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

Supplementary Materials

A Mechanistic Study of the Addition of Alcohol to a Five-Membered Ring Silene via a Photochemical Reaction

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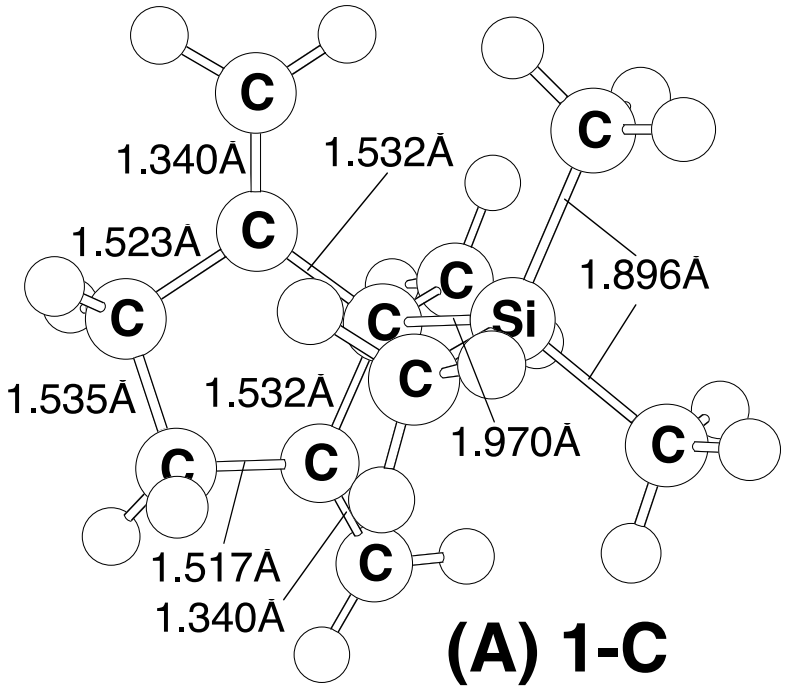
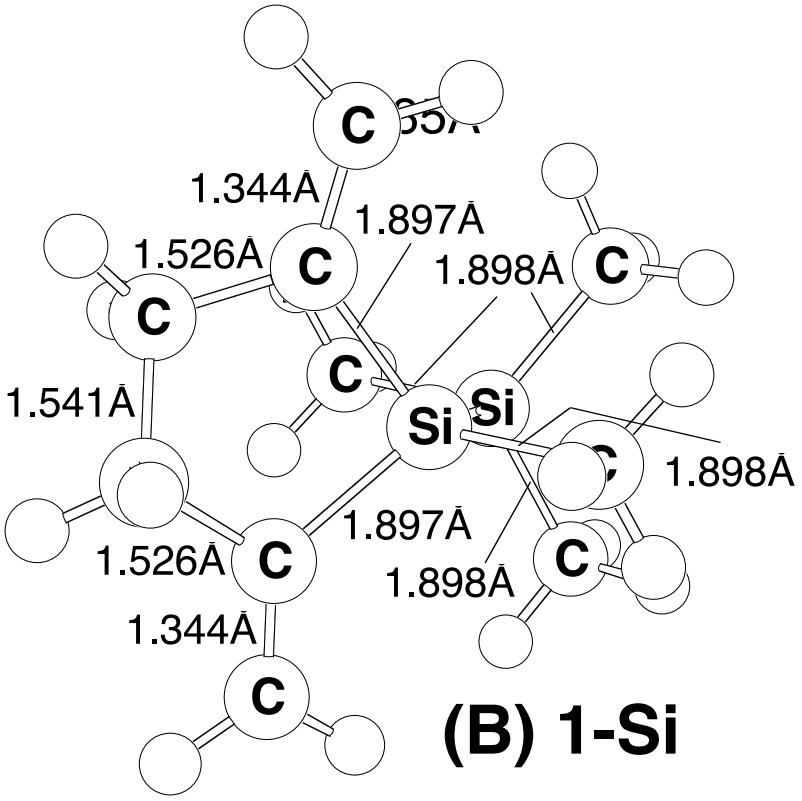
The fixed geometrical parameters are shown below:



