

1. Geometries

*** BeH ***

BERYLLIUM	4.0	0.000000	0.000000	0.0000
HYDROGEN	1.0	0.000000	0.000000	1.3426

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*** CH ***

CARBON	6.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.0000	1.1199

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*** CH2 (1A1) ***

CARBON	6.0	0.000000	0.000000	0.173491
HYDROGEN	1.0	0.863117	0.000000	-0.520473
HYDROGEN	1.0	-0.863117	0.000000	-0.520473

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*** CH2 (3B1) ***

CARBON	6.0	0.000000	0.000000	0.105335
HYDROGEN	1.0	0.988771	0.000000	-0.316004
HYDROGEN	1.0	-0.988771	0.000000	-0.316004

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*** CH3 ***

CARBON	6.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	1.0761	0.0000	0.0000
HYDROGEN	1.0	-0.53805	-0.93193	0.0000
HYDROGEN	1.0	-0.53805	0.93193	0.0000

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*** CH3CH2 - transition state ***

CARBON	6.0	-0.258719	-0.816829	0.000000
CARBON	6.0	-0.250987	0.674191	0.000000
HYDROGEN	1.0	0.758830	-1.225939	0.000000
HYDROGEN	1.0	-0.758830	-1.213866	0.883419

HYDROGEN	1.0	-0.758830	-1.213866	-0.883419
HYDROGEN	1.0	-0.170021	1.225939	-0.924320
HYDROGEN	1.0	-0.170021	1.225939	0.924320

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*** CH3Cl ***

CARBON	6.0	0.000000	0.000000	1.121004
CHLORINE	17.0	0.000000	0.000000	-0.654596
HYDROGEN	1.0	1.030550	0.000000	1.467371
HYDROGEN	1.0	-0.515275	0.892483	1.467371
HYDROGEN	1.0	-0.515275	-0.892483	1.467371

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*** CH3F ***

CARBON	6.0	-0.632074	0.000001	-0.000000
FLUORINE	9.0	0.749117	0.000002	-0.000002
HYDROGEN	1.0	-0.983182	-0.338489	0.972625
HYDROGEN	1.0	-0.983222	1.011553	-0.193172
HYDROGEN	1.0	-0.983203	-0.673084	-0.779437

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*** CH3FCl -- transition state ***

CHLORINE	17.0	1.454749	-0.001237	-0.000040
FLUORINE	9.0	-0.323587	0.004631	0.000124
CARBON	6.0	-2.387418	-0.002147	-0.000073
HYDROGEN	1.0	-2.495086	-0.855361	-0.649404
HYDROGEN	1.0	-2.497313	-0.138673	1.063139
HYDROGEN	1.0	-2.501537	0.986269	-0.413734

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*** CH3SH ***

CARBON	6.0	-0.047746	1.150109	0.000000
SULFUR	16.0	-0.047746	-0.663637	0.000000
HYDROGEN	1.0	1.278061	-0.829659	0.000000
HYDROGEN	1.0	-1.091202	1.456430	0.000000

HYDROGEN	1.0	0.431778	1.545383	0.891004
HYDROGEN	1.0	0.431778	1.545383	-0.891004

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*** CH4 ***

CARBON	6.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.6276	0.6276	0.6276
HYDROGEN	1.0	0.6276	-0.6276	-0.6276
HYDROGEN	1.0	-0.6276	0.6276	-0.6276
HYDROGEN	1.0	-0.6276	-0.6276	0.6276

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*** Cl2 ***

CHLORINE	17.0	0.0000	0.0000	0.0000
CHLORINE	17.0	0.0000	0.0000	1.9879

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*** ClCH3Cl- -- transition state ***

CHLORINE	17.0	0.000025	0.019526	2.322499
CARBON	6.0	0.000513	0.000486	-0.000089
HYDROGEN	1.0	0.761278	-0.750733	0.006377
HYDROGEN	1.0	-1.030451	-0.282724	0.002147
HYDROGEN	1.0	0.270728	1.034927	-0.008697
CHLORINE	17.0	-0.000297	-0.019784	-2.322458

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*** ClF ***

FLUORINE	9.0	0.0000	0.0000	0.0000
CHLORINE	17.0	0.0000	0.0000	1.6283

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*** ClO ***

OXYGEN	8.0	0.0000	0.0000	0.0000
CHLORINE	17.0	0.0000	0.0000	1.5696

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*** CN ***

CARBON	6.0	0.0000	0.0000	0.0000
NITROGEN	7.0	0.0000	0.0000	1.1718

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*** CO ***

CARBON	6.0	0.0000	0.0000	0.0000
OXYGEN	8.0	0.0000	0.0000	1.1283

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*** CO2 ***

CARBON	6.0	0.0000	0.0000	0.0000
OXYGEN	8.0	0.0000	0.0000	1.15996
OXYGEN	8.0	0.0000	0.0000	-1.15996

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*** CS ***

CARBON	6.0	0.0000	0.0000	0.0000
SULFUR	16.0	0.0000	0.0000	1.5349

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*** F2 ***

FLUORINE	9.0	0.0000	0.0000	0.0000
FLUORINE	9.0	0.0000	0.0000	1.4119

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*** FCH3Cl- -- transition state ***

FLUORINE	9.0	0.000000	0.000000	-2.537929
CARBON	6.0	0.000000	0.000000	-0.488372
HYDROGEN	1.0	1.062087	0.000000	-0.614972
HYDROGEN	1.0	-0.531044	0.919794	-0.614972
HYDROGEN	1.0	-0.531044	-0.919794	-0.614972
CHLORINE	17.0	0.000000	0.000000	1.624501

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*** H2 ***

HYDROGEN	1.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.0000	0.7414

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*** H2CCH2 ***

CARBON	6.0	0.665593	0.000000	0.000000
CARBON	6.0	-0.665593	0.000000	0.000000
HYDROGEN	1.0	1.231668	0.921495	0.000000
HYDROGEN	1.0	1.231668	-0.921495	0.000000
HYDROGEN	1.0	-1.231668	0.921495	0.000000
HYDROGEN	1.0	-1.231668	-0.921495	0.000000

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*** H2CO ***

OXYGEN	8.0	0.000000	0.000000	0.674622
CARBON	6.0	0.000000	0.000000	-0.529707
HYDROGEN	1.0	0.000000	0.935488	-1.109367
HYDROGEN	1.0	0.000000	-0.935488	-1.109367

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*** H2NNH2 ***

NITROGEN	7.0	0.709861	-0.100341	-0.075134
NITROGEN	7.0	-0.709861	0.100341	-0.075134
HYDROGEN	1.0	1.049529	-0.372881	0.838343
HYDROGEN	1.0	1.138255	0.781853	-0.312407
HYDROGEN	1.0	-1.049529	0.372881	0.838343
HYDROGEN	1.0	-1.138255	-0.781853	-0.312407

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*** H2O ***

OXYGEN	8.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.75751	0.58717
HYDROGEN	1.0	0.0000	-0.75751	0.58717

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*** H2S ***

SULFUR	16.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.9616	0.9269

HYDROGEN 1.0 0.0000 -0.9616 0.9269

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*** H3CCH3 ***

CARBON	6.0	-0.763092	0.000000	0.000000
CARBON	6.0	0.763092	0.000001	-0.000001
HYDROGEN	1.0	1.158312	-0.443642	-0.914097
HYDROGEN	1.0	-1.158309	-1.013325	-0.074640
HYDROGEN	1.0	1.158311	-0.569815	0.841253
HYDROGEN	1.0	1.158308	1.013455	0.072848
HYDROGEN	1.0	-1.158310	0.442020	0.914883
HYDROGEN	1.0	-1.158310	0.571304	-0.840243

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*** H3COH ***

CARBON	6.0	-0.046423	0.663069	0.000000
OXYGEN	8.0	-0.046423	-0.755063	0.000000
HYDROGEN	1.0	-1.086956	0.975938	0.000000
HYDROGEN	1.0	0.860592	-1.057039	0.000000
HYDROGEN	1.0	0.438145	1.071594	0.889539
HYDROGEN	1.0	0.438145	1.071594	-0.889539

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*** HC2H4 - transition state ***

CARBON	6.0	-0.567877	0.000051	-0.218958
CARBON	6.0	0.751139	-0.000036	0.041932
HYDROGEN	1.0	-1.493884	-0.000488	1.531765
HYDROGEN	1.0	-1.101691	0.920651	-0.408626
HYDROGEN	1.0	-1.102022	-0.920234	-0.409110
HYDROGEN	1.0	1.299128	-0.922344	0.173763
HYDROGEN	1.0	1.298899	0.922325	0.174363

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*** HCCH ***

CARBON	6.0	0.000000	0.000000	-0.601571
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CARBON	6.0	0.000000	0.000000	0.601571
HYDROGEN	1.0	0.000000	0.000000	1.664176
HYDROGEN	1.0	0.000000	0.000000	-1.664176

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*** HCl ***

CHLORINE	17.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.0000	1.2746

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*** HClH -- transition state ***

HYDROGEN	1.0	0.000000	0.000000	1.485800
CHLORINE	17.0	0.000000	0.000000	0.000000
HYDROGEN	1.0	0.000000	0.000000	-1.485800

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*** HCN ***

CARBON	6.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.0000	1.06501
NITROGEN	7.0	0.0000	0.0000	-1.15324

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*** HCN -- transition state ***

CARBON	6.0	0.080319	0.620258	0.000000
NITROGEN	7.0	0.080319	-0.568095	0.000000
HYDROGEN	1.0	-1.044148	0.255121	0.000000

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*** HCO ***

CARBON	6.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	1.1191	0.0000	0.0000
OXYGEN	8.0	-0.6646	0.9695	0.0000

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*** HF ***

FLUORINE	9.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.0000	0.9168

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*** HN2 ***
NITROGEN  7.0  -0.062442   0.659491   0.000000
NITROGEN  7.0  -0.062442  -0.518709   0.000000
HYDROGEN  1.0   0.874194  -0.985478   0.000000
--
*** HN2 -- transition state ***
NITROGEN  7.0   0.084563  -0.642934   0.000000
NITROGEN  7.0   0.084563   0.479877   0.000000
HYDROGEN  1.0  -1.183883   1.141399   0.000000
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** HN2O -- transition state ***
HYDROGEN  1.0  -0.303286  -1.930712   0.000000
OXYGEN     8.0  -0.861006  -0.621526   0.000000
NITROGEN  7.0   0.000000   0.257027   0.000000
NITROGEN  7.0   1.027333   0.729104   0.000000
--
*** HNC ***
CARBON     6.0   0.000000   0.000000  -0.737248
NITROGEN  7.0   0.000000   0.000000   0.432089
HYDROGEN  1.0   0.000000   0.000000   1.426960
--
*** HOCH3F- -- transition state ***
FLUORINE   9.0   1.850614  -0.013179  -0.000128
CARBON     6.0   0.090857   0.010586   0.000269
HYDROGEN   1.0   0.040907   1.079548  -0.011749
HYDROGEN   1.0   0.037163  -0.528013  -0.922944
HYDROGEN   1.0   0.037486  -0.507463   0.935132
OXYGEN     8.0  -1.892801   0.103266  -0.000118
HYDROGEN   1.0  -2.173821  -0.815112   0.000039
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*** HOCH4 -- transition state ***

CARBON	6.0	-1.211487	0.007968	0.000407
OXYGEN	8.0	1.293965	-0.108694	0.000133
HYDROGEN	1.0	0.009476	-0.118020	0.002799
HYDROGEN	1.0	-1.525529	-0.233250	1.010070
HYDROGEN	1.0	-1.430665	1.033233	-0.278082
HYDROGEN	1.0	-1.552710	-0.710114	-0.737702
HYDROGEN	1.0	1.416636	0.849894	-0.000591

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*** HOCl ***

OXYGEN	8.0	1.091852	-0.117250	0.000000
HYDROGEN	1.0	1.368603	0.805753	0.000000
CHLORINE	17.0	-0.594319	0.007779	0.000000

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*** HOH -- transition state ***

HYDROGEN	1.0	0.000000	0.000000	-0.860287
OXYGEN	8.0	0.000000	0.000000	0.329024
HYDROGEN	1.0	0.000000	0.000000	-1.771905

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*** Li2 ***

LITHIUM	3.0	0.0000	0.0000	0.0000
LITHIUM	3.0	0.0000	0.0000	2.6730

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*** LiF ***

FLUORINE	9.0	0.0000	0.0000	0.0000
LITHIUM	3.0	0.0000	0.0000	1.5639

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*** LiH ***

LITHIUM	3.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.0000	1.5957

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*** N2 ***

NITROGEN	7.0	0.0000	0.0000	0.5488
NITROGEN	7.0	0.0000	0.0000	-0.5488

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*** N2O ***

NITROGEN	7.0	0.0	0.0	-1.195674
NITROGEN	7.0	0.0	0.0	-0.075111
OXYGEN	8.0	0.0	0.0	1.111937

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*** Na2 ***

SODIUM	11.0	0.0000	0.0000	0.0000
SODIUM	11.0	0.0000	0.0000	3.0789

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*** NaCl ***

SODIUM	11.0	0.0000	0.0000	0.0000
CHLORINE	17.0	0.0000	0.0000	2.3608

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*** NH ***

NITROGEN	7.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.0000	1.0362

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*** NH2 ***

NITROGEN	7.0	0.000000	0.000000	0.141904
HYDROGEN	1.0	-0.801783	0.000000	-0.496664
HYDROGEN	1.0	0.801783	0.000000	-0.496664

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*** NH3 ***

NITROGEN	7.0	0.000000	0.000000	0.112890
HYDROGEN	1.0	0.000000	0.938024	-0.263409
HYDROGEN	1.0	0.812353	-0.469012	-0.263409
HYDROGEN	1.0	-0.812353	-0.469012	-0.263409

--

*** O2 ***

OXYGEN	8.0	0.0000	0.0000	0.0000
OXYGEN	8.0	0.0000	0.0000	1.2075

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*** O3 ***

OXYGEN	8.0	0.00000000	0.00000000	0.44434005
OXYGEN	8.0	1.08339666	0.00000000	-0.22217002
OXYGEN	8.0	-1.08339666	0.00000000	-0.22217002

