Supported Neodymium Catalysts for MMA Polymerization: On the Origin of Surface-Induced Stereoselectivity

Iker Del Rosal, Mathieu Tschan, Régis M. Gauvin,* Laurent Maron* and Christophe M. Thomas*

Electronic Supplementary Information

Table of contents

General considerations

Manipulations were carried out under an argon atmosphere in a glove-box or by using Schlenk techniques. Solvents were dried using conventional reagents and stored in the glove-box over 3Å molecular sieves. MMA was dried over CaH_2, vacuum distilled, degassed with argon and stored in the glove box freezer at –40 °C. Supported catalyst was prepared according to reported procedure[1]. Liquid-state NMR analyses were run on a on a Bruker AC-500 spectrometer. Size exclusion chromatography (SEC) of PHBs was performed in THF at 20°C using a Waters SIS HPLC pump, a Waters 410 refractometer, a DAD-UV detector and Waters styragel columns (HR2, HR3, HR4, HR5E) or PL-GEL Mixte B and 100A columns. The number average molecular masses (M_n) and polydispersity index (M_w/M_n) of the resultant polymers were calculated with reference to a polystyrene calibration.

Polymer Synthesis

In a typical experiment (Table 1, entry 2), in the glovebox, silica-supported neodymium borohydride (0.05 g containing 0.017 mmol of Nd) was suspended in toluene (5 mL) at –40 °C. To this solution was added rapidly the desired amount of MMA (8.5 mmol, 0.851 g) . The reaction solution was quickly removed from the glovebox and the mixture was immediately stirred at 30 °C. Conversion was monitored by comparing the relative magnitude of peaks corresponding to the methyl hydrogen for MMA and PMMA. After the desired reaction time, the mixture was quenched with acidic methanol (0.5 mL of a 1.2 M HCl solution in MeOH), and the polymer was precipitated with excess methanol (ca. 20 mL). The polymer was then dried under vacuum to constant weight.

Methodological Details

All DFT calculations were performed with Gaussian 03.[2] Calculations were carried out at the DFT level of theory using the hybrid functional B3PW91.[3] Geometry optimizations were achieved without any symmetry restriction. Calculations of vibrational frequencies were systematically done in order to characterize the nature of stationary points. Stuttgart effective core potentials and their associated basis set were used for silicon and lanthanum.[4] The basis sets were augmented by a set of polarization functions (ζ_d=0.284 for Si and ζ_f=1.000 for La). Hydrogen and oxygen atoms were treated with 6-31G(d,p) double-ζ basis sets.[5] The electron density and partial charge distribution were examined in terms of localized electron-pair bonding units by using the NBO program.[6] Through this method, the input atomic orbital basis set is transformed via natural atomic orbitals (NAOs) and natural hybrid orbitals (NHOs) into natural bond orbitals (NBOs), which correspond to the localized one center ("lone pair") and two-center ("bond") elements of the Lewis structure.

1 N. Ajellal, G. Durieux, L. Delevoye, G. Tricot, C. Dujardin, C. M. Thomas and R. M. Gauvin, *Chem. Commun.* 2010, **46**, 1032.

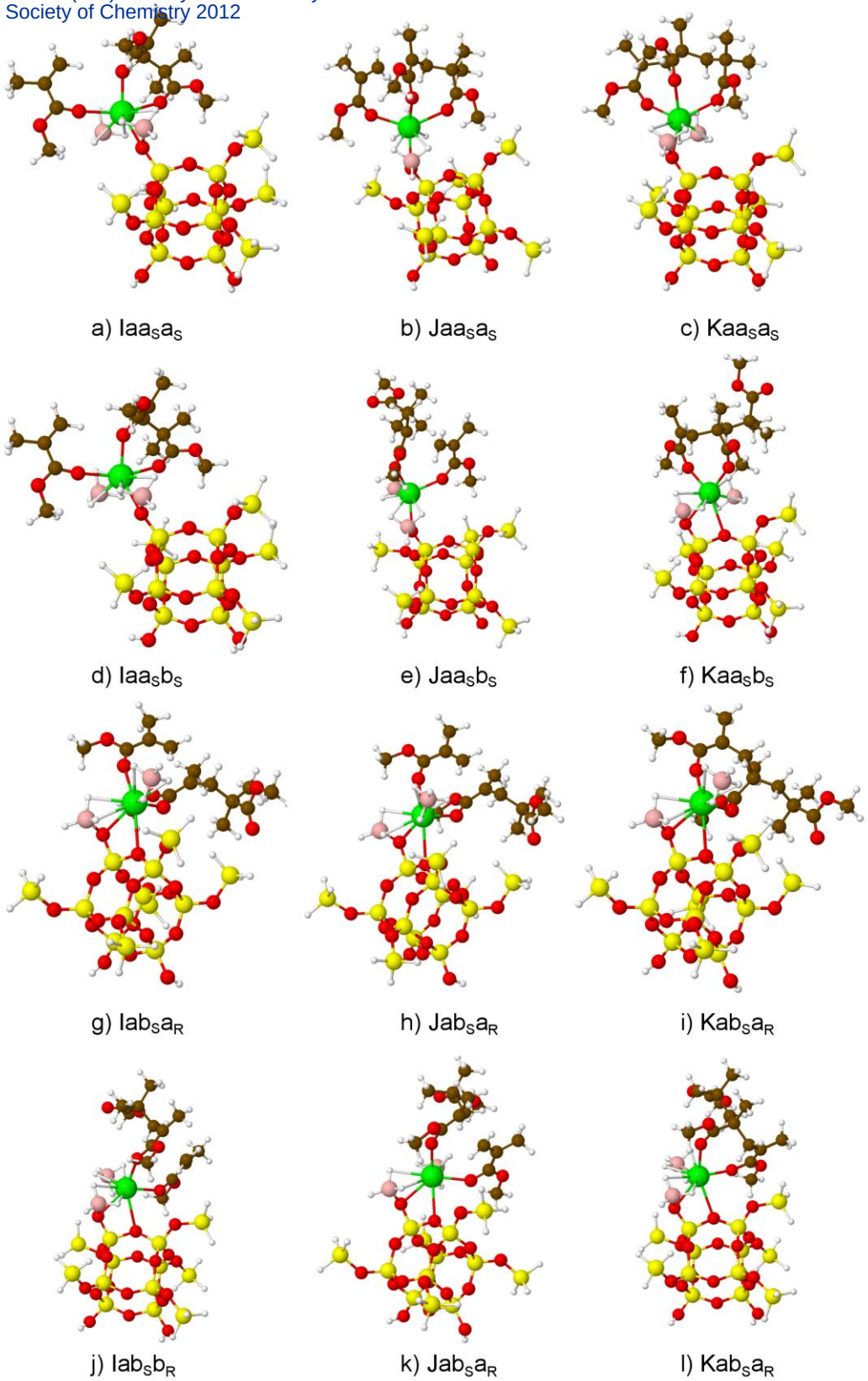
2 M. J. Frisch *et al*. Gaussian 03 (Revision B.05), 2003.

3 J. P. Perdew, in *Electronic structure of solids* ; P. Ziesche, H. Eschrig, Eds.; Akademie: Berlin, 1991; Chapter Unified Theory of Exchange and Correlation Beyond the Local Density Approximation; J. P. Perdew, K. Burke, Y. Wang, *Phys. Rev. B,* 1996, **54**, 16533; K. Burke, J. P. Perdew, Y. Wang, in *Electronic density functional theory: recent progress and new directions*; J. F. Dobson, G. Vignale, M. P. Mas, Eds.; Plenum: New-York, 1998; Chapter Derivation of a Generalized Gradient Approximation: the PW91 Density Functional; J. P. Perdew, J. A Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, C. Fiolhais, *Phys. Rev. B,* 1992, **46**, 6671; J. P. Perdew, K. Burke, Y. Wang, *Phys. Rev. B,* 1998, **57**, 14999; J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, C. Fiolhais, *Phys. Rev. B,* 1993, **48**, 4978.

4 W. Küechle, M. Dolg, H. Stoll, H. Preuss, *Mol. Phys.*, 1991, **74**, 1245.

5 P. C. Harihara, J. A. Pople, *Theo. Chim. Acta,* 1973, **28**, 213; W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257.

6 A. E. Reed, F. Weinhold, *J. Chem. Phys.,* 1983, **78**, 4066; A. E. Reed, L. A. Curtiss, F. Weinhold, *Chem. Rev.*, 1988, **88**, 899.



FigS1. Optimized structures of grafted complexes **I** to **K** involved in the second propagation step of MMA polymerization mediated by $La(BH_4)_2$@**c**-1.

Cartesian coordinates of the optimized structures.

c model of $SiO_{2\text{-}700}$

G = -1652.405143 u.a.

O	-0.423835	0.563122	4.079551
Si	-0.491608	0.775965	2.459560
O	0.606501	1.930531	2.010321
Si	1.593069	2.311002	0.744225
O	2.913724	3.030044	1.407873
O	-0.145029	-0.655275	1.709236
Si	-0.538937	-1.516624	0.354808
O	-0.446536	-3.118042	0.678115
O	-2.021579	1.260411	2.063465
Si	-2.797148	2.197604	0.944651
O	-1.786387	3.398524	0.419509
Si	-0.708401	3.724398	-0.791018
O	-1.099257	2.860804	-2.150272
Si	-0.757104	1.418724	-2.884600
O	0.773440	0.934616	-2.496323
Si	1.556029	0.019937	-1.356243
O	2.046239	0.954546	-0.089928
O	0.532025	-1.182137	-0.856813
O	-2.080850	-1.137386	-0.121557
Si	-2.850075	-0.095565	-1.155315
O	-1.858509	0.272195	-2.422325
O	2.933382	-0.619586	-1.986997
O	-4.133375	2.858973	1.619384
O	-3.299116	1.264726	-0.324865
O	0.820569	3.342864	-0.297177
O	-4.180891	-0.804398	-1.812819
O	-0.782291	5.323454	-1.130497
O	-0.839853	1.621395	-4.506592
H	3.634515	3.200510	0.794387
Si	-4.459494	4.279592	2.473018
H	-4.942296	-0.852263	-1.227225
Si	-0.932235	6.232899	-2.545475
Si	-1.885950	1.075969	-5.716048
H	2.798144	-1.283355	-2.669583
Si	0.660980	1.016235	5.293577
Si	-1.527313	-4.298775	1.212883
H	-0.701822	-5.438199	1.701661
H	-2.377532	-3.767788	2.318660
H	-2.391632	-4.741076	0.080311
H	0.225393	0.299057	6.524769
H	2.049255	0.613148	4.927299
H	0.597306	2.490282	5.510738
H	-1.466839	1.768594	-6.966855
H	-1.753677	-0.400652	-5.881180
H	-3.296054	1.427423	-5.381373
H	-0.797728	7.659499	-2.138296
H	0.145025	5.870771	-3.511942
H	-2.268805	6.000877	-3.166012
H	-5.715313	4.034326	3.236170
H	-3.341252	4.595739	3.408593
H	-4.654912	5.405955	1.515244

$(BH_4)_2(THF)_2La$@c-1

G = -2116.993107 u.a.

O	3.580071	7.305140	11.649270
H	0.283240	5.779995	9.271393
H	3.203250	3.909772	2.462951
Si	5.437774	9.721739	8.666031
H	2.512126	8.603438	0.867177
B	3.033255	9.716843	0.677201
O	3.613737	9.257500	4.826768
Si	4.434494	8.493606	5.974255
O	5.683251	7.592771	5.316550
Si	6.203840	4.616032	7.221577
Si	7.218851	7.103964	5.667383
O	7.207206	5.589739	6.336209
Si	3.456266	5.992216	7.591509
O	3.451638	7.443858	6.825409
C	2.800930	4.656603	3.152091
O	4.458367	8.755584	9.592726
H	0.838111	4.543735	2.217989
C	0.984373	6.045473	3.767310
O	2.008236	6.892358	3.174136
C	1.271359	4.658720	3.217656
Si	4.438368	7.242085	10.255589
O	5.978944	6.735196	10.588328
Si	7.204395	5.872440	9.878244
O	6.558625	4.776363	8.828907
O	6.402489	3.057672	6.762660
Si	7.720553	2.076628	6.374094
La	2.080242	9.451612	3.167408
O	1.996889	5.269988	7.362102
Si	0.831602	4.675483	8.433445
C	3.114529	6.077315	2.695727
O	5.099192	9.565907	7.065991
O	7.024992	9.344580	8.952939
Si	8.209276	8.367635	8.331672
O	9.693021	9.029439	8.596009
O	5.188330	11.285157	9.102644
Si	4.432983	12.014990	10.423019
O	3.699657	6.183055	9.220518
O	8.240357	6.916015	9.118462
O	8.039256	5.026599	11.015481
O	4.621201	5.005038	6.950584
O	8.103171	7.031683	4.287406
Si	7.951416	7.741663	2.763315
O	7.946785	8.163549	6.710960
Si	3.837543	6.732917	13.217197
O	2.445244	11.943959	3.661139
C	2.031336	13.027754	2.784800
C	2.337720	14.313048	3.548765
C	3.476751	13.886664	4.479601
C	3.051533	12.480861	4.865623
B	-0.569112	9.532985	3.603128
H	8.915388	2.453020	7.184190
H	8.803651	5.491889	11.368069
H	9.867184	9.838997	8.107105
H	9.235613	7.487252	2.052589
H	6.823524	7.110421	2.018157

H	7.715441	9.209311	2.890998
H	8.028291	2.215126	4.920973
H	7.314103	0.675384	6.676099
H	4.945917	11.448200	11.704216
H	4.764296	13.466216	10.339899
H	2.955210	11.827704	10.340869
H	4.130607	5.270549	13.197532
H	4.969846	7.468232	13.852048
H	2.576320	6.993999	13.966099
H	-0.246505	4.096978	7.581826
H	1.416757	3.614510	9.303445
H	3.441079	9.824781	-0.446203
H	2.155915	10.561913	0.927471
H	3.940862	9.855002	1.510691
H	4.042042	6.472447	3.119325
H	3.145112	6.170924	1.604899
H	3.224415	4.470383	4.144058
H	0.869861	3.871853	3.860928
H	0.014580	6.458831	3.484061
H	1.095348	6.077912	4.856326
H	3.859872	11.807393	5.152408
H	2.295462	12.493895	5.660766
H	4.430729	13.863054	3.941708
H	3.588901	14.538818	5.349529
H	2.609840	15.131244	2.877278
H	1.467666	14.629878	4.133667
H	0.969614	12.897612	2.555992
H	2.610205	12.942010	1.860070
H	-0.290932	8.767974	2.665747
H	-1.751569	9.586229	3.800830
H	0.041475	9.138713	4.611195
H	-0.105585	10.647006	3.302318

$(BH_4)_2(THF)_2La$@c-2

G = -2116.918240 u.a.

O	0.875083	-0.509056	3.950937
Si	1.111687	0.852686	4.821636
O	0.462368	2.186194	4.099421
Si	-0.782874	3.288996	4.251426
O	-1.688032	2.833180	5.556668
Si	-2.125951	2.792525	7.151363
O	-3.613790	2.110331	7.330657
Si	0.461010	-0.860839	2.348409
O	0.573045	0.576344	6.348069
Si	0.491233	1.281657	7.849807
O	-1.027011	1.905092	8.038645
O	2.767879	1.174419	4.874358
Si	3.314559	2.720666	4.915877
O	2.444561	3.685944	5.861815
Si	1.856933	3.943285	7.439112
O	0.275839	4.388532	7.280794
Si	-1.003210	5.393627	7.591071
O	-2.281846	4.337053	7.740058
O	0.699612	0.079643	8.951038
Si	1.353801	0.001417	10.500445
O	1.721378	2.384067	8.070392
O	4.906596	2.498543	5.732555
O	3.797066	3.298248	3.484781
Si	3.499855	4.663355	2.490550
La	3.271284	7.058744	7.000586
B	3.216327	9.756099	6.865375
O	-1.671001	3.098455	2.871737
O	-0.168901	4.807169	4.306653
Si	0.018861	6.309653	5.062938
O	-0.450240	7.422228	3.926217
Si	-1.271897	7.294492	2.475781
O	1.499123	6.567122	5.639531
O	2.827621	4.977803	8.162085
O	-1.151809	6.375799	6.281403
O	-0.831164	6.254128	8.979472
Si	-1.794813	6.431664	10.357422
H	0.825825	-2.289145	2.132445
H	-2.166421	3.884076	2.618480
H	-1.840445	8.633447	2.153421
H	0.913522	1.163230	11.327493
H	4.837991	5.097779	2.003720
H	-3.616342	1.149126	7.308363
H	-1.895863	5.133910	11.086309
H	-2.394710	6.302900	2.567541
H	-0.354244	6.859819	1.379300
H	-1.002789	-0.665193	2.153165
H	2.665878	4.188853	1.351866
H	2.818796	5.718204	3.275774
H	1.228378	0.011494	1.412831
H	-1.104611	7.437818	11.214337
H	-3.153618	6.919181	9.986524
H	0.872344	-1.271515	11.106332
H	2.846123	-0.013957	10.422609
H	3.191789	10.957962	6.886631
H	3.042462	9.291703	5.735028
H	2.329032	9.280641	7.602387
C	6.236699	2.741077	5.107430
C	7.165803	2.853957	6.302086
C	6.483869	2.014961	7.388572
C	5.019731	2.351484	7.205898
H	4.316494	1.569946	7.493266
H	4.733067	3.311619	7.642962
H	6.655630	0.945240	7.230783
H	6.823775	2.275373	8.393662
H	7.236284	3.901671	6.607631
H	8.167130	2.492259	6.056269
H	6.153369	3.656099	4.524569
H	6.427487	1.874267	4.472079
H	4.306849	9.322729	7.277904
B	5.595008	6.223571	5.830845
H	4.677815	5.448027	5.532525
H	6.630158	5.916796	5.289953
H	5.262698	7.360294	5.482460
H	5.713610	6.205018	7.063984
O	3.652200	7.553874	9.556568
C	3.209783	6.716627	10.651748
C	4.059507	7.151832	11.832510
C	4.150093	8.662237	11.603837
C	4.258700	8.767751	10.083799
H	3.329433	5.680780	10.335661
H	2.144828	6.909800	10.835532

H	5.052135	6.690018	11.780034
H	3.607741	6.885680	12.792024
H	5.000238	9.129286	12.107852
H	3.237569	9.153520	11.958562
H	3.735442	9.626699	9.659516
H	5.299509	8.789363	9.744665

$(BH_4)_2(THF)_2La$@c-3

G = -2116.934971 u.a.