(A) 1-C



(B) 1-Si

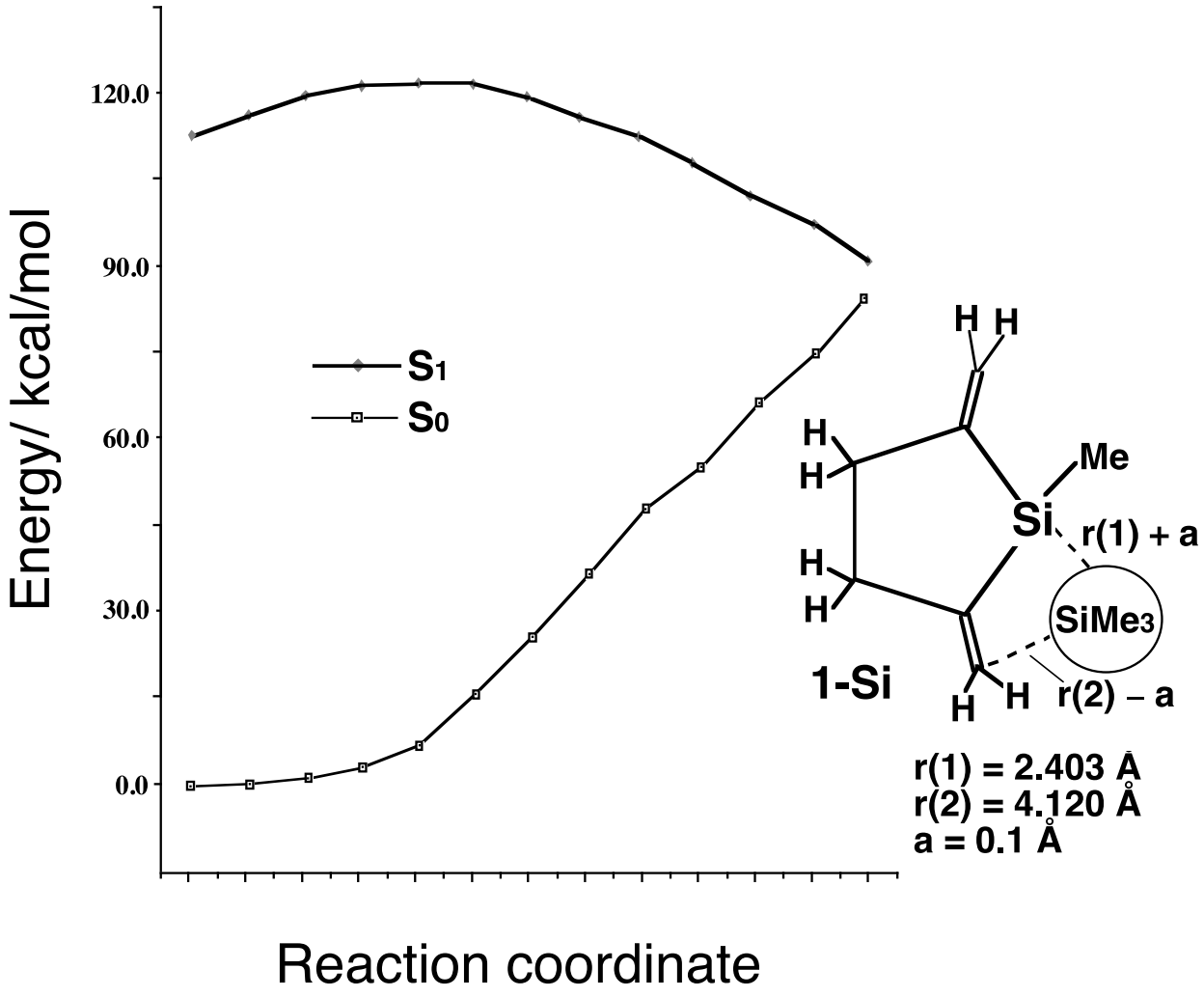


Figure SA: The behavior of the ground-state (starting from reactant, **1-Si**, CAS(6,6)/6-311G(d)) and lowest energy singlet state (starting from the FC point at the S_1 state, CAS(6,6)/6-311G(d)) along the reaction coordinate towards the conical intersection point (**S_0/S_1-CI-Si**). From this scan, it is apparent to see that that stretching the r(1) coordinate on the S_1 surface and a steepest ascent reaction path toward **S_0/S_1-CI-Si**. Moreover, both curves stop at an abrupt conical intersection. The reason for this is because the force constant is not real zero at the conical intersection point, since the conical intersection point is not a true minimum at the excited state surface. For details, interesting readers can find in ref. (8).

(1) **1-C**

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-3.068472	1.236522	1.121254
6	-2.128325	0.680407	1.044869
1	-1.607348	0.762584	2.004770
6	-1.241191	1.176702	-0.067276
6	-2.384882	-0.784551	0.706173
1	-2.485036	-1.384670	1.616431
1	-3.310828	-0.873944	0.125056
6	-1.216542	-1.222846	-0.143385
6	-0.428552	0.000863	-0.619374
6	-0.255289	0.030364	-2.153426
1	0.310193	0.907593	-2.486918
1	-1.229156	0.053779	-2.657358
1	0.280682	-0.851641	-2.521700
14	1.452971	0.027490	0.286223
6	2.272223	1.664804	-0.135557
1	3.286713	1.698437	0.272885
1	1.710232	2.503327	0.285058
1	2.336705	1.800281	-1.218897
6	2.470036	-1.391723	-0.402712
1	3.492570	-1.347285	-0.015521
1	2.519390	-1.344887	-1.494181
1	2.044885	-2.357076	-0.115597
6	1.247135	-0.150286	2.139741
1	2.224340	-0.232670	2.625198
1	0.669825	-1.045712	2.387272
1	0.735755	0.718904	2.562511
6	-1.295075	2.429667	-0.542878
1	-1.953642	3.170630	-0.099386
1	-0.684933	2.754695	-1.378956
6	-1.002063	-2.508017	-0.462756
1	-1.651608	-3.294160	-0.089014
1	-0.186716	-2.811857	-1.110534

CASSCF(6,6)/6-311G(d) = -717.1565338385
MP2(6,6)/6-311++G(3df,3pd)//CASSCF(6,6)/6-311G(d)= -719.472515

(2) **FC-C**

CASSCF(6,6)/6-311G(d) = -716.988897098

MP2(6,6)/6-311++G(3df,3pd)//CASSCF(6,6)/6-311G(d)= -719.3281791

(3) **S1/S0-CI-C**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.297175	0.004719	-0.005226
6	0.708668	-0.400186	1.710245
6	2.227736	-0.251167	1.795679
6	2.749600	-0.136870	0.358379
6	1.614118	0.466662	-0.439480
1	3.644528	0.471315	0.300102
1	3.004397	-1.114806	-0.033507
1	2.464801	0.656638	2.344226
1	2.682554	-1.076909	2.334273
14	0.030156	-2.084810	0.926746
6	1.074126	-3.008902	-0.355011
1	2.073657	-3.229154	0.009499
1	1.156218	-2.500152	-1.307190
1	0.592241	-3.970618	-0.525921
6	0.181547	-3.225375	2.468178
1	-0.456766	-2.883879	3.280877
1	1.199209	-3.260357	2.853045
1	-0.106645	-4.249359	2.234907
6	-1.818405	-2.155946	0.521959
1	-2.433719	-1.615237	1.236347
1	-2.129395	-3.197361	0.571114
1	-2.048779	-1.784148	-0.469521
6	-0.887039	0.924800	-0.158186
1	-0.689230	1.931167	0.210752
1	-1.775606	0.552556	0.332075
1	-1.128151	1.002279	-1.215181
6	-0.069619	0.198878	2.690217
1	0.371769	0.731040	3.516451
1	-1.143216	0.174229	2.663270
6	1.819968	1.345956	-1.447515
1	1.013143	1.775505	-2.012075

