-2.026996000	0.267742000	-0.018441000
6	-2.077970000	0.212481000	1.438907000
1	-1.087777000	0.400202000	1.857656000
1	-2.755295000	0.984461000	1.811010000
1	-2.431100000	-0.766519000	1.813073000
6	-3.349475000	0.090134000	-0.604764000
1	-4.028560000	0.850629000	-0.212259000
1	-3.295855000	0.210866000	-1.689430000
1	-3.787934000	-0.901993000	-0.388817000

CH3

E(RB3LYP) = -287.680472569

6	0.904220000	0.000145000	-0.011677000
6	0.170856000	1.189498000	-0.008209000
6	-1.220862000	1.137516000	0.002469000
7	-1.922327000	-0.000105000	0.007926000
6	-1.220622000	-1.137654000	0.002468000
6	0.171034000	-1.189401000	-0.008209000

CH2OH

E(RB3LYP) = -362.915519853

6	0.000000000	0.507648000	0.000000000
6	1.371034000	0.239074000	0.000000000
6	1.801710000	-1.083488000	0.000000000
7	0.973395000	-2.133631000	0.000000000
6	-0.335452000	-1.867625000	0.000000000
6	-0.870854000	-0.579728000	0.000000000

1	0.674939000	2.150199000	-0.016730000
1	-1.800725000	2.056571000	0.003265000
1	-1.800345000	-2.056795000	0.003261000
1	0.675267000	-2.150034000	-0.016725000
6	2.411056000	0.000082000	0.007573000
1	2.781815000	-0.008679000	1.038160000
1	2.815634000	-0.881657000	-0.493990000
1	2.815613000	0.890013000	-0.479216000

1	2.099615000	1.043827000	0.000000000
1	2.864182000	-1.311099000	0.000000000
1	-0.996982000	-2.729721000	0.000000000
1	-1.941108000	-0.423544000	0.000000000
6	-0.490873000	1.934689000	0.000000000
1	-0.092076000	2.447380000	0.886274000
1	-0.092076000	2.447380000	-0.886274000
8	-1.912666000	1.960319000	0.000000000
1	-2.207380000	2.875223000	0.000000000

OMe

E(RB3LYP) = -362.910884511

6	0.000000000	0.525325000	0.000000000
6	-1.368724000	0.232495000	0.000000000
6	-1.762016000	-1.096816000	0.000000000
7	-0.913163000	-2.135224000	0.000000000
6	0.386049000	-1.837791000	0.000000000
6	0.902654000	-0.541289000	0.000000000
1	-2.092286000	1.038100000	0.000000000
1	-2.819623000	-1.344917000	0.000000000
1	1.070685000	-2.681894000	0.000000000
1	1.973662000	-0.392081000	0.000000000
8	0.342842000	1.835920000	0.000000000
6	1.725586000	2.180059000	0.000000000
1	2.228613000	1.800157000	0.894897000
1	2.228613000	1.800157000	-0.894897000
1	1.758450000	3.267788000	0.000000000

NH2

E(RB3LYP) = -303.732399761

6	0.001785000	0.930828000	0.000000000
6	0.002805000	0.196899000	1.196036000
6	0.002805000	-1.190358000	1.135127000
7	0.002276000	-1.899104000	0.000000000
6	0.002805000	-1.190358000	-1.135127000
6	0.002805000	0.196899000	-1.196036000
1	0.006938000	0.701232000	2.156568000
1	0.002145000	-1.766172000	2.056876000
1	0.002145000	-1.766172000	-2.056876000
1	0.006938000	0.701232000	-2.156568000
7	0.048743000	2.312460000	0.000000000
1	-0.226668000	2.786469000	0.845899000
1	-0.226668000	2.786469000	-0.845899000

N(C3H7)2

E(RB3LYP) = -539.657510480

6	-0.865493000	-0.069694000	0.246404000
6	-1.891512000	0.899398000	0.321466000
6	-3.196617000	0.546887000	0.005527000
7	-3.589865000	-0.670393000	-0.384282000
6	-2.618250000	-1.587146000	-0.460923000
6	-1.281382000	-1.354808000	-0.170917000
1	-1.692694000	1.915642000	0.628935000
1	-3.977246000	1.300529000	0.074557000
1	-2.924073000	-2.580181000	-0.780890000
1	-0.578181000	-2.167577000	-0.285834000
7	0.448920000	0.211018000	0.563505000
6	1.392447000	-0.885795000	0.802784000
1	2.083440000	-0.562755000	1.587290000
1	0.845510000	-1.738339000	1.218882000
6	2.203636000	-1.344335000	-0.417956000
1	2.806665000	-0.508316000	-0.783375000
1	1.521096000	-1.610965000	-1.230859000
6	0.833548000	1.560879000	0.989419000
1	0.136167000	1.916333000	1.759035000
1	1.807528000	1.475497000	1.476637000
6	0.935746000	2.615023000	-0.126646000
1	-0.028046000	2.715323000	-0.632770000
1	1.125936000	3.577314000	0.363817000
6	2.026336000	2.345214000	-1.164926000
1	3.011599000	2.252316000	-0.695808000
1	1.827787000	1.425903000	-1.720057000
1	2.081050000	3.162254000	-1.889071000
6	3.111231000	-2.531929000	-0.083475000
1	3.819499000	-2.279814000	0.712381000
1	2.530753000	-3.396680000	0.253407000
1	3.691689000	-2.843026000	-0.955382000

Substituted Pyrenes

SO2CN

E(RB3LYP) = -1256.78770585

6	0.973082000	2.467162000	-0.096664000
6	0.229721000	1.238810000	-0.144421000

C(CN)3

E(RB3LYP) = -931.985777311

6	0.976939000	-2.448810000	0.000010000
6	0.242663000	-1.213352000	-0.000005000

6	2.327936000	2.462940000	0.001034000
6	0.938601000	0.000014000	-0.092739000
6	3.070840000	1.234895000	0.056502000
6	2.358822000	-0.000006000	0.007322000
6	-1.166752000	1.223674000	-0.242280000
6	0.229688000	-1.238757000	-0.144493000
6	3.070808000	-1.234929000	0.056435000
6	-1.166781000	-1.223579000	-0.242364000
6	-1.828878000	0.000058000	-0.286094000
1	-1.725651000	2.149819000	-0.295501000
6	0.973018000	-2.467136000	-0.096804000
1	-1.725691000	-2.149714000	-0.295668000
6	4.469164000	1.209373000	0.154637000
6	4.469129000	-1.209452000	0.154571000
6	5.156370000	-0.000048000	0.203473000
1	2.875644000	3.398472000	0.038364000
6	2.327870000	-2.462954000	0.000899000
1	0.426736000	-3.402861000	-0.138531000
1	5.014585000	-2.146109000	0.192506000
1	6.237705000	-0.000068000	0.279180000
1	2.875558000	-3.398500000	0.038179000
1	5.014639000	2.146016000	0.192622000
1	0.426830000	3.402907000	-0.138336000
16	-3.609813000	0.000078000	-0.390244000
8	-4.073276000	-1.274235000	-0.913796000
6	-4.066208000	-0.000216000	1.344832000
7	-4.384225000	-0.000417000	2.455064000
8	-4.073267000	1.274563000	-0.913383000

6	2.335443000	-2.456988000	0.000018000
6	0.967190000	0.015703000	-0.000012000
6	3.093622000	-1.236232000	0.000011000
6	2.390878000	0.004196000	-0.000005000
6	-1.155923000	-1.179557000	-0.000012000
6	0.263791000	1.253767000	-0.000028000
6	3.113144000	1.233201000	-0.000013000
6	-1.140071000	1.246314000	-0.000035000
6	-1.830226000	0.040711000	-0.000028000
1	-1.706563000	-2.114052000	-0.000009000
6	1.015685000	2.476906000	-0.000038000
1	-1.670798000	2.190527000	-0.000049000
6	4.495181000	-1.222204000	0.000019000
6	4.515511000	1.196697000	-0.000004000
6	5.194409000	-0.017851000	0.000012000
1	2.875008000	-3.398072000	0.000030000
6	2.375149000	2.464777000	-0.000030000
1	0.474897000	3.416943000	-0.000051000
1	5.069800000	2.129012000	-0.000010000
1	6.278363000	-0.026871000	0.000018000
1	2.928882000	3.397594000	-0.000036000
1	5.034728000	-2.163141000	0.000032000
1	0.421882000	-3.380460000	0.000015000
6	-3.386866000	0.008307000	0.000001000
6	-3.872908000	-0.705781000	-1.205870000
7	-4.228075000	-1.266987000	-2.146210000
6	-3.872854000	-0.705396000	1.206122000
7	-4.227969000	-1.266301000	2.146661000
6	-3.973997000	1.365573000	-0.000207000
7	-4.427780000	2.423093000	-0.000364000

NO2

E(RB3LYP) = -820.479711527

6	2.465572000	-0.247298000	0.000000000
6	1.236769000	0.498172000	0.000000000
6	2.462839000	-1.605701000	0.000000000
6	-0.000006000	-0.215184000	0.000000000
6	1.235235000	-2.352210000	0.000000000
6	0.000000000	-1.638675000	0.000000000
6	1.220285000	1.897055000	0.000000000
6	-1.236777000	0.498178000	0.000000000
6	-1.235232000	-2.352219000	0.000000000
6	-1.220290000	1.897059000	0.000000000
6	0.000000000	2.561473000	0.000000000
1	2.139180000	2.467482000	0.000000000
6	-2.465575000	-0.247304000	0.000000000
1	-2.139179000	2.467494000	0.000000000
6	1.209629000	-3.753965000	0.000000000
6	-1.209624000	-3.753974000	0.000000000
6	0.000005000	-4.442835000	0.000000000
1	3.398861000	-2.153997000	0.000000000
6	-2.462832000	-1.605710000	0.000000000
1	-3.401062000	0.301180000	0.000000000
1	-2.146232000	-4.300988000	0.000000000
1	0.000013000	-5.526903000	0.000000000
1	-3.398862000	-2.153993000	0.000000000
1	2.146237000	-4.300981000	0.000000000
1	3.401046000	0.301209000	0.000000000
7	0.000000000	4.041361000	0.000000000
8	1.084276000	4.611799000	0.000000000
8	-1.084275000	4.611800000	0.000000000