C	0.179073	-0.111736	4.473097
O	1.048925	0.898012	5.060652
C	0.646920	2.221794	4.605952
C	-0.132172	1.960660	3.329909
C	-0.865913	0.662182	3.675487
La	2.454834	0.602538	7.172077
O	4.717917	0.074257	5.868145
O	3.739290	2.254347	8.881948
Si	3.416131	3.562575	7.826774
O	3.290709	2.810059	6.426491
Si	4.804426	1.374713	9.809883
O	4.110561	-0.111852	9.483233
Si	4.279760	-1.644220	10.245537
O	4.779930	1.991914	11.333892
Si	3.924695	3.357296	11.818753
O	4.432396	4.646495	10.930058
Si	4.391708	5.652706	9.616663
O	4.531434	4.749286	8.207911
O	4.310554	3.661913	13.378700
Si	3.973606	2.965953	14.880851
O	2.340456	2.971807	11.607944
Si	0.882066	3.753213	11.533000
O	-0.121992	3.027448	10.459158
Si	-0.419511	2.451949	8.906038
O	-0.587635	3.830933	7.934922
Si	0.623242	4.931914	7.788091
O	0.736727	5.417807	6.221173
Si	0.820083	6.945696	5.502134
O	1.150244	5.358188	11.213880
Si	1.425076	6.527811	10.079529
O	0.451889	6.276552	8.755709
O	0.243891	3.621181	13.052278
O	0.998910	8.005542	10.671824
O	3.041724	6.603746	9.675022
O	5.691092	6.653314	9.677350
Si	7.103085	6.800071	8.767300
B	6.858082	1.128075	9.348782
O	1.995987	4.216930	8.395188
B	2.053797	-2.099160	6.948422
O	0.687319	1.430835	8.329637
O	-1.935471	1.785295	8.965307
Si	-3.061033	1.634728	10.199855
H	5.277625	2.759245	15.574642
H	-0.662175	3.933247	13.132948
H	-4.275502	1.008632	9.600205
H	6.783143	7.254107	7.382251
H	5.048045	-2.542740	9.344377
H	1.727206	8.484283	11.078104
H	1.972370	7.721356	6.044818
H	-3.426263	2.968323	10.769623
H	-2.543849	0.762604	11.297220
H	3.127270	3.910838	15.661457
H	5.033225	-1.423977	11.514947
H	2.914843	-2.156479	10.518832
H	3.274735	1.659113	14.713027
H	1.017007	6.700795	4.044248
H	-0.451315	7.692649	5.723242
H	7.940620	7.822179	9.455814
H	7.831590	5.498444	8.713013
H	1.924570	-3.289840	6.837249
H	2.993550	-1.823536	7.715468
H	1.038986	-1.558240	7.396796
H	2.327858	-1.574694	5.858606
H	1.554861	2.814708	4.492810
H	0.016998	2.678154	5.376429
H	0.548794	1.810587	2.484412
H	-0.807780	2.784193	3.085209
H	-1.202694	0.105173	2.797296
H	-1.741091	0.876682	4.297829
H	-0.241736	-0.718770	5.277635
H	0.801021	-0.750906	3.838661
H	7.066737	0.351018	8.464965
H	7.714880	1.822133	9.806869
H	6.063748	1.996494	8.866709
H	6.339354	0.541901	10.311732
C	5.451986	-1.178623	5.911506
C	6.552727	-1.057541	4.858268
C	6.735950	0.457837	4.732887
C	5.306765	0.949801	4.876381
H	4.750832	-1.996038	5.727060
H	5.862178	-1.284229	6.920812
H	6.219933	-1.479624	3.903734
H	7.464366	-1.581256	5.157195
H	7.188320	0.760668	3.784776
H	7.356129	0.843405	5.549325
H	4.753468	0.838844	3.933642
H	5.186478	1.971228	5.238495

Initiation step of MMA polymerization mediated by $(BH_4)_2La$@c-1

A

G = -1997,979477 u.a.

C	-0.462622	-4.157105	15.674993
C	0.544059	-4.944643	15.269633
C	0.791262	-6.329669	15.798789
C	1.454017	-4.427452	14.223164
O	2.327642	-5.325128	13.816338
C	3.275305	-4.934326	12.802981
O	1.430123	-3.279051	13.753005
La	0.920364	-1.016632	12.862754
O	4.900750	-1.787047	13.234578
Si	5.840579	-1.069725	14.457341
O	0.790026	-1.223929	10.585980
Si	2.228205	-1.287087	9.880244
O	2.548711	-0.045955	8.835252
Si	3.647988	1.067779	8.308524

O	4.430727	0.491966	6.970967
Si	4.784104	-0.957552	6.273168
O	4.738076	-0.704445	4.649235
O	2.897091	2.469825	7.936568
Si	1.280775	2.960681	7.833369
O	4.758776	1.374534	9.498477
Si	6.201589	0.768541	10.028337
O	7.078889	1.956481	10.725760
Si	6.788867	3.579534	11.113319
B	2.048140	1.109723	13.995879
O	3.281835	-1.199639	11.226699
Si	4.853804	-1.587241	11.604798
O	5.225632	-3.033409	10.894536
Si	5.991452	-3.630628	9.551239
O	6.674246	-5.059014	9.968918
Si	8.179698	-5.775359	9.682238
O	2.557146	-2.718883	9.102039
Si	3.430983	-3.301309	7.823141
O	4.886593	-3.884617	8.352223
O	5.923267	-0.420143	11.153451
O	7.064904	0.129662	8.773827
Si	7.344544	-1.311481	8.007360
O	6.294020	-1.463302	6.738470
O	8.903097	-1.388426	7.489799
O	7.167240	-2.581860	9.050521
O	3.680540	-2.119477	6.695558
O	2.615871	-4.539014	7.125556
Si	1.009566	-5.062501	7.174740
B	-1.632524	-1.130380	13.594425
H	0.540451	2.089045	6.876036
H	0.643568	2.901666	9.179488
H	1.309463	4.363928	7.335302
H	-2.782972	-1.145453	13.931122
H	-1.318950	-2.142745	12.949943
H	-1.375826	-0.145742	12.878346
H	-0.874775	-1.056320	14.578368
H	0.877058	-6.094455	6.108639
H	5.751595	0.412468	14.387095
H	7.256124	-1.517436	14.307078
H	5.280484	-1.578460	15.740060
H	9.234518	-5.070614	10.465553
H	9.211062	-0.613120	7.011108
H	4.795775	-1.500636	4.112933
H	0.714076	-5.666399	8.507101
H	0.081368	-3.925280	6.914055
H	8.055521	-7.186580	10.144366
H	8.506380	-5.735977	8.228037
H	8.010253	4.051822	11.823333
H	6.582978	4.368549	9.864812
H	5.595760	3.692657	11.998540
H	0.056702	-6.576720	16.567963
H	0.723487	-7.076749	15.001794
H	1.792045	-6.418145	16.233352
H	-1.160373	-4.500859	16.432720
H	-0.630762	-3.169251	15.259096
H	3.869772	-5.824676	12.607774
H	2.752925	-4.619563	11.898063
H	3.905364	-4.124121	13.171348
H	2.111650	1.171137	12.757170
H	2.551337	2.069558	14.509104
H	0.854535	0.994554	14.312393
H	2.616770	0.052483	14.334414

B

G = -1997,949157 u.a.

C	0.273728	-3.671637	15.773700
C	0.549143	-4.751949	14.912072
C	-0.239130	-6.033689	14.943655
C	1.489774	-4.518960	13.897664
O	1.797858	-5.569570	13.124842
C	2.735283	-5.366999	12.068093
O	2.029991	-3.382163	13.654390
La	1.658599	-1.120028	13.026204
O	4.537676	-1.357149	13.274043
Si	5.486006	-1.026220	14.666694
O	0.888797	-1.243611	10.845162
Si	2.153934	-1.315270	9.864545
O	2.339224	-0.090169	8.767355
Si	3.499298	0.974633	8.253286
O	4.336828	0.342313	6.977396
Si	4.779422	-1.104820	6.329510
O	4.725223	-0.909822	4.698344
O	2.795911	2.373977	7.791833
Si	1.201052	2.939251	7.726361
O	4.559588	1.286631	9.488424
Si	6.082784	0.901959	9.997177
O	6.871997	2.227615	10.526814
Si	6.419317	3.777773	11.042803
B	2.188605	1.375317	13.822491
O	3.425709	-1.194505	11.004695
Si	4.925538	-1.398149	11.656828
O	5.553968	-2.865099	11.252392
Si	6.126776	-3.504768	9.823368
O	6.835816	-4.930667	10.185428
Si	8.352251	-5.620329	9.884775
O	2.361194	-2.762708	9.074586
Si	3.464810	-3.392244	8.010355
O	4.876768	-3.755920	8.784369
O	5.961047	-0.187049	11.257437
O	6.961468	0.222706	8.777233
Si	7.341750	-1.230768	8.080567
O	6.314381	-1.506839	6.814178
O	8.907085	-1.230099	7.580438
O	7.234680	-2.466451	9.172950
O	3.750332	-2.319443	6.787452
O	2.863562	-4.781091	7.387521
Si	1.301946	-5.373347	7.119049
B	-0.798593	-1.535606	14.635725
H	0.398643	2.091328	6.798331
H	0.597394	2.924630	9.088771
H	1.283102	4.333172	7.208578
H	-1.871470	-1.191964	15.042896
H	-0.562043	-2.737657	15.178039
H	-0.769513	-1.806757	13.439556
H	0.130567	-0.847332	15.040034
H	1.443670	-6.494822	6.148986

H	5.847115	0.414582	14.691377
H	6.704380	-1.882627	14.616647
H	4.625964	-1.394671	15.822228
H	9.406125	-4.871014	10.626587
H	9.182439	-0.440309	7.105542
H	4.893136	-1.706748	4.186885
H	0.728448	-5.873344	8.401447
H	0.430356	-4.304696	6.551187
H	8.268943	-7.022170	10.380539
H	8.642623	-5.604393	8.422456
H	7.654921	4.396990	11.597950
H	5.926174	4.566539	9.877943
H	5.364869	3.682286	12.090444
H	-0.853731	-6.084451	15.846757
H	-0.907439	-6.137754	14.079201
H	0.421641	-6.906744	14.940356
H	-0.374133	-3.862368	16.628181
H	1.078696	-2.976407	15.996382
H	2.883238	-6.349878	11.620466
H	2.339697	-4.676919	11.317963
H	3.684295	-4.983089	12.449632
H	2.778162	1.104478	12.764838
H	2.427690	2.488654	14.198402
H	0.975584	1.201016	13.616961
H	2.536378	0.533198	14.673556

C

G = -1997,951082 u.a.

B	2.114190	1.273151	13.915936
Si	5.488387	-1.192816	14.606205
La	1.657174	-1.168330	12.912142
O	1.905310	-3.327815	13.699934
H	-0.791918	-2.795853	14.970343
C	-0.041591	-3.496463	15.655583
C	0.390001	-4.667704	14.926769
C	-0.337968	-5.973530	15.088115
C	1.388682	-4.484868	13.991922
O	1.840983	-5.569005	13.324841
C	2.842711	-5.371836	12.336004
O	0.903411	-1.265418	10.716586
Si	4.934484	-1.409703	11.574332
Si	2.187287	-1.308585	9.760327
O	5.973480	-0.193332	11.203662
O	5.546318	-2.869078	11.124810
O	2.441234	-2.744575	8.966940
Si	3.537395	1.015478	8.200113
O	2.380047	-0.067398	8.682729
O	4.543612	-1.415821	13.189947
O	3.428894	-1.172426	10.938166
B	-1.025197	-1.559600	14.298589
O	4.390237	0.415174	6.919603
Si	4.840795	-1.020842	6.250747
O	3.808391	-2.243815	6.677087
Si	3.531372	-3.347935	7.874349
O	2.920734	-4.715410	7.216058
Si	1.365624	-5.369161	7.086629
O	2.827782	2.419402	7.761969
Si	1.230908	2.979502	7.707922
O	4.582976	1.309905	9.452425
Si	6.103950	0.921953	9.966964
O	6.996307	0.272320	8.741764
Si	7.388857	-1.167939	8.023676
O	7.279531	-2.419059	9.097973
Si	6.167476	-3.480327	9.703824
O	4.952793	-3.729362	8.622942
O	4.802009	-0.797919	4.622777
O	6.371653	-1.426124	6.745393
O	6.881582	2.239696	10.531986
Si	6.418949	3.770090	11.095123
O	6.885410	-4.900397	10.069699
Si	8.370018	-5.621186	9.693214
O	8.957601	-1.153063	7.534946
H	0.431174	2.147810	6.763218
H	0.627613	2.934294	9.070116
H	1.306929	4.384435	7.220001
H	-2.152619	-1.348872	14.633747
H	-0.861340	-1.964208	13.163813
H	-0.183215	-0.822883	14.767826
H	1.468308	-6.486934	6.107513
H	5.900676	0.231812	14.702112
H	6.677106	-2.087200	14.522103
H	4.604591	-1.583730	15.735121
H	9.466676	-4.929114	10.428430
H	9.226988	-0.365836	7.052429
H	4.937078	-1.593498	4.099613
H	0.922628	-5.886061	8.413151
H	0.408771	-4.336778	6.593887
H	8.263035	-7.038181	10.138579
H	8.615541	-5.556698	8.223882
H	7.647113	4.376162	11.680199
H	5.930537	4.594411	9.953125
H	5.356689	3.636098	12.130935
H	-0.412433	-6.268245	16.142113
H	-1.363565	-5.922043	14.695319
H	0.175826	-6.774340	14.553909
H	-0.715425	-3.692919	16.492023
H	0.738309	-2.792906	15.944140
H	3.102657	-6.370265	11.981834
H	2.466233	-4.778257	11.496425
H	3.729794	-4.886014	12.750754
H	2.842846	1.048378	12.937399
H	2.305776	2.362382	14.379713
H	0.939593	1.135515	13.530883
H	2.329940	0.383922	14.760944

D

G = -1997,942345 u.a.

B	1.802295	1.047407	14.447750
Si	5.838680	-1.706123	14.463277
La	2.024190	-1.221080	13.070362
O	1.983396	-3.127682	14.223377
H	-1.308319	-3.010682	14.169908
C	-0.747855	-3.183153	15.128659
C	0.145104	-4.379421	15.073877
C	-0.434698	-5.701193	15.489814
C	1.432266	-4.250332	14.669948

O	2.276070	-5.324933	14.763567
C	3.171495	-5.513624	13.682618
O	1.048455	-1.166920	10.896989
Si	5.124585	-1.404725	11.448854
Si	2.258169	-1.178897	9.853129
O	6.166363	-0.193140	11.079358
O	5.653263	-2.859581	10.902490
O	2.465162	-2.590273	9.004839
Si	3.546250	1.171052	8.293120
O	2.392669	0.097911	8.806863
O	4.820570	-1.491755	13.088656
O	3.589726	-1.071814	10.941336
B	-0.831691	-2.127250	12.466260
O	4.296798	0.602047	6.936477
Si	4.671420	-0.812147	6.179250
O	3.649292	-2.036975	6.622806
Si	3.435784	-3.177498	7.798324
O	2.727438	-4.491728	7.132470
Si	1.291849	-5.338132	7.427487
O	2.851852	2.612565	7.968419
Si	1.256122	3.167211	7.848548
O	4.680544	1.389539	9.484032
Si	6.229017	0.964278	9.872430
O	7.024665	0.347559	8.568357
Si	7.333999	-1.069573	7.765702
O	7.273315	-2.356803	8.800969
Si	6.184096	-3.430832	9.425537
O	4.907180	-3.620852	8.408527
O	4.525133	-0.524553	4.567938
O	6.226624	-1.254201	6.552420
O	7.060615	2.250245	10.433992
Si	6.651111	3.761656	11.082374
O	6.902759	-4.868846	9.703705
Si	8.350651	-5.600274	9.217776
O	8.865151	-1.067796	7.170689
H	0.503267	2.347205	6.856113
H	0.594297	3.096808	9.181977
H	1.347902	4.580063	7.387297
H	-1.906738	-2.232003	11.965497
H	-0.037865	-3.014037	12.394381
H	-0.588073	-1.092361	13.035697
H	1.268519	-6.458312	6.446354
H	6.976688	-0.753556	14.354721
H	6.319228	-3.113707	14.476766
H	4.976637	-1.407305	15.634224
H	9.496783	-4.959581	9.923526
H	9.102574	-0.293947	6.651177
H	4.523524	-1.310371	4.013426
H	1.289504	-5.871908	8.820065
H	0.117488	-4.443502	7.219326
H	8.238177	-7.032893	9.607393
H	8.519602	-5.473989	7.741850
H	7.908433	4.314871	11.656628
H	6.140656	4.647897	9.998342
H	5.619261	3.598386	12.146050
H	-0.727016	-5.700126	16.549612
H	-1.341974	-5.936848	14.915777
H	0.280235	-6.511909	15.341949
H	-1.540709	-3.302814	15.875851
H	-0.212579	-2.256911	15.360832
H	3.746867	-6.411799	13.915759
H	2.631987	-5.671937	12.738255
H	3.859021	-4.669967	13.563984
H	2.993599	0.750274	14.225436
H	1.710285	2.052118	15.094873
H	1.238934	1.153496	13.348763
H	1.298077	0.081595	15.048395

E

G = -1997,984098 u.a.