1	2.816465	1.606136	-1.757705

Derivative Coupling

-1	-0.0217420798	-0.0539829755	-0.0318060066
-2	-0.0037651738	0.0530440494	0.0656320669
-3	0.0030803587	-0.0015339996	0.0036029117
-4	-0.0005236623	0.0002077465	-0.0020608756
-5	0.0039383927	0.0081234476	0.0093907307
-6	-0.0001853401	-0.0000122701	0.0006576914
-7	-0.0002455116	-0.0000491623	0.0003483027
-8	-0.0003430563	-0.0009266806	0.0000807948
-9	-0.0002221952	-0.0003024288	0.0002131613
-10	-0.0124392384	0.0129333270	-0.0487260268
-11	0.0012015744	-0.0034031370	0.0033415036
-12	0.0007914605	-0.0011721619	-0.0005831123
-13	-0.0011619950	0.0011070981	0.0020093059
-14	0.0005980443	-0.0011670252	0.0001661638
-15	0.0039458654	0.0067172461	0.0048569859
-16	-0.0000848718	-0.0003830423	0.0003352702
-17	-0.0001745385	-0.0008105658	0.0008016766
-18	0.0000797424	0.0017482022	-0.0026342538
-19	-0.0004373297	-0.0032134053	0.0035489181
-20	-0.0010587744	-0.0001514150	0.0000723093
-21	-0.0013284839	-0.0003637633	0.0006071214
-22	0.0021017518	0.0002481944	0.0008805386
-23	0.0054616351	0.0053480221	0.0140507493
-24	-0.0028397679	0.0041143997	-0.0003471479
-25	-0.0009726367	-0.0000926857	-0.0010746468
-26	0.0023573919	-0.0026851471	0.0003907092
-27	0.0255392432	-0.0202454554	-0.0292010819
-28	-0.0001188732	-0.0014051659	0.0024549757
-29	-0.0003715904	0.0007684291	-0.0015482995
-30	-0.0013659107	-0.0007430655	0.0052878431
-31	0.0000539525	0.0004661178	0.0002997185
-32	0.0002316171	-0.0021827277	-0.0010479976

Unscaled Gradient Difference

-1	-0.0172088328	-0.0012100563	-0.0939510934
-2	-0.0038409218	-0.1072592944	0.0949872310
-3	-0.0019990022	0.0106736328	0.0000099847
-4	-0.0000584801	-0.0012867054	0.0006810040
-5	-0.0199067249	0.0179765704	0.0200213745
-6	-0.0001305747	0.0004804434	0.0000118315
-7	-0.0000729987	0.0001492914	-0.0000066556
-8	0.0031060595	0.0014658401	0.0002735117
-9	-0.0030271400	-0.0007105967	-0.0007963628
-10	0.0136998453	0.0389881956	0.0244411515
-11	0.0034352965	0.0064018871	-0.0004519810
-12	-0.0002476312	-0.0002818674	0.0000687866
-13	0.0001562122	-0.0006145418	-0.0006531508
-14	-0.0014149817	0.0012024873	0.0012600908

-15	-0.0045263993	-0.0086835162	-0.0039564464
-16	-0.0002911067	-0.0003463017	0.0006663375
-17	0.0006444761	0.0003525096	-0.0000831453
-18	0.0000832273	-0.0024467882	0.0035158748
-19	0.0013224317	0.0031222185	-0.0000930540
-20	-0.0002267120	-0.0002063874	0.0001431492
-21	0.0008520047	-0.0001019903	0.0000868982
-22	-0.0004455804	0.0000731966	-0.0003070100
-23	0.0113873176	0.0225444356	0.0044189621
-24	-0.0066309068	0.0024114491	-0.0062688329
-25	0.0005350882	-0.0019462732	0.0003814413
-26	0.0030638410	-0.0020384366	-0.0010256411
-27	0.0188114176	0.0053089812	-0.0289818053
-28	-0.0003958307	0.0167093081	-0.0079651209
-29	-0.0003541498	-0.0076320964	0.0048228388
-30	0.0037260540	0.0097622782	-0.0074980473
-31	-0.0000219871	0.0020622520	0.0019561724
-32	-0.0000233107	-0.0049201250	-0.0057082940

CASSCF(6,6)/6-311G(d) = -716.9878509272
MP2(6,6)/6-311++G(3df,3pd)//CASSCF(6,6)/6-311G(d)= -719.3198029

(4) **Int-C**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.911044	0.015129	-0.075642
1	-3.624368	-0.065201	-0.905601
6	-2.443557	-1.498583	0.193127
1	-3.230721	-2.199644	-0.104577
1	-2.220724	-1.654870	1.257794
6	-1.176125	-1.675447	-0.627069
1	-1.402509	-2.062095	-1.626361
1	-0.485712	-2.362218	-0.131460
6	-0.655309	-0.273484	-0.729634
6	-1.589712	0.646999	-0.427743
6	-1.474278	2.135274	-0.518284
1	-2.295205	2.535347	-1.121607
1	-0.538036	2.461908	-0.977023
1	-1.529405	2.582167	0.478945
6	0.743242	-0.043313	-1.222649
1	0.804193	0.897178	-1.780953
1	1.006993	-0.828313	-1.941909

14	2.088079	0.002418	0.130687
6	3.748984	0.307824	-0.697337
1	3.738280	1.256532	-1.241930
1	3.978196	-0.493405	-1.406010
1	4.548789	0.347639	0.047944
6	2.150588	-1.625650	1.055563
1	2.287734	-2.460519	0.362038
1	1.225956	-1.792068	1.615867
1	2.982211	-1.632568	1.766538
6	1.732707	1.399602	1.332235
1	1.673079	2.356408	0.805234
1	2.524943	1.471472	2.083311
1	0.784578	1.233956	1.852164
6	-3.467175	0.464869	1.060183
1	-4.546306	0.448554	1.183051
1	-2.865006	0.806568	1.898423

CASSCF(6,6, + 6,4)/6-311G(d) = -717.17768504
MP2(6,6, + 6,4)/6-311++G(3df,3pd)//CASSCF(6,6, + 6,4)/6-311G(d)= -719.452360622

(5) **CH3OH**

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.000000	0.000000	2.000000
6	1.385642	0.000000	2.210512
1	-0.455560	0.000000	2.826900
1	1.647942	0.000000	3.287333
1	1.827084	0.881563	1.759173
1	1.827084	-0.881563	1.759173

CASSCF(6,4)/6-311G(d) = -115.0498058
MP2(6,4)/6-311++G(3df,3pd)//CASSCF(6,4)/6-311G(d)= -115.4382962

(6) **Cpx-C**

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	2.880600	-1.298637	2.147573
6	2.412692	-0.491394	1.596230