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*** OH- ***

OXYGEN	8.0	0.000000	0.000000	0.106894
HYDROGEN	1.0	0.000000	0.000000	-0.855149

--

*** OH ***

OXYGEN	8.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.0000	0.9697

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*** P2 ***

PHOSPHORUS	15.0	0.0000	0.0000	0.0000
PHOSPHORUS	15.0	0.0000	0.0000	1.8934

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*** PH2 ***

PHOSPHORUS	15.0	0.000000	0.000000	-0.115657
HYDROGEN	1.0	1.020130	0.000000	0.867427
HYDROGEN	1.0	-1.020130	0.000000	0.867427

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*** PH3 ***

PHOSPHORUS	15.0	0.000000	0.000000	0.127520
HYDROGEN	1.0	1.187921	0.000000	-0.637602
HYDROGEN	1.0	-0.593960	-1.028770	-0.637602

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HYDROGEN      1.0      -0.593960      1.028770      -0.637602
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*** S2 ***
SULFUR      16.0      0.0000 0.0000 0.0000
SULFUR      16.0      0.0000 0.0000 1.8892
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*** SH ***
SULFUR      16.0      0.000000      0.000000      0.078835
HYDROGEN     1.0      0.000000      0.000000     -1.261367
--
*** SH3 -- transition state ***
HYDROGEN     1.0      1.262097     -0.220097      0.000000
SULFUR      16.0      0.000000      0.223153      0.000000
HYDROGEN     1.0     -0.500576     -1.115445      0.000000
HYDROGEN     1.0     -0.761521     -2.234913      0.000000
--
*** Si2 ***
SILICON      14.0 0.0000 0.0000 0.0000
SILICON      14.0 0.0000 0.0000 2.2460
--
*** Si2H6 ***
SILICON      14.0      0.000000      0.000000      1.170305
SILICON      14.0      0.000000      0.000000     -1.170305
HYDROGEN      1.0      1.388110      0.000000      1.685486
HYDROGEN      1.0     -0.694055      1.202138      1.685486
HYDROGEN      1.0     -0.694055     -1.202138      1.685486
HYDROGEN      1.0     -1.388110      0.000000     -1.685486
HYDROGEN      1.0      0.694055      1.202138     -1.685486
HYDROGEN      1.0      0.694055     -1.202138     -1.685486
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*** SiH2 (1A1) ***

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SILICON	14.0	0.000000	0.000000	0.130965
HYDROGEN	1.0	0.000000	1.094746	-0.916757
HYDROGEN	1.0	0.000000	-1.094746	-0.916757

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*** SiH2 (3B1) ***

SILICON	14.0	0.0000	0.0000	0.0000
HYDROGEN	1.0	0.0000	0.0000	-1.514
HYDROGEN	1.0	0.0000	1.5130	0.0555

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*** SiH3 ***

SILICON	14.0	0.000000	0.000000	0.079177
HYDROGEN	1.0	0.000000	1.407982	-0.369492
HYDROGEN	1.0	1.219348	-0.703991	-0.369492
HYDROGEN	1.0	-1.219348	-0.703991	-0.369492

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*** SiH4 ***

SILICON	14.0	0.000000	0.000000	0.000000
HYDROGEN	1.0	0.852576	0.852576	0.852576
HYDROGEN	1.0	-0.852576	-0.852576	0.852576
HYDROGEN	1.0	-0.852576	0.852576	-0.852576
HYDROGEN	1.0	0.852576	-0.852576	-0.852576

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*** SiO ***

SILICON	14.0	0.0000	0.0000	0.0000
OXYGEN	8.0	0.0000	0.0000	1.5097

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*** SO ***

SULFUR	16.0	0.0000	0.0000	0.0000
OXYGEN	8.0	0.0000	0.0000	1.4811

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*** SO2 ***

SULFUR	16.0	0.0000	0.0000	0.0000
OXYGEN	8.0	0.0000	1.2349	0.72264
OXYGEN	8.0	0.0000	-1.2349	0.72264
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2.1 Estat values (tab-delimited text format, copy and paste into Excel for table format)

	pc-0	pc-1[sp]	pc-2[sp]	pc-3[sp]	pc-4[sp]	pc-0[spd_2]	pc-1	pc-1[spd_2]	pc-1[spd_3]
	pc-2[spd_1]	pc-2[spd]	pc-2[spd_3]	pc-3[spd_2]	pc-3[spd]	pc-4[spd]	pc-2	pc-3[spdf]	
	pc-4[spdf]	pc-3	pc-4[spdfg]	cc-pVDZ[sp]	cc-pVTZ[sp]	cc-pVQZ[sp]	cc-pV5Z[sp]		
	cc-pVDZ	cc-pVTZ[spd]	cc-pVQZ[spd]	cc-pV5Z[spd]	cc-pVTZ	cc-pVQZ[spdf]	cc-		
	pV5Z[spdf]	cc-pVQZ	cc-pV5Z[spdfg]	STO-3G	6-31G	6-311G	6-31G(d,p)	6-311G(d,p)	
	6-31G(2d,2p)	6-311G(2d,2p)	6-311G(2df,2pd)						
al	0.023947229	0.023463206	0.02352473	0.023837722	0.023882051	0.024229997			
	0.023686921	0.023711534	0.023677644	0.023744886	0.023769767	0.02373654			
	0.024094025	0.024059147	0.024088451	0.023770759	0.02405753	0.024086758			
	0.02405755	0.024086787	0.023748294	0.023781652	0.023891402	0.023974458			
	0.023956512	0.023975424	0.024091891	0.02417716	0.023981326	0.02409539			
	0.024179431	0.024095537	0.024179141	0.023878211	0.023880499	0.02389162			
	0.024140604	0.024151452	0.024084291	0.024096599	0.024100714				
b	0.033407902	0.033033329	0.033653477	0.034571962	0.034573461	0.033603371			
	0.033182507	0.033200229	0.033160038	0.033803019	0.03382625	0.033786685			
	0.034763205	0.034725552	0.034725794	0.033830637	0.034731815	0.034732517			
	0.034731819	0.034732526	0.033617256	0.034244955	0.034546146	0.034567649			
	0.033769055	0.034399009	0.034700571	0.034720818	0.03440473	0.034707252			
	0.034727715	0.034707261	0.034727715	0.040248038	0.034408542	0.034349537			
	0.034578648	0.034536962	0.034539454	0.034487976	0.034494121				
be	0.016716313	0.040347093	0.042485674	0.043805705	0.043794894	0.045793086			
	0.040347093	0.04260212	0.043796987	0.040285473	0.042485674	0.043674011			
	0.042690949	0.043805705	0.043794894	0.042485673	0.043805705	0.043794894			
	0.043805705	0.043794894	0.04304756	0.043564795	0.043796741	0.043813221			
	0.04304756	0.043564795	0.043796741	0.043813221	0.043564795	0.043796741			
	0.043813221	0.043796741	0.043813221	0.05174911	0.04508512	0.04373382			
	0.04508512	0.043733819	0.04508512	0.04373382	0.04373382				
beh	0.015834792	0.020755323	0.020283072	0.02068722	0.020657536	0.024356729			
	0.020368779	0.024695366	0.025415559	0.020004334	0.026044088	0.025335969			

	0.024870522	0.026820054	0.026856898	0.026374866	0.027594859	0.027629736
	0.027605081	0.027655576	0.020492979	0.020578281	0.020651493	0.020665306
	0.025438994	0.026705036	0.026850797	0.026864551	0.027359624	0.027592638
	0.027659238	0.027624353	0.027659238	0.022311326	0.020395784	0.020558032
	0.022415465	0.025279899	0.026657834	0.026634685	0.02727024	
c	0.018655592	0.01822672	0.01870756	0.019181181	0.01918072	0.018797856
	0.018355965	0.018337497	0.018309636	0.018843034	0.018826098	0.018800023
	0.019312924	0.019288711	0.019287619	0.018829953	0.019293554	0.019292741
	0.019293557	0.019292744	0.018553734	0.019022378	0.019164616	0.019177195
	0.01866875	0.019132933	0.019273426	0.019284905	0.019137264	0.019278422
	0.019290042	0.019278425	0.019290042	0.020327714	0.018743489	0.019039114
	0.018877145	0.019181858	0.018832905	0.01913765	0.019142199	
ch	0.037476068	0.038619415	0.039378688	0.039807492	0.039736407	0.040976331
	0.04038315	0.04129242	0.041531832	0.041057405	0.041981236	0.042294738
	0.042553409	0.04278573	0.042790559	0.042235655	0.043046699	0.043065615
	0.043048631	0.043066653	0.039091504	0.039672586	0.039855236	0.039763253
	0.041498933	0.042563016	0.042785024	0.042799848	0.042826571	0.04306833
	0.043072804	0.043070767	0.0430728	0.042393871	0.039375284	0.039873638
	0.041470937	0.041994116	0.042670541	0.042695186	0.042918225	
ch2_sing	0.05398307	0.056457556	0.057196474	0.057524493	0.057391253	0.057560777
	0.058180466	0.059339992	0.060013454	0.058915951	0.060163994	0.060817647
	0.06092185	0.061358299	0.061393285	0.060783525	0.061987061	0.062049842
	0.061998536	0.062056798	0.056829317	0.057266322	0.057588992	0.057425644
	0.059389497	0.06100122	0.061361615	0.061375457	0.061634975	0.062037368
	0.062059297	0.062048718	0.062059298	0.06024085	0.057211429	0.057655207
	0.059559069	0.059992277	0.061218454	0.061286457	0.061837002	
ch2_trip	0.037947575	0.040845483	0.040968793	0.041378537	0.041286391	0.035635325
	0.03805355	0.037882337	0.037847402	0.038319029	0.038251657	0.038360358
	0.038804896	0.038789561	0.038791428	0.038329893	0.038744015	0.038749795
	0.038745346	0.038749839	0.040828193	0.040972882	0.041400629	0.041331424
	0.038195839	0.038527834	0.03878493	0.038802978	0.03853346	0.038740625

	0.038750614	0.038742349	0.038750615	0.042703758	0.040519704	0.041235692
	0.038170531	0.038734144	0.038314128	0.038638875	0.038609429	
ch3	0.05592419	0.061258589	0.060857351	0.061467336	0.061353141	0.053736332
	0.058363899	0.058111127	0.058166287	0.058422348	0.058534491	0.058748016
	0.059310001	0.059321397	0.059339572	0.058761767	0.059353973	0.059371043
	0.05936192	0.059373809	0.060976046	0.060875211	0.061459846	0.061405724
	0.058157876	0.058994849	0.059323313	0.05934078	0.059071925	0.059360881
	0.059374861	0.059367747	0.059374861	0.061861039	0.060361893	0.061441911
	0.058196161	0.058946739	0.058428778	0.05912676	0.059171154	
ch3ch2	0.121971592	0.13381804	0.132087958	0.133052553	0.132760844	0.118718895
	0.127893894	0.127132973	0.127097062	0.1273482	0.127527118	0.127909646
	0.128872316	0.128848668	0.1288603	0.127887999	0.128894591	0.128918748
	0.128904969	0.128921423	0.132564916	0.132008814	0.133047733	0.132889908
	0.126622782	0.128214525	0.12886005	0.128863666	0.128332141	0.128899127
	0.128924849	0.128903876	0.128924847	0.128639646	0.131114378	0.133158503
	0.126630038	0.128178874	0.126777428	0.128446214	0.128525718	
ch3cl	0.08239057	0.09177557	0.089317609	0.089832903	0.089760707	0.079465424
	0.087207901	0.086271154	0.086104281	0.086145369	0.086022411	0.086246246
	0.087037221	0.087002293	0.087050727	0.086421656	0.08717215	0.087193128
	0.087191372	0.087207432	0.090532958	0.08942342	0.089850048	0.089855658
	0.085724379	0.086560373	0.087010912	0.087043765	0.086766682	0.087173665
	0.087219351	0.087199066	0.087219762	0.086118673	0.089227734	0.090341063
	0.085986005	0.086851938	0.085458741	0.086747421	0.086860698	
ch3f	0.089277926	0.097985901	0.096519198	0.097107575	0.096907857	0.086302706
	0.09321464	0.092917909	0.092938372	0.092581864	0.092724879	0.092954253
	0.09371685	0.093695132	0.093729114	0.092953504	0.093761431	0.093794345
	0.093769164	0.093796296	0.097114904	0.096622886	0.097168457	0.097027989
	0.092515137	0.093230104	0.093710929	0.093721104	0.093343512	0.093781975
	0.093800187	0.093784011	0.093800231	0.094127104	0.096378469	0.097477315
	0.092494963	0.09341791	0.092356584	0.093520399	0.09353423	

ch3fc1	0.110649396	0.119052947	0.120368002	0.119978593	0.119747027	0.102824438
	0.11155598	0.110584711	0.110654631	0.112222167	0.111639607	0.111541511
	0.112357785	0.11216429	0.112141966	0.111861451	0.11221109	0.112176201
	0.112162981	0.11214742	0.119677645	0.11984376	0.120499619	0.120175402
	0.111933779	0.112258264	0.112337296	0.112242274	0.112237509	0.112361699
	0.112256901	0.112328942	0.112256678	0.128280085	0.119455327	0.12030734
	0.11222276	0.113691191	0.111888412	0.112689426	0.112691978	
ch3sh	0.102482964	0.112347161	0.10985128	0.110408523	0.110373831	0.096705882
	0.105006417	0.103847067	0.103515347	0.103951958	0.103564854	0.103734677
	0.104665751	0.104560144	0.104577716	0.103856232	0.104618049	0.104630205
	0.104621113	0.1046345	0.111030547	0.109951106	0.110538121	0.11051628
	0.103219555	0.104095726	0.104597784	0.104607116	0.104179009	0.104644379
	0.104671487	0.104655101	0.104672854	0.106123972	0.109528623	0.111067862
	0.103568964	0.104604078	0.10297451	0.104420726	0.104350671	
ch4	0.075997284	0.08442169	0.082884848	0.083828485	0.083692476	0.075024584
	0.082127725	0.081417159	0.081558561	0.081722926	0.08190797	0.08222965
	0.082946348	0.082956746	0.082997578	0.082342955	0.08313602	0.083164076
	0.083156132	0.083174589	0.083469183	0.082761883	0.083737627	0.083704975
	0.080796699	0.082399359	0.082944703	0.082962376	0.08265502	0.083119817
	0.083172405	0.083134795	0.083172399	0.078462814	0.082473878	0.083753667
	0.081143975	0.082082698	0.080929814	0.08243623	0.082674999	
c12	0.027853824	0.030197756	0.029206111	0.029017696	0.028622837	0.022469607
	0.024299951	0.023763984	0.023502684	0.023893492	0.02341686	0.023286366
	0.023304272	0.023292115	0.023289859	0.023544851	0.023304832	0.02331199
	0.023284883	0.023276038	0.030054615	0.029341314	0.028935878	0.028871329
	0.02393409	0.023372625	0.0233733	0.023355574	0.023423471	0.023401331
	0.023340289	0.023371725	0.023337496	0.028542327	0.030321407	0.029533998
	0.024994599	0.024486472	0.023773545	0.023602266	0.023661918	
clch3cl-	0.078147161	0.083385504	0.082677188	0.083220991	0.083075367	0.073949525
	0.079445034	0.078738203	0.078710934	0.079321452	0.079243049	0.079279874
	0.080226063	0.079991953	0.080029483	0.079492721	0.080125382	0.080141927