B	1.239343	1.045392	13.593595
Si	5.007976	-2.623403	14.169890
La	1.417849	-1.423804	12.629179
O	1.274036	-2.894587	14.246288
H	-0.714995	-3.192543	17.328140
C	0.240878	-2.790550	16.965183
C	1.107369	-3.882665	16.410816
C	1.465863	-5.000411	17.346739
C	1.550618	-3.847510	15.139137
O	2.425315	-4.811704	14.673713
C	1.906376	-5.609908	13.618477
O	0.660887	-1.183705	10.027791
Si	4.614343	-1.734074	11.234718
Si	2.103972	-1.175728	9.284538
O	5.738014	-0.545889	11.145257
O	5.124035	-3.119370	10.522376
O	2.417190	-2.487862	8.341150
Si	3.624960	1.315062	8.250408
O	2.386071	0.226888	8.475335
O	4.123798	-2.020222	12.800179
O	3.145223	-1.238847	10.630514
B	-0.069838	-2.430836	10.527009
O	4.532891	0.878633	6.944544
Si	4.985439	-0.447427	6.077209
O	3.869460	-1.665059	6.208867
Si	3.490610	-2.958573	7.161980
O	2.809424	-4.115591	6.236917
Si	1.383335	-5.030300	6.292662
O	3.006954	2.803480	8.013258
Si	1.452553	3.479229	7.965444
O	4.581881	1.321908	9.602247
Si	6.037014	0.769861	10.156400
O	7.010685	0.305104	8.911023
Si	7.379533	-1.022661	7.989268
O	7.119193	-2.413790	8.843939
Si	5.928392	-3.526377	9.115738
O	4.862534	-3.556418	7.862670
O	5.096980	0.041186	4.513220
O	6.446790	-1.007287	6.624248
O	6.809994	1.915995	11.018610
Si	6.350703	3.206410	12.019496
O	6.573590	-5.007662	9.332278
Si	8.125017	-5.677756	9.215344
O	8.977972	-1.033630	7.613476
H	0.670719	2.862120	6.856053
H	0.765249	3.259637	9.268696

H	1.649531	4.933269	7.714406
H	-0.808646	-2.930174	9.724445
H	0.779128	-3.249647	10.939250
H	-0.712291	-2.053306	11.531848
H	1.465160	-5.977028	5.146129
H	6.258420	-1.814817	14.247731
H	5.326520	-4.052674	13.932269
H	4.135816	-2.391466	15.343477
H	9.014758	-5.070427	10.245952
H	9.320579	-0.213092	7.246697
H	5.159389	-0.668699	3.867307
H	1.309686	-5.777822	7.579917
H	0.203255	-4.133028	6.143610
H	7.959986	-7.135808	9.465950
H	8.680396	-5.442135	7.852255
H	7.577394	3.603617	12.763581
H	5.863702	4.334646	11.176871
H	5.285063	2.762948	12.962111
H	1.996005	-4.618909	18.230943
H	0.565037	-5.505138	17.722903
H	2.102229	-5.744694	16.865622
H	0.718756	-2.302625	17.826349
H	0.023080	-2.022968	16.220417
H	2.687263	-6.324234	13.349283
H	1.010780	-6.154322	13.944464
H	1.651103	-5.009963	12.736131
H	1.836763	0.297758	14.384285
H	1.100312	2.148036	14.041513
H	1.865388	1.051660	12.522334
H	0.131925	0.511876	13.361558

BH_3 trapped on the silica surface

G = -1997.947927 u.a.

H	1.713909	-0.180072	13.440017
H	3.887902	0.629913	15.656966
H	2.642388	-1.380909	14.329059
C	1.742149	-0.750422	14.378658
C	2.917579	1.146215	15.619934
H	2.938034	1.776853	14.719866
H	-0.517057	2.228918	17.228451
C	-0.163559	1.591063	18.050475
H	-0.978599	0.933648	18.374255
O	0.994632	0.864922	17.675481
C	0.863628	0.088866	16.550264
La	-1.862238	-2.131965	16.730757
O	-3.715836	-1.435609	18.035704
Si	-4.033230	-2.659303	18.994158
O	-3.180707	-3.952356	18.315043
O	-3.248066	-2.483511	20.535255
O	-5.574503	-3.151333	19.270522
Si	-6.456409	-4.552289	19.068134
O	-7.873903	-4.218265	18.337093
Si	-8.741549	-2.809455	17.964813
C	1.781997	0.165957	15.565482
O	-0.178679	-0.748398	16.565426
O	-1.173612	-4.823757	17.030936
Si	-0.210067	-5.769700	15.953247
B	-2.740797	-2.786354	14.294317
Si	-2.211199	-5.279597	18.258992
O	-1.329764	-5.485474	19.626966
Si	-1.622741	-5.902086	21.210547
O	-2.577534	-7.250612	21.237016
Si	-4.181267	-7.647388	21.259187
O	-4.811122	-7.664477	19.727437
Si	-4.701440	-7.001934	18.221671
O	-5.614241	-5.624998	18.128650
Si	-3.384455	-3.358098	22.008475
O	-3.103779	-2.371379	23.264199
Si	-1.792730	-1.603989	24.029102
O	-3.104312	-6.611099	17.896418
O	-5.192265	-8.105599	17.127839
Si	-6.058148	-8.072970	15.669884
O	-0.198040	-6.204743	21.939212
Si	0.588235	-7.579122	22.541622
O	-2.373826	-4.652688	21.983637
O	-4.947662	-3.854600	22.083084
Si	-5.935563	-5.185645	22.002986
O	-7.094459	-5.112146	23.163182
O	-6.729027	-5.214735	20.557865
O	-5.013089	-6.550032	22.178856
O	-4.250528	-9.147873	21.921670
H	-8.890977	-1.968671	19.186852
H	-8.028563	-2.051555	16.898597
H	-10.073140	-3.266568	17.481265
H	-2.216162	-1.443133	25.449420
H	-1.085181	-6.317477	14.886075
H	0.423290	-6.858582	16.747559
H	0.803600	-4.825939	15.417118
H	0.708263	-8.605831	21.466960
H	-5.098771	-9.594414	21.843050
H	-6.778766	-4.949145	24.056852
H	-0.577794	-2.460115	23.946887
H	-1.564653	-0.275791	23.402228
H	1.935596	-7.121955	22.978185
H	-0.176091	-8.130448	23.696358
H	-5.863622	-9.412452	15.050063
H	-7.501347	-7.837203	15.957230
H	-5.523610	-7.001602	14.782486
H	2.848280	1.794546	16.494466
H	0.868923	-1.406395	14.391879
H	0.127637	2.222337	18.892686
H	-1.551173	-3.116519	14.462963
H	-3.104986	-3.030197	13.178318
H	-3.424279	-3.368604	15.145784
H	-2.802675	-1.564129	14.533729
B	-1.718373	-1.837732	20.361925
H	-1.114508	-2.277795	21.310404
H	-1.279006	-2.341076	19.333164
H	-1.857389	-0.649870	20.323062

Comparison of the catalytic properties of the different MMA isomers

MMA_{cis}

G = -345,567234 u.a.

C	1.268400	0.045218	3.496167

O	1.203809	0.079530	2.069537
C	-0.035936	-0.057725	1.553195
O	-1.025252	-0.200345	2.241348
C	-0.013850	-0.010309	0.058971
C	1.298429	0.177572	-0.646185
C	-1.189710	-0.141014	-0.565599
H	2.322135	0.164378	3.748869
H	0.676128	0.855675	3.929214
H	0.887580	-0.906006	3.877288
H	1.156547	0.191996	-1.729714
H	1.778393	1.114373	-0.344726
H	1.999472	-0.625838	-0.397147
H	-1.261644	-0.117739	-1.649022
H	-2.101334	-0.273976	0.008001

MMA_{trans}

G = -345,56778 u.a.

C	1.214293	0.034325	3.532276
O	1.223217	0.076754	2.104877
C	0.013362	-0.061944	1.526370
O	-1.010763	-0.212006	2.162179
C	0.056602	-0.013735	0.035871
C	-1.276586	-0.170488	-0.634368
C	1.211332	0.156510	-0.618942
H	2.253616	0.154386	3.838659
H	0.599749	0.841268	3.940399
H	0.818024	-0.919979	3.889503
H	-1.175595	-0.126782	-1.721283
H	-1.740059	-1.123356	-0.359059
H	-1.969364	0.612966	-0.310550
H	1.238158	0.190884	-1.704695
H	2.151306	0.264891	-0.089676

A_{trans}

G = -1997,981354 u.a.

C	2.262807	-5.316312	12.195430
O	2.161294	-5.308667	13.633254
C	1.699444	-4.216552	14.204309
C	1.619316	-4.252821	15.683068
C	1.042329	-3.037501	16.347221
O	1.353468	-3.230993	13.538767
La	0.364760	-1.093163	12.772729
O	2.870359	-0.990056	11.369453
Si	4.409893	-1.383506	11.856377
O	5.503295	-0.196743	11.522136
Si	5.860675	1.048577	10.486470
O	4.463870	1.668110	9.858284
Si	3.460049	1.390247	8.569322
O	2.726621	2.795894	8.176572
Si	1.114812	3.295918	8.046565
O	4.341951	-1.617746	13.480321
Si	5.340917	-1.080855	14.743170
O	0.450437	-1.049730	10.483931
Si	1.951160	-1.043031	9.922851
O	2.402096	-2.429965	9.128602
Si	3.370373	-2.963416	7.902509
O	4.782155	-3.555744	8.530284
Si	5.760239	-3.329059	9.840558
O	6.431201	-4.759831	10.267744
Si	7.958266	-5.458817	10.069461
B	1.025924	1.089389	14.145654
C	2.053181	-5.336564	16.342324
O	2.333505	0.251652	8.966751
O	4.361969	0.868594	7.285371
Si	4.805756	-0.544783	6.567241
O	4.912699	-0.218797	4.958984
O	6.270255	-1.062911	7.149093
Si	7.207048	-0.936295	8.507495
O	6.841651	0.479330	9.285123
O	3.684069	-1.736457	6.835666
O	8.805401	-0.975725	8.124113
O	6.955619	-2.240356	9.492039
O	4.855248	-2.799913	11.125451
O	2.642234	-4.199647	7.113182
Si	1.347012	-4.334092	6.036456
O	6.656896	2.211110	11.313291
Si	6.300755	3.803072	11.767341
B	-2.108407	-1.900359	13.313517
H	-0.173042	0.790416	14.278771
H	1.688529	0.101073	14.517326
H	1.305510	2.074123	14.770028
H	1.247361	1.237693	12.933153
H	0.718734	-5.662220	6.283334
H	4.804888	-1.719003	15.978151
H	5.286657	0.401952	14.856748
H	6.741596	-1.534703	14.503412
H	0.403962	2.470534	7.028061
H	1.162151	4.719918	7.612805
H	0.435534	3.179000	9.368063
H	-2.068574	-0.796110	12.737476
H	-1.534778	-2.714569	12.573546
H	-1.428366	-1.785068	14.347953
H	1.865932	-4.268984	4.639135
H	8.946405	-4.778786	10.954915
H	9.154404	-0.157911	7.757368
H	5.172924	-0.963738	4.409319
H	0.358311	-3.241084	6.264066
H	7.810657	-6.886967	10.468128
H	8.393654	-5.363804	8.646424
H	7.440925	4.248538	12.616196
H	6.195349	4.664330	10.554664
H	5.028502	3.845527	12.542338
H	2.004866	-5.381070	17.426126
H	2.462306	-6.195571	15.822693
H	2.611657	-6.315675	11.941847
H	1.285741	-5.124912	11.747656
H	2.981829	-4.565008	11.865402
H	1.033197	-3.163081	17.431684
H	1.625160	-2.139592	16.114369
H	0.013852	-2.855542	16.016423
H	-3.234072	-2.227628	13.562955

B_{trans}

G = -1997,936685 u.a.

C	1.606509	-5.840083	12.402794
O	0.942174	-5.454599	13.614080

C	1.254978	-4.261121	14.123490
C	0.479872	-3.806846	15.229262
C	1.027278	-2.721026	16.129238
O	2.171616	-3.563338	13.584325
La	1.035484	-1.436623	13.129792
O	3.228414	-1.078341	11.513559
Si	4.837392	-1.306041	11.891800
O	5.759242	-0.008355	11.464054
Si	5.904837	1.243839	10.388186
O	4.404328	1.708324	9.871715
Si	3.332258	1.319017	8.671677
O	2.439510	2.642678	8.328085
Si	0.782972	2.977386	8.246734
O	4.854873	-1.493607	13.519382
Si	6.011140	-1.225693	14.728716
O	0.776055	-1.389832	10.877071
Si	2.201429	-1.235246	10.148455
O	2.697821	-2.574094	9.311175
Si	3.637082	-3.034837	8.031487
O	5.142362	-3.459090	8.561814
Si	6.209661	-3.131110	9.778464
O	7.055798	-4.484103	10.135954
Si	8.642462	-4.999100	9.863055
B	1.415397	0.939071	14.251095
C	-0.848075	-4.233436	15.344867
O	2.347741	0.090286	9.174525
O	4.168458	0.858354	7.322985
Si	4.706021	-0.504907	6.572210
O	4.652976	-0.180875	4.960714
O	6.256178	-0.862296	7.038099
Si	7.285173	-0.622263	8.312997
O	6.835471	0.756139	9.113656
O	3.737790	-1.804522	6.926411
O	8.839563	-0.486721	7.793963
O	7.257870	-1.937201	9.311551
O	5.386938	-2.664628	11.137261
O	2.981167	-4.353763	7.316128
Si	1.710021	-4.622728	6.237758
O	6.645503	2.500070	11.125061
Si	6.138570	4.011245	11.695783
B	-1.799021	-2.443627	13.644858
H	0.314269	0.448251	14.562858
H	2.286503	0.118822	14.592995
H	1.587680	2.004820	14.771321
H	1.445950	1.018279	13.014040
H	1.237179	-6.015617	6.474024
H	5.495756	-1.901058	15.951632
H	6.166042	0.236279	14.967673
H	7.316464	-1.822197	14.321364
H	0.117361	2.044039	7.292495
H	0.671198	4.379300	7.756492
H	0.169314	2.851611	9.599268
H	-2.924899	-2.202924	13.304818
H	-1.087875	-2.958518	12.785950
H	-1.258952	-1.504325	14.234423
H	2.210096	-4.485521	4.838715
H	9.587460	-4.202468	10.697463
H	9.075311	0.379745	7.449342
H	4.991561	-0.880750	4.394699
H	0.602804	-3.652469	6.478426
H	8.686057	-6.432492	10.266647
H	8.993022	-4.859751	8.420147
H	7.299800	4.578118	12.436959
H	5.783806	4.892065	10.546088
H	4.968306	3.854404	12.605314
H	-1.391382	-4.021197	16.263568
H	-1.158737	-5.135378	14.826438
H	1.249153	-6.846922	12.189303
H	1.344965	-5.166954	11.582124
H	2.689487	-5.838689	12.539618
H	0.910674	-3.003111	17.181681
H	2.097699	-2.564788	15.965365
H	0.513738	-1.749642	16.036165
H	-1.775167	-3.381427	14.556976

C_{trans}

G = -1997,946592 u.a.