1	2.876827	0.441831	1.884925
6	0.878375	-0.494481	1.839419
1	0.505269	0.515919	1.945300
1	0.601169	-1.062763	2.718994
6	0.308014	-1.125605	0.571614
6	2.553641	-0.768028	0.100270
6	1.241184	-1.271949	-0.369427
6	-1.155659	-1.452585	0.491991
1	-1.496498	-1.811449	1.462934
1	-1.327256	-2.261815	-0.214546
6	1.079585	-1.829278	-1.758294
1	1.816167	-2.605868	-1.938879
1	1.223704	-1.054976	-2.507415
1	0.095669	-2.253050	-1.905060
14	-2.290572	-0.000269	-0.025545
6	-4.050133	-0.696228	-0.045554
1	-4.344259	-1.063022	0.936142
1	-4.146391	-1.520920	-0.749294
1	-4.766397	0.069455	-0.337558
6	-1.816796	0.622507	-1.738086
1	-2.565602	1.319223	-2.112029
1	-1.725490	-0.182190	-2.464069
1	-0.872173	1.153223	-1.676206
6	-2.175612	1.425343	1.198973
1	-2.971763	2.146605	1.020395
1	-1.226525	1.935884	1.068633
1	-2.260034	1.093452	2.231882
1	1.988182	3.229655	-1.543075
6	1.688432	3.198273	-0.501858
1	1.085081	4.066024	-0.287141
1	2.576648	3.226641	0.118986
8	0.869960	2.045867	-0.213140
1	1.354318	1.226614	-0.377771
6	3.636439	-0.566264	-0.631672
1	4.540826	-0.178171	-0.202123
1	3.665281	-0.796707	-1.679483

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(7) **Cis-TS-C**

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	2.361594	-2.920997	-0.701692
6	1.900967	-2.187812	-0.032792
1	1.814753	-2.628579	0.966971
6	0.529320	-1.760188	-0.529944
1	-0.240983	-2.407578	-0.099580
1	0.474662	-1.884935	-1.618853
6	2.657640	-0.901259	0.054614
6	1.708786	0.236440	0.327146
6	0.340383	-0.261739	-0.206806
6	-0.813537	-0.069054	0.800874
1	-0.730167	0.900352	1.300634
1	-0.804509	-0.841854	1.577795
6	1.861558	0.843041	1.707895
8	2.041063	1.428216	-0.918988
6	1.683095	2.684047	-0.568105
1	2.384017	3.078556	0.170724
1	0.659898	2.703858	-0.186564
1	1.730715	3.311637	-1.462095
1	1.646110	0.101676	2.485581
1	2.884322	1.202141	1.870944
1	1.200869	1.698007	1.875497
14	-2.595171	-0.012536	0.025142
6	-3.813678	0.453974	1.371812
1	-4.829132	0.515922	0.969497
1	-3.557349	1.425129	1.805440
1	-3.807431	-0.291025	2.172930
6	-2.592020	1.301991	-1.319106
1	-3.587217	1.400589	-1.762404
1	-1.886634	1.040404	-2.113303
1	-2.300854	2.272587	-0.906825
6	-3.047904	-1.672986	-0.704912
1	-4.073451	-1.660175	-1.086101
1	-2.975883	-2.461953	0.049556
1	-2.383487	-1.930807	-1.534721
6	3.983123	-0.806338	-0.114753
1	4.518458	0.131040	-0.017729
1	4.578813	-1.695420	-0.305841

1	0.540363	0.530491	-1.165476

(8) **Tran-TS-C**

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-2.295743	-2.190531	-1.500140
6	-1.788851	-1.970135	-0.555453
1	-1.696732	-2.895747	0.023961
6	-2.521509	-0.924655	0.244086
6	-0.407264	-1.371236	-0.811473
6	-0.229639	-0.304530	0.276273
6	-1.648073	0.295268	0.400348
6	-1.844257	1.236437	1.580614
1	-2.887132	1.553584	1.680311
1	-1.255131	2.150825	1.459403
1	-1.555850	0.755028	2.520749
8	-1.835134	1.208247	-1.063115
6	-3.097871	1.860683	-1.078379
1	-3.135807	2.644174	-0.318441
1	-3.915736	1.150546	-0.943431
1	-3.217978	2.336322	-2.055773
6	-3.716057	-1.148970	0.810488
1	-4.212430	-0.404489	1.423483
1	-4.235379	-2.091691	0.663947
1	0.363133	-2.146068	-0.760786
1	-0.368794	-0.926931	-1.813665
14	2.688440	0.086247	0.033288
6	3.098326	-0.830387	-1.549082
1	2.865037	-0.215043	-2.423062
1	2.533443	-1.762916	-1.626216
1	4.163398	-1.079058	-1.582499
6	2.959502	-1.031471	1.511460
1	2.679734	-0.522582	2.438622
1	4.011393	-1.323039	1.586364
1	2.361020	-1.943221	1.426281
6	3.821938	1.583347	0.176064
1	3.679540	2.254789	-0.675738

1	4.869987	1.270616	0.197653
1	3.609061	2.139847	1.093496
1	0.047008	-0.964712	1.474791
1	0.837590	1.507824	0.744310
6	0.885011	0.712131	-0.007176
1	0.731733	1.190142	-0.981352

(9) **Cis-Pro-C**

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-1.952131	2.399261	-1.071430
6	-1.248102	1.853277	-0.455749
1	-0.621448	2.571984	0.058708
6	-0.396043	0.866632	-1.305090
1	0.562941	1.284247	-1.572251
1	-0.932517	0.606794	-2.203886
6	-1.973252	0.969786	0.558616
6	-1.696583	-0.480862	0.185422
6	-0.273492	-0.401015	-0.421821
1	-0.114623	-1.283393	-1.026400
6	0.828199	-0.272810	0.656507
1	0.801859	-1.159436	1.288492
1	0.597347	0.568148	1.310410
6	-1.889061	-1.505862	1.297315
8	-2.498053	-0.830913	-0.978024
6	-3.928242	-0.823889	-0.855243
1	-4.291669	0.112141	-0.451530
1	-4.284484	-1.636911	-0.234395
1	-4.313453	-0.955646	-1.855794
1	-1.265975	-1.274557	2.148455
1	-2.918757	-1.529473	1.632498
1	-1.635168	-2.490649	0.922971
14	2.625053	-0.110826	0.055388
6	3.740634	-0.852944	1.390940
1	4.791417	-0.759640	1.123665
1	3.531086	-1.910600	1.539107
1	3.599591	-0.352274	2.347246