CN

E(RB3LYP) = -708.182361633

6	-2.464095000	0.105180000	0.000000000
6	-1.235600000	0.851008000	0.000000000
6	-2.462022000	-1.253375000	0.000000000
6	0.000000000	0.137318000	0.000000000
6	-1.234814000	-2.000411000	0.000000000
6	-0.000006000	-1.286654000	0.000000000
6	-1.216653000	2.249555000	0.000000000
6	1.235596000	0.850983000	0.000000000
6	1.234799000	-2.000416000	0.000000000
6	1.216680000	2.249539000	0.000000000
6	0.000026000	2.942549000	0.000000000
1	-2.148335000	2.802434000	0.000000000
6	2.464102000	0.105157000	0.000000000
1	2.148384000	2.802382000	0.000000000
6	-1.209399000	-3.402306000	0.000000000
6	1.209379000	-3.402303000	0.000000000
6	-0.000015000	-4.091561000	0.000000000
1	-3.398457000	-1.801053000	0.000000000
6	2.462027000	-1.253389000	0.000000000
1	3.400265000	0.652862000	0.000000000
1	2.146255000	-3.948966000	0.000000000
1	-0.000003000	-5.175626000	0.000000000
1	3.398438000	-1.801109000	0.000000000
1	-2.146289000	-3.948946000	0.000000000
1	-3.400276000	0.652854000	0.000000000
6	0.000008000	4.374622000	0.000000000
7	-0.000008000	5.530313000	0.000000000

N(CF3)2

E(RB3LYP) = -1345.56677409

6	-1.529603000	2.409286000	0.079524000
6	-0.842770000	1.148409000	0.028997000
6	-2.887002000	2.470804000	0.086055000
6	-1.613001000	-0.050924000	-0.015006000
6	-3.690929000	1.280985000	0.043220000
6	-3.035936000	0.015290000	-0.007374000
6	0.555617000	1.062925000	0.024363000
6	-0.958148000	-1.316883000	-0.066064000

CHO

E(RB3LYP) = -729.273851790

6	1.953789000	-1.411656000	0.000000000
6	1.419817000	-0.076158000	0.000000000
6	1.137685000	-2.497095000	0.000000000
6	0.000000000	0.093601000	0.000000000
6	-0.293108000	-2.358240000	0.000000000
6	-0.853816000	-1.046154000	0.000000000
6	2.240243000	1.053807000	0.000000000
6	-0.562447000	1.405013000	0.000000000

6	-3.806200000	-1.183980000	-0.049901000
6	0.441858000	-1.359334000	-0.073639000
6	1.177287000	-0.181000000	-0.027837000
1	1.151602000	1.966755000	0.062949000
6	-1.759701000	-2.508400000	-0.108149000
1	0.960952000	-2.309367000	-0.113066000
6	-5.092671000	1.320719000	0.050078000
6	-5.205524000	-1.093630000	-0.040781000
6	-5.837594000	0.145572000	0.008708000
1	-3.389972000	3.431220000	0.124799000
6	-3.116961000	-2.443446000	-0.100547000
1	-1.256255000	-3.468310000	-0.146440000
1	-5.795141000	-2.003538000	-0.072872000
1	-6.920501000	0.196000000	0.015029000
1	-3.707685000	-3.352835000	-0.132599000
1	-5.595105000	2.281298000	0.088736000
1	-0.938523000	3.318080000	0.113195000
7	2.630676000	-0.282474000	-0.029647000
6	3.336352000	0.083745000	-1.213346000
9	2.523443000	-0.036303000	-2.269744000
9	3.792823000	1.363341000	-1.196592000
9	4.406944000	-0.698128000	-1.426751000
6	3.272763000	-0.120781000	1.229684000
9	4.586523000	-0.359201000	1.146043000
9	3.131296000	1.125275000	1.752779000
9	2.739955000	-0.968109000	2.125364000

6	-2.270491000	-0.877341000	0.000000000
6	0.299199000	2.508653000	0.000000000
6	1.685374000	2.338133000	0.000000000
1	3.319664000	0.951952000	0.000000000
6	-1.992151000	1.544010000	0.000000000
1	-0.117363000	3.511841000	0.000000000
6	-1.153691000	-3.464505000	0.000000000
6	-3.090728000	-2.015255000	0.000000000
6	-2.535455000	-3.291139000	0.000000000
1	1.557129000	-3.497584000	0.000000000
6	-2.805786000	0.455546000	0.000000000
1	-2.413033000	2.543846000	0.000000000
1	-4.168354000	-1.891361000	0.000000000
1	-3.185114000	-4.159111000	0.000000000
1	-3.883748000	0.577787000	0.000000000
1	-0.731605000	-4.463745000	0.000000000
1	3.031471000	-1.533876000	0.000000000
6	2.558626000	3.533672000	0.000000000
8	3.769407000	3.511147000	0.000000000
1	2.013340000	4.501723000	0.000000000

NHNO2
E(RB3LYP) = -875.830647370

6	0.797426000	2.539152000	-0.003554000
6	-0.033276000	1.373084000	-0.124527000
6	2.147520000	2.432083000	0.110925000
6	0.585033000	0.089145000	-0.121241000
6	2.800204000	1.152474000	0.115298000
6	1.999564000	-0.021530000	-0.002741000
6	-1.426959000	1.455898000	-0.228975000
6	-0.218797000	-1.082773000	-0.238616000
6	2.616764000	-1.307033000	-0.002693000
6	-1.606979000	-0.960544000	-0.369854000
6	-2.200458000	0.300767000	-0.352448000
1	-1.905957000	2.429751000	-0.209398000
6	0.431549000	-2.364804000	-0.237203000
1	-2.219031000	-1.844975000	-0.475501000
6	4.191347000	1.018152000	0.231173000
6	4.011375000	-1.390998000	0.115835000
6	4.786467000	-0.240194000	0.231322000
1	2.759844000	3.323058000	0.201935000
6	1.781583000	-2.469831000	-0.124188000
1	-0.182754000	-3.254189000	-0.325857000
1	4.484804000	-2.367018000	0.116873000
1	5.863450000	-0.325013000	0.321767000
1	2.254785000	-3.446093000	-0.123486000
1	4.803756000	1.908989000	0.321230000
1	0.323559000	3.515003000	-0.003801000
7	-3.601692000	0.462405000	-0.543088000
1	-3.941615000	1.387188000	-0.773425000
7	-4.553042000	-0.163760000	0.266241000
8	-5.657822000	0.364333000	0.263802000
8	-4.233664000	-1.183771000	0.848262000

COCH3
E(RB3LYP) = -768.606325391

6	-0.334328000	-2.478527000	-0.000041000
6	0.437478000	-1.264972000	-0.000023000
6	-1.692434000	-2.450117000	-0.000049000
6	-0.254040000	-0.016161000	-0.000014000
6	-2.415769000	-1.207702000	-0.000040000
6	-1.677644000	0.013094000	-0.000022000
6	1.834254000	-1.269271000	-0.000009000
6	0.486355000	1.201817000	0.000004000
6	-2.366045000	1.262500000	-0.000012000
6	1.886229000	1.148122000	0.000008000
6	2.564510000	-0.075203000	0.000005000
1	2.380062000	-2.205488000	-0.000007000
6	-0.234162000	2.445272000	0.000016000
1	2.436851000	2.081459000	0.000023000
6	-3.816588000	-1.153686000	-0.000047000
6	-3.768606000	1.265364000	-0.000020000
6	-4.481318000	0.069908000	-0.000037000
1	-2.259253000	-3.375238000	-0.000061000
6	-1.592911000	2.473512000	0.000007000
1	0.332796000	3.370399000	0.000030000
1	-4.296716000	2.212922000	-0.000012000
1	-5.565309000	0.091468000	-0.000042000
1	-2.120556000	3.421489000	0.000015000
1	-4.382351000	-2.079235000	-0.000060000
1	0.195898000	-3.424717000	-0.000047000
6	4.063715000	-0.162249000	0.000023000
8	4.621993000	-1.243608000	-0.000054000
6	4.873902000	1.121089000	0.000216000
1	4.647498000	1.727099000	-0.881947000
1	4.647500000	1.726824000	0.882570000
1	5.932050000	0.865153000	0.000180000

OCF3
E(RB3LYP) = -1028.30478291

6	-0.868112000	-2.445625000	-0.210256000
6	-0.147401000	-1.206071000	-0.298726000
6	-2.215330000	-2.465420000	-0.032350000
6	-0.873793000	0.017474000	-0.198009000
6	-2.975247000	-1.251057000	0.072343000
6	-2.286494000	-0.005446000	-0.014045000
6	1.241460000	-1.165260000	-0.485686000
6	-0.186087000	1.264093000	-0.286780000

Cl
E(RB3LYP) = -1075.53866972

6	2.461568000	-0.010284000	0.000000000
6	1.232242000	0.733635000	0.000000000
6	2.462445000	-1.369482000	0.000000000
6	0.000000000	0.016374000	0.000000000
6	1.237641000	-2.119988000	0.000000000
6	0.002132000	-1.407797000	0.000000000
6	1.211941000	2.135568000	0.000000000
6	-1.234434000	0.729839000	0.000000000

6	-3.013847000	1.217216000	0.083496000
6	1.203634000	1.266967000	-0.470052000
6	1.882037000	0.061833000	-0.557486000
1	1.814003000	-2.079872000	-0.575012000
6	-0.945073000	2.479698000	-0.186967000
1	1.750846000	2.198451000	-0.546443000
6	-4.365778000	-1.248237000	0.255102000
6	-4.403604000	1.169450000	0.265755000
6	-5.068452000	-0.050484000	0.350531000
1	-2.743335000	-3.410863000	0.034139000
6	-2.292304000	2.455681000	-0.009742000
1	-0.417378000	3.424861000	-0.255237000
1	-4.959716000	2.097819000	0.340634000
1	-6.143175000	-0.067922000	0.491719000
1	-2.849731000	3.383466000	0.064842000
1	-4.892730000	-2.194075000	0.321985000
1	-0.311114000	-3.373138000	-0.287163000
8	3.270246000	0.096907000	-0.819077000
6	4.117598000	-0.009013000	0.223254000
9	5.362141000	0.094856000	-0.247399000
9	3.933945000	0.955440000	1.150207000
9	4.011817000	-1.191271000	0.870620000

6	-1.231189000	-2.123703000	0.000000000
6	-1.218391000	2.131868000	0.000000000
6	-0.004270000	2.806463000	0.000000000
1	2.140515000	2.693015000	0.000000000
6	-2.461533000	-0.017763000	0.000000000
1	-2.148668000	2.686480000	0.000000000
6	1.214426000	-3.522203000	0.000000000
6	-1.203804000	-3.525809000	0.000000000
6	0.006360000	-4.213830000	0.000000000
1	3.400585000	-1.914552000	0.000000000
6	-2.458328000	-1.376928000	0.000000000
1	-3.398834000	0.528231000	0.000000000
1	-2.140161000	-4.073645000	0.000000000
1	0.007961000	-5.297957000	0.000000000
1	-3.394725000	-1.924995000	0.000000000
1	2.152425000	-4.067233000	0.000000000
1	3.397278000	0.538439000	0.000000000
17	-0.006895000	4.566850000	0.000000000