C	2.111730	-5.440208	12.417243
O	1.198778	-5.069063	13.454886
C	1.462739	-3.930033	14.128404
C	0.452946	-3.388150	14.927221
C	0.814900	-2.506970	16.107050
O	2.563695	-3.295399	13.897404
La	1.350003	-1.286954	13.296507
O	3.334372	-0.967088	11.499150
Si	4.946234	-1.167041	11.884273
O	5.822596	0.145241	11.413388
Si	5.818816	1.336733	10.258138
O	4.259850	1.633019	9.795229
Si	3.181000	1.199783	8.617952
O	2.250069	2.491829	8.253748
Si	0.593931	2.829483	8.299543
O	4.943025	-1.302312	13.517104
Si	5.755030	-2.273371	14.649219
O	0.880891	-1.519952	11.061474
Si	2.235336	-1.309517	10.224496
O	2.788456	-2.661684	9.444787
Si	3.705085	-3.136383	8.153413
O	5.244603	-3.464394	8.654336
Si	6.336709	-3.024789	9.812528
O	7.260315	-4.313078	10.213513
Si	8.783752	-4.877150	9.745282
B	1.417326	1.176809	14.341846
C	-0.922483	-3.966423	14.922390
O	2.230694	-0.041418	9.161930
O	4.005978	0.734148	7.263953
Si	4.595763	-0.626265	6.549185
O	4.476872	-0.374466	4.928480
O	6.176536	-0.883247	6.976088
Si	7.228472	-0.528600	8.204704
O	6.729293	0.853522	8.966934
O	3.709853	-1.959052	6.989055
O	8.753918	-0.322924	7.626267
O	7.304087	-1.805388	9.250872
O	5.538864	-2.535690	11.180361
O	3.089269	-4.516954	7.523068

Si	1.860804	-4.873242	6.420401
O	6.498687	2.691570	10.865641
Si	5.978013	3.949668	11.872327
B	-1.909345	-2.130357	13.559720
H	0.414472	0.543970	14.719789
H	2.412300	0.495299	14.653220
H	1.463652	2.265354	14.842593
H	1.373674	1.237619	13.105063
H	1.421729	-6.267357	6.708274
H	5.013340	-2.129410	15.930943
H	7.145700	-1.754149	14.805950
H	5.790020	-3.691360	14.202035
H	-0.145457	1.889708	7.407859
H	0.445081	4.227366	7.807627
H	0.084439	2.716453	9.696114
H	-3.093728	-2.160277	13.718183
H	-1.416875	-2.678141	12.619220
H	-1.306424	-1.249154	14.128432
H	2.397614	-4.784834	5.031067
H	9.845420	-4.090482	10.435954
H	8.955308	0.572406	7.338153
H	4.900010	-1.043036	4.381867
H	0.719212	-3.926896	6.583715
H	8.846752	-6.304580	10.166828
H	8.947090	-4.768642	8.266616
H	7.185114	4.436123	12.597487
H	5.411461	5.042584	11.031334
H	4.954529	3.453637	12.835206
H	-1.242061	-4.357258	15.899121
H	-1.065031	-4.735034	14.165131
H	1.770477	-6.416131	12.071075
H	2.083835	-4.726161	11.589223
H	3.131914	-5.510456	12.799489
H	0.679704	-3.053946	17.051372
H	1.866230	-2.197875	16.089444
H	0.188659	-1.606753	16.191778
H	-1.732597	-3.178142	14.767237

TS $A_{trans} \rightarrow A_{cis}$

G = -1997,97316 u.a.

La	0.739690	-1.222663	12.707581
B	-1.743686	-1.893910	13.377238
H	-2.869631	-2.165298	13.688048
H	-1.252477	-2.740904	12.613953
H	-1.680322	-0.798224	12.790648
H	-1.005690	-1.808334	14.373783
H	0.371614	0.660977	14.251345
H	1.788180	1.036476	12.880523
B	1.585070	0.881157	14.094981
H	2.184064	-0.157012	14.437036
H	1.943339	1.833642	14.728917
O	0.670850	-1.093005	10.421120
Si	2.134177	-1.170738	9.772716
O	3.130646	-1.201528	11.168735
Si	4.667436	-1.668083	11.596660
O	4.643810	-1.911894	13.221750
Si	5.619221	-1.286409	14.464481
H	5.511698	0.195701	14.523424
H	5.103555	-1.899971	15.720963
H	7.034174	-1.703206	14.243125
O	5.801173	-0.530900	11.230843
O	5.020158	-3.102585	10.854508
H	6.755911	4.263103	10.156768
O	4.800450	1.391100	9.612832
O	2.443068	-2.573188	8.936285
O	2.552416	0.107748	8.811587
Si	3.349166	-3.155126	7.682675
Si	3.726004	1.181602	8.369808
O	3.062314	2.633423	8.025106
H	0.564695	-5.460609	8.216216
Si	1.486395	3.191667	7.763299
H	0.810975	2.357329	6.727765
H	1.622032	4.595560	7.284897
H	0.715675	3.150968	9.038341
O	2.516274	-4.331920	6.905579
Si	0.897586	-4.819879	6.910240
H	0.000292	-3.653795	6.670721
H	0.762726	-5.812764	5.807887
O	4.753372	-3.817912	8.257474
Si	5.813910	-3.666384	9.511790
Si	6.186868	0.693341	10.178711
O	6.418624	-5.139922	9.892486
O	7.077986	1.806176	10.976327
Si	6.852943	3.432437	11.391303
H	5.620812	3.587201	12.215272
H	8.056078	3.820951	12.178951
O	1.635904	-3.492772	13.303608
C	1.768470	-4.362091	14.172379
O	2.485862	-5.442137	13.977040
C	3.130562	-5.592937	12.690659
C	1.106368	-4.311143	15.511728
C	1.785501	-3.826044	16.553162
O	4.534797	0.615502	7.043669
Si	4.865144	-0.813841	6.295307
O	6.329999	-1.399330	6.808206
Si	7.329946	-1.347597	8.124307
O	8.904136	-1.479850	7.669224
O	7.083867	0.074066	8.938248
O	7.050413	-2.645753	9.109582
O	3.701115	-1.950898	6.606447
Si	7.887740	-5.926359	9.601091
C	-0.311602	-4.810019	15.549096
O	4.908276	-0.487161	4.684407
H	8.960635	-5.323084	10.442416
H	9.261265	-0.713227	7.211155
H	4.919642	-1.262208	4.115112
H	7.673415	-7.349405	9.988165
H	8.251578	-5.833458	8.158252
H	-0.712232	-4.728132	16.561699
H	-0.953318	-4.230697	14.876671
H	-0.362340	-5.860310	15.239048
H	1.317518	-3.749211	17.530161
H	2.812800	-3.484981	16.468613
H	3.641268	-6.552418	12.742614
H	2.380434	-5.595373	11.897771
H	3.840601	-4.782260	12.526470

*First propagation step of MMA polymerization mediated by $(BH_4)_2La$@**c**-1*

Faa$_S$

G = -2343,558763 u.a.

H	-1.975443	-4.651227	16.359879
C	-1.554607	-4.101445	15.523311
H	-0.472135	-4.047765	15.459044
C	-2.355928	-3.524474	14.616416
H	-4.190490	-4.142691	15.534403
C	-3.856918	-3.575564	14.662757
H	-4.287398	-2.570457	14.717169
C	-1.714185	-2.795163	13.499136
O	-2.581578	-2.270605	12.650639
C	-2.046778	-1.534370	11.534344
H	-2.916808	-1.201077	10.970824
H	-1.412965	-2.176815	10.919322
O	-0.495248	-2.670176	13.351075
H	9.811167	-3.644817	7.095802
La	1.884108	-2.563770	12.649969
H	1.132832	-0.170293	12.355071
H	9.913817	-5.597650	8.565165
H	1.782938	1.180613	13.704962
B	1.814590	0.026172	13.374375
H	1.381479	-0.714944	14.268080
H	5.301637	-2.334200	15.111071
H	5.737390	-4.476642	13.969021
Si	5.780732	-2.995865	13.873467
H	7.155708	-2.536349	13.521276
O	4.742053	-2.506388	12.591846
Si	5.012185	-1.914299	11.069122
H	2.970381	-0.346683	13.121393
H	2.325311	-4.450273	10.896877
B	1.163273	-4.232859	10.499925
H	0.415241	-4.334064	11.475966
O	1.079588	-2.745819	10.067005
O	7.863452	-4.107086	8.774859
Si	9.526058	-4.163390	8.464409
O	3.442293	-1.857752	10.536627
O	5.922874	-2.962637	10.190832
Si	2.356502	-2.113339	9.271262
O	3.036027	-3.124847	8.164620
Si	4.127084	-3.109202	6.914584
O	3.819974	-4.359531	5.910613
Si	2.935450	-5.799280	6.028654
H	0.855880	-5.002413	9.629154
Si	6.723529	-2.939232	8.730188
O	5.663080	-3.243845	7.507942
O	2.508099	-3.892432	14.324119
C	2.293641	-4.763325	15.309022
C	2.283124	-4.471036	16.629039
C	2.075062	-5.527637	17.676177
O	2.018121	-0.642586	8.603860
Si	2.817894	0.810466	8.456274
O	1.727371	2.025140	8.410268
Si	0.168878	2.240231	7.797208
O	7.436410	-1.462245	8.523596
Si	7.128827	0.005182	7.827455
O	8.597783	0.606632	7.400932
O	5.667573	-0.408532	11.069539
Si	5.395026	1.001576	10.216559
O	5.774878	2.283907	11.145714
Si	5.114531	3.129693	12.459272
O	3.980510	-1.705372	6.057490
Si	4.568506	-0.156160	6.051946
O	3.712206	0.817388	7.067532
O	1.996005	-6.044309	14.898951
C	2.884151	-6.607143	13.947867
C	2.467117	-3.065000	17.121826
O	3.809369	1.044858	9.754316
O	6.381064	1.029520	8.891621
O	6.163471	-0.193562	6.498603
O	4.398615	0.494584	4.551878
H	1.606521	-2.734473	17.721801
H	0.048188	1.610594	6.449979
H	-0.824634	1.632160	8.729227
H	-0.050744	3.709852	7.703028
H	3.299353	-6.599568	4.825815
H	8.613662	1.552648	7.227831
H	4.724648	-0.055267	3.833241
H	3.308520	-6.531638	7.271624
H	1.476601	-5.494973	6.022362
H	10.259583	-3.356894	9.481484
H	5.963103	4.344255	12.619782
H	3.707161	3.511227	12.161340
H	5.188642	2.284104	13.683121
H	2.913143	-5.548297	18.387704
H	1.173440	-5.328833	18.274318
H	1.974803	-6.520351	17.234880
H	3.345075	-2.984096	17.778550
H	2.594896	-2.354522	16.302538
H	2.527188	-7.621203	13.756090
H	2.889071	-6.049277	13.005311
H	3.908476	-6.655834	14.342541
H	-1.469789	-0.678688	11.892195
H	-4.266125	-4.048098	13.764102

Gaa$_S$

G = -2343,545087 u.a.

H	-0.520504	-2.719507	16.916809
C	-0.212131	-3.103318	15.933111
H	0.145650	-2.234235	15.368918
C	-1.395931	-3.708668	15.230003
H	-2.492189	-4.095406	17.044006
C	-2.420808	-4.481624	16.019201
H	-3.408414	-4.401432	15.557736
C	-1.591423	-3.461666	13.905916
O	-2.682615	-4.020596	13.301171
C	-3.138281	-3.413390	12.102245
H	-4.043291	-3.957160	11.823894
H	-2.404011	-3.497556	11.295322
O	-0.804555	-2.738793	13.128828
H	9.813054	-3.916926	7.108166
La	1.189127	-2.317430	12.235175
H	1.443276	0.110857	11.865614

H	9.794938	-5.883931	8.561396
H	1.943922	1.292689	13.421716
B	1.693631	0.168089	13.086137
H	0.719813	-0.291294	13.688943
H	5.825225	-1.334983	14.750062
H	5.880919	-3.775993	14.617587
Si	6.099256	-2.505282	13.871378
H	7.494170	-2.448477	13.347588
O	4.997060	-2.506784	12.581022
Si	5.069436	-1.911034	11.052987
H	2.657942	-0.592545	13.284112
H	1.960688	-4.300894	10.739108
B	0.995688	-3.984258	10.012425
H	-0.030245	-4.068315	10.683456
O	1.145131	-2.470007	9.684795
O	7.926279	-4.187743	8.899925
Si	9.550397	-4.416261	8.488767
O	3.475290	-1.827394	10.571688
O	5.881921	-2.954256	10.070561
Si	2.592767	-1.924433	9.136387
O	3.343249	-2.946291	8.090738
Si	4.407139	-2.954140	6.815623
O	4.012946	-4.150627	5.776484
Si	2.920292	-5.443666	5.781893
H	0.955850	-4.680830	9.035071
Si	6.858376	-2.961537	8.732034
O	5.940186	-3.204596	7.380739
O	1.868101	-3.952274	13.949729
C	1.432502	-4.624985	14.898301
C	1.026698	-4.021557	16.225871
C	0.697300	-5.097520	17.264513
O	2.417715	-0.426046	8.478084
Si	3.224785	1.022200	8.352749
O	2.142169	2.236212	8.224274
Si	0.454867	2.351891	8.193349
O	7.676212	-1.528434	8.617175
Si	7.495423	-0.037286	7.928966
O	9.019456	0.477959	7.590463
O	5.783666	-0.427277	11.039700
Si	5.696229	1.027456	10.238448
O	6.137233	2.231409	11.245898
Si	5.399099	3.255682	12.374798
O	4.331500	-1.515332	6.008161
Si	5.024159	-0.009208	6.031515
O	4.193006	1.016456	7.016442
O	1.302479	-5.927902	14.800138
C	1.616015	-6.535021	13.531266
C	2.185813	-3.144443	16.733576
O	4.149465	1.250998	9.702199
O	6.753218	1.014699	8.969793
O	6.592685	-0.152070	6.546337
O	4.964275	0.653364	4.528378
H	1.872730	-2.637100	17.651136
H	-0.077168	1.667478	6.979371
H	-0.125678	1.739193	9.421424
H	0.142324	3.806764	8.140778
H	3.183996	-6.202446	4.526982
H	9.093528	1.413574	7.380011
H	5.269679	0.078687	3.820253
H	3.159468	-6.312089	6.969411
H	1.522598	-4.927399	5.788867
H	10.421325	-3.701650	9.465507
H	6.388269	4.335987	12.649665
H	4.147998	3.828465	11.805604
H	5.109499	2.495548	13.622891
H	1.569653	-5.720298	17.486206
H	0.385416	-4.610815	18.193779
H	-0.110822	-5.751479	16.935271
H	3.072746	-3.743159	16.967006
H	2.462272	-2.380689	16.002354
H	1.475644	-7.603519	13.684669
H	0.936233	-6.165904	12.760998
H	2.647151	-6.314131	13.249927
H	-3.384624	-2.355557	12.253221
H	-2.201918	-5.556101	16.101403

Haa$_S$

G = -2343,574732 u.a.

H	-0.534264	-2.988205	16.933723
C	-0.417646	-2.957902	15.855265
H	0.155127	-2.124138	15.461877
C	-1.389159	-3.548792	15.067981
H	-2.299073	-4.584062	16.712240
C	-2.428051	-4.484312	15.631226
H	-3.443879	-4.120379	15.442150
C	-1.443172	-3.199301	13.688035
O	-2.514925	-3.661830	13.034296
C	-2.696687	-3.236307	11.680279
H	-3.627403	-3.702011	11.356191
H	-1.868723	-3.566571	11.049317
O	-0.605674	-2.473088	13.068557
H	9.914210	-3.782769	7.272136
La	1.671447	-2.385216	12.379156
H	1.090886	0.038058	12.271100
H	9.863316	-5.752060	8.722167
H	1.974004	1.287333	13.587350
B	1.883496	0.147728	13.221477
H	1.477135	-0.594697	14.126655
H	5.239124	-2.644705	15.009684
H	5.406481	-4.726612	13.709665
Si	5.618054	-3.255569	13.711250
H	7.032676	-2.931735	13.368328
O	4.617246	-2.561523	12.502384
Si	4.973893	-1.920540	11.016993
H	2.976180	-0.299370	12.846291
H	2.255182	-4.301557	10.695809
B	1.140414	-4.070252	10.186849
H	0.299949	-4.182014	11.082608
O	1.104514	-2.578847	9.773712
O	7.873580	-4.173313	8.857931
Si	9.544234	-4.300946	8.620425
O	3.437501	-1.757682	10.413418
O	5.870335	-2.982720	10.140134
Si	2.444779	-1.966493	9.065647
O	3.170789	-2.980846	7.993648
Si	4.312003	-2.975636	6.787495

O	3.994136	-4.180410	5.732665
Si	3.051742	-5.587009	5.761937
H	0.918348	-4.828551	9.280995
Si	6.786043	-2.960053	8.749194
O	5.813068	-3.200591	7.441831
O	2.225208	-3.866945	14.088412
C	1.704720	-4.509493	15.084567
C	1.573555	-4.024275	16.381787
C	1.152536	-4.952362	17.491465
O	2.195365	-0.476103	8.406648
Si	3.055498	0.951313	8.344397
O	2.010713	2.200639	8.248152
Si	0.327841	2.374328	8.267615
O	7.570596	-1.510659	8.631670
Si	7.365528	-0.012541	7.962475
O	8.881498	0.535102	7.641258
O	5.699503	-0.449522	11.104051
Si	5.527938	0.989489	10.270349
O	5.892872	2.235323	11.252964
Si	5.173033	3.113657	12.512306
O	4.262581	-1.542638	5.970397
Si	4.912347	-0.018562	6.032640
O	4.035278	0.968447	7.016451
O	1.166445	-5.724654	14.843063
C	1.343163	-6.296691	13.551705
C	2.343227	-2.802283	16.797733
O	3.978713	1.098712	9.707117
O	6.598644	1.011037	9.012744
O	6.474211	-0.132929	6.574042
O	4.863643	0.665805	4.539311
H	1.754015	-2.180712	17.485226
H	-0.257866	1.749932	7.045962
H	-0.241812	1.740206	9.489805
H	0.065173	3.839982	8.270523
H	3.429802	-6.356155	4.543362
H	8.945442	1.481402	7.481162
H	5.201106	0.112524	3.828697
H	3.349970	-6.379998	6.988180
H	1.606626	-5.226060	5.716101
H	10.265785	-3.538123	9.678894
H	6.019042	4.328156	12.687802
H	3.783834	3.493993	12.138488
H	5.185551	2.294899	13.756293
H	2.017596	-5.466861	17.933941
H	0.676063	-4.389460	18.303956
H	0.452637	-5.715831	17.147590
H	3.262993	-3.074866	17.334741
H	2.626620	-2.179835	15.946162
H	0.923592	-7.301200	13.620981
H	0.810693	-5.738267	12.776726
H	2.402258	-6.356349	13.284873
H	-2.781050	-2.147718	11.627204
H	-2.362689	-5.486801	15.194318

Faa_R

G = -2343,554186 u.a.