6	2.887005	-1.055107	-1.559344
1	3.932491	-1.020635	-1.860180
1	2.296860	-0.640290	-2.373129
1	2.610931	-2.102554	-1.453606
6	3.131634	1.696931	-0.178065
1	4.189862	1.765853	-0.424573
1	2.971843	2.267429	0.735285
1	2.578918	2.188763	-0.973857
6	-2.674914	1.400559	1.584180
1	-3.142764	0.732061	2.281379
1	-2.805176	2.450054	1.775575

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(10) **Tran-Pro-C**

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1.955374	2.397028	-1.071919
6	1.250075	1.853284	-0.455715
1	0.625027	2.573914	0.057978
6	1.973453	0.969257	0.559364
6	0.396119	0.867619	-1.304477
6	0.273325	-0.400419	-0.421732
6	1.696527	-0.481046	0.185300
6	-0.828211	-0.272148	0.656745
1	-0.597492	0.569113	1.310303
1	-0.801617	-1.158538	1.289026
6	1.889046	-1.506713	1.296527
1	2.918781	-1.530565	1.631604
1	1.635072	-2.491252	0.921602
1	1.266010	-1.275922	2.147843
8	2.497702	-0.830474	-0.978535
6	3.927914	-0.823607	-0.855941
1	4.284269	-1.637260	-0.235976
1	4.291472	0.112053	-0.451451
1	4.312947	-0.954415	-1.856680
6	2.673794	1.399439	1.586069
1	3.140591	0.730526	2.283565
1	2.803998	2.448815	1.778131

1	-0.562876	1.286196	-1.570121
1	0.931165	0.607906	-2.204167
14	-2.625095	-0.110739	0.055419
6	-3.740704	-0.854134	1.390213
1	-3.600476	-0.353754	2.346787
1	-3.530491	-1.911706	1.538059
1	-4.791430	-0.761474	1.122479
6	-2.886362	-1.054345	-1.559997
1	-2.296246	-0.638805	-2.373425
1	-3.931858	-1.019921	-1.860817
1	-2.609991	-2.101756	-1.454775
6	-3.132251	1.696894	-0.177587
1	-2.972168	2.267401	0.735700
1	-4.190598	1.765588	-0.423628
1	-2.580010	2.188908	-0.973610
1	0.113907	-1.282427	-1.026712

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(11) **1-Si**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
14	0.000000	0.000000	1.897399
6	1.897397	0.000000	1.955939
6	2.421500	0.229613	0.540110
6	1.409692	-0.347458	-0.468719
1	3.409779	-0.199339	0.400756
1	2.512681	1.301078	0.368331
1	1.519577	-1.430707	-0.494360
1	1.602237	0.013852	-1.474926
6	-1.006753	0.287758	-0.842983
1	-1.995574	0.531032	-0.491460
1	-0.878134	0.294027	-1.914431
6	2.707277	-0.182204	3.013867
1	3.782685	-0.180833	2.923246
1	2.324972	-0.330674	4.009863
14	-0.987378	-1.992867	2.799390
6	-0.183447	-3.516323	2.002157
1	-0.610156	-4.435901	2.396285
1	0.886774	-3.544567	2.189473
1	-0.328884	-3.524569	0.924914
6	-2.850892	-2.005090	2.424371
1	-3.355915	-1.151549	2.870273

1	-3.323698	-2.902716	2.816625
1	-3.042202	-1.977226	1.354659
6	-0.744759	-2.074025	4.683116
1	-1.181536	-1.211556	5.180759
1	0.308350	-2.108807	4.950544
1	-1.214489	-2.961772	5.100593
6	-0.769918	1.570495	2.633273
1	-0.627805	1.613648	3.710219
1	-1.839700	1.615517	2.443689
1	-0.320956	2.461588	2.204336

CASSCF(6,6)/6-311G(d) = -968.2299447955
MP2(6,6)/6-311++G(3df,3pd)//CASSCF(6,6)/6-311G(d)= -970.6065768

(12) **FC-Si**

CASSCF(6,6)/6-311G(d) = -967.9332495
MP2(6,6)/6-311++G(3df,3pd)//CASSCF(6,6)/6-311G(d)= -970.3083353

(13) **S1/S0-CI-Si**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.076788	0.147472	0.403990
14	0.272636	-0.430792	2.164534
6	2.152864	-0.499704	2.001339
6	2.521379	0.511271	0.921638
6	1.438694	0.495583	-0.180097
1	3.503585	0.316243	0.501368
1	2.561032	1.502316	1.368613
1	1.674519	-0.290675	-0.896389
1	1.425041	1.427877	-0.739977
6	3.060940	-1.253784	2.643351
1	4.115484	-1.198222	2.421352
1	2.780495	-1.952831	3.413087
6	-0.572795	-2.081388	2.588342
1	-1.646248	-2.016970	2.433756
1	-0.413322	-2.345515	3.629845
1	-0.191171	-2.892842	1.974837
14	-1.431959	2.415423	1.561840
6	-1.100835	0.512300	-0.252338
1	-1.079657	0.964151	-1.230567
6	-0.050513	3.481301	2.293486
1	0.762030	3.619369	1.586116
1	0.361168	3.039589	3.193326
1	-0.436367	4.469813	2.540150
6	-2.760861	1.959446	2.830747
1	-3.451450	1.217823	2.439754
1	-3.344260	2.842953	3.087165
1	-2.324924	1.563367	3.740439

6	-2.249611	3.412177	0.170376
1	-3.066817	2.868721	-0.293798
1	-1.540623	3.675373	-0.608963
1	-2.655494	4.340339	0.570860
1	-2.042984	0.073530	0.036712