	0.080141353	0.080148487	0.082731788	0.082821014	0.083428535	0.083202611
	0.078702516	0.079892276	0.080086534	0.080064461	0.080068607	0.080219361
	0.08020167	0.080228329	0.080196807	0.095070054	0.08193896	0.082900289
	0.078922577	0.079588608	0.078302594	0.079580086	0.079778401	
clf	0.041026399	0.043783459	0.044309707	0.043683136	0.043636962	0.035545064
	0.038608447	0.038015963	0.037874942	0.038399885	0.037768588	0.037527702
	0.037879318	0.037671759	0.037671919	0.037786836	0.037680739	0.037672829
	0.037643695	0.037644101	0.043946297	0.044179636	0.044020143	0.043736085
	0.038908562	0.037973098	0.037769975	0.0377468	0.037865202	0.037785342
	0.037713821	0.037754493	0.037713942	0.047330467	0.043920778	0.044218165
	0.038717503	0.039532344	0.038363941	0.038450438	0.0383096	
clo	0.044041693	0.048515941	0.047922104	0.046916191	0.046994327	0.040226394
	0.043660047	0.043247098	0.04315461	0.043411779	0.043008829	0.042861357
	0.042767227	0.042692614	0.04268309	0.042922774	0.042668912	0.042641142
	0.04264673	0.042629048	0.047630719	0.047625647	0.047152201	0.047120009
	0.042873529	0.042722965	0.042704833	0.042717543	0.042614635	0.042654258
	0.042639194	0.042640737	0.042647575	0.042024954	0.047597321	0.048049283
	0.042682825	0.043087361	0.043016438	0.043134796	0.042862248	
cn	0.16196372	0.164155458	0.164174917	0.16465792	0.164600462	0.146233071
	0.152359569	0.151009678	0.150749051	0.152696695	0.151693091	0.151554178
	0.152504462	0.152291362	0.152262327	0.1514419	0.151898595	0.15190552
	0.151881826	0.15189179	0.164415936	0.164943858	0.16486863	0.164727918
	0.152501986	0.152212729	0.15230991	0.15231075	0.151838244	0.151922838
	0.151907185	0.151909274	0.151907185	0.175497871	0.164351378	0.165276218
	0.152934342	0.153403494	0.152279826	0.152706678	0.152199894	
co	0.133747168	0.141009855	0.140372036	0.14071751	0.140585054	0.123930952
	0.131550077	0.131331682	0.131418602	0.131771442	0.131525774	0.131491552
	0.132258009	0.132186096	0.13219999	0.13112355	0.131757746	0.131800628
	0.131738112	0.131784866	0.140128829	0.140808279	0.140835636	0.140716433
	0.131258614	0.131807641	0.132209776	0.132226154	0.13137503	0.131748521

	0.131782374	0.131723548	0.131782373	0.138697542	0.139838313	0.141141584
	0.130836393	0.13258797	0.130745647	0.132208483	0.131700464	
co2	0.19401922	0.198241362	0.198876821	0.197501636	0.196993881	0.16950326
	0.177799837	0.176507561	0.176718778	0.178542046	0.176833548	0.176487015
	0.177311971	0.176957352	0.176951034	0.176184032	0.176301226	0.176334604
	0.176271491	0.176312997	0.197422602	0.198310273	0.198055735	0.197379311
	0.177698743	0.176960785	0.177130262	0.17704186	0.176269851	0.176394728
	0.176334732	0.176368055	0.176334732	0.211008163	0.197436424	0.198402014
	0.177207796	0.179049971	0.176386138	0.177950289	0.176953922	
cs	0.111112279	0.113972715	0.115071862	0.114720578	0.114391068	0.100015201
	0.104750118	0.103469546	0.103002055	0.10568875	0.104516978	0.104104008
	0.104962562	0.104569197	0.104507033	0.10465523	0.104569747	0.104546636
	0.104586331	0.104567292	0.114056367	0.114848154	0.114852293	0.114506752
	0.104168545	0.104357189	0.104495333	0.104523992	0.104390856	0.104521758
	0.104579909	0.104555394	0.104580321	0.110432983	0.113566028	0.114757625
	0.104962236	0.105559982	0.103851278	0.104408224	0.10445992	
f2	0.076212692	0.083979608	0.083479223	0.08324604	0.083084876	0.072466368
	0.078898178	0.07840682	0.078182943	0.079089702	0.078820502	0.078705139
	0.078983322	0.078988047	0.07899203	0.079057818	0.079112028	0.079088146
	0.079092742	0.079063577	0.083617358	0.084163009	0.083473995	0.083380216
	0.080067405	0.078969344	0.079007569	0.079034895	0.079145917	0.079150094
	0.079127482	0.079131608	0.079127482	0.082175288	0.083574052	0.084443313
	0.078856022	0.080971453	0.07863279	0.079273254	0.079333796	
fch3cl-	0.074162432	0.078582431	0.076783442	0.077570872	0.077503282	0.07160976
	0.076113793	0.075957964	0.075669171	0.075054737	0.075627671	0.075849439
	0.076701209	0.07670544	0.076782657	0.075907289	0.076965512	0.077031862
	0.076979785	0.077035234	0.078496041	0.077509491	0.077920714	0.077598426
	0.075919868	0.076599277	0.076913024	0.076798898	0.076866786	0.077179813
	0.077067976	0.077195733	0.077067835	0.140211957	0.078403318	0.078771977
	0.076557845	0.077034689	0.076348289	0.077274853	0.077519974	

h2	0.019268536	0.019572049	0.019803768	0.020194116	0.020177714	0.017976478
	0.01821756	0.018186564	0.018161404	0.018449519	0.018356777	0.018384082
	0.018573907	0.018552805	0.018556267	0.01850715	0.018543204	0.018545657
	0.018543915	0.018545674	0.019627521	0.019944503	0.020173049	0.020190752
	0.018214612	0.018383473	0.018543341	0.018557644	0.018473768	0.018532994
	0.018545534	0.018533824	0.018545534	0.020585785	0.019522162	0.019944695
	0.018267389	0.018461761	0.018221656	0.018384938	0.01845573	
h2cch2	0.140914936	0.150544404	0.149848389	0.150728277	0.150517393	0.135059512
	0.143114029	0.142356526	0.142361365	0.14313626	0.143045278	0.143343526
	0.144359666	0.144278262	0.144269963	0.143150534	0.144108671	0.144125958
	0.144113901	0.144124312	0.149956357	0.150211477	0.150880964	0.150683547
	0.142725064	0.143896378	0.144357323	0.144296075	0.14378112	0.144182303
	0.144136498	0.144183181	0.1441365	0.160755726	0.149396034	0.15124812
	0.143272198	0.144408497	0.143539813	0.144551854	0.144339947	
h2co	0.133438215	0.148367374	0.149427202	0.151249582	0.15124598	0.127068591
	0.144056699	0.144254847	0.144681147	0.145456106	0.145452188	0.145574005
	0.147370346	0.147339846	0.147399	0.145245052	0.147089733	0.14718197
	0.147073882	0.147171244	0.145746301	0.141343296	0.141552272	0.141309302
	0.141885361	0.146090485	0.147160424	0.147375549	0.145862658	0.146922276
	0.147133468	0.146904559	0.147133469	0.142910602	0.140123889	0.141717661
	0.141904585	0.145324959	0.142092536	0.145381944	0.145174528	
h2nnh2	0.126678143	0.140719184	0.136325415	0.137249419	0.137104055	0.124980445
	0.134455667	0.133526015	0.133875122	0.133294321	0.133961512	0.134260401
	0.135047344	0.135081964	0.135058244	0.134074176	0.135065943	0.135080234
	0.135051088	0.135072485	0.138738226	0.136279689	0.137098205	0.137186966
	0.132902594	0.134139246	0.13497325	0.135037297	0.134186494	0.134971905
	0.135059521	0.134956069	0.13505952	0.119826156	0.136782587	0.137344356
	0.132293559	0.134095629	0.132698945	0.13434554	0.134299176	
h2o	0.051649395	0.057247521	0.054843322	0.055146545	0.055121582	0.050162789
	0.053290081	0.05308699	0.053152734	0.052874703	0.053282065	0.053315677
	0.053635121	0.053634687	0.053642747	0.053297533	0.053714317	0.053739252

	0.053712832	0.053738228	0.056483942	0.054846316	0.055090308	0.055162694
	0.053037035	0.053280979	0.053615314	0.053635474	0.053371237	0.053715071
	0.053740247	0.053714986	0.053740247	0.049596585	0.05533487	0.055459159
	0.052470525	0.053461136	0.05289842	0.053512919	0.053572776	
h2s	0.039358174	0.040557966	0.040340369	0.040344976	0.040394547	0.033530216
	0.034909481	0.034343946	0.034082621	0.034843002	0.034285406	0.034157144
	0.034595437	0.034471134	0.034452809	0.034237714	0.034398805	0.034395864
	0.034383495	0.034388011	0.04045688	0.040270921	0.040604483	0.040440126
	0.034400401	0.03433868	0.034519496	0.034501232	0.034274832	0.0344411
	0.034423779	0.034432909	0.034425105	0.042475168	0.040065826	0.040402308
	0.034659154	0.03480407	0.034130784	0.034493579	0.034392555	
h3cch3	0.141201176	0.155830641	0.1530475	0.154333137	0.154043091	0.13883936
	0.150139088	0.14897818	0.148895559	0.149079004	0.149311866	0.149810916
	0.150932709	0.150919563	0.150955832	0.149912572	0.151110962	0.151144435
	0.151129324	0.151151848	0.153934528	0.152913075	0.154248932	0.154142157
	0.147770772	0.150087135	0.150908739	0.150924925	0.150367801	0.151089913
	0.151150754	0.151099534	0.151150746	0.145572348	0.152123236	0.154379251
	0.148077841	0.149750756	0.147880427	0.150213178	0.150468356	
h3coh	0.111667424	0.123410193	0.120616377	0.121295514	0.121108544	0.109190987
	0.117829604	0.117305087	0.117284372	0.117057709	0.117461927	0.117736099
	0.11857438	0.118563055	0.118594122	0.117786272	0.118729295	0.11876518
	0.118733047	0.118765512	0.121728128	0.120416672	0.12128752	0.121204136
	0.116510048	0.117874897	0.118570142	0.118575941	0.118097772	0.118738305
	0.118771326	0.118735441	0.118771322	0.109518706	0.120382688	0.121562845
	0.116146095	0.117815454	0.116491143	0.118138908	0.118278798	
hc2h4	0.144929908	0.154800666	0.154122833	0.155005009	0.154767278	0.139043301
	0.147315418	0.146547155	0.146538653	0.147374753	0.147294677	0.147563267
	0.148578507	0.148483277	0.148473405	0.147393118	0.148310364	0.148327563
	0.14831463	0.148325283	0.154167995	0.15445903	0.155121513	0.154934485
	0.146882907	0.148100459	0.148542996	0.148503049	0.14798028	0.14837377

	0.148338345	0.148373034	0.148338344	0.164889239	0.153560738	0.155422404
	0.147389776	0.148548555	0.147606392	0.148673284	0.148468771	
hcch	0.14924101	0.155075242	0.154820669	0.155697538	0.155531778	0.140660541
	0.146863633	0.146523292	0.146668244	0.147530474	0.147371971	0.147652204
	0.148519757	0.148448575	0.148452268	0.14710857	0.148000174	0.148014669
	0.147991488	0.148011771	0.154903815	0.155510385	0.155867665	0.155698848
	0.147421502	0.148192222	0.14848723	0.14849118	0.147753702	0.148041632
	0.148019036	0.14803845	0.148019032	0.171517227	0.155030223	0.15630534
	0.148006567	0.148861479	0.148621013	0.148962223	0.148342937	
hcl	0.019510972	0.02029153	0.020165434	0.020216429	0.020239215	0.016808375
	0.017545917	0.017241279	0.017148256	0.017559022	0.017276141	0.017177833
	0.017421361	0.017358694	0.017353206	0.01728954	0.017358222	0.017352834
	0.017347484	0.017348197	0.020282463	0.020151969	0.020318622	0.020261217
	0.01731039	0.017273014	0.017382765	0.017371043	0.017282314	0.017371823
	0.017360111	0.017369015	0.017361364	0.019736913	0.020060821	0.020146565
	0.017467294	0.017498777	0.017171767	0.017333759	0.017324045	
hclh	0.037466926	0.039953654	0.040765592	0.040575909	0.040421451	0.036107567
	0.03771836	0.037199257	0.037147542	0.038489211	0.037925603	0.037585676
	0.037627633	0.037522563	0.037416201	0.037878062	0.037466044	0.03736493
	0.037466014	0.03735453	0.040409073	0.040847949	0.040602968	0.040498352
	0.037567871	0.037660456	0.037570807	0.037494108	0.037588225	0.037480075
	0.037413173	0.03747959	0.03741298	0.056784991	0.040133773	0.041030634
	0.037756576	0.03830852	0.037360471	0.037886813	0.0378085	
hcn	0.152935072	0.159289022	0.159502943	0.160735445	0.160619801	0.141505987
	0.148937076	0.148301232	0.148406868	0.150889838	0.150498119	0.150613544
	0.15201165	0.151879943	0.151877934	0.150173342	0.151437833	0.151461671
	0.15142354	0.151452454	0.158947375	0.159913167	0.160206581	0.160055171
	0.149205017	0.151293065	0.151805913	0.151899301	0.150848622	0.151365928
	0.151449889	0.151355859	0.151449888	0.165242684	0.158921455	0.160298396
	0.149257208	0.151411419	0.149308402	0.151252868	0.150728431	