C	1.557240	-6.471359	13.605844
O	1.209849	-5.906064	14.882955
C	1.393542	-4.610053	15.039794
O	1.871830	-3.910299	14.132432
La	1.232807	-2.220179	12.440963
B	2.149867	0.049153	13.538006
C	1.012542	-4.116882	16.380999
C	0.231455	-5.032288	17.277998
C	1.386271	-2.872475	16.710319
O	-0.806133	-2.318255	13.248956
C	-1.772760	-2.594339	14.123788
O	-1.912803	-3.947696	14.389867
C	-2.415628	-4.692031	13.286873
B	0.969455	-3.912459	10.235257
O	1.140808	-2.405210	9.894580
Si	2.575531	-1.895818	9.281692
O	3.537247	-1.829360	10.663118
Si	5.153504	-1.982986	11.042471
O	5.918698	-0.522295	11.010974
Si	5.823594	0.944065	10.234040
O	6.362219	2.122487	11.224789
Si	5.719033	3.179192	12.380936
C	-2.545020	-1.692671	14.761208
C	-2.353166	-0.218557	14.556585
C	-3.627768	-2.105081	15.716104
O	3.235492	-2.919610	8.179015
Si	4.206724	-2.939905	6.833100
O	3.696183	-4.095577	5.797893
Si	2.781437	-5.513360	5.926836
O	2.399100	-0.381589	8.655525
Si	3.244108	1.041510	8.504555
O	4.253251	1.222424	9.799486
O	4.126820	-1.486930	6.052620
Si	4.864076	-0.002276	6.058097
O	6.457159	-0.197098	6.470107
Si	7.442560	-0.134333	7.798962
O	6.795727	0.920180	8.898929
O	5.764598	-3.254995	7.289826
Si	6.761003	-3.051100	8.591526
O	7.801254	-4.310104	8.673049
Si	9.473203	-4.484712	8.496730
O	4.129312	1.028793	7.111817
O	4.728518	0.688494	4.572492
O	2.194759	2.291440	8.467576
Si	0.512661	2.450510	8.396434
O	5.854637	-3.026375	9.976750
O	5.190417	-2.616962	12.554085
Si	6.242952	-2.432475	13.870401
O	7.617608	-1.642294	8.450439
O	8.959185	0.342056	7.378875
H	-0.051334	-3.975114	10.916395
H	0.907071	-4.616446	9.263698
H	1.937455	-4.242136	10.951554
H	5.928936	-3.548980	14.805636
H	6.009884	-1.119871	14.532439
H	-0.110693	1.833432	9.601745
H	7.656812	-2.536531	13.405974
H	0.237280	3.913445	8.362973
H	1.333534	-5.170474	6.002343
H	3.061045	-6.297150	4.690674

H	3.194720	-6.287919	7.131912
H	-0.010287	1.798994	7.160725
H	5.496511	2.444586	13.657396
H	4.444547	3.768857	11.885054
H	6.743749	4.244329	12.573393
H	1.268976	-0.440271	14.251554
H	2.563614	1.086289	13.978995
H	3.056202	-0.788606	13.416345
H	1.656826	0.212441	12.402325
H	1.136217	-2.456790	17.681344
H	1.940737	-2.239107	16.025953
H	0.051283	-4.554150	18.243074
H	-0.734837	-5.270244	16.822671
H	1.349885	-7.535974	13.699093
H	2.613695	-6.298977	13.391464
H	9.908949	-3.984412	7.161328
H	9.748683	-5.944128	8.614214
H	-3.262239	0.245813	14.148982
H	9.047985	1.278549	7.178295
H	4.951686	0.110660	3.836757
H	10.182327	-3.740847	9.577587
H	-3.447583	-1.693343	16.719679
H	-4.606238	-1.718206	15.397822
H	-3.699684	-3.190374	15.804415
H	-2.144571	0.291069	15.507703
H	-1.528239	-0.005528	13.874508
H	-2.467017	-5.736334	13.604609
H	-3.421714	-4.348823	13.012304
H	-1.762801	-4.609086	12.410313
H	0.948031	-6.028176	12.815690
H	0.758893	-5.975853	17.447403

Gaa_R

G = -2343,542848 u.a.

C	2.440118	-6.216493	13.289475
O	1.705612	-5.844689	14.459724
C	1.509569	-4.542153	14.680677
O	1.981389	-3.698365	13.861996
La	1.233479	-2.030447	12.268305
B	1.625537	0.516038	13.016358
C	0.797490	-4.250944	15.890703
C	0.322732	-5.394532	16.749133
C	0.549349	-2.941098	16.208070
O	-0.780770	-2.261100	13.334362
C	-1.454341	-2.648742	14.376743
O	-1.948145	-3.915417	14.358055
C	-2.069977	-4.558461	13.097038
B	0.572153	-3.573919	10.029059
O	0.868382	-2.103804	9.654046
Si	2.312545	-1.733242	8.982692
O	3.273946	-1.617291	10.354185
Si	4.719507	-1.752298	11.140322
O	5.547834	-0.334762	11.139331
Si	5.590529	1.039300	10.192998
O	6.018689	2.318379	11.106858
Si	5.308992	3.342041	12.256137
C	-1.646038	-1.923638	15.535550
C	-1.233324	-0.484066	15.613199
C	-2.567986	-2.414440	16.616834
O	2.920691	-2.898118	7.988813
Si	4.211273	-3.091709	6.961848
O	3.928171	-4.368498	5.983710
Si	2.720205	-5.549537	5.873185
O	2.283859	-0.270992	8.225603
Si	3.271686	1.062415	8.099013
O	4.101151	1.258062	9.515189
O	4.390159	-1.738138	6.033392
Si	5.179737	-0.281082	6.024184
O	6.685486	-0.493043	6.683685
Si	7.476621	-0.330448	8.127211
O	6.739157	0.851671	9.021347
O	5.593443	-3.367100	7.822274
Si	6.561749	-3.130324	9.132795
O	7.520886	-4.433260	9.355476
Si	9.152920	-4.782353	9.079532
O	4.344672	0.864296	6.861335
O	5.296434	0.274325	4.481651
O	2.359654	2.382273	7.805058
Si	0.702279	2.720751	7.743037
O	5.632953	-2.966632	10.505479
O	4.179014	-2.166383	12.650266
Si	4.999220	-2.479337	14.120343
O	7.482866	-1.773053	8.933867
O	9.059446	0.042937	7.887898
H	-0.354125	-3.516297	10.834231
H	0.304089	-4.271945	9.088395
H	1.575129	-4.019741	10.631011
H	5.158024	-3.950411	14.281774
H	4.180960	-1.898401	15.213789
H	0.047752	2.322296	9.021150
H	6.338797	-1.829714	14.047788
H	0.591675	4.191558	7.538247
H	1.407199	-4.911289	5.574211
H	3.127498	-6.441898	4.751771
H	2.643503	-6.322841	7.145168
H	0.081744	1.993467	6.598430
H	5.063174	2.583606	13.514330
H	4.038545	3.904780	11.721444
H	6.300948	4.428247	12.494159
H	1.776465	-0.280494	13.960779
H	1.795589	1.650155	13.371910
H	2.424607	0.192991	12.132404
H	0.481211	0.344776	12.572283
H	0.139937	-2.687479	17.179402
H	1.004659	-2.130679	15.649721
H	-0.141752	-5.010811	17.660730
H	-0.417950	-6.010147	16.229351
H	2.479223	-7.305291	13.308342
H	3.450163	-5.801039	13.317071
H	9.539445	-4.386077	7.694839
H	9.294394	-6.254800	9.253731
H	-2.114233	0.173579	15.614114
H	9.226765	0.956305	7.636977
H	5.617122	-0.369146	3.842868
H	9.998122	-4.062098	10.074350
H	-2.152988	-2.206904	17.612723

H	-3.534918	-1.891887	16.575389
H	-2.763356	-3.484957	16.542513
H	-0.691242	-0.272186	16.546065
H	-0.599866	-0.184842	14.776923
H	-2.591233	-5.496414	13.296463
H	-2.653461	-3.954417	12.395200
H	-1.098232	-4.773895	12.644353
H	1.934845	-5.872929	12.383280
H	1.147818	-6.054455	17.037418

Haa_R

G = -2343,574408 u.a.

C	2.493783	-6.194377	13.165313
O	1.634648	-5.886204	14.247733
C	1.423759	-4.565293	14.545823
O	1.885497	-3.689367	13.672184
La	1.343077	-2.050181	12.205167
B	1.350765	0.534638	12.949796
C	0.764397	-4.285150	15.703601
C	0.409177	-5.398044	16.657268
C	0.468518	-2.856798	16.072920
O	-0.775018	-2.358109	13.460127
C	-1.403843	-2.718790	14.461916
O	-2.517397	-3.413712	14.346059
C	-2.934497	-3.769086	13.015062
B	0.476547	-3.478304	9.957396
O	0.857618	-2.039191	9.559976
Si	2.315431	-1.697916	8.917197
O	3.250023	-1.559510	10.316492
Si	4.701071	-1.678895	11.108187
O	5.525258	-0.261592	11.089367
Si	5.594293	1.094376	10.117734
O	6.009187	2.387801	11.017477
Si	5.273630	3.419450	12.143435
C	-1.002526	-2.366066	15.881892
C	-1.050677	-0.829700	16.010918
C	-1.946882	-2.991915	16.913559
O	2.957054	-2.887583	7.974648
Si	4.252207	-3.104596	6.958366
O	3.969276	-4.390654	5.993455
Si	2.911235	-5.712469	6.033918
O	2.324120	-0.254169	8.125998
Si	3.311024	1.077428	7.988192
O	4.116014	1.305125	9.413978
O	4.446986	-1.769024	6.007951
Si	5.245033	-0.317316	5.975543
O	6.739601	-0.518804	6.663535
Si	7.508619	-0.326717	8.115049
O	6.761600	0.878491	8.971140
O	5.626076	-3.370644	7.837199
Si	6.571148	-3.105380	9.157580
O	7.526017	-4.403528	9.415511
Si	9.194883	-4.677875	9.471579
O	4.405107	0.852828	6.773635
O	5.387969	0.199563	4.421996
O	2.403653	2.391141	7.654813
Si	0.751462	2.703940	7.462071
O	5.612848	-2.908322	10.508460
O	4.122373	-2.057787	12.614973
Si	4.874404	-2.558248	14.080950
O	7.493470	-1.749003	8.956684
O	9.096691	0.034156	7.894324
H	-0.384641	-3.351937	10.838851
H	0.063196	-4.143052	9.045291
H	1.472532	-4.009469	10.485723
H	4.990443	-4.037989	14.099584
H	4.043579	-2.037363	15.192810
H	0.017700	2.374842	8.716784
H	6.232017	-1.939544	14.096766
H	0.642263	4.158608	7.162765
H	1.519758	-5.253600	5.763569
H	3.369932	-6.633702	4.956718
H	2.986632	-6.390311	7.359539
H	0.212679	1.902257	6.325734
H	4.950228	2.657561	13.382134
H	4.042072	4.015809	11.555879
H	6.278371	4.479861	12.435642
H	1.608109	-0.226940	13.897601
H	1.339332	1.680356	13.309905
H	2.199563	0.333731	12.072922
H	0.251090	0.190720	12.485817
H	0.705301	-2.679523	17.133006
H	1.119050	-2.185881	15.500402
H	0.425669	-5.038639	17.693743
H	-0.587829	-5.830032	16.487723
H	2.512339	-7.284878	13.108842
H	3.513054	-5.827302	13.331515
H	9.822797	-4.282580	8.178542
H	9.362233	-6.139307	9.703415
H	-2.074380	-0.451844	15.916960
H	9.272921	0.935816	7.609492
H	5.694588	-0.467268	3.800443
H	9.799742	-3.904272	10.593818
H	-1.599717	-2.727777	17.917484
H	-2.967603	-2.615324	16.799901
H	-1.977582	-4.079770	16.839524
H	-0.678999	-0.546731	17.000933
H	-0.426934	-0.340251	15.259019
H	-3.850183	-4.343546	13.145930
H	-3.122796	-2.869840	12.425054
H	-2.166097	-4.370052	12.525733
H	2.124866	-5.791216	12.216661
H	1.120314	-6.224813	16.576082

Fab_S

G = -2343,558832 u.a.

La	1.666517	-2.067576	12.971465
Si	2.063866	-1.591034	9.588534
O	3.549547	-1.393584	6.281014
B	2.118946	0.453040	13.806562
H	2.316794	1.577618	14.180792
H	3.176964	-0.128769	13.525067
H	1.406377	0.436893	12.789277
O	0.731400	-2.009304	10.430466
H	1.685325	-3.936868	11.150884
Si	1.794953	-5.259875	6.266614

B	0.563529	-3.499295	10.818583
H	-0.145104	-3.501499	11.828925
H	0.399543	-4.755380	6.402431
H	1.932415	-6.065866	5.021037
C	-1.810010	-1.629599	14.218823
O	-2.571931	-0.606352	13.868507
C	-2.011110	0.337188	12.937441
H	-1.799023	-0.155426	11.985730
H	-1.092820	0.768979	13.340160
H	-4.555065	-2.104274	14.853338
C	-3.838617	-2.184892	15.677113
H	-2.249634	-4.361829	16.229729
C	-1.806442	-3.656370	15.533157
H	-0.821159	-3.899202	15.150139
H	2.301436	-2.468271	18.122035
C	-2.468783	-2.546618	15.175697
H	-3.832694	-1.216973	16.188625
C	2.898017	-2.944724	17.330539
H	3.891079	-3.128369	17.765120
O	2.098532	-3.532932	14.583885
H	3.011109	-2.222704	16.519372
H	1.587485	-5.622264	13.179799
C	1.632073	-6.222892	14.094822
H	0.978847	-7.090569	13.980168
H	1.569444	-6.169775	17.485408
H	1.324795	-4.895795	18.693259
C	2.006043	-5.265962	17.912988
H	2.937969	-5.541980	18.426951
O	1.158612	-5.511784	15.228190
C	1.888902	-4.393196	15.578465
O	2.858697	-3.953376	6.093337
Si	3.481021	-2.826949	7.098012
O	5.000950	-3.283195	7.562883
O	4.521297	-2.546287	12.736263
O	5.407861	-3.117958	10.236911
Si	5.522774	-3.381794	13.856942
Si	8.672443	-4.923135	8.403947
H	5.347744	-2.730986	15.177546
Si	6.144622	-3.205937	8.745652
Si	4.790846	-1.951005	11.215345
O	3.229673	-1.563781	10.809599
O	2.509830	-2.676139	8.434096
O	1.972142	-0.065347	8.966792
O	7.110161	-1.880665	8.537852
O	5.729750	-0.602427	11.204693
Si	5.685164	0.861704	10.401747
O	6.349066	2.017286	11.338506
Si	5.939992	2.903742	12.724874
C	2.257248	-4.219672	16.865619
O	-0.669855	-1.774302	13.769315
Si	3.020963	1.216784	8.798715
O	3.818541	1.102350	7.357723
Si	4.416482	0.018821	6.271515
O	5.998803	-0.326962	6.619936
Si	7.057350	-0.360931	7.890651
O	8.588823	-0.041702	7.386312
O	7.049452	-4.564505	8.718889
O	2.175076	2.613349	8.842085
Si	0.579911	3.070807	8.528870
O	4.114609	1.219860	10.035312
O	6.587473	0.752418	9.022658
O	4.288011	0.735754	4.797866
H	0.102626	2.456346	7.256003
H	-0.298945	2.644497	9.656306
H	0.582737	4.555608	8.416306
H	0.084345	-4.173118	9.945973
H	6.930082	-3.245920	13.380424
H	5.115713	-4.809857	13.872157
H	9.541329	-4.302468	9.444929
H	8.777643	0.887976	7.227544
H	4.447729	0.153272	4.049377
H	2.171337	-6.075792	7.455673
H	8.782913	-6.407247	8.458907
H	9.056350	-4.425006	7.052091
H	7.023731	3.913358	12.888962
H	4.626557	3.575926	12.527348
H	5.898468	1.994929	13.904055
H	2.663597	-6.567731	14.247911
H	1.552250	-0.222819	14.676809
H	-2.776028	1.101664	12.810451
H	-4.198426	-2.943044	16.375985

Gab$_S$

G = -2343,551004 u.a.