Derivative Coupling

-1	0.0176133953	-0.0178053768	0.0135468373
-2	0.0110466846	-0.0176295083	-0.0203857882
-3	0.0011913321	0.0024552305	0.0027173984
-4	-0.0011232288	-0.0001372821	-0.0013083364
-5	-0.0006806164	-0.0026481997	-0.0008155374
-6	0.0000266563	-0.0001190269	0.0005187534
-7	-0.0001293377	0.0002100630	0.0002602445
-8	0.0018986752	0.0010884988	-0.0007689219
-9	0.0002938233	0.0009722059	0.0006049574
-10	-0.0006765342	-0.0004050139	0.0009128673
-11	-0.0003836635	-0.0002911824	-0.0004380095
-12	0.0001232774	0.0000750480	0.0001506692
-13	-0.0027451486	0.0033213014	0.0054669344
-14	-0.0000099679	-0.0003804479	-0.0000745322
-15	-0.0003634518	-0.0007299630	-0.0000210188
-16	0.0009663297	0.0023184402	-0.0006529491
-17	-0.0186141060	0.0118856758	-0.0233345819
-18	-0.0058673311	0.0059084532	0.0109200427
-19	-0.0003656477	0.0006698326	0.0005166052
-20	0.0008933921	-0.0016234835	0.0016473899
-21	-0.0000919074	-0.0001766343	-0.0002091815
-22	0.0016565321	0.0012394403	0.0016654380
-23	0.0004047826	-0.0012553471	0.0009625110
-24	0.0002080310	0.0025557767	0.0028394552
-25	0.0003109874	-0.0000180432	-0.0006099974
-26	0.0001898768	-0.0011107760	0.0018692444
-27	-0.0011935875	-0.0004437515	0.0023317611
-28	-0.0040417343	0.0102229304	0.0063710228
-29	-0.0000692368	-0.0006994254	0.0002890732
-30	0.0006072215	-0.0002930458	0.0001217550
-31	-0.0019296334	0.0021389295	-0.0035780295
-32	0.0008541357	0.0007046815	-0.0015160766

Unscaled Gradient Difference

-1	-0.0669283148	0.0338201114	-0.0916714886
-2	-0.0161671113	0.0000443063	0.0170536382

-3	-0.0038679434	0.0104877494	0.0026674977
-4	0.0007275717	0.0028559897	-0.0014190376
-5	0.0053984498	-0.0098278397	-0.0080381179
-6	0.0002032433	-0.0000116537	0.0005989876
-7	0.0006172094	-0.0003253457	0.0007417154
-8	0.0043990503	0.0017609967	0.0001444795
-9	-0.0010842644	-0.0017909305	0.0015229570
-10	-0.0011361928	-0.0021131899	0.0027647967
-11	-0.0009358206	-0.0008712145	-0.0014843798
-12	0.0002502387	0.0007071730	0.0004829409
-13	0.0017226452	0.0036553463	0.0023033978
-14	0.0006743610	0.0008134139	-0.0002773468
-15	0.0001568696	-0.0008565798	0.0001441636
-16	0.0008820168	0.0000082331	-0.0015356312
-17	0.0182059029	-0.0004661881	0.0876435212
-18	0.0764507496	-0.0803175571	-0.0157045576
-19	0.0006180989	-0.0005788582	-0.0013027257
-20	-0.0110723697	0.0221680271	0.0020227381
-21	0.0008645269	-0.0000411877	-0.0006106795
-22	-0.0016226134	-0.0018541098	-0.0000940082
-23	0.0069228056	0.0053473720	0.0023792937
-24	-0.0137889414	0.0233440606	0.0014603727
-25	-0.0000869233	-0.0009176513	-0.0003959045
-26	-0.0077019314	-0.0022267163	0.0053063367
-27	0.0028551419	0.0001679913	-0.0015633723
-28	0.0056427029	-0.0155137139	-0.0127667447
-29	-0.0012537652	0.0014678505	-0.0016834157
-30	-0.0009710572	0.0014223515	-0.0016605853
-31	0.0030039152	-0.0043669645	0.0044665583
-32	-0.0029782509	0.0140087280	0.0085046005

CASSCF(6,6)/6-311G(d) = -968.0703069636
MP2(6,6)/6-311++G(3df,3pd)//CASSCF(6,6)/6-311G(d)= -970.468129

(14) **Int-Si**

Atomic Number	.	Coordinates (Angstroms) X	Y	Z
6		0.000000	0.000000	0.000000
14		0.000000	0.000000	1.736310
6		1.872722	0.000000	1.998197
6		2.410207	0.354840	0.613797
6		1.449979	-0.163282	-0.470888
1		3.426037	-0.004800	0.459114
1		2.431027	1.438477	0.531775
1		1.671010	-1.210435	-0.659611
1		1.618044	0.362957	-1.409676
6		2.628767	-0.249918	3.079691
1		3.707580	-0.227169	3.040350

1	2.196349	-0.478282	4.038724
6	-1.371038	0.137286	3.021821
1	-1.478832	-0.782377	3.586743
1	-2.320371	0.356961	2.544842
1	-1.159296	0.937485	3.724721
6	-1.112728	0.028288	-1.017110
1	-0.829289	0.645181	-1.873127
1	-1.991655	0.508460	-0.593190
14	-1.713296	-1.659234	-1.665667
6	-2.191211	-2.776970	-0.225834
1	-2.888904	-2.288501	0.445461
1	-1.332312	-3.078332	0.365155
1	-2.673054	-3.683359	-0.588015
6	-0.427175	-2.530419	-2.736167
1	-0.122360	-1.913124	-3.576203
1	-0.847358	-3.446634	-3.142568
1	0.467733	-2.804929	-2.185024
6	-3.250478	-1.350333	-2.721360
1	-3.015528	-0.776088	-3.612223
1	-4.007500	-0.800846	-2.173641
1	-3.703591	-2.284239	-3.051941

CASSCF(6,6, + 6,4)/6-311G(d) = -968.1881512
MP2(6,6, + 6,4)/6-311++G(3df,3pd)//CASSCF(6,6, + 6,4)/6-311G(d)= -970.5804374

(15) **CH3OH**

Atomic Number	.	Coordinates (Angstroms) X	Y	Z
8		0.000000	0.000000	2.000000
6		1.385642	0.000000	2.210512
1		-0.455560	0.000000	2.826900
1		1.647942	0.000000	3.287333
1		1.827084	0.881563	1.759173
1		1.827084	-0.881563	1.759173

CASSCF(6,4)/6-311G(d) = -115.0498058
MP2(6,4)/6-311++G(3df,3pd)//CASSCF(6,4)/6-311G(d)= -115.4382962

(16) **Cpx-Si**

Atomic Number	.	Coordinates (Angstroms) X	Y	Z
6		-2.346161	1.426175	0.365269
6		-1.263647	2.421272	-0.043610
6		-0.124695	1.728366	-0.821247