NHCN

E(RB3LYP) = -763.543276059

6	0.573871000	2.559653000	0.000041000
6	-0.330568000	1.442565000	-0.000025000
6	1.920659000	2.375964000	0.000158000
6	0.214634000	0.125301000	0.000034000
6	2.498985000	1.061059000	0.000221000
6	1.625224000	-0.065718000	0.000157000
6	-1.720041000	1.608562000	-0.000136000
6	-0.662102000	-0.998453000	-0.000031000
6	2.166885000	-1.384644000	0.000217000
6	-2.047918000	-0.794917000	-0.000154000
6	-2.564967000	0.498691000	-0.000201000
1	-2.136812000	2.611090000	-0.000160000
6	-0.087870000	-2.316043000	0.000029000
1	-2.717685000	-1.647354000	-0.000215000
6	3.884944000	0.847730000	0.000344000
6	3.559719000	-1.548158000	0.000340000
6	4.406441000	-0.443158000	0.000403000
1	2.587488000	3.231925000	0.000206000
6	1.259235000	-2.497815000	0.000148000
1	-0.756314000	-3.170244000	-0.000020000
1	3.974452000	-2.550585000	0.000386000
1	5.480674000	-0.588881000	0.000498000
1	1.673794000	-3.500511000	0.000192000
1	4.552240000	1.703159000	0.000393000
1	0.158632000	3.561988000	-0.000004000
7	-3.965358000	0.718915000	-0.000288000
1	-4.297931000	1.671745000	-0.000621000
6	-4.878725000	-0.248400000	-0.000421000
7	-5.667355000	-1.098294000	-0.000768000

SiH3

E(RB3LYP) = -906.634482096

6	-0.051302000	2.460123000	-0.006728000
6	0.694677000	1.231862000	-0.006757000
6	-1.410492000	2.461170000	-0.001228000
6	-0.021504000	0.000046000	-0.002760000
6	-2.159660000	1.234928000	0.002890000
6	-1.446162000	0.000008000	0.001124000
6	2.096667000	1.204501000	-0.013566000
6	0.694832000	-1.231955000	-0.006976000
6	-2.159670000	-1.234921000	0.002766000
6	2.096466000	-1.204509000	-0.013917000
6	2.812437000	0.000103000	-0.013651000
1	2.627380000	2.152284000	-0.023380000
6	-0.051317000	-2.460264000	-0.007106000
1	2.626780000	-2.152663000	-0.024154000
6	-3.561940000	1.209489000	0.007522000
6	-3.561838000	-1.209527000	0.007417000
6	-4.251171000	0.000015000	0.010019000
1	-1.957124000	3.398468000	-0.000321000
6	-1.410421000	-2.461240000	-0.001495000
1	0.497068000	-3.396537000	-0.010920000
1	-4.108632000	-2.146525000	0.008796000
1	-5.335402000	-0.000024000	0.013541000
1	-1.957090000	-3.398518000	-0.000654000
1	-4.108732000	2.146488000	0.008976000
1	0.497127000	3.396368000	-0.010403000
14	4.695056000	0.000044000	0.015797000
1	5.204242000	1.250811000	-0.604197000
1	5.212050000	-1.175620000	-0.731971000
1	5.213946000	-0.074110000	1.408195000

CH2F

E(RB3LYP) = -754.506018299

6	-0.160165000	-2.371340000	0.000000000
6	-0.805688000	-1.087977000	0.000000000
6	1.195105000	-2.480595000	0.000000000
6	0.006669000	0.081753000	0.000000000
6	2.039661000	-1.318783000	0.000000000
6	1.426647000	-0.031111000	0.000000000
6	-2.202684000	-0.955046000	0.000000000
6	-0.609628000	1.367848000	0.000000000
6	2.236637000	1.142654000	0.000000000
6	-2.007043000	1.451205000	0.000000000
6	-2.800484000	0.302016000	0.000000000
1	-2.825186000	-1.841260000	0.000000000
6	0.232434000	2.532888000	0.000000000
1	-2.472674000	2.433142000	0.000000000
6	3.439975000	-1.404991000	0.000000000

CH=CH2

E(RB3LYP) = -693.335296362

6	-0.137302000	2.516905000	-0.000068000
6	0.685344000	1.338983000	-0.000019000
6	-1.494214000	2.430648000	-0.000108000
6	0.049281000	0.065084000	-0.000014000
6	-2.163078000	1.159377000	-0.000105000
6	-1.371209000	-0.026990000	-0.000060000
6	2.084731000	1.399157000	0.000020000
6	0.847435000	-1.117949000	0.000025000
6	-2.003922000	-1.305537000	-0.000061000
6	2.240040000	-1.005070000	0.000066000
6	2.877441000	0.244448000	0.000082000
1	2.566754000	2.372026000	0.000013000
6	0.180001000	-2.392474000	0.000016000
1	2.830843000	-1.914181000	0.000069000
6	-3.561238000	1.043410000	-0.000148000

6	3.631985000	1.006011000	0.000000000
6	4.223446000	-0.254738000	0.000000000
1	1.664566000	-3.458808000	0.000000000
6	1.587103000	2.424794000	0.000000000
1	-0.238346000	3.510491000	0.000000000
1	4.251287000	1.896795000	0.000000000
1	5.304228000	-0.340946000	0.000000000
1	2.206574000	3.315674000	0.000000000
1	3.909973000	-2.382781000	0.000000000
1	-0.781660000	-3.260564000	0.000000000
6	-4.301404000	0.457651000	0.000000000
1	-4.641475000	0.996104000	0.889827000
1	-4.641475000	0.996108000	-0.889824000
9	-4.947910000	-0.781932000	-0.000002000

C6H5

E(RB3LYP) = -847.027191005

6	1.113681000	-2.449027000	0.224154000
6	0.367396000	-1.226016000	0.106962000
6	2.472938000	-2.450121000	0.226193000
6	1.085496000	0.000000000	0.000000000
6	3.223199000	-1.229724000	0.112980000
6	2.509569000	0.000000000	0.000000000
6	-1.032723000	-1.200461000	0.103594000
6	0.367394000	1.226014000	-0.106962000
6	3.223198000	1.229725000	-0.112980000
6	-1.032724000	1.200458000	-0.103594000
6	-1.746127000	-0.000002000	-0.000001000
1	-1.572656000	-2.135159000	0.210252000
6	1.113678000	2.449026000	-0.224154000
1	-1.572659000	2.135155000	-0.210251000
6	4.625418000	-1.204372000	0.111057000
6	4.625417000	1.204375000	-0.111056000
6	5.314936000	0.000001000	0.000000000
1	3.018851000	-3.383680000	0.314893000
6	2.472936000	2.450121000	-0.226193000
1	0.565425000	3.381331000	-0.311222000
1	5.172107000	2.137481000	-0.197607000
1	6.399183000	0.000001000	0.000000000
1	3.018846000	3.383681000	-0.314892000
1	5.172109000	-2.137478000	0.197607000
1	0.565427000	-3.381332000	0.311222000
6	-3.232408000	-0.000002000	0.000000000
6	-3.952803000	-0.963913000	-0.720746000
6	-3.952801000	0.963912000	0.720746000
1	-3.416908000	-1.703639000	-1.304698000
1	-3.416902000	1.703638000	1.304696000
6	-5.345273000	-0.964016000	-0.721164000
6	-5.345270000	0.964019000	0.721165000
1	-5.882044000	-1.712993000	-1.292923000
1	-5.882039000	1.712997000	1.292924000
6	-6.047914000	0.000002000	0.000001000
1	-7.132016000	0.000003000	0.000001000

H

E(RB3LYP) = -615.916007870

6	2.460703000	-0.680663000	0.000000000
6	1.234018000	-1.428065000	0.000000000
6	2.461132000	0.678514000	0.000000000
6	0.000000000	-0.712527000	0.000000000
6	1.235192000	1.427113000	0.000000000
6	0.000319000	0.712830000	0.000000000
6	1.207800000	-2.830305000	0.000000000
6	-1.234878000	-1.426804000	0.000000000
6	-1.233969000	1.427912000	0.000000000
6	-1.210330000	-2.829322000	0.000000000
6	-0.001769000	-3.519704000	0.000000000
1	2.144678000	-3.377359000	0.000000000
6	-2.461364000	-0.678677000	0.000000000
6	-3.404071000	-1.370609000	-0.000104000
6	-4.170788000	-0.207646000	-0.000146000
1	-2.099517000	3.331192000	-0.000145000
6	-1.175704000	-2.480837000	-0.000023000
1	0.787101000	-3.291803000	0.000044000
1	-3.889221000	-2.341004000	-0.000105000
1	-5.252741000	-0.277983000	-0.000179000
1	-1.660206000	-3.451708000	-0.000026000
1	-4.167047000	1.943405000	-0.000182000
1	0.349487000	3.486597000	-0.000073000
6	4.341720000	0.395528000	0.000157000
6	5.262277000	-0.573438000	0.000437000
1	5.007901000	-1.627510000	0.000690000
1	6.318766000	-0.333917000	0.000373000
1	4.687419000	1.426944000	-0.000151000

SiMe3

E(RB3LYP) = -1024.65330044

6	-0.933075000	-2.453319000	0.000014000
6	-0.191957000	-1.221477000	0.000004000
6	-2.292169000	-2.461246000	0.000017000
6	-0.915547000	0.006282000	0.000000000
6	-3.048069000	-1.238535000	0.000012000
6	-2.340166000	-0.000283000	0.000003000
6	1.208971000	-1.184880000	-0.000003000
6	-0.203885000	1.239438000	-0.000008000
6	-3.059096000	1.231521000	-0.000002000
6	1.199430000	1.217089000	-0.000012000
6	1.927900000	0.020322000	-0.000010000
1	1.737853000	-2.134703000	-0.000001000
6	-0.955132000	2.464298000	-0.000013000
1	1.720437000	2.169666000	-0.000017000
6	-4.450188000	-1.219469000	0.000014000
6	-4.461578000	1.199700000	0.000000000
6	-5.145144000	-0.012781000	0.000008000
1	-2.834210000	-3.401289000	0.000025000
6	-2.314703000	2.460536000	-0.000011000
1	-0.410612000	3.403010000	-0.000019000
1	-5.012617000	2.134271000	-0.000005000
1	-6.229428000	-0.017845000	0.000010000
1	-2.864926000	3.395812000	-0.000015000
1	-4.992928000	-2.158886000	0.000021000
1	-0.380470000	-3.387311000	0.000018000
14	3.826255000	0.001752000	-0.000003000
6	4.441007000	-0.901209000	-1.542214000
1	4.105363000	-0.398295000	-2.453835000
1	5.534926000	-0.940265000	-1.563278000
1	4.073281000	-1.930941000	-1.579126000
6	4.440982000	-0.901263000	1.542187000
1	5.534915000	-0.939708000	1.563609000
1	4.104746000	-0.398779000	2.453826000
1	4.073830000	-1.931215000	1.578700000
6	4.486420000	1.771056000	0.000023000
1	4.163616000	2.327480000	-0.884916000
1	4.163733000	2.327421000	0.885041000
1	5.580918000	1.762395000	-0.000051000