hcn_ts	0.15051948	0.154557627	0.155228925	0.155128157	0.154815411	0.135939883
	0.141539044	0.140602454	0.140457298	0.142275132	0.141435412	0.141486063
	0.142438016	0.142037488	0.142023445	0.141162767	0.141692371	0.141707999
	0.141682133	0.141859513	0.154222093	0.155267646	0.155514634	0.155031845
	0.141364546	0.142004868	0.142274266	0.142291349	0.141614849	0.14185735
	0.141869353	0.141847629	0.141869353	0.157034585	0.154891402	0.1554046
	0.141749322	0.142739462	0.140966695	0.142332411	0.141857083	
hco	0.126208786	0.131851369	0.131804396	0.131882051	0.131747282	0.120684758
	0.125452896	0.125670041	0.125719243	0.12575597	0.125749069	0.125704049
	0.126179469	0.126113824	0.12612526	0.125404784	0.125795895	0.125841349
	0.125777977	0.125828653	0.131638244	0.132131096	0.132141865	0.131899202
	0.125407454	0.125890596	0.126157544	0.126150637	0.125564366	0.125824142
	0.125828983	0.125804112	0.125829007	0.138174984	0.131290898	0.132504199
	0.125055976	0.126436261	0.125070508	0.12632577	0.125944074	
hf	0.02473757	0.02721696	0.025848141	0.02605759	0.02607487	0.023066603
	0.024425207	0.024386032	0.024286707	0.024236765	0.024252125	0.024228239
	0.024426196	0.024390229	0.024397457	0.024217117	0.024424943	0.024441041
	0.024422073	0.024438431	0.0269558	0.025941163	0.026071917	0.026090908
	0.024523905	0.024285609	0.024415543	0.024402115	0.024330637	0.024458855
	0.024446414	0.024456122	0.024446414	0.025820354	0.026434575	0.026339322
	0.02437556	0.02462085	0.024420169	0.024470863	0.024504932	
hn2	0.133444391	0.139507351	0.139400734	0.139344211	0.139079039	0.12419871
	0.130308403	0.129477082	0.129366879	0.130629222	0.130006307	0.12989666
	0.130563045	0.130350287	0.13030581	0.129592763	0.129936955	0.129928668
	0.129914392	0.129909477	0.13944683	0.139444309	0.139653799	0.139257345
	0.130439368	0.130361433	0.130456831	0.130382792	0.129911815	0.130022627
	0.129941956	0.129997122	0.129941965	0.13894791	0.138620176	0.139835637
	0.130098766	0.131476221	0.129721869	0.130813526	0.130345039	
hn2_ts	0.166025614	0.170742901	0.170760407	0.170711798	0.170579706	0.151802816
	0.158734108	0.157620855	0.157241579	0.159054661	0.158408049	0.158242507
	0.158946739	0.158758599	0.158699647	0.15784149	0.158149031	0.1581309

	0.158118555	0.158103629	0.170341842	0.170999698	0.171030223	0.170752986
	0.158598807	0.158706627	0.15880039	0.158800602	0.158058721	0.158185254
	0.158152117	0.15815227	0.158152117	0.171681892	0.170040637	0.171189817
	0.158396634	0.159835758	0.157904949	0.159186621	0.158445025	
hn2o	0.23920568	0.244225292	0.242511935	0.241539033	0.241167215	0.21606184
	0.226442133	0.224663451	0.223898031	0.226099271	0.224953159	0.224580109
	0.225263786	0.224893418	0.224798481	0.223830712	0.224029633	0.22400968
	0.22398444	0.223975456	0.24337294	0.242737164	0.242568576	0.241506179
	0.226259722	0.225470035	0.225258113	0.224970365	0.224394195	0.224284855
	0.224059663	0.224238716	0.224059662	0.256566379	0.243169014	0.24295534
	0.22620794	0.227412338	0.225455365	0.226225102	0.225109574	
hnc	0.136899749	0.14725691	0.146046664	0.147042581	0.146932647	0.130594624
	0.139928551	0.139689609	0.139930863	0.140053709	0.14012104	0.140269529
	0.14132414	0.141270437	0.141249319	0.139614706	0.140739934	0.140758507
	0.1407299	0.140753743	0.146471217	0.146923756	0.147130258	0.14704024
	0.139904962	0.140944086	0.14128764	0.141279043	0.140411326	0.140737457
	0.140750766	0.140734279	0.140750765	0.145154161	0.145399637	0.147387177
	0.139027184	0.141325138	0.139346777	0.141342531	0.140711749	
hoch3f-	0.114977324	0.122424009	0.121217192	0.122039612	0.121888934	0.111354578
	0.118099638	0.118018241	0.118114908	0.117795882	0.118245865	0.118514449
	0.11942262	0.119443702	0.119504653	0.118552206	0.119656074	0.119714264
	0.119669642	0.119716398	0.122233598	0.121733981	0.122232744	0.121985206
	0.117967046	0.119108581	0.119561423	0.119504208	0.119363518	0.119793432
	0.119737255	0.119804009	0.11973726	0.155209403	0.121106615	0.122570257
	0.117469038	0.119193017	0.117783423	0.119471301	0.119696867	
hoch4	0.114942892	0.127268208	0.124942033	0.126032196	0.125846203	0.113638942
	0.122898542	0.122486394	0.122553116	0.122313502	0.122791924	0.123104278
	0.123942198	0.123969456	0.123998115	0.123140232	0.124122481	0.124152999
	0.124136362	0.124160305	0.125341995	0.124860203	0.12582297	0.125903928
	0.121062821	0.122996111	0.123820565	0.123961155	0.123205089	0.1239935

	0.124145392	0.124004988	0.124145388	0.116333228	0.123890973	0.12567102
	0.120996593	0.122589533	0.121455103	0.123030469	0.123139375	
hoc1	0.067158329	0.07332268	0.071860601	0.071534455	0.071455587	0.062221566
	0.067111128	0.066401411	0.066310214	0.066548508	0.066236868	0.066113787
	0.066447447	0.066384499	0.066408089	0.066267916	0.066415421	0.066425619
	0.066397313	0.066407975	0.072448319	0.071855436	0.071752471	0.071604016
	0.066566511	0.066330472	0.066417895	0.066446939	0.066267812	0.066452565
	0.066445548	0.066436294	0.066447306	0.069052047	0.071749847	0.072054324
	0.066252656	0.067207065	0.0663179	0.066707444	0.066580776	
hoh	0.039554655	0.041305808	0.040641978	0.041046342	0.040951697	0.03873325
	0.040456299	0.0405423	0.040381693	0.040331479	0.040440414	0.040424283
	0.040632785	0.040646154	0.040643341	0.040427406	0.040600138	0.040600167
	0.040596634	0.040597514	0.040606327	0.040975322	0.04102374	0.040963799
	0.039964372	0.040438509	0.040610189	0.040649035	0.040402286	0.04055689
	0.040594284	0.040551793	0.040594284	0.04010326	0.039717216	0.040913045
	0.039570248	0.040317078	0.039976491	0.040409024	0.040332633	
hooh	0.104915964	0.115266209	0.111852228	0.112147566	0.112167018	0.100584655
	0.107524088	0.106822842	0.106892439	0.106782454	0.106866257	0.106857826
	0.107473781	0.107434761	0.107438502	0.106898489	0.107496391	0.107516887
	0.107477955	0.107502259	0.114006449	0.112169164	0.112174068	0.112290669
	0.107226633	0.106967981	0.107413704	0.107439361	0.107064861	0.107497433
	0.107510256	0.107475619	0.107510257	0.106492908	0.112876779	0.113106707
	0.106457795	0.107911895	0.106751739	0.107411873	0.10739545	
li2	0.011254632	0.009481579	0.009387493	0.008883123	0.008866027	0.01000794
	0.009481579	0.009482342	0.00939336	0.010291681	0.009366809	0.009207499
	0.008959146	0.00883422	0.008824158	0.009366809	0.008834489	0.00882276
	0.008834489	0.00882276	0.010020126	0.008875959	0.008873842	0.008867499
	0.008951535	0.008837762	0.008831085	0.008825232	0.008846338	0.008830242
	0.008826205	0.008830321	0.008826204	0.012940383	0.009835783	0.008873838
	0.009797179	0.008815981	0.009861812	0.008813055	0.008833116	

lif	0.011806698	0.014049442	0.014650251	0.01475945	0.014787087	0.012544658
	0.01401422	0.014021816	0.014062849	0.014477709	0.014673443	0.014721781
	0.014742943	0.014843727	0.014875013	0.014678441	0.014960382	0.014999979
	0.014960712	0.015000311	0.013458728	0.014249767	0.014596331	0.014749261
	0.014259743	0.014642732	0.014802123	0.014853595	0.014759757	0.014939303
	0.015000567	0.014947482	0.015000518	0.013254864	0.013266986	0.013937819
	0.013702057	0.014227132	0.014220308	0.014593083	0.014787001	
lih	0.01522843	0.016550549	0.016544414	0.016648085	0.016649146	0.01542279
	0.016383871	0.016221854	0.016312089	0.01610111	0.016148998	0.016173545
	0.015865289	0.016381571	0.016383195	0.016146239	0.016378787	0.016383271
	0.016378839	0.01638294	0.017126503	0.016693384	0.016681319	0.016655272
	0.016529468	0.016358226	0.0163771	0.016382734	0.016327237	0.016378547
	0.016384377	0.01637943	0.016384364	0.02016644	0.016568644	0.016630007
	0.016187667	0.016367343	0.016015212	0.016317946	0.016321857	
mg	0.027743339	0.028466384	0.030844702	0.031216732	0.031232501	0.032830319
	0.028466384	0.030805938	0.030918698	0.028554659	0.030844702	0.03097564
	0.030922491	0.031216732	0.031232501	0.030844703	0.031216732	0.031232501
	0.031216732	0.031232501	0.031139841	0.031353808	0.031410732	0.03141964
	0.031139842	0.031353809	0.031410733	0.031419642	0.031353809	0.031410733
	0.031419642	0.031410733	0.031419642	0.033054083	0.031408579	0.031272518
	0.031408578	0.03127252	0.031408579	0.031272519	0.03127252	
n2	0.15517836	0.161617018	0.161933925	0.162026499	0.161948442	0.140536281
	0.14874875	0.147596839	0.147388626	0.149344094	0.148678876	0.148582119
	0.149347835	0.149161796	0.14913196	0.14811574	0.14853776	0.148552549
	0.148509802	0.148527146	0.160974747	0.16210856	0.162253236	0.16206524
	0.148467928	0.148895662	0.149137147	0.149182092	0.148246961	0.148507951
	0.148526348	0.148477174	0.14852635	0.156775455	0.160981136	0.162202205
	0.148436061	0.149994136	0.147858492	0.149272513	0.148531367	
n2o	0.23223889	0.23746297	0.236470578	0.235878785	0.235576338	0.206115594
	0.217065592	0.215151652	0.214322133	0.217285027	0.215809522	0.215391749
	0.216256329	0.215792569	0.215723623	0.214694241	0.214901477	0.214902591

	0.214862138	0.214874134	0.236527461	0.236301966	0.236521888	0.235828265
	0.216574412	0.215966934	0.215969306	0.215843052	0.214874945	0.214972723
	0.214899631	0.214933035	0.214899636	0.243641019	0.236100176	0.236564264
	0.216043377	0.218261659	0.215098952	0.216676986	0.21553142	
na2	0.011978571	0.011171012	0.010757586	0.010781403	0.010779754	0.012071589
	0.011171012	0.011059023	0.011034294	0.010895582	0.010627797	0.010735483
	0.010752563	0.010572624	0.010554811	0.0106278	0.010575359	0.010557963
	0.010575362	0.010557963	0.010833391	0.010788631	0.010784916	0.010775834
	0.01077477	0.010686829	0.010673017	0.010613848	0.010684197	0.010670646
	0.010615262	0.010670367	0.010615263	0.017500107	0.010874275	0.01082206
	0.010771294	0.010691222	0.010732756	0.010609381	0.010624064	
nacl	0.002930422	0.006192098	0.006324713	0.00638002	0.006405013	0.002450805
	0.007872322	0.007599573	0.007978187	0.007719402	0.00782825	0.007964751
	0.00773384	0.008087893	0.008143677	0.008410681	0.008231204	0.008281355
	0.008349313	0.00840267	0.005673004	0.002033811	0.002009712	0.008119027
	0.008231915	0.007602527	0.007699575	0.008155454	0.008220939	0.008290672
	0.008424144	0.008408278	0.008423718	0.015559124	0.005553052	0.009984497
	0.007935398	0.01001097	0.007270475	0.007817056	0.007971204	
nh	0.025462997	0.027336661	0.027141705	0.027408054	0.027362923	0.024678931
	0.025760922	0.025636912	0.025660751	0.025921327	0.025898739	0.025895436
	0.026165716	0.026142405	0.026143158	0.025872755	0.026106864	0.026109965
	0.026104936	0.026107799	0.02749761	0.027265978	0.027430009	0.027392059
	0.025982301	0.026045073	0.026160949	0.026154435	0.026011639	0.02612506
	0.026114212	0.026123381	0.026114213	0.02710083	0.026918104	0.027537938
	0.02579553	0.026194117	0.025896362	0.026171142	0.026124649	
nh2	0.047665231	0.051971382	0.050830192	0.051199879	0.051116934	0.045639977
	0.048661005	0.048317286	0.048432192	0.048481627	0.048611176	0.048676841
	0.049088686	0.049054284	0.04905741	0.048660453	0.049095673	0.049104829
	0.049096056	0.049105087	0.051781048	0.050963836	0.051185477	0.051162118
	0.048585485	0.048832652	0.04905743	0.049060202	0.048864114	0.049106073