6	0.087428	0.299219	-0.290710
14	-1.446940	-0.252720	0.377141
1	-0.836115	2.832308	0.867006
1	-1.684635	3.250124	-0.604432
1	-0.355536	1.731204	-1.889632
1	0.780045	2.317389	-0.718389
6	-1.748037	-1.515276	1.751178
1	-2.799854	-1.644406	1.994793
1	-1.337548	-2.495570	1.523301
1	-1.253818	-1.150026	2.645780
6	-3.638184	1.719827	0.506322
1	-4.016255	2.716194	0.350861
1	-4.362475	0.986365	0.815675
6	1.274855	-0.484554	-0.831838
1	1.091938	-1.551338	-0.716757
1	1.384181	-0.331298	-1.910267
14	2.960932	-0.208891	-0.010573
6	3.553963	1.591470	-0.058949
1	2.954670	2.239101	0.573382
1	4.582387	1.658436	0.290589
1	3.530125	1.991329	-1.071399
6	2.896805	-0.802478	1.787345
1	2.698305	-1.871265	1.840282
1	3.835733	-0.614092	2.302508
1	2.107350	-0.296602	2.332939
6	4.233920	-1.246421	-0.967574
1	4.312980	-0.920476	-2.004926
1	5.224768	-1.169570	-0.526776
1	3.963640	-2.301321	-0.980382
8	-2.599462	-1.280440	-1.030670
1	-2.130931	-1.387209	-1.851163
6	-3.858945	-1.956455	-0.955464
1	-4.649064	-1.222539	-0.978273
1	-3.882903	-2.507580	-0.028377
1	-3.960981	-2.639958	-1.787273

CASSCF(12,10)/6-311G(d) = -1083.2615991

MP2(12,10)/6-311++G(3df,3pd)//CASSCF(12,10)/6-311G(d)= -1086.04556391

(17) **Cis-TS-Si**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.568724
6	1.509202	0.000000	2.102467
6	2.228545	-1.106759	1.288111
14	1.718978	-0.572130	-0.482184
1	-0.481022	-0.896676	1.909791

1	-0.530553	0.847823	1.958066
1	1.980774	0.939617	1.887250
1	1.529728	-0.159886	3.156263
6	1.943298	-1.856123	-1.908176
1	1.545179	-1.463025	-2.824442
1	2.987238	-2.069425	-2.036972
1	1.423220	-2.757888	-1.648614
6	-1.033600	0.315029	-0.813773
1	-1.979396	0.605715	-0.401921
1	-0.916057	0.275098	-1.877748
6	3.688461	-1.553944	1.500693
1	3.943969	-2.275303	0.746234
1	4.357007	-0.717230	1.405026
14	4.048662	-2.416990	3.208164
6	3.754358	-1.257448	4.731470
1	2.732612	-0.948949	4.771173
1	4.002967	-1.785663	5.632673
1	4.381947	-0.390813	4.645981
6	2.896433	-3.963371	3.359599
1	3.098303	-4.641578	2.552357
1	3.078308	-4.460082	4.293838
1	1.869442	-3.654562	3.315712
6	5.892275	-3.004018	3.212870
1	6.538788	-2.156360	3.086949
1	6.116921	-3.486859	4.145046
1	6.053469	-3.695890	2.408035
8	2.868986	0.750439	-0.089627
1	3.529112	0.795999	1.432791
6	3.136773	1.560168	-1.245448
1	2.425641	2.363277	-1.286712
1	3.064776	0.975715	-2.143061
1	4.129756	1.961601	-1.180146

-1	0.00	-0.03	0.01
-2	-0.02	-0.04	0.00
-3	-0.04	0.01	0.04
-4	0.05	0.09	0.00
-5	0.06	0.03	0.05
-6	-0.03	-0.04	-0.02
-7	-0.10	-0.05	-0.12
-8	-0.13	0.02	-0.05
-9	-0.11	0.06	0.03
-10	-0.02	-0.03	0.02
-11	-0.08	0.12	0.11
-12	-0.08	-0.18	-0.15
-13	-0.15	-0.01	-0.14
-14	0.02	0.01	0.00
-15	-0.10	-0.21	-0.09
-16	-0.03	-0.17	-0.02
-17	0.02	-0.07	0.03
-18	-0.19	-0.20	0.08
-19	0.11	-0.22	-0.17

-20	0.02	0.03	0.02
-21	-0.03	0.00	0.00
-22	-0.08	-0.05	-0.04
-23	-0.10	-0.01	0.01
-24	-0.10	0.04	-0.03
-25	0.00	-0.01	-0.01
-26	-0.04	0.09	-0.12
-27	0.01	-0.18	-0.13
-28	-0.04	-0.10	0.03
-29	-0.01	-0.03	-0.03
-30	0.03	-0.09	-0.10
-31	-0.06	-0.09	-0.05
-32	-0.13	-0.08	-0.04
-33	0.01	0.09	0.00
-34	-0.15	-0.20	0.03
-35	-0.02	0.00	-0.07
-36	0.07	0.07	-0.05
-37	-0.26	-0.05	-0.04
-38	0.07	-0.19	-0.28

CASSCF(12,10)/6-311G(d) = -1083.22079531
MP2(12,10)/6-311++G(3df,3pd)//CASSCF(12,10)/6-311G(d)= -1086.002001

(17) **Cis-Pro-Si**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.522174
6	1.439362	0.000000	2.045770
6	2.336073	-0.974698	1.243419
14	1.562972	-0.926576	-0.501741
1	-0.487312	-0.914157	1.856669
1	-0.584294	0.819872	1.930671
1	1.844715	0.999331	1.904770
1	1.482182	-0.190650	3.111197
6	1.154001	-2.549280	-1.346757
1	0.752561	-2.407346	-2.345625
1	2.047744	-3.162631	-1.447640
1	0.424878	-3.119225	-0.787933
6	-0.995812	0.489885	-0.743459
1	-1.849831	0.992393	-0.315077
1	-0.997675	0.401184	-1.816366
6	2.646389	-2.315324	1.917724
1	3.214865	-2.939122	1.228070
1	3.345803	-2.120854	2.737053
14	1.376427	-3.428454	2.771622
6	0.723938	-2.614294	4.339005
1	0.119634	-1.730433	4.175476

1	0.109012	-3.309842	4.905100
1	1.545578	-2.325818	4.991723
6	-0.067299	-3.966057	1.685903
1	0.270609	-4.487501	0.795771
1	-0.715786	-4.646857	2.235794
1	-0.687875	-3.138128	1.355967
6	2.334952	-4.955444	3.329665
1	3.112279	-4.684834	4.038782
1	1.687643	-5.674236	3.827386
1	2.815709	-5.470318	2.502132
8	2.662055	-0.059231	-1.420609
1	3.287127	-0.470328	1.105146
6	2.513827	0.146811	-2.834574
1	1.673541	0.797125	-3.051019
1	2.387748	-0.794047	-3.358451
1	3.420876	0.621965	-3.185097