SMe

E(RB3LYP) = -1053.45287927

6	-0.151899000	-2.374396000	0.000107000
6	0.490440000	-1.089012000	0.000086000
6	-1.507092000	-2.487622000	0.000029000
6	-0.326279000	0.076238000	-0.000020000
6	-2.355468000	-1.329005000	-0.000079000
6	-1.744838000	-0.040224000	-0.000102000
6	1.887742000	-0.955356000	0.000166000
6	0.289891000	1.362723000	-0.000044000
6	-2.557694000	1.131752000	-0.000208000
6	1.684232000	1.454544000	0.000039000
6	2.485539000	0.305639000	0.000144000
1	2.489043000	-1.855406000	0.000246000
6	-0.555629000	2.526647000	-0.000152000

1	-2.147998000	-3.375069000	0.000000000
1	-0.002093000	-4.603998000	0.000000000
6	1.210381000	2.829632000	0.000000000
6	-1.207842000	2.830179000	0.000000000
6	0.001559000	3.519602000	0.000000000
1	3.399098000	1.224320000	0.000000000
6	-2.461032000	0.680543000	0.000000000
1	-3.398210000	-1.226166000	0.000000000
1	-2.144954000	3.376896000	0.000000000
1	0.001574000	4.603859000	0.000000000
1	-3.397647000	1.228363000	0.000000000
1	2.148102000	3.375270000	0.000000000
1	3.397918000	-1.227658000	0.000000000

1	2.148913000	2.435247000	0.000020000
6	-3.755702000	-1.418590000	-0.000161000
6	-3.952276000	0.991901000	-0.000288000
6	-4.541787000	-0.270314000	-0.000264000
1	-1.972952000	-3.467640000	0.000048000
6	-1.909736000	2.415159000	-0.000230000
1	-0.086729000	3.504987000	-0.000170000
1	-4.573555000	1.881369000	-0.000369000
1	-5.622391000	-0.358546000	-0.000326000
1	-2.530854000	3.304961000	-0.000311000
1	-4.223405000	-2.397556000	-0.000142000
1	0.470587000	-3.263236000	0.000188000
16	4.247928000	0.579910000	0.000237000
6	4.949231000	-1.099813000	0.000315000
1	4.666034000	-1.652783000	-0.896109000
1	6.030454000	-0.958837000	0.000366000
1	4.665944000	-1.652736000	0.896740000

OH

E(RB3LYP) = -691.163168957

6	0.324198000	2.463091000	0.000024000
6	1.076847000	1.237948000	0.000015000
6	-1.034930000	2.457739000	0.000016000
6	0.362107000	0.003193000	0.000046000
6	-1.780790000	1.229762000	0.000015000
6	-1.061656000	-0.001897000	0.000035000
6	2.476161000	1.225236000	-0.000021000
6	1.083406000	-1.225941000	0.000031000
6	-1.772816000	-1.238106000	0.000009000
6	2.484922000	-1.198293000	-0.000018000
6	3.168190000	0.016442000	-0.000008000
1	3.037282000	2.152227000	-0.000055000
6	0.340606000	-2.455896000	0.000022000
1	3.038187000	-2.133450000	-0.000001000
6	-3.182623000	1.199813000	-0.000023000
6	-3.175400000	-1.217675000	-0.000028000
6	-3.869764000	-0.011354000	-0.000042000
1	-1.584123000	3.393654000	0.000007000
6	-1.019075000	-2.460350000	0.000010000
1	0.889849000	-3.391714000	0.000034000
1	-3.718365000	-2.157048000	-0.000047000
1	-4.953923000	-0.014702000	-0.000071000
1	-1.561440000	-3.400233000	-0.000004000
1	-3.731689000	2.135621000	-0.000037000
1	0.867836000	3.401890000	0.000044000
8	4.536604000	0.084438000	-0.000045000
1	4.907270000	-0.804025000	-0.000002000

CH2NMe2

E(RB3LYP) = -789.239624863

6	-0.962671000	2.534570000	-0.085130000
6	-0.107408000	1.385955000	-0.196785000
6	-2.309270000	2.403085000	0.051595000
6	-0.699148000	0.091196000	-0.158944000
6	-2.934243000	1.110348000	0.092530000
6	-2.109408000	-0.048369000	-0.013847000
6	1.284932000	1.494053000	-0.335045000
6	0.130507000	-1.064285000	-0.263242000
6	-2.697889000	-1.347211000	0.025070000
6	1.513831000	-0.902157000	-0.406035000
6	2.097747000	0.366700000	-0.444017000
1	1.734424000	2.482522000	-0.355095000
6	-0.492095000	-2.359706000	-0.219953000
1	2.152414000	-1.776159000	-0.475389000
6	-4.320714000	0.947533000	0.233652000
6	-4.088237000	-1.459287000	0.167660000
6	-4.887205000	-0.323169000	0.270294000
1	-2.939357000	3.282749000	0.133051000
6	-1.837657000	-2.493795000	-0.083385000
1	0.140755000	-3.237446000	-0.299373000
1	-4.539707000	-2.445392000	0.197477000
1	-5.960694000	-0.429852000	0.379574000
1	-2.288923000	-3.480194000	-0.053476000
1	-4.951456000	1.826563000	0.314735000
1	-0.509481000	3.520148000	-0.113323000
6	3.594432000	0.512611000	-0.645212000
1	3.833222000	0.269642000	-1.686746000
1	3.878269000	1.572341000	-0.499576000
7	4.387924000	-0.377715000	0.200794000
6	4.297174000	-0.024234000	1.613015000
1	3.254483000	-0.028558000	1.934476000
1	4.840877000	-0.759926000	2.210346000
1	4.720835000	0.975133000	1.827314000
6	5.774309000	-0.443141000	-0.241913000
1	6.321654000	-1.164145000	0.370153000
1	5.818440000	-0.777186000	-1.281477000
1	6.296847000	0.529589000	-0.170065000

CH3

E(RB3LYP) = -655.243497740

6	0.311798000	-2.458574000	-0.005840000
6	1.058215000	-1.230496000	-0.005075000
6	-1.047720000	-2.460166000	-0.001715000
6	0.340127000	0.000041000	-0.002042000
6	-1.798131000	-1.234734000	0.001540000
6	-1.084297000	-0.000005000	0.000351000
6	2.459573000	-1.201984000	-0.009761000
6	1.058105000	1.230569000	-0.005086000
6	-1.798196000	1.234686000	0.001546000
6	2.459544000	1.202140000	-0.009774000
6	3.171049000	0.000137000	-0.009348000
1	3.001568000	-2.143164000	-0.015469000

CH2OH

E(RB3LYP) = -730.474321914

6	0.366016000	-2.352013000	0.000000000
6	-0.540462000	-1.238417000	0.000000000
6	1.713394000	-2.166412000	0.000000000
6	0.000000000	0.077078000	0.000000000
6	2.287326000	-0.850219000	0.000000000
6	1.410410000	0.273926000	0.000000000
6	-1.935771000	-1.405472000	0.000000000
6	-0.882274000	1.197687000	0.000000000
6	1.946314000	1.595419000	0.000000000
6	-2.262476000	0.975251000	0.000000000
6	-2.801822000	-0.315926000	0.000000000
1	-2.308503000	-2.426013000	0.000000000

6	0.311666000	2.458608000	-0.005844000
1	3.001472000	2.143345000	-0.015498000
6	-3.200470000	-1.209392000	0.005110000
6	-3.200548000	1.209268000	0.005121000
6	-3.890274000	-0.000077000	0.007099000
1	-1.593430000	-3.398101000	-0.001231000
6	-1.047862000	2.460148000	-0.001707000
1	0.859625000	3.395237000	-0.008750000
1	-3.747123000	2.146511000	0.006188000
1	-4.974535000	-0.000103000	0.009876000
1	-1.593631000	3.398050000	-0.001212000
1	-3.746983000	-2.146672000	0.006167000
1	0.859776000	-3.395191000	-0.008746000
6	4.681205000	-0.000050000	0.022006000
1	5.050626000	-0.008653000	1.053314000
1	5.090014000	-0.880342000	-0.479355000
1	5.089923000	0.888373000	-0.464767000

6	-0.312401000	2.518239000	0.000000000
1	-2.930458000	1.832201000	0.000000000
6	3.673491000	-0.631111000	0.000000000
6	3.337704000	1.764251000	0.000000000
6	4.188690000	0.661333000	0.000000000
1	2.382416000	-3.020631000	0.000000000
6	1.033261000	2.706094000	0.000000000
1	-0.984188000	3.370231000	0.000000000
1	3.749256000	2.768018000	0.000000000
1	5.262409000	0.811561000	0.000000000
1	1.444724000	3.710135000	0.000000000
1	4.344338000	-1.483743000	0.000000000
1	-0.046775000	-3.355581000	0.000000000
6	-4.314890000	-0.447230000	0.000000000
1	-4.708978000	0.072403000	0.881779000
1	-4.708978000	0.072403000	-0.881779000
8	-4.849190000	-1.764299000	0.000000000
1	-4.140799000	-2.411459000	0.000000000

OCH3

E(RB3LYP) = -730.471925233

6	-0.226485000	2.530851000	0.000000000
6	0.617594000	1.365380000	0.000000000
6	-1.580621000	2.422063000	-0.000001000
6	-0.002418000	0.079167000	0.000000000
6	-2.231906000	1.140087000	-0.000001000
6	-1.421575000	-0.033698000	0.000000000
6	2.010178000	1.454878000	0.000000000
6	0.810818000	-1.087888000	0.000000000
6	-2.036434000	-1.320425000	0.000000000
6	2.210321000	-0.961388000	0.000001000
6	2.801873000	0.301823000	0.000001000
1	2.502287000	2.420551000	0.000000000
6	0.164438000	-2.370710000	0.000000000
1	2.812529000	-1.860442000	0.000001000
6	-3.626641000	1.004084000	-0.000001000
6	-3.437301000	-1.406375000	-0.000001000
6	-4.220367000	-0.256468000	-0.000001000
1	-2.199713000	3.313334000	-0.000001000
6	-1.191386000	-2.480672000	0.000000000
1	0.784090000	-3.261605000	0.000001000
1	-3.907304000	-2.384295000	-0.000001000
1	-5.301227000	-0.341611000	-0.000001000
1	-1.659328000	-3.459737000	0.000000000
1	-4.245136000	1.895556000	-0.000002000
1	0.244410000	3.508205000	-0.000001000
8	4.150360000	0.517968000	0.000001000
6	5.021993000	-0.603739000	0.000002000
1	4.881520000	-1.220413000	0.894482000
1	4.881521000	-1.220414000	-0.894477000
1	6.030993000	-0.194693000	0.000003000