La	0.781623	-1.495606	12.725370
Si	2.250680	-1.270638	9.634597
O	3.887224	-1.840113	6.505846
B	1.132844	0.974868	13.696336
H	1.303303	2.074019	14.146620
H	2.020307	0.672276	12.884599
H	0.045118	0.882720	13.105486
O	0.723413	-1.240800	10.207160
H	0.246009	-3.335766	10.904982
Si	1.377929	-5.001884	6.609788
B	-0.310692	-2.379976	10.341997
H	-1.157359	-1.921110	11.122460
H	0.373815	-3.931681	6.350801
H	1.422282	-5.957730	5.467873
C	-1.776826	-2.188144	15.069510
O	-2.623404	-1.316359	15.624950
C	-2.812021	-0.065368	14.956648
H	-3.232932	-0.219771	13.959725
H	-1.868593	0.478980	14.870992
H	-3.407013	-3.497828	17.000475
C	-2.320609	-3.604314	17.097612
H	-0.864791	-5.408749	15.596013
C	-0.857180	-4.405184	15.183646
H	-0.626433	-4.329982	14.127215
H	0.373174	-2.466482	16.725447
C	-1.629728	-3.420073	15.770005
H	-1.997905	-2.872126	17.845903
C	1.390735	-2.813020	16.480450
H	1.963133	-2.811767	17.415629
O	1.798916	-3.356156	13.667259
H	1.840565	-2.063203	15.822201
H	1.459721	-5.406285	12.069329

C	2.292458	-5.732398	12.699042
H	2.458233	-6.802114	12.565546
H	1.347071	-6.305103	16.299653
H	0.762191	-5.269426	17.615454
C	1.498539	-5.350295	16.807549
H	2.489266	-5.383100	17.282816
O	1.999659	-5.566631	14.084723
C	1.749598	-4.316387	14.526402
O	2.929861	-4.333656	6.714104
Si	3.624651	-3.105479	7.535686
O	5.059404	-3.635399	8.157307
O	4.649076	-1.795317	13.149152
O	5.217446	-2.979727	10.778008
Si	5.762304	-2.246357	14.345484
Si	8.338708	-5.517801	9.488114
H	5.386681	-1.511459	15.583244
Si	6.081729	-3.438062	9.438696
Si	4.708057	-1.600002	11.528467
O	3.121894	-1.298067	11.084710
O	2.618885	-2.620231	8.766507
O	2.570615	0.086323	8.770652
O	7.229738	-2.300558	9.085233
O	5.698584	-0.350788	11.134256
Si	6.070475	0.937772	10.164559
O	6.872310	2.064739	11.031674
Si	6.446993	3.515337	11.795403
C	1.379286	-4.179962	15.865380
O	-1.194373	-1.885710	13.983310
Si	3.636299	1.272520	8.315096
O	4.495218	0.772417	6.998137
Si	4.968413	-0.612090	6.239773
O	6.458199	-1.089469	6.785458
Si	7.425982	-0.971466	8.123210
O	9.013956	-0.965151	7.698535
O	6.807778	-4.861654	9.782864
O	2.818551	2.636597	7.953636
Si	1.185836	3.079163	7.883682
O	4.674762	1.591734	9.561989
O	7.048238	0.419943	8.939027
O	5.025259	-0.250676	4.637331
H	0.464214	2.208208	6.911748
H	0.569085	2.963337	9.235308
H	1.164927	4.494687	7.422027
H	-0.815736	-2.700297	9.301033
H	7.141016	-1.875128	13.913451
H	5.674363	-3.717595	14.562605
H	9.345772	-4.866147	10.373669
H	9.329251	-0.139887	7.318170
H	5.165551	-1.003674	4.055757
H	1.054622	-5.723631	7.872917
H	8.234441	-6.968671	9.808729
H	8.716711	-5.330372	8.057810
H	7.593229	3.863952	12.680446
H	6.246954	4.579402	10.770316
H	5.205156	3.331381	12.598510
H	3.192174	-5.179900	12.415350
H	1.140374	0.115863	14.594370
H	-3.513798	0.489931	15.578730
H	-2.116072	-4.602570	17.493560

Hab$_S$

G = -2343,571792 u.a.

La	1.266702	-1.864371	12.931276
Si	2.328479	-1.686285	9.669663
O	3.604779	-1.521026	6.304480
B	2.470554	0.336657	13.865283
H	3.019131	1.338896	14.231843
H	1.944028	0.498442	12.744349
H	1.578813	-0.017827	14.642074
O	0.907439	-2.017867	10.421019
H	1.577800	-3.946686	11.401202
Si	1.777576	-5.329012	6.416750
B	0.585309	-3.498407	10.789722
H	-0.355453	-3.434961	11.576932
H	0.414498	-4.756078	6.598684
H	1.826765	-6.161347	5.181803
C	-1.704568	-1.725846	14.756039
O	-2.501878	-0.631558	14.916057
C	-2.402412	0.396681	13.945869
H	-2.638150	0.030712	12.939726
H	-1.407716	0.853948	13.936056
H	-3.721912	-2.036368	16.414084
C	-3.052304	-2.892311	16.518814
H	-1.623098	-4.940780	15.508487
C	-1.051609	-4.022409	15.327316
H	-0.740242	-4.066284	14.276876
H	-0.228845	-2.492350	17.598238
C	-1.935345	-2.830409	15.515973
H	-2.693848	-2.896750	17.559749
C	0.581008	-2.770600	16.920793
H	1.507392	-2.840368	17.501885
O	1.866710	-3.684426	14.502965
H	0.685855	-1.963620	16.193846
H	2.496577	-5.992472	13.456045
C	2.853017	-6.106814	14.481500
H	3.054608	-7.152802	14.706433
H	-0.173179	-6.164980	16.908997
H	-0.816770	-4.896018	17.961386
C	0.038022	-5.184349	17.342832
H	0.911639	-5.281569	17.995291
O	1.827058	-5.711563	15.412822
C	1.384804	-4.473453	15.334794
O	2.895394	-4.079948	6.178549
Si	3.609164	-2.955738	7.123289
O	5.162972	-3.415843	7.451733
O	5.170316	-2.580373	12.723105
O	5.521870	-3.145843	10.114354
Si	6.278943	-2.273903	13.972184
Si	8.768950	-5.051677	8.209173
H	6.154026	-0.870373	14.447404
Si	6.288982	-3.291900	8.654206
Si	5.035548	-2.001089	11.194816
O	3.408967	-1.704094	10.964811
O	2.769045	-2.802076	8.547037
O	2.270302	-0.176653	9.013902
O	7.263239	-1.980367	8.393271

O	5.929115	-0.626193	11.027077
Si	5.927271	0.827853	10.225233
O	6.662906	1.948289	11.155863
Si	6.170059	3.358663	11.955786
C	0.249776	-4.118985	16.261494
O	-0.734625	-1.623168	13.866489
Si	3.222833	1.154253	8.731738
O	3.957181	1.011083	7.260510
Si	4.488378	-0.123548	6.190249
O	6.082934	-0.472723	6.472505
Si	7.191872	-0.482674	7.701251
O	8.703458	-0.192219	7.123588
O	7.198588	-4.649556	8.688666
O	2.302321	2.501711	8.759877
Si	0.665298	2.859067	8.535025
O	4.367359	1.283336	9.915221
O	6.773797	0.670029	8.815013
O	4.293165	0.536277	4.697276
H	0.148791	2.168969	7.317639
H	-0.112518	2.430025	9.732653
H	0.579732	4.336124	8.367329
H	0.331835	-4.180282	9.834746
H	7.663825	-2.543802	13.487742
H	5.928606	-3.228823	15.061651
H	9.757236	-4.431444	9.137926
H	8.871197	0.718907	6.865208
H	4.394376	-0.080263	3.966091
H	2.162464	-6.144324	7.603818
H	8.856526	-6.536872	8.286000
H	9.019894	-4.591705	6.813028
H	7.350883	3.808654	12.745163
H	5.803228	4.399027	10.951414
H	5.017131	3.069404	12.851015
H	3.748165	-5.499536	14.626545
H	3.270340	-0.605054	13.746947
H	-3.140251	1.146564	14.237834
H	-3.649548	-3.806052	16.392151

Fab_R

G = -2343,565076 u.a.

C	1.371796	-1.762404	18.240930
O	0.025582	-2.263368	18.343267
C	-0.674222	-2.359304	17.228140
C	-2.045058	-2.872276	17.438240
C	-2.835835	-3.002773	16.362248
O	-0.196564	-2.045297	16.129925
La	0.654927	-0.961033	14.082789
O	2.411292	-1.781615	12.605408
Si	3.275478	-1.559207	11.228556
O	2.700686	-0.143736	10.595712
Si	3.215629	1.157287	9.712697
O	2.951858	0.875658	8.106549
Si	2.810130	-0.378781	7.045053
O	2.282382	-1.760418	7.793007
Si	2.885708	-3.098006	8.553380
O	1.826323	-4.321004	8.305018
Si	1.941517	-6.006397	8.292191
O	-1.257723	-1.029467	13.009534
C	-2.528001	-1.282237	12.687723
O	-2.916378	-2.588488	12.927873
C	-2.220322	-3.556562	12.154463
B	1.246581	1.378229	15.244783
B	2.482820	-2.971134	13.590112
O	4.887021	-1.432455	11.579102
Si	6.356503	-1.711585	10.865394
O	7.460837	-2.084293	12.012991
Si	7.405105	-2.719742	13.577630
O	3.032845	-2.808015	10.174141
O	4.358903	-3.511305	7.920654
Si	5.968105	-3.235913	8.183588
O	6.485100	-1.936475	7.298330
Si	5.896112	-0.531337	6.663668
O	6.129432	0.727684	7.714812
Si	6.292673	1.002749	9.336440
O	6.881138	-0.352078	10.084301
O	6.788433	-4.573379	7.720253
Si	8.224408	-4.854501	6.875612
O	6.232436	-2.962216	9.792297
C	-3.417149	-0.382023	12.225766
C	-3.046950	1.061950	12.054634
C	-4.827031	-0.762845	11.877323
O	7.332974	2.245097	9.566420
Si	8.877555	2.388353	10.235175
O	4.828938	1.425706	9.979011
O	2.356145	2.460031	10.195830
Si	2.706868	4.089192	10.481876
C	-2.467775	-3.209838	18.840556
O	1.707938	0.067158	5.908439
O	4.279261	-0.666852	6.335342
O	6.743222	-0.285954	5.275205
H	0.088233	1.014815	15.509942
H	1.496215	2.443475	15.735711
H	1.339769	1.418632	14.003060
H	2.024545	0.495409	15.642510
H	9.310253	3.790992	9.980348
H	1.336755	-3.447648	13.627276
H	3.291943	-3.807163	13.292922
H	2.727194	-2.471674	14.700047
H	6.787252	-1.730489	14.506790
H	6.629680	-3.992968	13.594866
H	8.819954	-2.974226	13.970118
H	2.955913	-6.472319	9.281284
H	2.313510	-6.467432	6.923354
H	0.592760	-6.527010	8.653696
H	1.395998	4.773997	10.653529
H	3.529511	4.223928	11.717299
H	3.440008	4.667389	9.317356
H	8.553587	-6.292753	7.083724
H	9.320079	-3.994739	7.410136
H	8.022621	-4.579935	5.424013
H	8.828415	2.126129	11.702646
H	9.817476	1.433760	9.579216
H	1.367693	-0.740742	17.854987
H	1.963831	-2.404208	17.584844
H	-2.402455	-2.336243	19.496895
H	-3.851588	-3.371259	16.472740

H	-2.513763	-2.753305	15.355327
H	-3.204910	1.388631	11.017686
H	-1.825719	-3.982777	19.274991
H	-3.673197	1.710724	12.683317
H	-2.002645	1.249982	12.310503
H	-2.355519	-3.370167	11.081448
H	-2.646920	-4.529191	12.409371
H	-5.009290	-1.827733	12.029767
H	-5.054837	-0.518815	10.830190
H	-5.549655	-0.202621	12.487668
H	6.517747	0.520555	4.802163
H	1.183322	-0.660380	5.561687
H	-1.146779	-3.569442	12.378819
H	1.762949	-1.786706	19.256526
H	-3.498064	-3.571479	18.848250

Gab_R

G = -2343,552491 u.a.

C	0.430615	-1.084437	18.549062
O	-0.859232	-1.567156	18.162353
C	-1.026824	-1.923746	16.886581
C	-2.329094	-2.399909	16.556447
C	-2.541823	-2.883840	15.279812
O	-0.045630	-1.838096	16.083796
La	0.827219	-0.932512	14.073768
O	2.507237	-1.786086	12.531486
Si	3.360424	-1.584828	11.143529
O	2.780001	-0.182017	10.488764
Si	3.291355	1.102384	9.578972
O	3.008525	0.791596	7.980952
Si	2.868629	-0.479959	6.942913
O	2.344434	-1.848049	7.718683
Si	2.946582	-3.173166	8.500505
O	1.878803	-4.397212	8.289741
Si	2.016981	-6.078884	8.193497
O	-1.130267	-1.183907	12.884526
C	-2.369432	-1.553533	12.924039
O	-2.777807	-2.470632	12.025292
C	-1.820432	-2.952960	11.084562
B	1.409173	1.550448	14.846694
B	2.570288	-2.977781	13.516067
O	4.974210	-1.454430	11.477707
Si	6.438315	-1.752893	10.759763
O	7.549768	-2.106825	11.905128
Si	7.506190	-2.737236	13.473622
O	3.103003	-2.851896	10.114472
O	4.411616	-3.611613	7.866166
Si	6.023722	-3.332810	8.110884
O	6.536112	-2.053974	7.193153
Si	5.949076	-0.657039	6.539985
O	6.186616	0.622701	7.564352
Si	6.366877	0.930264	9.178752
O	6.960364	-0.409465	9.948971
O	6.836307	-4.681833	7.669412
Si	8.279321	-4.985950	6.844225
O	6.299420	-3.022338	9.710552
C	-3.297625	-1.130949	13.874775
C	-2.986198	0.088826	14.689726
C	-4.749291	-1.509555	13.733176
O	7.412514	2.174448	9.368203
Si	8.913845	2.356231	10.122180
O	4.908360	1.366578	9.824802
O	2.441985	2.419154	10.038996
Si	2.820351	4.030869	10.385586
C	-3.412517	-2.365029	17.604717
O	1.760452	-0.025755	5.815432
O	4.328957	-0.800078	6.227051
O	6.789054	-0.434354	5.143517
H	0.278731	1.209061	15.231721
H	1.668042	2.672758	15.177870
H	1.428296	1.425860	13.608665
H	2.223228	0.735383	15.314684
H	9.344210	3.756529	9.851634
H	1.426495	-3.452871	13.549339
H	3.394255	-3.804483	13.237796
H	2.804195	-2.470022	14.628266
H	6.891998	-1.744421	14.400954
H	6.733054	-4.011507	13.498391
H	8.924431	-2.986829	13.856050
H	3.039006	-6.579207	9.157143
H	2.388472	-6.471278	6.803286
H	0.674488	-6.629258	8.534188
H	1.521287	4.723681	10.606819
H	3.668065	4.107510	11.608526
H	3.538393	4.643975	9.229455
H	8.599713	-6.421255	7.082971
H	9.373309	-4.120122	7.372224
H	8.091242	-4.738070	5.385984
H	8.782669	2.134160	11.591158
H	9.899477	1.395476	9.547740
H	0.684796	-0.171826	18.003643
H	1.198030	-1.841499	18.369814
H	-3.617882	-1.350064	17.961700
H	-3.460402	-3.414273	15.053161
H	-1.688978	-3.135490	14.658998
H	-3.844039	0.770402	14.708470
H	-3.137494	-2.959735	18.482959
H	-2.755821	-0.164158	15.738239
H	-2.135227	0.650164	14.291236
H	-1.417058	-2.137880	10.477896
H	-2.366792	-3.651314	10.449932
H	-4.877046	-2.475981	13.241064
H	-5.298558	-0.763576	13.141784
H	-5.234005	-1.555233	14.715098
H	6.640068	0.412865	4.713281
H	1.448999	-0.736832	5.247828
H	-0.995598	-3.474725	11.578580
H	0.350960	-0.873208	19.615119
H	-4.341779	-2.774030	17.200063

Hab_R

G = -2343,574336 u.a.

C	-0.319731	-2.678030	18.579752
O	-1.477353	-2.676512	17.761188
C	-1.296758	-2.465647	16.426197
C	-2.262734	-2.855294	15.553980

C	-2.060805	-2.579017	14.095183
O	-0.179786	-1.849008	16.074206
La	1.291489	-0.703038	14.856641
O	2.987159	-1.427316	13.209738
Si	3.553282	-1.428794	11.674499
O	2.781990	-0.171935	10.918767
Si	3.034187	0.980216	9.762371
O	2.419030	0.438698	8.325766
Si	2.173749	-0.991812	7.541916
O	1.886182	-2.212845	8.624904
Si	2.699181	-3.405874	9.435011
O	1.661192	-4.657890	9.616231
Si	1.836031	-6.317903	9.889320
O	-0.363090	-0.385097	13.027751
C	-1.520753	-0.621230	12.638976
O	-1.874321	-0.386331	11.397036
C	-0.873438	0.144739	10.501371
B	1.583377	1.732547	15.881628
B	3.434262	-2.344597	14.371926
O	5.189106	-1.198617	11.636851
Si	6.493156	-1.578542	10.688347
O	7.833428	-1.721433	11.609800
Si	8.195487	-2.305565	13.156663
O	3.169064	-2.849720	10.917957
O	4.020730	-3.899746	8.569931
Si	5.635669	-3.562696	8.444182
O	5.894324	-2.436198	7.256884
Si	5.119607	-1.169310	6.540958
O	5.489478	0.262406	7.286595
Si	5.973312	0.820897	8.766557
O	6.770475	-0.366707	9.595134
O	6.411798	-4.948337	8.056691
Si	7.634699	-5.367320	6.967463
O	6.203587	-2.996267	9.888193
C	-2.597402	-1.187284	13.538263
C	-2.802365	-0.159133	14.668577
C	-3.920023	-1.391604	12.791687
O	6.966491	2.101225	8.547623
Si	8.543638	2.479944	9.026512
O	4.645127	1.325879	9.617946
O	2.220970	2.333600	10.197664
Si	2.676279	3.942585	10.469061
C	-3.514524	-3.551461	16.006465
O	0.841518	-0.748162	6.605472
O	3.477920	-1.394142	6.606706
O	5.638251	-1.144882	4.980890
H	0.387859	1.468622	15.666308
H	1.717401	2.805601	16.397606
H	2.191090	1.657969	14.803419
H	2.019050	0.824473	16.620529
H	8.813523	3.848638	8.504482
H	2.455579	-3.048067	14.652571
H	4.408071	-3.003856	14.132180
H	3.644431	-1.577521	15.331129
H	7.768266	-1.309634	14.179347
H	7.514987	-3.611660	13.387195
H	9.674696	-2.480181	13.194116
H	3.032001	-6.585684	10.738540
H	1.969977	-7.019393	8.580030
H	0.595831	-6.764873	10.583145
H	1.433389	4.652582	10.880357
H	3.698551	4.012721	11.550837
H	3.215577	4.536785	9.211658
H	8.090985	-6.729943	7.359881
H	8.765189	-4.398598	7.058637
H	7.090722	-5.387830	5.579204
H	8.647544	2.465472	10.514001
H	9.505695	1.504841	8.436999
H	0.181660	-1.705234	18.581344
H	0.395662	-3.448944	18.268334
H	-4.410714	-2.918154	15.920180
H	-2.551231	-3.361626	13.503192
H	-0.991808	-2.660360	13.864006
H	-3.117275	0.807750	14.260801
H	-3.436581	-3.856036	17.051938
H	-3.581052	-0.518925	15.344352
H	-1.898447	-0.011266	15.262398
H	-0.475199	1.082732	10.890194
H	-1.391492	0.303087	9.557498
H	-3.803598	-2.070135	11.942142
H	-4.328027	-0.447813	12.417939
H	-4.649738	-1.829860	13.478555
H	5.462478	-0.325463	4.508952
H	0.593401	-1.496907	6.054879
H	-0.063278	-0.574726	10.378566
H	-0.672467	-2.902395	19.588163
H	-3.709598	-4.449445	15.404085

H_{syndio}

G = -2343,553124 u.a.