CASSCF(12,10)/6-311G(d) = -1083.3527370011
MP2(12,10)/6-311++G(3df,3pd)//CASSCF(12,10)/6-311G(d)= -1086.09997

(18) **Trans-TS-Si**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
1	0.000000	0.000000	1.095031
6	1.450304	0.000000	-0.549312
14	1.129338	-0.596969	-2.520689
6	-0.562085	-1.341310	-2.027192
6	-0.721626	-1.258658	-0.518293
1	-0.559036	0.880188	-0.334646
1	-0.288332	-2.154644	-0.056003
1	-1.780017	-1.218903	-0.236230
6	-1.480063	-1.825033	-2.874861
1	-2.421443	-2.227704	-2.500142
1	-1.339263	-1.883873	-3.951121
6	2.368251	-1.894952	-2.971523
1	3.375980	-1.473123	-3.035689
1	2.132561	-2.346858	-3.939902
1	2.391538	-2.696479	-2.226633
8	0.915241	0.671837	-3.603406
6	1.996930	1.219587	-4.180105
1	1.657490	2.016124	-4.851874
1	2.538446	0.489462	-4.791732
1	2.671424	1.672394	-3.447559
1	0.296684	1.336481	-3.215291
6	2.348695	1.237751	-0.380807
1	3.072718	1.281236	-1.202071
1	2.963460	1.071692	0.512861
14	1.666478	2.994377	-0.122805

6	0.760128	3.109981	1.510772
1	1.385822	2.737446	2.327298
1	-0.165412	2.528621	1.496958
1	0.498600	4.149483	1.730972
6	3.131367	4.177181	-0.092763
1	3.680744	4.131284	-1.037671
1	3.817818	3.917441	0.718407
1	2.791373	5.205790	0.058999
6	0.528489	3.496936	-1.523185
1	1.061036	3.497528	-2.477602
1	0.149517	4.509889	-1.354818
1	-0.333225	2.829930	-1.601739
1	2.096062	-1.065987	-0.114482
8	2.307053	-1.201649	1.313658
6	3.037572	-2.394061	1.562400
1	3.195860	-2.497678	2.637956
1	4.000992	-2.338204	1.050740
1	2.468225	-3.248094	1.188701

-1	0.00	-0.03	0.01
-2	-0.02	-0.04	0.00
-3	-0.04	0.01	0.04
-4	0.05	0.09	0.00
-5	0.06	0.03	0.05
-6	-0.03	-0.04	-0.02
-7	-0.10	-0.05	-0.12
-8	-0.13	0.02	-0.05
-9	-0.11	0.06	0.03
-10	-0.02	-0.03	0.02
-11	-0.08	0.12	0.11
-12	-0.08	-0.18	-0.15
-13	-0.15	-0.01	-0.14
-14	0.02	0.01	0.00
-15	-0.10	-0.21	-0.09
-16	-0.03	-0.17	-0.02
-17	0.02	-0.07	0.03
-18	-0.19	-0.20	0.08
-19	0.11	-0.22	-0.17
-20	0.02	0.03	0.02
-21	-0.03	0.00	0.00
-22	-0.08	-0.05	-0.04
-23	-0.10	-0.01	0.01
-24	-0.10	0.04	-0.03
-25	0.00	-0.01	-0.01
-26	-0.04	0.09	-0.12
-27	0.01	-0.18	-0.13
-28	-0.04	-0.10	0.03
-29	-0.01	-0.03	-0.03
-30	0.03	-0.09	-0.10
-31	-0.06	-0.09	-0.05
-32	-0.13	-0.08	-0.04

-33	0.01	0.09	0.00
-34	-0.15	-0.20	0.03
-35	-0.02	0.00	-0.07
-36	0.07	0.07	-0.05
-37	-0.26	-0.05	-0.04
-38	-0.26	-0.05	-0.04
-39	0.07	-0.19	-0.28
-40	0.03	-0.09	-0.10
-41	-0.06	-0.09	-0.05
-42	-0.13	-0.08	-0.04
-43	0.01	0.09	0.00
-44	-0.01	-0.03	-0.03

CASSCF(12,10)/6-311G(d) = - 1198.2819531

MP2(12,10)/6-311++G(3df,3pd)//CASSCF(12,10)/6-311G(d)= -1201.44739390

(19) **Trans-Pro-Si**

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.522174
6	1.439362	0.000000	2.045770
6	2.336073	-0.974698	1.243419
14	1.562972	-0.926576	-0.501741
1	-0.487312	-0.914157	1.856669
1	-0.584294	0.819872	1.930671
1	1.844715	0.999331	1.904770
1	1.482182	-0.190650	3.111197
6	1.154001	-2.549280	-1.346757
1	0.752561	-2.407346	-2.345625
1	2.047744	-3.162631	-1.447640
1	0.424878	-3.119225	-0.787933
6	-0.995812	0.489885	-0.743459
1	-1.849831	0.992393	-0.315077
1	-0.997675	0.401184	-1.816366
6	2.646389	-2.315324	1.917724
1	3.214865	-2.939122	1.228070
1	3.345803	-2.120854	2.737053
14	1.376427	-3.428454	2.771622
6	0.723938	-2.614294	4.339005
1	0.119634	-1.730433	4.175476
1	0.109012	-3.309842	4.905100
1	1.545578	-2.325818	4.991723
6	-0.067299	-3.966057	1.685903
1	0.270609	-4.487501	0.795771
1	-0.715786	-4.646857	2.235794
1	-0.687875	-3.138128	1.355967
6	2.334952	-4.955444	3.329665

1	3.112279	-4.684834	4.038782
1	1.687643	-5.674236	3.827386
1	2.815709	-5.470318	2.502132
8	2.662055	-0.059231	-1.420609
1	3.287127	-0.470328	1.105146
6	2.513827	0.146811	-2.834574
1	1.673541	0.797125	-3.051019
1	2.387748	-0.794047	-3.358451
1	3.420876	0.621965	-3.185097

CASSCF(12,10)/6-311G(d) = -1083.34886314

MP2(12,10)/6-311++G(3df,3pd)//CASSCF(12,10)/6-311G(d)= -1086.0948997