NH2

E(RB3LYP) = -671.292340571

6	-0.323944000	-2.457785000	-0.002586000
6	-1.072390000	-1.229745000	-0.003657000
6	1.035566000	-2.458508000	-0.000225000
6	-0.351205000	0.000027000	-0.002780000
6	1.786983000	-1.234078000	0.001344000
6	1.071568000	0.000002000	0.000066000
6	-2.470831000	-1.208030000	-0.004993000
6	-1.072305000	1.229717000	-0.003666000
6	1.786986000	1.234082000	0.001350000
6	-2.470889000	1.208105000	-0.005030000
6	-3.179334000	0.000120000	-0.004453000
1	-3.015821000	-2.147421000	-0.011970000
6	-0.323932000	2.457739000	-0.002579000
1	-3.015596000	2.147648000	-0.012115000
6	3.189066000	-1.208839000	0.003819000
6	3.189117000	1.208800000	0.003828000
6	3.880147000	-0.000008000	0.004955000
1	1.580477000	-3.397044000	-0.000038000
6	1.035619000	2.458487000	-0.000211000
1	-0.870399000	3.395263000	-0.004433000
1	3.735161000	2.146492000	0.004583000
1	4.964349000	-0.000031000	0.006626000
1	1.580503000	3.397037000	-0.000009000
1	3.735106000	-2.146533000	0.004564000
1	-0.870443000	-3.395292000	-0.004460000
7	-4.575595000	-0.000051000	-0.062702000
1	-5.027881000	0.837586000	0.272576000
1	-5.027626000	-0.837855000	0.272494000

N(C3H7)2

E(RB3LYP) = -907.215616236

6	-1.622073000	-2.429125000	-0.441573000
6	-0.778864000	-1.267805000	-0.337214000
6	-2.973739000	-2.336908000	-0.324307000
6	-1.399155000	-0.008200000	-0.108588000
6	-3.622951000	-1.076880000	-0.088926000
6	-2.811923000	0.091365000	0.019106000
6	0.612278000	-1.347935000	-0.463240000
6	-0.578386000	1.150341000	-0.005966000
6	-3.420354000	1.359829000	0.253595000
6	0.808621000	1.032899000	-0.130024000
6	1.436409000	-0.207714000	-0.370123000
1	1.042533000	-2.322230000	-0.648693000
6	-1.219792000	2.415843000	0.236046000
1	1.402832000	1.929817000	-0.016046000
6	-5.014270000	-0.953549000	0.038219000
6	-4.815441000	1.433406000	0.373437000
6	-5.601279000	0.288346000	0.266364000

1	-3.590285000	-3.226240000	-0.407314000
6	-2.570232000	2.514036000	0.358688000
1	-0.598840000	3.302146000	0.318655000
1	-5.281504000	2.396986000	0.551898000
1	-6.678657000	0.364669000	0.361516000
1	-3.032662000	3.479039000	0.539967000
1	-5.633944000	-1.840608000	-0.043383000
1	-1.154732000	-3.392489000	-0.619154000
7	2.821165000	-0.292373000	-0.505930000
6	3.588514000	0.893206000	-0.894320000
1	4.350867000	0.580357000	-1.616548000
1	2.930513000	1.580055000	-1.435910000
6	4.275686000	1.643684000	0.256799000
1	4.974533000	0.968166000	0.759370000
1	3.527365000	1.922990000	1.005440000
6	3.471984000	-1.595932000	-0.646471000
1	2.983697000	-2.182181000	-1.437823000
1	4.489903000	-1.406828000	-0.995519000
6	3.549167000	-2.439164000	0.638524000
1	2.542097000	-2.619729000	1.023998000
1	3.950844000	-3.420003000	0.356545000
6	4.412951000	-1.828827000	1.743882000
1	5.444038000	-1.676961000	1.407173000
1	4.017900000	-0.863094000	2.066520000
1	4.444695000	-2.483806000	2.618659000
6	5.019601000	2.889053000	-0.234162000
1	5.790293000	2.629091000	-0.967067000
1	4.337917000	3.600208000	-0.711631000
1	5.511935000	3.407453000	0.592371000

Substituted Butynes

SO2CN			
E(RB3LYP) = -757.550044613			
6	3.537075000	0.384495000	0.000238000
1	3.987365000	0.079500000	0.948338000
6	2.114032000	0.114198000	0.000441000
1	3.717989000	1.453691000	-0.140365000
6	0.926460000	-0.096746000	0.000082000
1	4.029640000	-0.157047000	-0.811593000
16	-0.728223000	-0.503511000	-0.000017000
8	-1.083761000	-1.107261000	1.266409000
6	-1.442017000	1.129365000	0.000023000
7	-1.936759000	2.172499000	0.000012000
8	-1.083665000	-1.107155000	-1.266521000
C(CN)3			
E(RB3LYP) = -432.757610960			
6	3.593504000	-0.000351000	0.000125000
1	3.977721000	0.902654000	-0.481081000
6	2.140473000	-0.000399000	0.000015000
1	3.977793000	-0.868583000	-0.541228000
6	0.939669000	-0.000511000	0.000041000
1	3.977590000	-0.035048000	1.022798000
6	-0.531293000	-0.000026000	-0.000004000
6	-1.046460000	-1.168745000	-0.763786000
7	-1.427213000	-2.077738000	-1.357634000
6	-1.046239000	-0.076830000	1.394094000
7	-1.426792000	-0.136474000	2.478306000
6	-1.045675000	1.245982000	-0.630473000
7	-1.425564000	2.215105000	-1.120754000
NO2			
E(RB3LYP) = -321.233771805			
6	-2.852403000	0.000571000	-0.000754000
1	-3.243248000	0.948038000	-0.379625000
6	-1.400936000	0.000487000	-0.002166000
1	-3.226414000	-0.141391000	1.017224000
6	-0.199884000	0.000015000	-0.001100000
1	-3.239524000	-0.812866000	-0.619667000
7	1.195160000	-0.000021000	-0.000012000
8	1.753933000	-1.092324000	0.000391000
8	1.753867000	1.092315000	0.000394000
CN			
E(RB3LYP) = -208.964154857			
6	2.468454000	-0.000075000	-0.000101000
1	2.854968000	0.488397000	0.898757000
6	1.018199000	0.000071000	0.000059000
1	2.854793000	0.534142000	-0.872629000
6	-0.189381000	0.000133000	0.000248000
1	2.854493000	-1.022909000	-0.026549000
6	-1.556313000	0.000058000	0.000034000
7	-2.715716000	-0.000107000	-0.000146000
N(CF3)2			
E(RB3LYP) = -846.337320026			
6	3.984914000	-0.173340000	0.031321000
1	4.324157000	-1.213084000	0.021850000
6	2.531588000	-0.124421000	-0.043914000
1	4.352848000	0.290228000	0.950576000
6	1.332809000	-0.093141000	-0.102452000
1	4.444331000	0.335169000	-0.820598000
7	-0.023675000	-0.021862000	-0.188272000
CHO			
E(RB3LYP) = -230.047296670			
6	-2.535125000	-0.125625000	0.000123000
1	-3.059623000	0.832263000	0.043192000
6	-1.094037000	0.057818000	0.000331000
1	-2.844209000	-0.727636000	0.859457000
6	0.107464000	0.182337000	0.000079000
1	-2.852315000	-0.651405000	-0.905174000
6	1.531895000	0.393275000	-0.000055000

6	-0.822401000	-1.209310000	-0.013970000
9	-0.029980000	-2.278707000	-0.044388000
9	-1.487368000	-1.207904000	1.158250000
9	-1.737080000	-1.334087000	-0.986305000
6	-0.623494000	1.272858000	-0.019930000
9	-1.939767000	1.208756000	-0.233665000
9	-0.429288000	1.769636000	1.217386000
9	-0.084973000	2.142843000	-0.882417000

NHNO2
E(RB3LYP) = -376.603067100

6	-3.324993000	0.209959000	0.047802000
1	-3.409834000	1.300532000	0.039988000
6	-1.921801000	-0.170981000	-0.002286000
1	-3.808680000	-0.155968000	0.957730000
6	-0.756079000	-0.469009000	-0.038226000
1	-3.875727000	-0.173675000	-0.815589000
7	0.538938000	-0.809464000	-0.107784000
1	0.884412000	-1.743153000	0.070917000
7	1.567542000	0.150058000	-0.000088000
8	2.690233000	-0.321274000	0.099566000
8	1.244980000	1.317311000	-0.042276000

COCH3
E(RB3LYP) = -269.384215340

6	-2.946620000	0.086909000	-0.000002000
1	-3.289273000	1.124916000	-0.000159000
6	-1.495065000	0.004851000	0.000003000
1	-3.358293000	-0.410319000	0.883053000
6	-0.291332000	-0.086710000	0.000001000
1	-3.358304000	-0.410596000	-0.882897000
6	1.156469000	-0.193546000	0.000000000
8	1.712109000	-1.274580000	-0.000001000
6	1.915725000	1.115626000	0.000000000
1	1.643383000	1.705967000	-0.880048000
1	1.643368000	1.705979000	0.880035000
1	2.987189000	0.917915000	0.000009000

OCF3
E(RB3LYP) = -529.063790066

6	3.566349000	0.206460000	0.000439000
1	4.190028000	-0.597687000	-0.399395000
6	2.161777000	-0.185571000	0.001649000
1	3.916283000	0.435566000	1.010462000
6	1.003956000	-0.491624000	0.000308000
1	3.722793000	1.091142000	-0.622559000
8	-0.247934000	-0.923034000	-0.000983000
6	-1.241370000	0.031076000	-0.000074000
9	-2.396976000	-0.620734000	-0.004967000
9	-1.181261000	0.811789000	1.085374000
9	-1.176197000	0.819302000	-1.079805000

Cl
E(RB3LYP) = -576.304403361

6	2.548059000	-0.000043000	-0.000362000
1	2.940390000	0.498436000	0.890522000
6	1.090993000	0.000160000	0.000386000
1	2.939550000	0.522324000	-0.877828000
6	-0.111317000	-0.000042000	0.000983000
1	2.939622000	-1.021092000	-0.014340000
17	-1.763880000	-0.000007000	-0.000259000