	0.049111801	0.049107598	0.049111802	0.04818931	0.050769106	0.051462716
	0.048263748	0.049008627	0.048411061	0.049016932	0.049007404	
nh3	0.069600431	0.077315726	0.074671735	0.075303576	0.075233876	0.069043891
	0.07415428	0.073531693	0.073895497	0.073593429	0.074134518	0.07439497
	0.074811354	0.074895988	0.074902178	0.07427701	0.074954278	0.074973701
	0.07495778	0.074977019	0.076241037	0.074627117	0.075157156	0.075257157
	0.073249584	0.074239824	0.07480124	0.074871493	0.074360977	0.074877343
	0.074963996	0.074884104	0.074964006	0.064618891	0.074842252	0.075321465
	0.072884961	0.074113912	0.073139807	0.07431928	0.074387808	
no	0.125987627	0.131211973	0.131132815	0.130809879	0.130586848	0.1148332
	0.121084639	0.120365336	0.120176421	0.12145581	0.120900873	0.120749286
	0.121240025	0.121078099	0.121041994	0.120389327	0.120590619	0.120593208
	0.12056137	0.120567485	0.130968216	0.130959224	0.13109782	0.130707597
	0.121402816	0.12107605	0.121156576	0.121106654	0.120550907	0.120645149
	0.120588136	0.120610001	0.120588135	0.133195095	0.130891691	0.131249523
	0.12110953	0.122335025	0.120809234	0.121553755	0.120988383	
o2	0.108077807	0.114554234	0.11203405	0.111364852	0.111096449	0.099623683
	0.105465748	0.104697433	0.104314439	0.105425025	0.105060688	0.104916677
	0.10514109	0.105018247	0.104955949	0.10438732	0.104657967	0.104643626
	0.104278462	0.104268835	0.114169097	0.112756299	0.112715398	0.11244913
	0.105953992	0.105028567	0.10506138	0.105006796	0.104706995	0.104705928
	0.104649819	0.1046656	0.104649819	0.111831765	0.114211759	0.113584142
	0.10542047	0.106498856	0.105079079	0.105470404	0.104858516	
o3	0.245603686	0.25554467	0.253137383	0.252829337	0.252581112	0.229060381
	0.239528307	0.237615152	0.236899883	0.23937865	0.238024186	0.237636244
	0.238612428	0.238197132	0.238099819	0.237173966	0.237372343	0.237351446
	0.2372849	0.237289096	0.255417946	0.253020859	0.253065811	0.252813574
	0.241287067	0.238368531	0.238363851	0.238172823	0.237642237	0.237479285
	0.237315685	0.237383049	0.237315686	0.26166884	0.255443884	0.254395947
	0.239325188	0.242178345	0.238622018	0.239196392	0.238404868	

oh-	0.020710714	0.02370872	0.023892395	0.023998242	0.023998695	0.021337203
	0.022072422	0.022228544	0.02235179	0.022260888	0.022287834	0.022250226
	0.022428829	0.022385232	0.0223796	0.02235294	0.022482818	0.022483798
	0.022482636	0.022483871	0.023834301	0.024072425	0.024063064	0.024027524
	0.022370375	0.022434221	0.022466658	0.022417166	0.022537012	0.022584542
	0.022528333	0.02258379	0.022528334	0.020076318	0.023505477	0.024325216
	0.022149698	0.024075506	0.02243041	0.022600121	0.022681151	
oh	0.024810978	0.027118139	0.026275352	0.026489353	0.026471254	0.023383727
	0.024784171	0.02461534	0.024620172	0.024756008	0.0247519	0.024719684
	0.024959382	0.024925389	0.024931899	0.02472118	0.024939562	0.02495008
	0.024938511	0.024948146	0.027001745	0.026354715	0.026496806	0.026500047
	0.024797056	0.024820083	0.024942676	0.024938236	0.024822701	0.024960758
	0.024954447	0.024959091	0.024954447	0.025590987	0.026364651	0.026696266
	0.024624293	0.025003958	0.024705447	0.024975296	0.02496645	
p2	0.105334513	0.107716797	0.10894046	0.108207758	0.108299657	0.090681204
	0.094337349	0.092833838	0.09122021	0.095159605	0.093624819	0.091924162
	0.09377999	0.092195084	0.092135227	0.093112334	0.091439344	0.091344437
	0.091419237	0.091308537	0.108342209	0.108583017	0.108650951	0.10855508
	0.092986921	0.092417809	0.092335511	0.092325431	0.091659194	0.091551901
	0.09150539	0.091517476	0.091489833	0.124848689	0.108682628	0.109144061
	0.096253866	0.09635783	0.092748655	0.092509762	0.091988134	
ph2	0.039590223	0.040829077	0.040639273	0.04060072	0.040639241	0.034110029
	0.035317107	0.034830861	0.034505108	0.035243303	0.034632435	0.034545722
	0.034943971	0.034878873	0.03486914	0.034600074	0.034785023	0.034794698
	0.034781524	0.034791874	0.040688296	0.040596025	0.040859993	0.040739853
	0.034895914	0.03479384	0.034955942	0.034924467	0.034706424	0.034856538
	0.034844431	0.034851208	0.034844908	0.042803737	0.040196278	0.040635458
	0.03502114	0.035151835	0.03459756	0.034825963	0.034745497	
ph3	0.056589709	0.057798361	0.057258118	0.057313057	0.057364028	0.047172944
	0.049095072	0.048414207	0.047987988	0.048932977	0.048165374	0.048056292
	0.048669293	0.048502869	0.048492997	0.048075103	0.048372133	0.048381092

	0.048365628	0.048378506	0.057460021	0.057195869	0.057685387	0.057499804
	0.048348691	0.048334477	0.048594015	0.048564262	0.048204248	0.04845139
	0.048440464	0.048440101	0.048440988	0.059141926	0.056834082	0.057279358
	0.04868526	0.048933034	0.048055409	0.048502092	0.048339777	
s2	0.055810624	0.058016282	0.057760369	0.056798304	0.056874311	0.04573657
	0.04789271	0.046884008	0.046120213	0.048013292	0.047010537	0.046292931
	0.046822054	0.046250885	0.046245871	0.046779142	0.045942131	0.045909246
	0.045920554	0.045880862	0.058071533	0.057271617	0.057085201	0.057042124
	0.04714291	0.046421678	0.046367853	0.046339801	0.046109799	0.046038267
	0.045980789	0.046013431	0.045978822	0.062584489	0.057883419	0.057644974
	0.048714651	0.048712372	0.046780288	0.046669617	0.046378728	
sh	0.020439333	0.021323821	0.021243999	0.021228282	0.021258569	0.018180121
	0.018801888	0.018549746	0.018424151	0.018801125	0.018526063	0.018503456
	0.01865565	0.018660927	0.018657465	0.018547734	0.018659354	0.018662989
	0.018654869	0.018660947	0.021305385	0.021206053	0.02134618	0.021289133
	0.018611288	0.01859961	0.018696119	0.018680894	0.018612607	0.018690864
	0.018682003	0.018691184	0.018683947	0.021293487	0.020998548	0.021277965
	0.018617492	0.018725276	0.018460915	0.018638915	0.018644898	
sh3	0.046512196	0.047786509	0.047164522	0.04714393	0.047201609	0.040162788
	0.041816112	0.04104678	0.040757498	0.041609244	0.041000023	0.04084077
	0.041263528	0.041126955	0.041122267	0.040987999	0.041083302	0.041081099
	0.041070728	0.041074429	0.047665477	0.047269464	0.047428273	0.047315018
	0.04131388	0.041114088	0.04121278	0.041178688	0.041067293	0.041152102
	0.041123745	0.04114415	0.041122938	0.049895585	0.046926933	0.047333639
	0.041402878	0.041609536	0.040844095	0.04120949	0.041119314	
si	0.01294271	0.012936546	0.012978871	0.013091263	0.013124473	0.013163755
	0.013151595	0.013150267	0.013102365	0.013193136	0.013192184	0.013143355
	0.013311248	0.013261022	0.013290314	0.013193875	0.013258843	0.013287074
	0.013258861	0.013287091	0.01307261	0.013109201	0.013152096	0.013183382
	0.013245247	0.013269109	0.013316796	0.013349147	0.013274148	0.013319572

	0.013350349	0.013320032	0.013350179	0.007711702	0.013131427	0.013146375
	0.013352786	0.013366589	0.013295747	0.01331004	0.013313731	
si2	0.09285119	0.090417238	0.091844537	0.091437031	0.091505281	0.085283688
	0.083881757	0.082364667	0.079781177	0.085031772	0.083429607	0.080619855
	0.079468841	0.080666666	0.080078368	0.082895211	0.080050604	0.079821725
	0.080023363	0.079776137	0.091317326	0.091536706	0.091811405	0.091763089
	0.081350478	0.080836026	0.080259708	0.080775238	0.080126208	0.080039177
	0.079980917	0.079990789	0.079990789	0.111718939	0.091739535	0.092154209
	0.085142705	0.085372965	0.081272268	0.08131495	0.080762465	
si2h6	0.111497436	0.112591147	0.111590459	0.111537512	0.111359354	0.093404547
	0.097187273	0.096311095	0.095752213	0.096782698	0.095544976	0.09565137
	0.096431256	0.096329934	0.09634667	0.095436279	0.096212434	0.096263735
	0.096217843	0.096300216	0.111463507	0.111163419	0.112155549	0.111878987
	0.095182519	0.095873401	0.096579101	0.096567603	0.095728726	0.096415582
	0.096450166	0.096405737	0.096453368	0.116798666	0.111263492	0.111917855
	0.096252526	0.096770709	0.095303701	0.096172362	0.096012153	
sih2_sing	0.045488105	0.046474495	0.046283109	0.046444085	0.046391451	0.047362055
	0.047183566	0.047949516	0.049738408	0.047254193	0.047919432	0.049958432
	0.048503115	0.050338224	0.050518118	0.048447218	0.050939857	0.051159677
	0.050954409	0.05117794	0.04636782	0.046365454	0.046624187	0.046581437
	0.04926497	0.050226555	0.050567168	0.05059091	0.050882187	0.051246742
	0.051277653	0.05125465	0.051282646	0.051821481	0.046142342	0.046644691
	0.047280026	0.047509601	0.049773192	0.050079245	0.050734377	
sih2_trip	0.037442074	0.038337532	0.037985796	0.038205484	0.03814981	0.031870555
	0.033347482	0.032961877	0.032582061	0.033181175	0.03266672	0.032470009
	0.033140501	0.032863841	0.032843989	0.032676879	0.032836832	0.032814129
	0.032843914	0.032820645	0.038033813	0.038004737	0.038329683	0.038282345
	0.032671166	0.032689791	0.032884313	0.032880517	0.032631098	0.032846472
	0.032853737	0.03284582	0.032851062	0.041434972	0.037613055	0.038266601
	0.032876824	0.033266402	0.03234091	0.032818819	0.032767853	

sih3	0.050240317	0.050593819	0.050053248	0.050288656	0.050133531	0.041835724
	0.043242797	0.042770833	0.042335367	0.043070841	0.042376322	0.042255956
	0.042931878	0.042709796	0.04270481	0.042285524	0.042598581	0.042596433
	0.042600167	0.042605082	0.049998029	0.049973005	0.05042474	0.050305939
	0.042231631	0.042442756	0.042779264	0.042771358	0.042310167	0.042647595
	0.042656532	0.042639538	0.042656823	0.053582451	0.049837222	0.050323197
	0.042751367	0.04305957	0.042156969	0.042584082	0.042487136	
sih4	0.064352762	0.064537679	0.063840165	0.06410999	0.0639075	0.053862858
	0.055678428	0.055255164	0.054961976	0.055512114	0.05483641	0.054950574
	0.055512791	0.055443442	0.055465594	0.054811658	0.05543299	0.055458663
	0.055437359	0.05548181	0.063785059	0.063721445	0.06430729	0.064142246
	0.054558984	0.055098275	0.055561881	0.055567022	0.055064486	0.055521393
	0.055552169	0.055518446	0.055553663	0.067925346	0.063761909	0.064116419
	0.055102855	0.055496815	0.05465427	0.055202373	0.055201377	
sio	0.124172194	0.13123563	0.129482747	0.129672111	0.129780635	0.115449714
	0.123223291	0.122896386	0.123110723	0.122404971	0.12187931	0.121942875
	0.122361389	0.122424038	0.122503134	0.121318465	0.121972391	0.122056985
	0.12195827	0.122038755	0.130491861	0.130573853	0.129812572	0.129877949
	0.123436937	0.122532242	0.12253949	0.122606294	0.121974626	0.122108111
	0.122121596	0.122088984	0.122126018	0.154850189	0.130905056	0.130338232
	0.122297913	0.123611649	0.122446354	0.122861108	0.122419381	
so	0.078191359	0.080653084	0.081098513	0.080746949	0.080582412	0.063561495
	0.066404178	0.063743878	0.062362877	0.066553485	0.063646925	0.06200998
	0.063730882	0.062047138	0.061913476	0.062934962	0.061137633	0.060980912
	0.061105063	0.060955006	0.081137472	0.081285995	0.080849666	0.080788206
	0.06660391	0.06320245	0.06245225	0.062176573	0.062339747	0.061526208
	0.061210945	0.061492047	0.061182918	0.085361399	0.081536498	0.081688683
	0.067846665	0.068953403	0.064724617	0.064621495	0.063822648	
so2	0.165233094	0.169157839	0.172048496	0.170855182	0.170060252	0.12946776
	0.137635792	0.133435061	0.132164009	0.137827029	0.133306118	0.131835547
	0.133559137	0.132101441	0.131971752	0.131659923	0.13026453	0.130200199

0.130213246	0.13014703	0.170278621	0.171759673	0.170928249	0.17059002
0.136805041	0.133033875	0.132351807	0.132216853	0.131153297	0.130578496
0.130361393	0.130555761	0.130368643	0.222532683	0.171267096	0.172092721
0.137831538	0.140636501	0.134417433	0.134421244	0.132468098	