La	0.595653	-1.117013	11.858667
H	-0.891509	-2.657061	10.602141
B	0.106884	-3.083278	9.981321
H	0.928491	-3.452663	10.847663
H	-0.203418	-3.986410	9.255918
H	0.309007	1.161413	12.828259
O	0.679430	-1.859147	9.262141
B	-0.358349	1.364302	11.799784
H	-1.242582	0.480478	11.772251
H	-0.845284	2.459136	11.791217
H	0.379817	1.174781	10.823163
O	2.798215	-0.974846	10.380504
Si	2.246803	-1.621769	8.906147
H	3.083189	4.103408	11.263643
Si	4.362842	4.497777	10.609861
Si	3.447527	0.812861	7.420013
H	4.100115	5.096566	9.270857
H	3.586845	-1.968765	15.111075
H	2.685760	0.327781	15.133180
Si	3.641365	-0.617785	14.503503
H	3.056820	-6.545866	8.848337
O	3.150178	-0.753625	12.846932
Si	4.057922	-0.789241	11.448311
H	2.144106	-5.790499	6.705818
O	2.462232	-0.491765	7.732170
O	3.890569	1.503684	8.859257

H	0.064831	1.972005	6.946224
H	0.862991	0.897627	4.897712
H	1.035377	3.325025	5.150146
Si	1.081601	2.016539	5.858421
O	2.638352	1.904254	6.521376
H	4.026711	-7.353383	6.751304
O	3.112967	-2.986062	8.596198
Si	3.377128	-6.200900	7.434657
O	4.512051	-4.941655	7.392052
Si	4.588125	-3.415487	7.958891
O	0.201478	-1.979664	13.835173
C	-0.103015	-2.519778	15.018217
O	-1.129201	-1.907858	15.688275
H	-1.957562	-0.189325	16.338350
C	-1.109536	-0.490716	15.720287
H	-0.183742	-0.113605	16.176513
H	-1.223297	-0.049409	14.724672
C	0.482958	-3.615097	15.553626
C	0.117492	-4.091198	16.932539
H	-0.475787	-3.344741	17.462950
H	1.017870	-4.312268	17.519067
H	-0.474121	-5.017323	16.907151
C	1.508071	-4.398034	14.780210
H	2.450789	-4.446210	15.343305
H	1.720096	-3.885150	13.836299
C	1.134097	-5.866980	14.417129
C	-0.251046	-5.943854	13.773101
C	2.199570	-6.402354	13.438058
C	1.269129	-6.728908	15.672204
O	0.219568	-7.549910	15.875143
C	0.332997	-8.402495	17.016713
O	5.055982	-2.087682	11.439275
Si	6.331949	-2.616598	10.497617
O	7.283639	-1.319447	10.121150
Si	7.496250	-0.221485	8.903936
O	7.073115	-0.886054	7.450471
Si	5.781579	-0.985563	6.415551
O	6.283890	-0.950095	4.852420
O	4.859056	0.617446	11.203345
Si	5.173298	1.613096	9.895066
O	6.568543	1.127258	9.167369
O	5.750171	-3.321544	9.129495
O	4.969222	-2.398175	6.715444
O	4.800077	0.323796	6.613280
O	5.363764	3.139494	10.432046
O	7.164885	-3.702205	11.380936
Si	8.793497	-3.969116	11.764664
O	9.092248	0.162312	8.936968
H	9.618747	-3.948888	10.523197
H	8.850056	-5.309793	12.408129
H	5.026357	-0.070098	14.503375
H	3.199634	-6.332599	13.875434
H	9.352480	0.895098	8.370882
H	6.706679	-1.755590	4.540238
H	9.261070	-2.916064	12.710457
H	5.118482	5.451547	11.467418
H	-0.500475	-6.968704	13.485678
H	-1.030413	-5.578366	14.445878
H	-0.267635	-5.322017	12.871793
H	2.010228	-7.449834	13.179020
H	2.177421	-5.818608	12.511671
H	-0.579991	-8.998158	17.033696
H	1.211323	-9.047863	16.932223
H	0.421785	-7.811459	17.931958
O	2.240216	-6.720137	16.400295

A'$_{BH4}$

G = -2343,559798 u.a.

C	1.590708	-2.233548	17.087867
O	0.590374	-2.992210	16.423371
C	1.040820	-3.735112	15.346603
C	0.793319	-5.060641	15.302477
C	1.133741	-5.877221	14.090299
O	1.643224	-3.020883	14.397544
La	1.826382	-1.443218	12.843893
B	2.930003	0.784776	13.881390
B	0.588851	-2.385088	10.492773
O	1.219946	-0.993136	10.225479
Si	2.704119	-0.945540	9.549494
O	3.117883	0.569327	9.044288
Si	4.480392	1.524282	9.108695
O	5.384457	1.289993	7.745054
Si	5.785596	0.130618	6.644907
O	7.160069	-0.667149	7.109971
Si	8.004638	-1.073144	8.474713
O	9.614017	-1.170012	8.156698
O	3.684064	-1.324722	10.869041
Si	5.020156	-2.150067	11.404925
O	5.408202	-3.395353	10.406469
Si	6.252835	-3.594231	8.986685
O	5.277812	-3.281367	7.690418
Si	4.009186	-2.385462	7.121574
O	4.565353	-0.976645	6.464921
O	4.412400	-2.715026	12.837318
Si	5.054439	-3.719161	14.077458
O	-0.366734	-0.427755	13.416062
C	-1.519205	0.015044	13.438667
C	-2.565578	-0.407986	14.396456
C	-2.223592	-1.294739	15.342592
O	2.950471	-2.052688	8.355106
O	6.282537	-1.117387	11.601284
Si	6.732346	0.345303	10.932243
O	7.570898	1.213477	12.025501
Si	7.276762	2.072859	13.457199
C	0.125581	-5.785516	16.435312
O	4.040136	3.093843	9.210189
Si	2.865581	4.074465	8.496546
O	5.372275	1.146840	10.444220
O	6.754498	-5.146718	8.950995
Si	7.156966	-6.266284	7.749673
O	7.549119	-2.574234	8.987486
O	7.726036	0.067640	9.642637
O	3.240388	-3.238121	5.960118
Si	1.705479	-3.937226	5.803683
O	6.028467	0.927284	5.227293
O	-1.933379	0.938472	12.588413

C	-0.978813	1.424280	11.625440
C	-3.938838	0.186008	14.253966
H	-0.197552	-2.215951	11.429067
H	1.491452	-3.144530	10.895844
H	0.034687	-2.849552	9.532464
H	4.768524	-3.052689	15.372090
H	6.524747	-3.821047	13.848363
H	4.413859	-5.054174	13.977533
H	1.820419	-6.698446	14.340544
H	2.583338	3.622005	7.103258
H	1.615582	4.016638	9.308927
H	3.407074	5.461541	8.491926
H	1.691328	-4.583026	4.461031
H	7.985719	-7.312472	8.409578
H	10.076818	-0.326857	8.156823
H	6.185012	0.360985	4.465852
H	1.496315	-4.956209	6.870438
H	0.655869	-2.881843	5.878843
H	5.911148	-6.868191	7.194092
H	7.930978	-5.601268	6.661360
H	8.581788	2.690401	13.827040
H	6.252479	3.125217	13.215073
H	6.831562	1.132188	14.522615
H	-0.835511	-6.217449	16.120287
H	0.740608	-6.627812	16.783167
H	-0.063560	-5.125151	17.282993
H	0.235959	-6.346735	13.663075
H	1.598742	-5.273305	13.308471
H	1.094544	-1.717711	17.912918
H	2.373587	-2.889064	17.492395
H	2.049991	-1.490136	16.427507
H	-1.522848	2.156864	11.031304
H	-0.137235	1.895274	12.138617
H	-0.617949	0.608513	10.995213
H	-4.608329	-0.220035	15.015364
H	-3.913912	1.275472	14.358967
H	-4.364287	-0.028098	13.268285
H	-2.959825	-1.631255	16.066983
H	-1.220737	-1.702823	15.431467
H	2.095970	0.285048	14.649466
H	3.782313	-0.086621	13.652754
H	2.354381	1.031943	12.809939
H	3.422915	1.775142	14.350179

B'$_{BH4}$

G = -2343,529391 u.a.

C	-0.553383	-3.613543	16.253451
O	-0.485514	-4.755730	15.421287
C	0.641699	-4.866153	14.642611
C	1.257677	-6.062611	14.529830
C	2.390789	-6.276794	13.570880
O	0.998736	-3.747880	14.009053
La	1.337011	-1.994407	12.747053
B	2.777000	0.007345	14.555528
B	0.356085	-2.772043	10.260946
O	0.939788	-1.347788	10.125690
Si	2.463198	-1.146919	9.588095
O	2.751441	0.397682	9.089866
Si	3.988854	1.506489	9.170765
O	5.009118	1.314612	7.888810
Si	5.607850	0.190876	6.841709
O	7.031272	-0.433896	7.413919
Si	7.811025	-0.709830	8.848126
O	9.439745	-0.634154	8.652072
O	3.338426	-1.414142	11.012980
Si	4.759532	-2.026029	11.622213
O	5.337070	-3.226141	10.662968
Si	6.317279	-3.389032	9.327031
O	5.416060	-3.236670	7.950156
Si	4.094874	-2.495076	7.286735
O	4.534101	-1.050817	6.616366
O	4.182489	-2.637609	13.050259
Si	4.987905	-3.205481	14.466467
O	-0.452625	-0.603982	13.370274
C	-0.834329	0.613725	13.487528
C	-0.415743	1.468636	14.519245
C	0.409960	0.891266	15.503830
O	2.947177	-2.239106	8.456875
O	5.873519	-0.844113	11.849800
Si	6.222324	0.637314	11.169834
O	6.874106	1.595786	12.315992
Si	6.511445	3.114009	12.974181
C	0.800249	-7.264281	15.304734
O	3.363683	3.014148	9.161964
Si	1.954513	3.735539	8.563389
O	4.823990	1.302213	10.583691
O	7.010972	-4.863662	9.378434
Si	6.916519	-6.284428	8.466072
O	7.490412	-2.233558	9.390170
O	7.311160	0.426868	9.947266
O	3.486041	-3.460974	6.121566
Si	1.977147	-4.161510	5.795503
O	5.849833	0.985411	5.423772
O	-1.664379	1.123826	12.568022
C	-2.118344	0.248454	11.531958
C	-0.685478	2.947604	14.470198
H	-0.510881	-2.689426	11.139537
H	1.257879	-3.517333	10.701440
H	-0.096852	-3.211691	9.239261
H	5.744568	-2.075759	15.066963
H	5.916488	-4.296440	14.053635
H	3.917758	-3.704904	15.362544
H	3.280457	-6.670203	14.083365
H	1.673417	3.251380	7.180575
H	0.809441	3.411283	9.460996
H	2.208412	5.202622	8.557540
H	2.110998	-4.799738	4.456160
H	7.753809	-7.287971	9.178480
H	9.798487	0.253401	8.550622
H	6.099190	0.426551	4.682287
H	1.661774	-5.185242	6.830274
H	0.923164	-3.108296	5.763175
H	5.501816	-6.749650	8.387553
H	7.451033	-6.042572	7.095532
H	7.501881	3.331022	14.065763
H	6.663728	4.162688	11.925507

H	5.122773	3.124282	13.514349
H	0.412141	-8.046974	14.639197
H	1.635146	-7.716342	15.859361
H	0.013725	-7.009305	16.016299
H	2.128409	-7.016929	12.800811
H	2.676338	-5.355654	13.057658
H	-1.456610	-3.729142	16.858236
H	0.316878	-3.546770	16.919736
H	-0.635506	-2.685566	15.673117
H	-2.817765	0.841115	10.943815
H	-1.288234	-0.083460	10.902811
H	-2.623307	-0.623829	11.952347
H	-0.734877	3.370780	15.479215
H	0.091843	3.497919	13.920245
H	-1.638571	3.153240	13.974291
H	0.652659	1.497160	16.375808
H	0.271972	-0.161983	15.731931
H	1.770047	0.771316	15.061801
H	2.459978	-1.112587	14.938681
H	2.663775	0.188071	13.348515
H	3.812499	0.408416	15.020068

C'$_{BH4}$

G = -2343,528877 u.a.

C	-0.479424	-3.533794	16.420514
O	-0.529074	-4.662477	15.568460
C	0.523968	-4.803754	14.697750
C	1.081454	-6.020353	14.519925
C	2.121303	-6.264593	13.466954
O	0.870257	-3.690571	14.049482
La	1.215154	-1.957878	12.756723
O	3.243587	-1.404697	11.039021
Si	4.651945	-2.036479	11.658880
O	5.227494	-3.242914	10.707813
Si	6.209334	-3.413578	9.375885
O	5.330003	-3.241550	7.988137
Si	4.015377	-2.497830	7.314183
O	4.466870	-1.057396	6.643428
Si	5.549238	0.174816	6.878697
O	6.964635	-0.461312	7.459194
Si	7.731491	-0.748585	8.897834
O	9.362282	-0.689892	8.710024
O	-0.519310	-0.526829	13.361751
C	-0.905053	0.702581	13.460727
C	-0.483184	1.563733	14.467509
C	0.372090	0.995612	15.465731
B	2.628767	0.074851	14.598756
B	0.253134	-2.745386	10.271108
O	0.851088	-1.328991	10.130401
Si	2.379990	-1.139334	9.605353
O	2.685195	0.401898	9.106657
Si	3.930134	1.501007	9.200728
O	3.318084	3.013863	9.190525
Si	1.920820	3.750092	8.581765
O	-1.743524	1.191279	12.528289
C	-2.205706	0.292902	11.520080
C	0.643714	-7.214946	15.317071
O	2.864899	-2.236904	8.480736
O	3.405126	-3.451998	6.140313
Si	1.971291	-4.329561	5.918840
O	5.776820	-0.864905	11.897405
Si	6.141993	0.610856	11.212901
O	6.794837	1.564508	12.363088
Si	6.456450	3.095158	13.004278
O	4.056303	-2.641621	13.081472
Si	4.838546	-3.292694	14.474080
O	7.234624	0.388426	9.997490
O	4.752785	1.286999	10.619745
O	7.399104	-2.271471	9.437997
O	6.854952	-4.908725	9.456722
Si	7.536197	-6.006567	8.364808
O	4.958635	1.302471	7.926243
O	5.805432	0.966639	5.461640
C	-0.753552	3.042622	14.421590
H	-0.620654	-2.649118	11.141791
H	1.144926	-3.495157	10.723557
H	-0.195191	-3.189148	9.249242
H	5.458707	-2.171664	15.229763
H	5.881073	-4.248379	14.006434
H	3.774159	-3.970418	15.251784
H	3.036373	-6.694305	13.899250
H	1.643979	3.265262	7.198633
H	0.767046	3.441916	9.473709
H	2.192255	5.214036	8.573053
H	2.120458	-5.016942	4.605697
H	8.405937	-6.911697	9.164966
H	9.725304	0.186805	8.553279
H	5.985049	0.399334	4.706021
H	1.812237	-5.328148	7.012877
H	0.809016	-3.397972	5.886800
H	6.448978	-6.782775	7.703166
H	8.342661	-5.281872	7.340012
H	7.453379	3.313123	14.088468
H	6.617154	4.129662	11.941529
H	5.071559	3.129834	13.550619
H	0.174688	-7.974422	14.674605
H	1.502643	-7.705249	15.797259
H	-0.074653	-6.941893	16.091232
H	1.767927	-6.987077	12.716941
H	2.396017	-5.349591	12.937222
H	-1.340993	-3.614479	17.086929
H	0.439867	-3.524807	17.022836
H	-0.551912	-2.593428	15.862158
H	-2.911568	0.870746	10.922288
H	-1.384704	-0.056291	10.887965
H	-2.711053	-0.570171	11.961927
H	-0.966635	3.440510	15.420200
H	0.099531	3.610214	14.021951
H	-1.613391	3.261117	13.785323
H	0.593208	1.627484	16.327696
H	0.170182	-0.033187	15.756168
H	1.576239	0.857551	15.038313
H	2.336844	-1.036861	14.998923
H	2.509001	0.275066	13.401925
H	3.582449	0.579093	15.120097

*Second propagation step of MMA polymerization mediated by $(BH_4)_2La$@**c**-1*

Iaa_Sa_S

G = -2689,149697 u.a.