NHCN
E(RB3LYP) = -264.309297914

6	2.930164000	-0.380974000	0.000000000
1	2.983343000	-1.473374000	0.000042000
6	1.537853000	0.049182000	-0.000001000
1	3.460596000	-0.022273000	0.886513000
6	0.385715000	0.390980000	0.000000000
1	3.460578000	-0.022340000	-0.886550000
7	-0.913414000	0.784676000	-0.000001000
1	-1.129814000	1.772342000	0.000005000
6	-1.940619000	-0.075044000	0.000000000
7	-2.837070000	-0.807422000	0.000000000

SiH3
E(RB3LYP) = -407.429583072

6	2.668741000	0.000012000	-0.000075000
1	3.059680000	-0.956500000	-0.358728000
6	1.213557000	-0.000061000	0.000098000
1	3.059756000	0.167692000	1.007581000
6	0.001838000	0.000049000	0.000151000
1	3.059575000	0.788871000	-0.649183000
14	-1.821482000	0.000001000	-0.000031000
1	-2.327725000	1.261200000	0.596080000
1	-2.327713000	-1.146954000	0.794010000
1	-2.327636000	-0.114323000	-1.390381000

CH2F
E(RB3LYP) = -255.286260547

6	-2.611975000	-0.177546000	0.000045000
1	-3.100398000	0.307311000	-0.849782000
6	-1.179030000	0.081241000	0.000440000
1	-3.080837000	0.188688000	0.917536000
6	0.007871000	0.282951000	0.000167000
1	-2.805694000	-1.251697000	-0.070438000
6	1.436237000	0.545827000	-0.000107000
1	1.735162000	1.105860000	-0.890524000
1	1.735461000	1.106217000	0.889984000
9	2.177522000	-0.650136000	-0.000005000

CH=CH2
E(RB3LYP) = -194.118714993

6	-2.569281000	0.159489000	0.000027000
1	-2.883130000	0.707133000	-0.893906000
6	-1.129955000	-0.060926000	-0.000061000
1	-2.877421000	0.743389000	0.872766000
6	0.066007000	-0.230382000	0.000000000
1	-3.113862000	-0.788801000	0.021241000
6	1.466213000	-0.478657000	0.000008000
6	2.414064000	0.467336000	0.000010000
1	2.165016000	1.522032000	-0.000003000
1	3.463985000	0.200474000	0.000004000
1	1.763132000	-1.525390000	-0.000009000

C6H5
E(RB3LYP) = -347.812391303

6	-4.058050000	0.000062000	0.000058000
1	-4.451139000	1.020374000	-0.027043000
6	-2.601484000	0.000292000	-0.000065000
1	-4.452184000	-0.487102000	0.897181000
6	-1.394305000	-0.000159000	-0.000081000
1	-4.452270000	-0.534220000	-0.869744000

SiMe3
E(RB3LYP) = -525.450949882

6	3.645511000	-0.000377000	-0.000267000
1	4.039359000	-0.867865000	-0.538046000
6	2.189122000	-0.001490000	-0.001164000
1	4.037513000	-0.032162000	1.020619000
6	0.976188000	-0.002147000	-0.001608000
1	4.037968000	0.899827000	-0.482428000

6	0.034001000	-0.000167000	-0.000040000
6	0.751182000	-1.209566000	-0.000023000
6	0.750962000	1.209388000	-0.000009000
1	0.206251000	-2.145981000	-0.000010000
1	0.205887000	2.145718000	-0.000021000
6	2.142082000	-1.205625000	0.000019000
6	2.141814000	1.205763000	0.000019000
1	2.680575000	-2.146775000	0.000064000
1	2.680097000	2.147035000	0.000019000
6	2.843072000	0.000128000	0.000036000
1	3.927142000	0.000254000	0.000070000

H

E(RB3LYP) = -116.692792927

6	1.238325000	0.000002000	0.000037000
1	1.629429000	0.945856000	0.385108000
6	-0.218483000	-0.000003000	-0.000144000
1	1.629595000	-0.139502000	-1.011550000
6	-1.420722000	0.000009000	0.000036000
1	1.629337000	-0.806380000	0.626715000
1	-2.483085000	-0.000022000	0.000153000

OH

E(RB3LYP) = -191.925356551

6	-1.990063000	0.010013000	0.001185000
1	-2.374556000	0.957909000	-0.386681000
6	-0.529862000	-0.003100000	-0.000349000
1	-2.393345000	-0.125859000	1.009084000
6	0.670882000	-0.006830000	-0.000097000
1	-2.389843000	-0.789416000	-0.629583000
8	1.983708000	-0.102463000	0.000257000
1	2.382345000	0.776567000	0.000687000

CH3

E(RB3LYP) = -156.026788189

6	-2.060916000	-0.000059000	0.000001000
1	-2.455947000	-0.414332000	0.932377000
6	-0.602113000	0.000135000	0.000004000
1	-2.455965000	-0.600494000	-0.824871000
6	0.602106000	0.000110000	-0.000019000
1	-2.456216000	1.014422000	-0.107479000
6	2.060910000	-0.000059000	0.000001000
1	2.455974000	-0.699463000	-0.742799000
1	2.456217000	0.992858000	-0.234210000
1	2.456012000	-0.293750000	0.977059000

OMe

E(RB3LYP) = -231.236918292

6	2.576043000	0.203926000	0.000190000
1	3.132513000	-0.624351000	-0.448615000
6	1.142358000	-0.073928000	0.002573000
1	2.961665000	0.352932000	1.013359000
6	-0.035595000	-0.317164000	0.000513000
1	2.803895000	1.103755000	-0.579056000
8	-1.304082000	-0.625670000	-0.000718000
6	-2.208248000	0.500905000	-0.000011000
1	-2.050270000	1.106500000	0.895421000
14	-0.864993000	-0.000321000	-0.000329000
6	-1.471028000	1.180410000	-1.340298000
1	-1.113972000	0.873450000	-2.327389000
1	-2.565067000	1.206834000	-1.371177000
1	-1.115191000	2.198472000	-1.158616000
6	-1.468211000	0.572775000	1.692506000
1	-2.562221000	0.587519000	1.733046000
1	-1.111422000	-0.092400000	2.483918000
1	-1.109876000	1.581187000	1.917846000
6	-1.474720000	-1.750314000	-0.349996000
1	-1.121137000	-2.104526000	-1.322419000
1	-1.118372000	-2.451263000	0.410070000
1	-2.568857000	-1.787715000	-0.355857000

SMe

E(RB3LYP) = -554.233986385

6	-2.982873000	0.250589000	0.000219000
1	-3.164702000	1.325608000	-0.093192000
6	-1.553406000	-0.026934000	0.000700000
1	-3.458308000	-0.087227000	0.926125000
6	-0.365296000	-0.254260000	0.000189000
1	-3.483815000	-0.242795000	-0.838287000
16	1.277268000	-0.667513000	-0.000084000
6	2.062916000	0.993513000	-0.000002000
1	1.781820000	1.545666000	0.895610000
1	3.139058000	0.815543000	-0.000178000
1	1.781618000	1.545968000	-0.895362000

CH2NMe2

E(RB3LYP) = -290.020124675

6	3.523076000	0.181806000	-0.179632000
1	3.627981000	1.008394000	-0.888535000
6	2.120002000	-0.168550000	0.006877000
1	4.092069000	-0.666202000	-0.571846000
6	0.959501000	-0.455483000	0.151276000
1	3.985102000	0.488806000	0.763206000
6	-0.440825000	-0.830043000	0.350347000
1	-0.594634000	-1.842031000	-0.038856000
1	-0.646505000	-0.879514000	1.438838000
7	-1.390596000	0.056528000	-0.330248000
6	-1.332017000	1.423359000	0.172523000
1	-0.319397000	1.814157000	0.064650000
1	-2.007828000	2.053456000	-0.410246000
1	-1.622009000	1.498736000	1.238114000
6	-2.741074000	-0.483167000	-0.257607000
1	-3.421403000	0.159208000	-0.821183000
1	-2.769162000	-1.480301000	-0.704254000
1	-3.122028000	-0.557942000	0.779143000

CH2OH

E(RB3LYP) = -231.258146126

6	-2.631936000	-0.187716000	-0.000040000
1	-3.123208000	0.293827000	-0.850445000
6	-1.199159000	0.076950000	0.000554000
1	-3.103908000	0.179491000	0.915819000
6	-0.013175000	0.281570000	0.000166000
1	-2.824151000	-1.262362000	-0.067963000
6	1.417540000	0.555929000	-0.000129000
1	1.670973000	1.153497000	-0.886732000
1	1.671372000	1.154129000	0.885937000
8	2.147779000	-0.676755000	0.000029000
1	3.087068000	-0.464943000	-0.000153000

NH2

E(RB3LYP) = -172.064256323

6	-2.020688000	-0.000609000	-0.005165000
1	-2.407420000	0.944647000	-0.398457000
6	-0.561316000	-0.000618000	-0.001300000
1	-2.434340000	-0.135800000	0.999408000
6	0.643658000	-0.000382000	0.006581000
1	-2.414712000	-0.800554000	-0.639756000
7	1.998637000	0.000114000	0.081660000
1	2.447754000	0.837149000	-0.266732000
1	2.448334000	-0.836587000	-0.266778000

1	-2.051768000	1.106575000	-0.895665000
1	-3.210726000	0.077510000	0.000707000

N(C3H7)2
E(RB3LYP) = -407.997383829

6	-0.910502000	-3.502167000	-0.095758000
1	-1.944807000	-3.631307000	-0.430350000
6	-0.585827000	-2.086911000	0.052827000
1	-0.794585000	-4.056050000	0.841520000
6	-0.320702000	-0.911556000	0.140650000
1	-0.267751000	-3.976768000	-0.844256000
7	-0.033552000	0.406437000	0.218132000
6	1.373439000	0.739928000	0.507357000
1	1.439480000	1.831766000	0.525462000
1	1.658279000	0.379785000	1.509931000
6	2.345757000	0.190978000	-0.535436000
1	2.059071000	0.575748000	-1.519634000
1	2.245976000	-0.897209000	-0.582721000
6	-1.029226000	1.235179000	0.926828000
1	-1.077459000	0.951434000	1.990139000
1	-0.665883000	2.266266000	0.879245000
6	-2.426176000	1.159549000	0.309397000
1	-2.780292000	0.124939000	0.352257000
1	-3.097388000	1.742094000	0.950538000
6	-2.496386000	1.677682000	-1.129501000
1	-2.182971000	2.725303000	-1.188670000
1	-1.846760000	1.097176000	-1.787931000
1	-3.516427000	1.613860000	-1.518059000
6	3.796956000	0.566981000	-0.222435000
1	3.933624000	1.652929000	-0.196515000
1	4.111924000	0.169782000	0.747589000
1	4.476834000	0.167216000	-0.979041000