2.2 Hartree-Fock energies (tab-delimited text format, copy and paste into Excel for table format)

	pc-0	pc-1[sp]	pc-2[sp]	pc-3[sp]	pc-4[sp]	pc-0[spd_2]	pc-1	pc-1[spd_2]	pc-1[spd_3]
	pc-2[spd_1]	pc-2[spd]	pc-2[spd_3]	pc-3[spd_2]	pc-3[spd]	pc-4[spd]	pc-2	pc-3[spdf]	
	pc-4[spdf]	pc-3	pc-4[spdfg]	cc-pVDZ[sp]	cc-pVTZ[sp]	cc-pVQZ[sp]	cc-pV5Z[sp]		
	cc-pVDZ	cc-pVTZ[spd]	cc-pVQZ[spd]	cc-pV5Z[spd]	cc-pVTZ	cc-pVQZ[spdf]	cc-		
	pV5Z[spdf]	cc-pVQZ	cc-pV5Z[spdfg]	STO-3G	6-31G	6-311G	6-31G(d,p)	6-311G(d,p)	
	6-31G(2d,2p)	6-311G(2d,2p)	6-311G(2df,2pd)						
al	-241.7520298	-241.8575087	-241.8681299	-241.8701537	-241.8703755	-241.7520424	-		
	241.8575107	-241.857522	-241.8575521	-241.8681321	-241.8681432	-241.8681755	-		
	241.8701671	-241.8701991	-241.8704538	-241.8681496	-241.8702174	-241.8704743	-		
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	-111.1503515	-111.1617298	-111.1664238	-111.2182266	-111.2234982	-111.2248704 -
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290.6126015	-290.6163602	-290.6195082	-290.6277016	-290.6323083	-290.6347438	-
290.635174	-290.6372308	-290.637838	-290.6337015	-290.6387314	-290.6392336	-
290.6388151	-290.6395182	-290.5891207	-290.5954005	-290.5979537	-290.5994191	-
290.6288067	-290.6392416	-290.64317	-290.643913	-290.6409719	-290.6445385	-
290.6452328	-290.6445945	-290.6452332	-287.3045262	-290.565769	-290.5903976	-
290.6084883	-290.6305658	-290.6123366	-290.6345543	-290.6360034		
sih4	-291.0482559	-291.1824933	-291.196809	-291.2028387	-291.2045432	-291.1189127 -
291.2347754	-291.2393517	-291.241998	-291.2501737	-291.2559972	-291.2577895	-
291.2585671	-291.260213	-291.2607373	-291.2577869	-291.262033	-291.2623796	-
291.262146	-291.2627694	-291.1990796	-291.2054893	-291.208161	-291.2100719	-
291.2499882	-291.2614757	-291.2659495	-291.2668505	-291.2635927	-291.2675505	-
291.2683701	-291.2676133	-291.2683488	-287.9178288	-291.1736032	-291.2002934	-
291.2301092	-291.2531743	-291.2340452	-291.2569837	-291.2587597		
sio	-363.3821569	-363.691249	-363.75821	-363.7676222	-363.7682692	-363.4706117 -
363.7653832	-363.7732838	-363.7770672	-363.8248048	-363.8334815	-363.8365779	-
363.8410173	-363.8439127	-363.8449698	-363.8378493	-363.8479828	-363.8488895	-
363.8483294	-363.8492865	-363.730831	-363.7592508	-363.7722175	-363.773752	-
363.8006103	-363.8389316	-363.8484108	-363.8505104	-363.8432392	-363.8522441	-
363.8547436	-363.8524679	-363.8547418	-359.4351684	-363.7008242	-363.7514243	-
363.7765804	-363.8155974	-363.7842592	-363.8281748	-363.8315415		
so	-471.8451575	-472.2063015	-472.2781592	-472.2914276	-472.2937541	-471.9538171 -
472.2959664	-472.3085301	-472.3156902	-472.3627913	-472.3757822	-472.3811182	-
472.3850783	-472.390204	-472.3918722	-472.3834104	-472.3976208	-472.3990802	-
472.3982443	-472.3995718	-472.2542004	-472.2835267	-472.295279	-472.297674	-
472.3422361	-472.3838036	-472.3937557	-472.3963722	-472.3909925	-472.4011971	-
472.4042781	-472.4016624	-472.4042892	-466.976015	-472.2205123	-472.2670744	-
472.3108101	-472.3513005	-472.3185471	-472.3658643	-472.3744614		

so2	-546.2972015	-546.8667803	-547.0025985	-547.0269904	-547.0348877	-546.6135581	-
547.1247919	-547.1620767	-547.1775439	-547.2376362	-547.2751515	-547.2877125	-	
547.2906238	-547.3023313	-547.305635	-547.2921238	-547.3186847	-547.3212049	-	
547.3200465	-547.3222663	-546.9511622	-547.0046028	-547.0298872	-547.0351388	-	
547.2102089	-547.2880389	-547.3041896	-547.3089434	-547.3033485	-547.3205489	-	
547.3262727	-547.3214694	-547.3261831	-540.5533506	-546.9032531	-546.981956	-	
547.1654659	-547.2232385	-547.187209	-547.2602191	-547.2792377			

2.3 Full valence CASSCF energies (tab-delimited text format, copy and paste into Excel for table format)

	pc-0	pc-1[sp]	pc-2[sp]	pc-3[sp]	pc-4[sp]	pc-0[spd_2]	pc-1	pc-1[spd_2]	pc-1[spd_3]
	pc-2[spd_1]	pc-2[spd]	pc-2[spd_3]	pc-3[spd_2]	pc-3[spd]	pc-4[spd]	pc-2	pc-3[spdf]	
	pc-4[spdf]	pc-3	pc-4[spdfg]	cc-pVDZ[sp]	cc-pVTZ[sp]	cc-pVQZ[sp]	cc-pV5Z[sp]		
	cc-pVDZ	cc-pVTZ[spd]	cc-pVQZ[spd]	cc-pV5Z[spd]	cc-pVTZ	cc-pVQZ[spdf]	cc-		
	pV5Z[spdf]	cc-pVQZ	cc-pV5Z[spdfg]	STO-3G	6-31G	6-311G	6-31G(d,p)	6-311G(d,p)	
	6-31G(2d,2p)	6-311G(2d,2p)	6-311G(2df,2pd)						
al	-241.775977	-241.8809719	-241.8916546	-241.8939915	-241.8942576	-241.7762724	-		
	241.8811976	-241.8812335	-241.8812298	-241.891877	-241.891913	-241.891912	-		
	241.8942611	-241.8942582	-241.8945423	-241.8919204	-241.8942749	-241.8945611	-		
	241.8942749	-241.8945611	-241.8938683	-241.898849	-241.9002804	-241.9006519	-		
	241.8941025	-241.8991166	-241.9005707	-241.9009443	-241.8991222	-241.9005796	-		
	241.9009569	-241.9005797	-241.9009587	-239.050347	-241.8780493	-241.8938555	-		
	241.8783111	-241.894117	-241.8782857	-241.8940928	-241.8940977				
b	-24.49670439	-24.54894121	-24.5602318	-24.56310452	-24.56362204	-24.49691841	-		
	24.54910309	-24.54913401	-24.54914156	-24.56039422	-24.56043261	-24.56043854	-		
	24.56332315	-24.56333084	-24.56385146	-24.56043701	-24.56333712	-24.5638582	-		
	24.56333713	-24.56385821	-24.5601812	-24.56234258	-24.56344374	-24.56360349	-		
	24.56035996	-24.56254556	-24.56366504	-24.5638302	-24.5625513	-24.56367174	-		
	24.56383712	-24.56367175	-24.56383712	-24.18923664	-24.55375655	-24.56115072	-		
	24.5539424	-24.56136116	-24.55393957	-24.5613392	-24.56134536				
be	-14.55417822	-14.60543561	-14.61333839	-14.616189	-14.61668649	-14.58325499	-		
	14.60543561	-14.60769064	-14.60888551	-14.61113819	-14.61333839	-14.61452672	-		
	14.61507424	-14.616189	-14.61668649	-14.61333838	-14.616189	-14.61668649	-		
	14.616189	-14.61668649	-14.61538519	-14.61643826	-14.61676487	-14.61682526	-		
	14.61538519	-14.61643826	-14.61676487	-14.61682526	-14.61643826	-14.61676487	-		
	14.61682526	-14.61676487	-14.61682526	-14.40362959	-14.61184915	-14.61560776	-		
	14.61184915	-14.61560776	-14.61184915	-14.61560776	-14.61560776				

beh	-15.09492405	-15.15534709	-15.16530193	-15.16899755	-15.16957817	-15.13869674	-
15.15744832	-15.16508347	-15.16836518	-15.16577392	-15.17533635	-15.17547159	-	
15.17546466	-15.17924653	-15.17986244	-15.17578905	-15.18012499	-15.1807046	-	
15.18013942	-15.18074287	-15.16575559	-15.16828986	-15.16952413	-15.16971945	-	
15.17487517	-15.17853278	-15.17982249	-15.18000265	-15.17942422	-15.18064766	-	
15.18086801	-15.18068647	-15.18086801	-14.95672145	-15.16306731	-15.16774626	-	
15.16969533	-15.17648793	-15.17424044	-15.17822668	-15.17893964			
c	-37.59576263	-37.68532207	-37.70414271	-37.7072733	-37.70776098	-37.59592985	-
37.68546967	-37.68546541	-37.68547901	-37.70429747	-37.70429607	-37.70430822	-	
37.70743888	-37.70745347	-37.70794279	-37.70429993	-37.70745832	-37.70794793	-	
37.70745833	-37.70794793	-37.70094503	-37.70568461	-37.70739895	-37.70774885	-	
37.70108663	-37.70584097	-37.70757181	-37.70792772	-37.70584532	-37.70757682	-	
37.70793288	-37.70757683	-37.70793288	-37.21872028	-37.69560914	-37.70383964	-	
37.69576221	-37.70400634	-37.69574692	-37.70398589	-37.70399045			
ch	-38.18958744	-38.27996912	-38.30027425	-38.30471544	-38.30543967	-38.21038272	-
38.29505648	-38.29778193	-38.29908389	-38.31554732	-38.31792985	-38.31882655	-	
38.32121199	-38.32185258	-38.32235655	-38.31859534	-38.32239117	-38.32290445	-	
38.32240454	-38.32291607	-38.29525061	-38.30195813	-38.3043752	-38.30525502	-	
38.31027903	-38.31919029	-38.32169047	-38.32223287	-38.31973763	-38.32225534	-	
38.32283623	-38.32226784	-38.32283623	-37.81111884	-38.28953359	-38.30034859	-	
38.3044478	-38.31531332	-38.30811138	-38.31743529	-38.3179668			
ch2_sing	-38.81319921	-38.90108955	-38.92124976	-38.92677496	-38.92771457	-	
38.84448572	-38.92692326	-38.93111924	-38.93278201	-38.94768503	-38.95171861	-	
38.95336353	-38.9552355	-38.95641901	-38.95696078	-38.95305183	-38.95747126	-	
38.95802184	-38.95751246	-38.95805464	-38.91514393	-38.92298952	-38.92607083	-	
38.92736052	-38.94048614	-38.95295557	-38.95604817	-38.95674232	-38.95400122	-	
38.95715554	-38.95793168	-38.9571914	-38.95793168	-38.43212417	-38.91029218	-	
38.92174267	-38.93551162	-38.94740691	-38.94110662	-38.95134651	-38.95236294		
ch2_trip	-38.85271784	-38.93347483	-38.95620694	-38.96082722	-38.96149037	-38.867434	
	-38.94631844	-38.94779984	-38.94819946	-38.969041	-38.9697513	-38.97019839	-
38.97299576	-38.97315156	-38.97362016	-38.97048576	-38.97364254	-38.97405615	-	

38.97367717	-38.97408074	-38.94933037	-38.95727934	-38.96039954	-38.96120178	-
38.95959509	-38.97023672	-38.9729011	-38.97348613	-38.97072917	-38.97337448	-
38.97401891	-38.97339654	-38.97401891	-38.47194047	-38.94744875	-38.9562581	-
38.95811455	-38.96732146	-38.95912586	-38.96880967	-38.96924266		
ch3	-39.50668164	-39.58919795	-39.61258836	-39.61772685	-39.61843506	-39.52694731 -
39.60723955	-39.60933254	-39.60972148	-39.63016388	-39.6311865	-39.63170518	-
39.63455733	-39.63475435	-39.63524977	-39.6323095	-39.63553849	-39.63593015	-
39.63560284	-39.6359746	-39.60344746	-39.61348141	-39.61712776	-39.61798193	-
39.61776684	-39.63137805	-39.63436458	-39.63503949	-39.63211281	-39.63512035	-
39.63589716	-39.63516305	-39.63589716	-39.13400963	-39.6038114	-39.61283831	-
39.61839519	-39.62764087	-39.61938339	-39.6301489	-39.63079752		
ch3ch2	-78.50211775	-78.66465967	-78.70961328	-78.72089145	-78.72263044	-
78.55132057	-78.70285888	-78.70668853	-78.70875976	-78.74634106	-78.74844585	-
78.74988368	-78.75557486	-78.75607886	-78.75709088	-78.75128156	-78.75786324	-
78.75865148	-78.75804295	-78.75877654	-78.69506738	-78.71336878	-78.71937503	-
78.72163118	-78.72621107	-78.74960114	-78.7552659	-78.75664377	-78.75155927	-
78.75715504	-78.75863253	-78.75730367	-78.75863253	-77.78623829	-78.69610825	-
78.71250053	-78.72742499	-78.74321091	-78.72893933	-78.74786034	-78.74937293	
ch3cl	-498.8572581	-499.1275071	-499.1800964	-499.1928961	-499.1939638	-
498.9129297	-499.1746198	-499.1804691	-499.1830218	-499.2207487	-499.2252243	-
499.2268474	-499.2336451	-499.2347421	-499.2358546	-499.2291296	-499.2375775	-
499.2384908	-499.2378132	-499.2386569	-499.1612201	-499.1893404	-499.1963368	-
499.1983009	-499.2052955	-499.2322769	-499.2389411	-499.240644	-499.2354317	-
499.242057	-499.2436714	-499.2423112	-499.2436614	-493.8119132	-499.1428317	-
499.177674	-499.1819674	-499.2173894	-499.1853111	-499.2222188	-499.2255823	
ch3f	-138.6874923	-139.0491481	-139.1417427	-139.1567988	-139.1585725	-138.7487518 -
139.0958581	-139.099559	-139.1038935	-139.185177	-139.1885723	-139.189684	-
139.1988753	-139.1995936	-139.2006923	-139.1921979	-139.2023762	-139.2033587	-
139.2025904	-139.2035279	-139.0993147	-139.1397209	-139.1530032	-139.1570753	-
139.1374908	-139.1849007	-139.1968034	-139.2000629	-139.1878716	-139.1997709	-