Substituted Butadienes

SO2CN
E(RB3LYP) = -796.913415616

6	0.471097000	-0.030474000	-0.692650000
1	0.414711000	0.189530000	-1.751978000
6	1.583333000	-0.029999000	0.055301000
1	1.498047000	-0.282249000	1.109472000
6	2.903965000	0.281609000	-0.456543000
1	2.987227000	0.528569000	-1.510964000
6	3.994522000	0.275444000	0.320277000
1	3.937134000	0.030934000	1.375836000
1	4.973450000	0.514843000	-0.076742000
16	-1.076545000	-0.491119000	0.022852000
8	-0.889530000	-0.897606000	1.406112000
6	-1.906236000	1.096559000	0.082597000
7	-2.445205000	2.117493000	0.115855000
8	-1.829158000	-1.290520000	-0.928128000

C(CN)3
E(RB3LYP) = -472.108456783

6	0.117067000	0.000853000	1.263069000
6	1.454059000	0.000716000	1.182033000
1	1.984593000	0.001439000	2.131104000
1	-0.380460000	0.001677000	2.223392000
6	2.289691000	-0.000178000	-0.006303000
1	1.813860000	-0.000880000	-0.981294000
6	3.626729000	-0.000142000	0.060734000
1	4.147691000	0.000543000	1.012840000
1	4.237273000	-0.000797000	-0.833705000
6	-0.854314000	0.000056000	0.055676000
6	-0.664000000	1.209240000	-0.781713000
7	-0.497700000	2.156860000	-1.414001000
6	-0.663324000	-1.209412000	-0.781114000
7	-0.496632000	-2.157232000	-1.412993000
6	-2.245877000	-0.000311000	0.561383000
7	-3.314689000	-0.000617000	0.987719000

NHNO2
E(RB3LYP) = -360.602745747

6	-0.487791000	0.964856000	0.000214000
6	0.850731000	0.847885000	0.000033000
1	1.374520000	1.801600000	0.000104000
1	-0.997695000	1.916150000	0.000381000
6	1.700711000	-0.326865000	-0.000313000
1	1.227698000	-1.298613000	-0.000494000
6	3.036887000	-0.211600000	-0.000358000
1	3.528295000	0.756530000	-0.000128000
1	3.677223000	-1.085458000	-0.000590000
7	-1.441209000	-0.133032000	0.000086000
8	-1.039427000	-1.293975000	0.000307000
8	-2.626174000	0.193395000	0.000027000

CN
E(RB3LYP) = -248.310070862

6	0.815662000	1.006455000	0.000006000
6	-0.525168000	0.854772000	0.000117000
1	-1.131036000	1.756658000	0.000242000
1	1.256779000	1.996523000	0.000041000
6	-1.234613000	-0.408893000	0.000082000
1	-0.635508000	-1.315220000	-0.000039000
6	-2.571563000	-0.493515000	0.000190000
1	-3.197197000	0.393475000	0.000314000
1	-3.077983000	-1.450966000	0.000161000
6	1.733645000	-0.080429000	-0.000162000
7	2.496740000	-0.950116000	-0.000301000

N(CF3)2 E(RB3LYP) = -885.692109056 6 -0.807967000 -0.048526000 1.161282000 6 -2.118996000 -0.070986000 0.901006000 1 -2.783862000 -0.078521000 1.761023000 1 -0.422377000 -0.039506000 2.174766000 6 -2.742666000 -0.089859000 -0.410776000 1 -2.083678000 -0.085785000 -1.272326000 6 -4.069623000 -0.112551000 -0.582652000 1 -4.753338000 -0.115680000 0.260395000 1 -4.511491000 -0.128446000 -1.571534000 7 0.179458000 -0.019522000 0.098632000 6 0.813428000 1.246603000 -0.083360000 9 -0.100717000 2.168374000 -0.426176000 9 1.415517000 1.704446000 1.043794000 9 1.746264000 1.197873000 -1.039516000 6 0.974912000 -1.195561000 -0.078600000 9 2.113264000 -1.197659000 0.659519000 9 0.260871000 -2.266678000 0.288301000 9 1.343025000 -1.360817000 -1.357494000	CHO E(RB3LYP) = -269.396712262 6 -0.852252000 1.060520000 0.000211000 6 0.491583000 0.898778000 0.000077000 1 1.100193000 1.801790000 0.000069000 1 -1.250803000 2.070845000 0.000284000 6 1.230164000 -0.349001000 -0.000097000 1 0.658505000 -1.268706000 -0.000100000 6 2.571571000 -0.373727000 -0.000224000 1 3.157725000 0.540611000 -0.000195000 1 3.121116000 -1.307528000 -0.000339000 6 -1.869015000 -0.002856000 0.000187000 8 -1.663280000 -1.201725000 -0.000152000 1 -2.912811000 0.374509000 0.000574000
NHNO2 E(RB3LYP) = -415.961801769 6 0.216123000 0.847183000 0.009480000 6 1.560733000 0.781089000 -0.011209000 1 2.081633000 1.731549000 -0.048562000 1 -0.318616000 1.785572000 -0.003188000 6 2.377234000 -0.416891000 0.012623000 1 1.874878000 -1.381080000 0.062229000 6 3.717084000 -0.412859000 -0.018587000 1 4.279538000 0.513946000 -0.065786000 1 4.286750000 -1.333445000 0.002487000 7 -0.626825000 -0.257246000 0.061134000 1 -0.322933000 -1.218106000 0.002439000 7 -2.000555000 -0.152334000 -0.001914000 8 -2.602458000 -1.220314000 -0.035504000 8 -2.487121000 0.967501000 -0.004246000	COCH3 E(RB3LYP) = -308.731838400 6 -0.389825000 0.952512000 0.000087000 6 0.960144000 0.884179000 0.000047000 1 1.500652000 1.829749000 0.000073000 1 -0.844545000 1.938713000 0.000100000 6 1.794265000 -0.303707000 -0.000020000 1 1.293701000 -1.263436000 -0.000046000 6 3.133172000 -0.224678000 -0.000063000 1 3.647696000 0.731950000 -0.000035000 1 3.753184000 -1.113372000 -0.000189000 6 -1.339230000 -0.188252000 0.000001000 8 -0.990810000 -1.357757000 0.000112000 6 -2.809962000 0.189485000 -0.000108000 1 -3.046746000 0.796261000 0.880132000 1 -3.046670000 0.795882000 -0.880632000 1 -3.422183000 -0.710923000 0.000048000
OCF3 E(RB3LYP) = -568.423370544 6 0.380575000 1.583323000 -0.002682000 6 1.568230000 0.966085000 -0.000062000 1 2.388657000 1.679667000 0.006170000 1 0.320437000 2.661665000 0.000017000 6 1.977895000 -0.429498000 -0.003928000 1 1.224524000 -1.204132000 -0.012576000 6 3.267643000 -0.790476000 0.001906000 1 4.066894000 -0.056051000 0.010417000 1 3.559800000 -1.833369000 -0.001592000 8 -0.933813000 1.118596000 -0.010441000 6 -1.305538000 -0.174804000 0.000450000 9 -2.638785000 -0.209201000 0.003035000 9 -0.873150000 -0.855129000 -1.082692000 9 -0.868359000 -0.838372000 1.091544000	Cl E(RB3LYP) = -615.664606880 6 0.747798000 0.921723000 -0.000004000 6 -0.585922000 0.836988000 0.000071000 1 -1.117244000 1.785989000 0.000144000 1 1.283841000 1.859667000 0.000009000 6 -1.392032000 -0.370526000 0.000070000 1 -0.861201000 -1.317210000 0.000033000 6 -2.730975000 -0.363785000 0.000109000 1 -3.296830000 0.562537000 0.000145000 1 -3.300201000 -1.285376000 0.000101000 17 1.826966000 -0.456001000 -0.000112000
NHCN E(RB3LYP) = -303.669328303 6 -0.222149000 0.801385000 -0.000020000 6 1.121609000 0.777267000 -0.000007000 1 1.615882000 1.742511000 0.000007000 1 -0.770297000 1.734079000 -0.000014000 6 1.970115000 -0.399423000 -0.000008000 1 1.492022000 -1.377663000 -0.000047000 6 3.309862000 -0.366075000 0.000035000 1 3.852852000 0.573472000 0.000072000 1 3.899047000 -1.274554000 0.000035000 7 -1.056232000 -0.328437000 -0.000056000 1 -0.648542000 -1.251796000 -0.000068000 6 -2.386757000 -0.249960000 0.000008000 7 -3.543346000 -0.175165000 0.000052000	SiH3 E(RB3LYP) = -446.760674163 6 -0.637872000 0.953426000 0.000015000 6 0.705651000 0.844078000 0.000075000 1 1.299648000 1.758360000 0.000095000 1 -1.032306000 1.969490000 -0.000069000 6 1.485564000 -0.385638000 0.000132000 1 0.941365000 -1.325432000 0.000461000 6 2.824568000 -0.407296000 -0.000129000 1 3.406042000 0.509588000 -0.000327000 1 3.378283000 -1.338495000 -0.000026000 14 -1.947523000 -0.384286000 -0.000036000 1 -1.369637000 -1.751575000 0.000014000 1 -2.812689000 -0.234685000 -1.200711000 1 -2.812854000 -0.234670000 1.200512000
CH2F E(RB3LYP) = -294.629763802	CH=CH2 E(RB3LYP) = -233.464719445

6	-0.773533000	1.096767000	0.000031000
6	0.556641000	0.918365000	0.000056000
1	1.163886000	1.821577000	0.000170000
1	-1.144967000	2.120149000	0.000108000
6	1.313034000	-0.328093000	-0.000050000
1	0.755547000	-1.256177000	-0.000157000
6	2.652030000	-0.357245000	-0.000024000
1	3.242074000	0.554492000	0.000090000
1	3.197830000	-1.293186000	-0.000115000
6	-1.892914000	0.107299000	-0.000136000
1	-2.523511000	0.245540000	0.886119000
1	-2.523065000	0.245304000	-0.886749000
9	-1.477705000	-1.228918000	0.000141000

6	-0.676410000	0.759176000	0.000159000
6	0.676453000	0.759200000	0.000037000
1	1.179011000	1.723513000	-0.000022000
1	-1.179088000	1.723418000	0.000192000
6	1.550145000	-0.399398000	-0.000017000
1	1.089278000	-1.382903000	0.000050000
6	2.888803000	-0.321129000	-0.000132000
1	3.400523000	0.636312000	-0.000194000
1	3.509636000	-1.208838000	-0.000165000
6	-1.550147000	-0.399439000	0.000261000
6	-2.888818000	-0.321096000	-0.000254000
1	-3.400477000	0.636373000	-0.000783000
1	-3.509678000	-1.208791000	-0.000162000
1	-1.089349000	-1.382971000	0.000758000

C6H5

E(RB3LYP) = -387.152227155

6	-0.840037000	1.265628000	0.410063000
6	-2.108877000	0.844426000	0.224638000
1	-2.900598000	1.551205000	0.463729000
1	-0.712794000	2.297341000	0.729592000
6	-2.559470000	-0.427397000	-0.316130000
1	-1.806458000	-1.098970000	-0.716153000
6	-3.848602000	-0.789868000	-0.380193000
1	-4.638083000	-0.151148000	0.003876000
1	-4.151253000	-1.734213000	-0.816526000
6	0.419584000	0.531443000	0.211091000
6	0.567839000	-0.834653000	0.505172000
6	1.548150000	1.231193000	-0.250943000
1	-0.264823000	-1.385170000	0.924796000
1	1.461356000	2.291915000	-0.462875000
6	1.785941000	-1.479763000	0.308661000
6	2.763098000	0.585272000	-0.453808000
1	1.879259000	-2.532823000	0.550486000
1	3.615796000	1.145226000	-0.821567000
6	2.886318000	-0.776657000	-0.179386000
1	3.833935000	-1.281091000	-0.330348000

SiMe3

E(RB3LYP) = -564.778182294

6	-0.281298000	1.244336000	0.000004000
6	-1.618136000	1.069654000	0.000021000
1	-2.266469000	1.946718000	0.000017000
1	0.051471000	2.283124000	-0.000015000
6	-2.323984000	-0.204488000	0.000023000
1	-1.722630000	-1.109704000	-0.000033000
6	-3.658595000	-0.317365000	0.000015000
1	-4.299691000	0.558832000	-0.000010000
1	-4.148959000	-1.283476000	-0.000056000
14	1.109247000	-0.037139000	-0.000005000
6	1.033399000	-1.124403000	-1.546065000
1	1.087986000	-0.517701000	-2.454709000
1	1.870771000	-1.829740000	-1.564152000
1	0.108586000	-1.705850000	-1.594599000
6	1.033284000	-1.124638000	1.545886000
1	1.870555000	-1.830100000	1.563818000
1	1.088014000	-0.518087000	2.454622000
1	0.108392000	-1.705960000	1.594387000
6	2.732217000	0.929464000	0.000154000
1	2.813376000	1.570387000	-0.883369000
1	2.813223000	1.570333000	0.883731000
1	3.594601000	0.255812000	0.000207000

H

E(RB3LYP) = -156.040812914

6	-1.846096000	-0.109663000	0.000028000
1	-2.017170000	-1.181684000	0.000317000
6	-0.608508000	0.399802000	-0.000055000
1	-0.476504000	1.480004000	-0.000117000
1	-2.722983000	0.526497000	0.000002000
6	0.608472000	-0.399856000	-0.000073000
1	0.476535000	-1.479899000	-0.000186000
6	1.846099000	0.109662000	0.000079000
1	2.017225000	1.181783000	0.000147000
1	2.723094000	-0.526372000	-0.000042000

SMe

E(RB3LYP) = -593.581433229

6	-0.232076000	0.841336000	-0.146795000
6	1.110451000	0.834688000	-0.046915000
1	1.612515000	1.798439000	-0.083672000
1	-0.762349000	1.783589000	-0.244190000
6	1.955622000	-0.335132000	0.101919000
1	1.453584000	-1.293081000	0.213042000
6	3.295298000	-0.298075000	0.122079000
1	3.839782000	0.634323000	0.008833000
1	3.884793000	-1.197768000	0.249949000
16	-1.262173000	-0.590553000	-0.227959000
6	-2.847884000	0.122480000	0.334563000
1	-3.133460000	0.968143000	-0.292923000
1	-3.595279000	-0.663817000	0.227634000
1	-2.793285000	0.427243000	1.379564000

OH

E(RB3LYP) = -231.287970220

6	-1.284629000	0.547671000	-0.000046000
6	0.044782000	0.720242000	-0.000003000
1	0.402963000	1.744366000	0.000059000
1	-1.968359000	1.390706000	0.000044000
6	1.024764000	-0.350328000	0.000001000
1	0.633683000	-1.363529000	-0.000004000
6	2.351509000	-0.160377000	0.000018000
1	2.784166000	0.835403000	0.000016000
1	3.042400000	-0.994715000	0.000029000
8	-1.861843000	-0.693269000	-0.000077000
1	-2.818666000	-0.609325000	0.000653000

CH2NMe2

E(RB3LYP) = -329.363931321

6	0.404498000	0.701707000	0.822879000
6	1.702674000	0.375453000	0.709918000
1	2.326730000	0.484063000	1.594792000
1	0.043379000	1.047451000	1.788350000
6	2.390683000	-0.112608000	-0.477384000
1	1.802925000	-0.258340000	-1.378921000
6	3.700503000	-0.390820000	-0.514220000
1	4.333066000	-0.257570000	0.358079000
1	4.178618000	-0.757184000	-1.414755000
6	-0.650064000	0.681259000	-0.248068000
1	-0.886145000	1.719251000	-0.514129000
1	-0.281236000	0.199059000	-1.170678000
7	-1.894717000	0.064238000	0.218708000
6	-1.746276000	-1.366876000	0.456164000

1	-0.933594000	-1.547414000	1.161895000
1	-2.668288000	-1.764286000	0.887176000
1	-1.527528000	-1.931628000	-0.470149000
6	-3.003054000	0.339669000	-0.684991000
1	-3.925146000	-0.077394000	-0.272867000
1	-3.137682000	1.418854000	-0.791793000
1	-2.855861000	-0.091236000	-1.693738000

CH3

E(RB3LYP) = -195.368388181

6	1.232088000	0.636897000	0.000033000
6	-0.108343000	0.730634000	-0.000156000
1	-0.545031000	1.727143000	-0.000283000
1	1.794519000	1.567935000	0.000080000
6	-1.063121000	-0.368151000	-0.000221000
1	-0.668172000	-1.380023000	-0.000715000
6	-2.392403000	-0.201550000	0.000205000
1	-2.839543000	0.787768000	0.000586000
1	-3.071161000	-1.045981000	0.000075000
6	2.066870000	-0.608995000	0.000113000
1	2.722204000	-0.632876000	0.878217000
1	1.474095000	-1.524195000	-0.000065000
1	2.722541000	-0.632788000	-0.877741000

CH2OH

E(RB3LYP) = -270.603128465

6	-0.739347000	1.115499000	-0.051624000
6	0.586801000	0.915626000	-0.148811000
1	1.201810000	1.759531000	-0.455728000
1	-1.116986000	2.111438000	-0.268106000
6	1.307809000	-0.319142000	0.130501000
1	0.719118000	-1.182384000	0.422536000
6	2.640522000	-0.422423000	0.041269000
1	3.257448000	0.419181000	-0.259651000
1	3.153874000	-1.349774000	0.265987000
6	-1.785220000	0.103224000	0.354094000
1	-1.740711000	-0.087758000	1.431171000
1	-2.781026000	0.513948000	0.145774000
8	-1.645649000	-1.184837000	-0.253396000
1	-1.591726000	-1.062188000	-1.207385000

OMe

E(RB3LYP) = -270.593241890

6	0.772724000	1.090742000	-0.000002000
6	-0.555521000	0.853058000	0.000017000
1	-1.141616000	1.768667000	0.000070000
1	1.114125000	2.119790000	0.000016000
6	-1.346376000	-0.367764000	-0.000039000
1	-0.838446000	-1.324163000	-0.000119000
6	-2.687805000	-0.375466000	0.000008000
1	-3.262696000	0.545257000	0.000097000
1	-3.246716000	-1.303191000	-0.000031000
8	1.858292000	0.283748000	-0.000045000
6	1.716466000	-1.132838000	0.000040000
1	1.191054000	-1.475585000	0.896001000
1	1.191172000	-1.475699000	-0.895946000
1	2.729865000	-1.531464000	0.000128000

NH2

E(RB3LYP) = -211.419368372

6	-1.275020000	0.573382000	0.000953000
6	0.067686000	0.725404000	0.005390000
1	0.443962000	1.742738000	0.010313000
1	-1.904353000	1.457122000	-0.001596000
6	1.045561000	-0.342751000	-0.003801000
1	0.672480000	-1.365754000	-0.025253000
6	2.377308000	-0.173648000	0.005534000
1	2.822384000	0.816266000	0.019526000
1	3.056077000	-1.017563000	-0.002873000
7	-1.990878000	-0.610575000	-0.068404000
1	-2.938246000	-0.585430000	0.273530000
1	-1.509371000	-1.467679000	0.156722000

N(C3H7)2

E(RB3LYP) = -447.344417184

6	0.303589000	-1.416162000	0.649786000
6	1.597096000	-1.614201000	0.286044000
1	1.985896000	-2.604605000	0.503273000
1	-0.226243000	-2.283833000	1.038215000
6	2.506744000	-0.715706000	-0.394821000
1	2.105898000	0.223552000	-0.764416000
6	3.798981000	-0.982966000	-0.649643000
1	4.265624000	-1.904600000	-0.315824000
1	4.421881000	-0.289011000	-1.200766000
7	-0.486063000	-0.283769000	0.603302000
6	0.070701000	1.052086000	0.834571000
1	-0.401910000	1.475169000	1.733159000
1	1.129906000	0.943930000	1.071222000
6	-0.111623000	2.030530000	-0.331533000
1	-1.178388000	2.126251000	-0.560408000
1	0.355259000	1.610895000	-1.228544000
6	-1.906287000	-0.466582000	0.921934000
1	-2.010906000	-0.960128000	1.901405000
1	-2.349504000	0.527558000	1.020639000
6	-2.693026000	-1.259752000	-0.130314000
1	-2.254545000	-2.258016000	-0.232963000
1	-3.705805000	-1.411965000	0.261059000
6	-2.759633000	-0.584302000	-1.501474000
1	-3.249078000	0.393136000	-1.438820000
1	-1.759602000	-0.433126000	-1.914064000
1	-3.327112000	-1.193529000	-2.209863000
6	0.478074000	3.410348000	-0.025802000
1	0.006401000	3.859892000	0.853928000
1	1.552891000	3.348868000	0.171516000

1	0.334085000	4.096183000	-0.864369000	