139.203188	-139.199967	-139.203188	-137.2623351	-139.089783	-139.13245	-
139.1306962	-139.171332	-139.1343496	-139.1769371	-139.1805057		
ch3fc1	-597.8398906	-598.3917127	-598.5013184	-598.5198683	-598.5218824	-
597.8931382	-598.4254531	-598.4310013	-598.4362942	-598.5367585	-598.5404063	-
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598.56278	-598.5614731	-598.5630142	-598.4578958	-598.5060911	-598.5210068	-598.52556
	-598.4878563	-598.542908	-598.5585128	-598.5625092	-598.5484293	-598.5637187 -
598.567685	-598.564067	-598.567686	-591.7225874	-598.4246674	-598.4903225	-
598.4560521	-598.5187351	-598.4589023	-598.5256184	-598.5308041		
ch3sh	-437.4959016	-437.7408948	-437.7885473	-437.802193	-437.8032698	-
437.5689021	-437.8025113	-437.8102029	-437.8143734	-437.8456187	-437.8519651	-
437.854517	-437.85993	-437.8617284	-437.8630418	-437.8562102	-437.8650282	-
437.8659906	-437.8653185	-437.8662004	-437.7734813	-437.7984649	-437.8052673	-
437.8077043	-437.8329515	-437.8594711	-437.866222	-437.8679325	-437.8629218	-
437.8696638	-437.8713097	-437.869901	-437.8713011	-433.0278382	-437.7551864	-
437.7886412	-437.8110247	-437.8447305	-437.8156672	-437.850514	-437.8547801	
ch4	-40.1613845	-40.246427	-40.27028291	-40.2764981	-40.27729867	-40.18714279 -
40.27064166	-40.2728953	-40.27329447	-40.29325779	-40.29462241	-40.2954587	-
40.29846044	-40.2987765	-40.29927707	-40.29624639	-40.29973991	-40.30015382	-
40.29984139	-40.30021575	-40.25972214	-40.27181031	-40.2757174	-40.27670636	-
40.27947004	-40.29513058	-40.29828451	-40.29901007	-40.29605651	-40.29928019	-
40.30012367	-40.29935556	-40.30012366	-39.80527199	-40.26296165	-40.27183365	-
40.28278949	-40.29107346	-40.28368402	-40.29449556	-40.29540661		
c12	-918.530687	-918.898872	-918.9552333	-918.9659428	-918.9681155	-918.5830658 -
918.9489594	-918.9547092	-918.9571439	-918.9980325	-919.0032887	-919.0045021	-
919.0136691	-919.0145139	-919.0158646	-919.0104385	-919.0220065	-919.0229897	-
919.0224273	-919.0234947	-918.9368379	-918.9679035	-918.9763587	-918.9773523	-
918.9886362	-919.0173125	-919.0242019	-919.0254916	-919.0245051	-919.0317298	-
919.0335699	-919.0322085	-919.0335722	-909.1550621	-918.8920257	-918.9448767	-
918.9342831	-918.9866104	-918.9435649	-918.9960818	-919.0034765		

clch3cl-	-958.1923435	-958.6725593	-958.7433059	-958.7581674	-958.7598253	-	
958.2283013	-958.7001145	-958.7046629	-958.707667	-958.7703634	-958.7739077	-	
958.7755636	-958.7860618	-958.7871249	-958.7886058	-958.7756827	-958.7886027	-	
958.7899312	-958.7887118	-958.7900155	-958.7116319	-958.7518125	-958.7657258	-	
958.7687932	-958.7360589	-958.7829555	-958.7954039	-958.7978622	-958.7844832	-	
958.7969444	-958.7996216	-958.7970484	-958.7996483	-948.2426078	-958.6702322	-	
958.7398728	-958.69337	-958.7642199	-958.6977998	-958.7706539	-958.7722964		
clf	-558.3265332	-558.7969426	-558.8882527	-558.9030196	-558.9047145	-558.3775117	-
558.8332593	-558.8392214	-558.8447283	-558.9258393	-558.9309367	-558.9328295	-	
558.9429383	-558.9447391	-558.9464812	-558.9374698	-558.950659	-558.9521029	-	
558.9512296	-558.952468	-558.8521194	-558.8919033	-558.9044951	-558.9086256	-	
558.8862997	-558.93358	-558.9477304	-558.9509794	-558.9405366	-558.9535839	-	
558.9571652	-558.9539869	-558.9571494	-552.586392	-558.8187282	-558.8743458	-	
558.8552001	-558.9062432	-558.8568692	-558.9133903	-558.9207666			
clo	-533.8052117	-534.1925523	-534.2695315	-534.2842615	-534.2849659	-533.8748776	-
534.2478128	-534.2560646	-534.2612064	-534.3206165	-534.3277654	-534.3300464	-	
534.3384112	-534.3407877	-534.3422936	-534.3343895	-534.3468603	-534.3482545	-	
534.3473923	-534.348642	-534.2425398	-534.276071	-534.2867748	-534.2891236	-	
534.2969546	-534.3344947	-534.3445025	-534.3468649	-534.3409522	-534.3506827	-	
534.3534305	-534.3510615	-534.3534055	-528.3796801	-534.2116817	-534.2572168	-	
534.2653636	-534.3079186	-534.2684385	-534.315625	-534.3234304			
cn	-92.04166973	-92.2754706	-92.32529001	-92.33537275	-92.33656523	-92.10561028	-
92.31527417	-92.31872356	-92.32118881	-92.3635769	-92.36619424	-92.36700237	-	
92.37312775	-92.37365298	-92.37469449	-92.36902811	-92.37590255	-92.37676899	-	
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sh3	-398.9888345	-399.1601052	-399.1828459	-399.1900267	-399.1905438	-399.0371705	-
399.1955908	-399.2015065	-399.2043465	-399.218153	-399.2227551	-399.2244329	-	
399.226831	-399.2285011	-399.2292475	-399.2251595	-399.2306052	-399.2311298	-	
399.2307211	-399.2312254	-399.1778394	-399.1904308	-399.1936797	-399.1955802	-	
399.2148726	-399.2290596	-399.2334072	-399.2343804	-399.2313287	-399.2355258	-	
399.2364043	-399.2355913	-399.2364063	-394.8377098	-399.1527469	-399.1827037	-	
399.1890239	-399.2182324	-399.1938161	-399.2213686	-399.2241562			
si	-288.7259416	-288.8463201	-288.8588286	-288.8613101	-288.8616167	-288.726188	-
288.8465393	-288.8465602	-288.8465522	-288.859047	-288.8590682	-288.859061	-	
288.8615565	-288.8615476	-288.8618726	-288.8590758	-288.8615701	-288.8618998	-	

288.8615702	-288.8618998	-288.8594933	-288.8652005	-288.8671707	-288.8675188	-
288.8597035	-288.865437	-288.8674255	-288.8677745	-288.865443	-288.867436	-
288.8677904	-288.8674369	-288.8677925	-288.8544845	-288.8415568	-288.8608234	-
288.8417824	-288.861048	-288.8417628	-288.8610292	-288.8610338		
si2	-577.5357302	-577.7648064	-577.7917319	-577.798983	-577.7994577	-577.5570046 -
577.784256	-577.7868402	-577.7898618	-577.8097591	-577.8120834	-577.8146394	-
577.8140657	-577.8201406	-577.8206156	-577.8138294	-577.8220398	-577.822927	-
577.8221961	-577.823112	-577.7937145	-577.806569	-577.8100616	-577.8107804	-
577.8158588	-577.8282543	-577.8314836	-577.832769	-577.8300602	-577.8340319	-
577.8349353	-577.8342461	-577.8349396	-571.2622609	-577.7590764	-577.7967404	-
577.7765879	-577.8143473	-577.780464	-577.8183022	-577.8205193		
si2h6	-581.084234	-581.3389692	-581.367683	-581.3801055	-581.3818955	-
581.1869432	-581.4165917	-581.4240312	-581.4289842	-581.4464201	-581.4550535	-
581.4588527	-581.461911	-581.4646751	-581.4658703	-581.4582403	-581.4679736	-
581.4687802	-581.4682058	-581.4694331	-581.3708614	-581.3856505	-581.3903134	-
581.3931233	-581.4463483	-581.4684605	-581.4764001	-581.4781279	-581.471755	-
581.4794481	-581.480983	-581.4796167	-581.4809525	-574.8472442	-581.3260786	-
581.3755537	-581.4081226	-581.4526188	-581.4144613	-581.4588535	-581.4624315	
sih2_sing	-289.89353	-290.0221212	-290.0364988	-290.0413022	-290.0421054	-
289.9368271	-290.0535455	-290.0574493	-290.0613382	-290.0677648	-290.0720284	-
290.0754233	-290.0754321	-290.0783262	-290.0789717	-290.0733171	-290.0800185	-
290.0806482	-290.0800785	-290.0808089	-290.0375149	-290.04452	-290.0467801	-
290.0477062	-290.0712153	-290.0809997	-290.0842966	-290.0849482	-290.082759	-
290.0859551	-290.0865946	-290.0859952	-290.086595	-286.7525737	-290.0159732	-
290.0392185	-290.0491316	-290.0705071	-290.0545211	-290.0758636	-290.0775588	
sih2_trip	-289.8713013	-289.9944987	-290.0087689	-290.0131379	-290.0138646	-
289.8998523	-290.0149592	-290.0175019	-290.0200085	-290.0295305	-290.0323102	-
290.0345079	-290.0354767	-290.037338	-290.0379173	-290.0331904	-290.0383149	-
290.0388477	-290.0383766	-290.0390023	-290.0097613	-290.0163873	-290.0188228	-
290.019697	-290.030827	-290.0399762	-290.0433787	-290.0439731	-290.0410285	-

290.0443225	-290.0448908	-290.0443665	-290.0448967	-286.7264722	-289.9888033	-
290.0117734	-290.0108071	-290.0323154	-290.0137221	-290.0353869	-290.0363634	
sih3	-290.4937839	-290.6236128	-290.6373494	-290.6426667	-290.6438857	-290.5385652 -
290.6558443	-290.6591311	-290.6618435	-290.6707724	-290.6746846	-290.6769998	-
290.6781059	-290.6799406	-290.6805428	-290.675987	-290.68133	-290.6818301	-
290.6814152	-290.6821232	-290.6391188	-290.6453735	-290.6483784	-290.649725	-
290.6710383	-290.6816844	-290.6859493	-290.6866844	-290.6832821	-290.6871861	-
290.6878894	-290.6872341	-290.68789	-287.3581086	-290.6156062	-290.6407208	-
290.6512396	-290.6736254	-290.6544936	-290.6771384	-290.6784905		
sih4	-291.1126086	-291.2470309	-291.2606492	-291.2669487	-291.2684507	-291.1727756 -
291.2904539	-291.2946069	-291.29696	-291.3056858	-291.3108336	-291.31274	-
291.3140799	-291.3156564	-291.3162029	-291.3125985	-291.317466	-291.3178382	-
291.3175833	-291.3182512	-291.2628646	-291.2692107	-291.2724683	-291.2742141	-
291.3045471	-291.316574	-291.3215114	-291.3224175	-291.3186572	-291.3230719	-
291.3239223	-291.3231317	-291.3239024	-287.9857542	-291.2373651	-291.2644098	-
291.285212	-291.3086711	-291.2886995	-291.3121861	-291.3139611		
sio	-363.5063291	-363.8224846	-363.8876927	-363.8972944	-363.8980498	-363.5860614 -
363.8886065	-363.8961802	-363.9001779	-363.9472098	-363.9553608	-363.9585207	-
363.9633787	-363.9663368	-363.967473	-363.9591678	-363.9699552	-363.9709465	-
363.9702877	-363.9713252	-363.8613228	-363.8898246	-363.9020301	-363.9036299	-
363.9240473	-363.9614638	-363.9709503	-363.9731167	-363.9652138	-363.9743522	-
363.9768652	-363.9745569	-363.9768678	-359.5900186	-363.8317292	-363.8817625	-
363.8988783	-363.939209	-363.9067055	-363.9510359	-363.9539609		
so	-471.9233488	-472.2869546	-472.3592577	-472.3721745	-472.3743366	-472.0173786 -
472.3623706	-472.372274	-472.3780531	-472.4293447	-472.4394292	-472.4431282	-
472.4488092	-472.4522512	-472.4537857	-472.4463453	-472.4587584	-472.4600612	-
472.4593493	-472.4605268	-472.3353379	-472.3648127	-472.3761287	-472.3784622	-
472.40884	-472.4470061	-472.456208	-472.4585488	-472.4533323	-472.4627233	-
472.4654891	-472.4631545	-472.4654721	-467.0613764	-472.3020488	-472.3487631	-
472.3786567	-472.4202539	-472.3832718	-472.4304858	-472.4382841		

so2	-546.4624346	-547.0359382	-547.174647	-547.1978455	-547.2049479	-546.7430259	-
547.2624277	-547.2955118	-547.3097079	-547.3754632	-547.4084576	-547.4195481	-	
547.4241829	-547.4344327	-547.4376068	-547.4237837	-547.4489492	-547.4514051	-	
547.4502597	-547.4524133	-547.1214408	-547.1763625	-547.2008155	-547.2057289	-	
547.347014	-547.4210728	-547.4365414	-547.4411603	-547.4345018	-547.4511274	-	
547.456634	-547.4520251	-547.4565518	-540.7758833	-547.0745202	-547.1540487	-	
547.3032975	-547.363875	-547.3216264	-547.3946404	-547.4117058			

3. Linear Regression Results - Delta Estat as a function of number of valence electrons (tab-delimited text format, copy and paste into Excel for table format)

	Intercept	95%CI	Slope	95%CI	R^2	
pc-0[sp]	0.002375149		0.00315964	0.000255171	0.00021434	0.06556194
pc-1[sp]	5.15361E-05		0.003023571	0.000499053	0.000205109	0.226644391
pc-2[sp]	-0.000268737		0.003306991	0.000475645	0.000224336	0.18203292
pc-3[sp]	-0.000330026		0.00314602	0.000483807	0.000213416	0.202812412
pc-4[sp]	-0.000244376		0.003114918	0.000469806	0.000211306	0.196601857
pc-0[spd_2]	4.51056E-05		0.001689958	0.000344321	0.000114641	0.308708766
pc-1[spd] = pc-1	0.001066711		0.000782219	1.04465E-05	5.30632E-05	0.001914985
pc-1[spd_2]	0.000687798		0.000454668	2.07984E-05	3.08432E-05	0.022014829
pc-1[spd_3]	0.000497169		0.000350664	2.71698E-05	2.37879E-05	0.060663017
pc-2[spd_1}]	0.0009076		0.000805725	2.66104E-05	5.46578E-05	0.011597856
pc-2[spd]	0.000413286		0.000387094	2.62439E-05	2.62592E-05	0.047116804
pc-2[spd_3]	0.00031546		0.000220165	1.71575E-05	1.49353E-05	0.06132539
pc-3[spd_2]	0.000314678		0.000362798	1.1102E-05	2.46111E-05	0.009973126
pc-3[spd]	2.40112E-05		0.000156988	1.73508E-05	1.06496E-05	0.116144462
pc-4[spd]	1.45633E-05		0.000142518	1.5913E-05	9.67E-06	0.118255757
pc-2[spdf] = pc-2	0.000527054		0.000307089	8.78E-06	2.08319E-05	0.008720192
pc-3[spdf]	4.58671E-05		3.15971E-05	1.02E-07	2.14E-06	0.000113076
pc-4[spdf]	3.27562E-05		2.7457E-05	5.09E-07	1.86E-06	0.003678496
pc-3[spdfg] = pc-3	3.91371E-05		3.00127E-05	8.47E-07	2.04E-06	0.00849605
pc-4[spdfg] = pc-4	2.27179E-05		2.85761E-05	1.28E-06	1.94E-06	0.021164084
STO-3G	-0.006031233		0.00655004	0.001296702	0.000444334	0.296569776
6-31G	-0.000403411		0.00325133	0.000482325	0.00022056	0.191422376
6-311G	-0.000551204		0.003219105	0.000525641	0.000218374	0.222895155
"6-31G(d,p)"	0.000498121		0.000831201	5.90603E-05	5.6386E-05	0.051513743
"6-311G(d,p)"	-8.79818E-05		0.000875104	9.7284E-05	5.93643E-05	0.117345675
"6-31G(2d,2p)"	0.000174452		0.000483239	5.8057E-05	3.27814E-05	0.134404482
"6-311G(2d,2p)"	-9.23154E-05		0.000343255	4.9891E-05	2.32853E-05	0.185177114

"6-311G(2df,2pd)"	-4.60946E-05	0.00022267	3.03696E-05	1.51052E-05	0.166742986
cc-pVDZ[sp]	-0.000255666	0.00311647	0.000491362	0.000211411	0.210994286
cc-pVTZ[sp]	-0.000295952	0.003256847	0.00048558	0.000220934	0.192984483
cc-pVQZ[sp]	-0.000342682	0.003177843	0.000499295	0.000215575	0.209836214
cc-pV5Z[sp]	-0.00035923	0.003152409	0.000485758	0.000213849	0.203458809
cc-pVDZ[spd] = cc-pVDZ	2.53693E-05	0.000618293	8.34841E-05	4.1943E-05	0.163966821
cc-pVTZ[spd]	6.95761E-05	0.000231388	2.86485E-05	1.56966E-05	0.141561416
cc-pVQZ[spd]	3.38E-06	0.000181795	2.07544E-05	1.23324E-05	0.122966956
cc-pV5Z[spd]	8.50E-06	0.000166965	1.87282E-05	1.13264E-05	0.119212374
cc-pVTZ[spdf] = cc-pVTZ	0.000152589	0.000137063	1.01367E-05	9.30E-06	0.055569412
cc-pVQZ[spdf]	-4.69E-06	2.85083E-05	4.08E-06	1.93E-06	0.180203573
cc-pV5Z[spdf]	2.98E-07	2.10E-06	7.55E-08	1.43E-07	0.013690629
cc-pVQZ[spdfg] = cc-pVQZ	-4.18E-06	2.60551E-05	3.37E-06	1.77E-06	0.152362207

4.1 CBS extrapolation parameters for static correlation energies calculated using correlation consistent basis sets

	-Es_infty	A	B	
al	0.024146184	-0.303128918	2.5	
b	0.03473193	-0.591292197	2.5	
be	0.043816089	-0.454175441	2.5	
beh	0.027655192	-0.535296131	2.5	
c	0.019291065	-0.278080082	2.5	
ch	0.043082793	-0.462032818	2.5	
ch2_sing	0.062072981	-0.790339225	2.5	
ch2_trip	0.038756192	-0.402102929	2.5	
ch3	0.059384849	-0.564609957	2.5	
ch3ch2	0.128940863	-1.098825973	2.5	
ch3cl	0.087229672	-0.836097963	2.5	
ch3f	0.093812542	-0.846667564	2.5	
ch3fcl	0.112293667	-0.096099706	2.5	
ch3sh	0.104686059	-0.915313801	2.5	
ch4	0.08317673	-0.943153396	2.5	
cl2	0.023350766	0.133496467	2.5	
clch3cl-	0.0802183	-0.267609748	2.5	
clf	0.037727454	0.251198104	2.5	
clo	0.042645629	-0.05635818	2.5	
cn	0.151911312	-0.13157038	2.5	
co	0.131771174	-0.718304389	2.5	
co2	0.176354295	-0.149856993	2.5	
cs	0.104576329	-0.33612142	2.5	
f2	0.079128721	0.031292753	2.5	
fch3cl-	0.077140773	-0.484824058	2.5	
h2	0.018542888	-0.125433727	2.5	
h2cch2	0.144175731	-0.708041831	2.5	

h2co	0.147075835	-2.203248442	2.5
h2nnh2	0.13504683	-1.558269011	2.5
h2o	0.053744116	-0.673979522	2.5
h2s	0.034435726	-0.289487187	2.5
h3cch3	0.151160148	-1.431992985	2.5
h3coh	0.118783498	-1.238699337	2.5
hc2h4	0.148371699	-0.703140769	2.5
hcch	0.148040605	-0.515815756	2.5
hcl	0.017368724	-0.155226548	2.5
hclh	0.037438449	0.274732723	2.5
hcn	0.151429758	-1.054288795	2.5
hcn_ts	0.141869871	-0.461268125	2.5
hco	0.125828392	-0.477726244	2.5
hf	0.024456445	-0.226102036	2.5
hn2	0.129970892	-0.102576626	2.5
hn2_ts	0.158156369	-0.176018842	2.5
hn2o	0.224134231	0.481359007	2.5
hnc	0.140757699	-0.625574388	2.5
hoch3f-	0.119787346	-0.759284749	2.5
hoch4	0.124117231	-1.654285833	2.5
hocl	0.066449826	-0.32889639	2.5
hoh	0.040581623	-0.326308865	2.5
hooh	0.107512853	-0.81005108	2.5
li2	0.008827362	0.034499936	2.5
lif	0.014984765	-0.409388528	2.5
lih	0.016384451	-0.103490172	2.5
mg	0.031418131	-0.116585761	2.5
n2	0.148514254	-0.485341135	2.5
n2o	0.21491744	-0.074230644	2.5
na2	0.010639733	0.084071345	2.5
nacl	0.008425065	-0.369072359	2.5

nh	0.026123383	-0.200788602	2.5
nh2	0.049120775	-0.462978014	2.5
nh3	0.074951018	-1.069338315	2.5
no	0.120600733	-0.088265911	2.5
o2	0.104321075	0.206018895	2.5
o3	0.237334767	0.559060696	2.5
oh-	0.022555674	-0.02970047	2.5
oh	0.02496266	-0.251971797	2.5
p2	0.091496082	0.296004722	2.5
ph2	0.03485425	-0.266036342	2.5
ph3	0.04845113	-0.445113767	2.5
s2	0.04599027	0.217932807	2.5
sh	0.018690755	-0.140362644	2.5
sh3	0.041136032	-0.122407475	2.5
si	0.013338505	-0.118158203	2.5
si2	0.079984734	0.255033331	2.5
si2h6	0.096461953	-1.325164703	2.5
sih2_sing	0.051286554	-0.730936329	2.5
sih2_trip	0.032858276	-0.409903841	2.5
sih3	0.04266368	-0.638502707	2.5
sih4	0.055557927	-0.892022698	2.5
sio	0.12211427	-0.254366771	2.5
so	0.061285758	1.921983474	2.5
so2	0.130427118	1.322372332	2.5

4.2 CBS extrapolation parameters for static correlation energies calculated using polarization consistent basis sets

	-E_infty	A	B	
al	0.024078883	-0.185649498	3.2	
b	0.034751335	-0.55369365	3.2	
be	0.043828117	-0.807182746	3.2	
beh	0.02765754	-0.771975074	3.2	
c	0.019302984	-0.284459128	3.2	
ch	0.043075298	-0.505157315	3.2	
ch2_sing	0.06205472	-0.765165474	3.2	
ch2_trip	0.038756515	-0.256614033	3.2	
ch3	0.059380869	-0.372455302	3.2	
ch3ch2	0.128935153	-0.629930474	3.2	
ch3cl	0.087216098	-0.477950475	3.2	
ch3f	0.093800637	-0.509770798	3.2	
ch3fcl	0.112161277	-0.180120775	3.2	
ch3sh	0.104644343	-0.474111045	3.2	
ch4	0.08318303	-0.505422342	3.2	
cl2	0.023274749	0.162538946	3.2	
clch3cl-	0.080158853	-0.400681177	3.2	
clf	0.037640865	0.087778316	3.2	
clo	0.042631648	0.175288309	3.2	
cn	0.151896367	-0.273424882	3.2	
co	0.13177554	-0.39265239	3.2	
co2	0.176294984	-0.067222451	3.2	
cs	0.104574943	0.048511279	3.2	
f2	0.079078282	-0.011956136	3.2	
fch3cl-	0.077031475	-0.676723907	3.2	
h2	0.018545613	-0.023151846	3.2	
h2cch2	0.144139797	-0.595043178	3.2	

h2co	0.147163489	-1.154870347	3.2
h2nnh2	0.135082998	-0.60693757	3.2
h2o	0.053734894	-0.263322901	3.2
h2s	0.034388946	-0.091001678	3.2
h3cch3	0.151166917	-0.754602814	3.2
h3coh	0.118770086	-0.592031225	3.2
hc2h4	0.148339762	-0.569416574	3.2
hcch	0.14802082	-0.548848301	3.2
hcl	0.017349087	-0.035818541	3.2
hclh	0.037399148	0.289345962	3.2
hcn	0.151465175	-0.77722357	3.2
hcn_ts	0.141785627	-0.376703261	3.2
hco	0.125812321	-0.24569144	3.2
hf	0.024434954	-0.131198476	3.2
hn2	0.129918664	-0.195929663	3.2
hn2_ts	0.158116662	-0.165302202	3.2
hn2o	0.223983023	-0.091488411	3.2
hnc	0.140766023	-0.692659978	3.2
hoch3f-	0.119717756	-0.701494566	3.2
hoch4	0.124170007	-0.619569025	3.2
hocl	0.06640562	-0.082939779	3.2
hoh	0.040600688	-0.104218287	3.2
hooh	0.107502935	-0.363791119	3.2
li2	0.008817065	0.330743392	3.2
lif	0.01498735	-0.18624612	3.2
lih	0.016385919	-0.144186746	3.2
mg	0.031232856	-0.233615137	3.2
n2	0.148527215	-0.247659394	3.2
n2o	0.214871958	-0.107018852	3.2
na2	0.010565179	0.037867926	3.2
nacl	0.008375821	0.020322854	3.2

nh	0.026111362	-0.143526475	3.2
nh2	0.049110019	-0.270466229	3.2
nh3	0.074982273	-0.424358723	3.2
no	0.120568213	-0.107651	3.2
o2	0.104271131	0.069988824	3.2
o3	0.237289444	-0.06949614	3.2
oh-	0.022486035	-0.080055139	3.2
oh	0.024948151	-0.136610435	3.2
p2	0.091325561	1.075850745	3.2
ph2	0.034790774	-0.114806731	3.2
ph3	0.048378513	-0.182618265	3.2
s2	0.045881622	0.540223146	3.2
sh	0.018660313	-0.067775521	3.2
sh3	0.041074415	-0.052012846	3.2
si	0.013274957	-0.049099559	3.2
si2	0.079833478	1.844220174	3.2
si2h6	0.096277386	-0.506810321	3.2
sih2_sing	0.051124195	-1.612552841	3.2
sih2_trip	0.032835334	-0.095011503	3.2
sih3	0.042609414	-0.19483863	3.2
sih4	0.055473823	-0.398743865	3.2
sio	0.122013817	-0.419134119	3.2
so	0.060987966	1.172677891	3.2
so2	0.130147993	0.910032664	3.2

5. Numerical Hartree-Fock energies for a selection of atoms and diatomics

	Num HF	N_nu	N_mu	R_infty	(Bohr)		Num HF	N_nu	N_mu	R_infty	(Bohr)
H	-0.500000	169	265	35		He	-2.861680	169	265	35	
Li	-7.432727	169	265	35		Na	-161.858912	169	265	35	
Be	-14.573023		169	265	35	Mg	-199.614636	169	265	35	
B	-24.529138		169	265	35	Al	-241.876861	169	265	35	
C	-37.688694		169	265	35	Si	-288.854547	169	265	35	
N	-54.400934		169	265	35	P	-340.718781	169	265	35	
O	-74.812396		169	265	35	S	-397.507281	169	265	35	
F	-99.411412		169	265	35	Cl	-459.483973	169	265	35	
F-	-99.459454		169	265	35	Cl-	-459.576925	169	265	35	
Ne	-128.547098		169	265	35	Ar	-526.817513	169	265	35	
H2	-1.133624	199	355	100		Na2	-323.717017	295	499	300	
HF	-100.070810		295	571	200	NaCl	-621.460596		295	523	300
LiF	-106.993356		295	559	300	FCI	-558.920172		295	571	350
F2	-198.773437		295	583	350	Cl2	-919.010838		295	553	350
N2	-108.993190		295	529	150	P2	-681.500255		295	541	300
CO	-112.790895		295	553	200	CS	-435.362393		295	559	300