C	-5.023676	-4.900008	12.926479
C	-3.557612	-4.792917	13.237642
C	-3.006684	-5.148395	14.407709
C	-2.655595	-4.258998	12.191061
O	-3.282120	-3.970345	11.062172
C	-2.486483	-3.418938	9.997801
O	-1.438201	-4.094715	12.315824
La	0.685701	-3.184139	13.309820
O	2.288798	-3.086310	11.399160
B	2.376799	-4.620495	11.644164
Si	3.442749	-2.301218	10.543557
O	3.594435	-2.959459	9.032402
Si	3.908846	-2.567448	7.459856
O	3.477505	-1.003527	7.142696
Si	4.122766	0.519546	7.243551
O	3.894931	1.187833	8.730456
Si	3.670961	0.783989	10.316080
O	5.130951	0.791662	11.106679
Si	6.734402	0.580992	10.772234
O	7.592390	1.555574	11.770657
Si	8.977443	1.367357	12.716072
O	4.901192	-2.399502	11.330731
Si	6.511360	-2.506660	10.990197
O	7.182737	-0.994015	11.035402
O	0.347483	-4.671543	14.997471
C	0.886176	-5.221289	16.068717
O	1.157779	-6.563475	15.989491
C	0.675595	-7.266201	14.860265
B	-0.575366	-0.797143	13.408825
O	2.984837	-0.716723	10.425542
O	2.672505	1.880531	10.997356
Si	2.703833	2.885464	12.353887
O	7.229564	-3.427848	12.142511
Si	8.183393	-4.823103	12.069713
O	6.764893	-3.202495	9.510449
Si	6.972665	-2.770047	7.927065
O	5.519548	-2.780590	7.142067
C	1.189282	-4.585716	17.233991
C	1.700873	-5.366080	18.417661
C	0.903690	-3.114894	17.368903
C	2.121347	-2.136184	17.310737
C	1.601078	-0.694551	17.140327
C	2.981157	-2.223182	18.575736
C	2.912709	-2.488373	16.065389
O	4.187061	-2.753262	16.256013
C	4.969368	-3.095137	15.093674
O	7.658660	-1.266457	7.831512
Si	7.191667	0.312459	7.703898
O	8.383516	1.051367	6.843535
O	7.972466	-3.865013	7.234681
Si	9.262229	-3.768904	6.147428
O	5.745897	0.442357	6.909640
O	7.046260	0.999611	9.203980
O	3.363782	1.497664	6.160032
O	3.029762	-3.522717	6.460726
Si	2.452183	-5.107623	6.546111
O	2.424912	-2.494013	14.928204
H	-3.627149	-5.540771	15.208452
H	-1.939537	-5.056976	14.597987
H	-5.564727	-5.305318	13.784186
H	-5.449047	-3.922176	12.679055
H	-3.177766	-3.273426	9.169306
H	-1.691653	-4.114554	9.720739
H	8.881966	-2.952939	4.957968
H	-0.757412	-1.332760	12.306325
H	9.560789	-5.168975	5.734270
H	-1.136986	0.261863	13.488107
H	-0.983640	-1.582428	14.283269
H	8.530366	-5.151356	13.481769
H	7.420329	-5.945256	11.453786
H	9.426836	-4.557890	11.289547
H	0.650162	-0.679214	13.559880
H	2.730124	-4.770915	12.819527
H	1.216917	-5.036181	11.532261
H	3.118622	-5.184694	10.884263
H	0.406688	-2.909655	18.329513
H	1.354620	3.505196	12.452452
H	3.005667	2.094816	13.581943
H	3.742300	3.942223	12.171526
H	2.198376	-5.538243	5.141942
H	8.240138	1.988024	6.678498
H	3.120719	1.063393	5.337109
H	3.458484	-6.001668	7.186700
H	1.177248	-5.134492	7.320415
H	10.450818	-3.168329	6.818417
H	10.072797	0.738534	11.921917
H	9.377814	2.735168	13.149814
H	8.670718	0.524422	13.908613
H	2.797394	-5.382551	18.500907
H	1.320434	-4.940481	19.355287
H	1.379132	-6.409762	18.366835
H	0.196678	-2.810285	16.588819
H	0.994022	-8.301339	15.002038
H	-0.418665	-7.235401	14.791013
H	1.097914	-6.885332	13.924749
H	-2.051839	-2.466722	10.309083
H	-5.201338	-5.551055	12.064455
H	3.807090	-1.506406	18.546781
H	2.358979	-1.987182	19.444860
H	3.402972	-3.218819	18.719439
H	2.421573	0.030919	17.130460
H	1.023589	-0.579673	16.219311
H	0.948770	-0.451501	17.985194
H	5.980362	-3.251088	15.465092
H	4.580042	-4.004743	14.633608
H	4.944485	-2.283131	14.366134

Jaa_Sa_S

G = -2689,127686 u.a.

C	-3.572131	-4.364834	15.415061

C	-2.347298	-3.555992	15.066487
C	-1.475937	-3.077233	16.040935
C	-2.092632	-3.239832	13.707237
O	-3.035723	-3.662765	12.850099
C	-2.882010	-3.301837	11.476314
O	-1.104699	-2.580624	13.248716
La	1.256585	-2.789466	13.115277
O	1.977345	-2.858850	10.719779
B	1.684581	-4.368403	10.881831
Si	3.271102	-2.207146	9.945024
O	3.800371	-3.190997	8.729453
Si	4.516775	-3.134487	7.238747
O	4.122225	-1.730852	6.461469
Si	4.670524	-0.174285	6.312279
O	4.033092	0.806311	7.470332
Si	3.425065	0.764004	9.006014
O	4.633916	1.130088	10.077394
Si	6.277818	1.013427	10.204213
O	6.845844	2.255971	11.104654
Si	6.119049	3.547828	11.919014
O	4.480943	-2.009291	11.068415
Si	6.127885	-1.952213	11.156848
O	6.688246	-0.410265	10.946021
O	0.752598	-4.739009	14.467966
C	0.214027	-5.090964	15.564433
O	-0.539220	-6.204484	15.578549
C	-0.675278	-6.914363	14.346908
B	1.607398	-0.176098	13.586016
O	2.816207	-0.738604	9.340816
O	2.252342	1.890831	9.123402
Si	0.655067	2.031387	9.654807
O	6.581889	-2.469817	12.650538
Si	7.661885	-1.822320	13.779865
O	6.783655	-2.958424	10.022657
Si	7.366857	-2.898204	8.475937
O	6.159370	-3.238990	7.402737
C	0.250717	-4.353618	16.762576
C	-0.330912	-4.961048	18.017236
C	1.311449	-3.285289	16.928362
C	2.816347	-3.688536	17.019753
C	3.610549	-2.441140	17.477238
C	3.050225	-4.839100	18.000602
C	3.360823	-3.999979	15.632548
O	4.134689	-5.062424	15.568000
C	4.734450	-5.363197	14.289265
O	8.003087	-1.401162	8.164058
Si	7.529422	0.047580	7.528300
O	8.872687	0.672752	6.813102
O	8.545229	-4.024832	8.329862
Si	10.128989	-4.013182	7.743555
O	6.325462	-0.175973	6.415162
O	6.984309	1.071453	8.711576
O	4.185056	0.442373	4.866298
O	3.986946	-4.378697	6.318543
Si	3.275712	-5.881335	6.623162
O	3.176017	-3.274173	14.650312
H	-1.817223	-3.067731	17.071719
H	-0.786716	-2.282421	15.769914
H	-3.640932	-4.496912	16.498196
H	-4.490506	-3.872172	15.075823
H	-3.757507	-3.710414	10.971223
H	-1.970555	-3.734182	11.054471
H	10.165250	-3.487747	6.348178
H	0.795527	-0.359610	12.667803
H	10.588818	-5.430464	7.768812
H	1.776468	0.990320	13.814887
H	1.162487	-0.772126	14.584316
H	7.143688	-0.534352	14.321436
H	7.751653	-2.832411	14.874078
H	9.005442	-1.621995	13.164870
H	2.665609	-0.738257	13.266995
H	2.384521	-4.778480	11.822617
H	0.502465	-4.422597	11.244583
H	1.864585	-5.011397	9.884605
H	1.090276	-2.745700	17.858001
H	-0.047491	0.721460	9.539656
H	0.645887	2.509122	11.064364
H	0.002894	3.036722	8.767259
H	3.519374	-6.709556	5.407736
H	8.791055	1.589971	6.535447
H	4.303612	-0.151372	4.119066
H	3.901120	-6.522965	7.814689
H	1.810679	-5.710101	6.836611
H	10.996772	-3.179325	8.624644
H	7.231357	4.296818	12.569451
H	5.408450	4.430927	10.949557
H	5.166660	3.042102	12.947537
H	0.355842	-5.652618	18.522289
H	-0.578519	-4.175761	18.742212
H	-1.244465	-5.519144	17.800186
H	1.244368	-2.515995	16.146396
H	-1.276111	-7.792477	14.586113
H	-1.183104	-6.309720	13.592500
H	0.300083	-7.220498	13.960311
H	-2.851771	-2.215546	11.359830
H	-3.562758	-5.361124	14.960046
H	4.116160	-5.049459	18.119066
H	2.646348	-4.565925	18.980223
H	2.558836	-5.757403	17.670802
H	4.686914	-2.641051	17.500631
H	3.428569	-1.590859	16.814361
H	3.298169	-2.167543	18.489868
H	5.377628	-6.222158	14.473656
H	3.957264	-5.613227	13.564223
H	5.312134	-4.510438	13.929021

Kaa_Sa_S

G = -2689,150823 u.a.

C	-3.437915	-3.948521	15.717037
C	-2.163402	-3.404062	15.130781
C	-1.081577	-2.884763	16.038174
C	-1.997138	-3.280713	13.780345
O	-2.987010	-3.762483	12.968559
C	-2.983310	-3.321260	11.619596
O	-0.958481	-2.753124	13.175359
La	1.298055	-2.772119	13.008583

O	2.058237	-2.979054	10.634583
B	1.936324	-4.493464	10.933366
Si	3.336451	-2.282349	9.871761
O	3.908907	-3.238682	8.653417
Si	4.645813	-3.136736	7.174902
O	4.200481	-1.743110	6.405951
Si	4.681823	-0.163069	6.271181
O	3.993246	0.782858	7.428516
Si	3.374244	0.702076	8.958865
O	4.557234	1.109669	10.043605
Si	6.202754	1.058825	10.186984
O	6.712469	2.315216	11.102634
Si	5.931458	3.577840	11.912993
O	4.531496	-2.049524	11.004013
Si	6.171872	-1.919002	11.114695
O	6.667026	-0.352945	10.920557
O	0.676028	-4.764687	14.477719
C	0.060639	-4.979186	15.525824
O	-0.507168	-6.148961	15.756968
C	-0.514897	-7.088358	14.666565
B	1.795619	-0.173944	13.458467
O	2.830628	-0.829868	9.271782
O	2.153342	1.775650	9.075853
Si	0.537915	1.842411	9.565362
O	6.625251	-2.424923	12.613529
Si	7.713757	-1.769065	13.729358
O	6.888446	-2.887204	9.983752
Si	7.474562	-2.789411	8.440225
O	6.288843	-3.172573	7.356642
C	-0.088053	-3.959270	16.637652
C	-0.716786	-4.577071	17.895354
C	1.258796	-3.241398	16.962827
C	2.612446	-3.991183	17.047651
C	3.609204	-3.050764	17.777275
C	2.547116	-5.324152	17.802305
C	3.232496	-4.153522	15.659809
O	4.066599	-5.169822	15.567113
C	4.781097	-5.325338	14.320669
O	8.046093	-1.264223	8.141150
Si	7.517656	0.169151	7.514278
O	8.839780	0.856966	6.817053
O	8.702332	-3.862596	8.297722
Si	10.240165	-3.818297	7.601597
O	6.334521	-0.095438	6.387985
O	6.919650	1.158127	8.701161
O	4.183038	0.441340	4.824428
O	4.186713	-4.400286	6.242437
Si	3.306252	-5.819923	6.499854
O	3.070295	-3.360309	14.731355
H	-1.518463	-2.356018	16.897424
H	-0.493578	-2.137123	15.492847
H	-3.754978	-3.352354	16.583731
H	-4.244813	-3.927173	14.980946
H	-3.865508	-3.773180	11.161466
H	-2.087027	-3.648924	11.084101
H	10.169719	-3.290785	6.208165
H	1.009480	-0.340852	12.511349
H	10.731498	-5.225239	7.591803
H	1.999456	0.990729	13.667409
H	1.278307	-0.726300	14.446576
H	7.181817	-0.497029	14.294676
H	7.840763	-2.788249	14.812069
H	9.043112	-1.538329	13.094557
H	2.840917	-0.780428	13.194361
H	2.643990	-4.725093	11.931229
H	0.758931	-4.660764	11.258066
H	2.253018	-5.196897	10.013517
H	1.103432	-2.758554	17.934258
H	-0.060264	0.477421	9.572148
H	0.467064	2.455826	10.919562
H	-0.172108	2.703499	8.575893
H	3.411325	-6.600342	5.234030
H	8.724986	1.775685	6.556648
H	4.344222	-0.137121	4.073216
H	3.892935	-6.596389	7.629260
H	1.879197	-5.495152	6.782150
H	11.148673	-2.967132	8.423027
H	7.012051	4.374005	12.561365
H	5.186868	4.428683	10.940187
H	5.000599	3.036464	12.942523
H	-0.124008	-5.395375	18.309124
H	-0.812138	-3.801450	18.661820
H	-1.715069	-4.963099	17.683846
H	1.405748	-2.414478	16.260133
H	-1.042549	-7.962250	15.045462
H	-1.040784	-6.657776	13.812728
H	0.505389	-7.347188	14.377008
H	-3.056503	-2.230017	11.551008
H	-3.353237	-4.989027	16.065170
H	3.540716	-5.766737	17.898548
H	2.153343	-5.153091	18.808325
H	1.903740	-6.054951	17.304693
H	4.614456	-3.482526	17.797360
H	3.658292	-2.071551	17.292178
H	3.279987	-2.908665	18.811111
H	5.458966	-6.161114	14.485951
H	4.079855	-5.549278	13.514423
H	5.332316	-4.415086	14.080138

Iaa_Sb_S

G = -2689,152671 u.a.

C	-2.857398	-3.053165	10.935601
O	-3.428839	-3.457576	12.192331
C	-2.607873	-3.531286	13.227605
C	-3.287893	-3.930617	14.481766
C	-4.772697	-4.157643	14.444848
O	-1.402019	-3.292545	13.115628
La	0.826601	-2.201260	13.532311
O	7.106282	-2.780972	11.626682
Si	8.009167	-4.210960	11.576166
O	0.851188	-3.386288	15.473241
C	1.573987	-3.735058	16.519945
O	1.909429	-5.062272	16.610656
C	1.272591	-5.963900	15.725759
O	4.732231	-1.745488	10.970216
Si	3.192880	-1.657497	10.355838

O	3.143066	-2.429313	8.892497
Si	3.309968	-2.121138	7.277028
O	4.876049	-2.398333	6.817280
Si	6.411343	-2.400563	7.424271
O	7.120508	-0.926725	7.167891
Si	6.691541	0.653568	6.960454
O	6.728817	1.444314	8.415529
Si	6.564735	1.131731	10.030638
O	7.528278	2.142479	10.886429
Si	9.142865	2.114932	11.377615
O	2.133024	-2.334444	11.404522
B	2.222860	-3.838869	11.784482
B	-0.510348	0.143326	13.443223
C	2.014139	-2.908264	17.507934
C	1.680802	-1.442258	17.450205
C	2.823897	-0.466567	17.017650
C	3.427400	-1.040198	15.748848
O	4.717529	-1.290038	15.797487
C	5.325461	-1.849607	14.615633
C	2.746296	-3.468684	18.700287
C	-2.531130	-4.064192	15.580946
Si	6.296549	-1.928510	10.482313
O	6.385228	-2.742049	9.043786
O	7.000778	-0.436769	10.344271
O	5.008229	1.411251	10.506444
Si	3.469949	1.397839	9.885026
O	2.580080	2.570297	10.593905
Si	2.755302	3.592820	11.926204
O	2.765723	-0.069990	10.171450
O	3.508138	1.704353	8.260933
Si	3.605924	0.930191	6.801600
O	5.176149	0.790673	6.311071
O	2.895462	-0.559438	6.935628
O	2.309973	-3.096702	6.423392
Si	1.755834	-4.681709	6.599920
O	2.864968	1.822540	5.635015
O	7.291545	-3.565824	6.686479
Si	8.375804	-3.590741	5.390739
O	7.795960	1.289961	5.921121
C	3.872218	-0.301144	18.122727
C	2.215712	0.907258	16.675085
O	2.778107	-1.236610	14.713332
H	-1.100273	1.189896	13.442266
H	0.718136	0.308740	13.400237
H	-0.818061	-0.559501	12.469997
H	2.745636	-3.892966	12.904522
H	1.049460	-4.219559	11.887105
H	0.557685	-4.695092	7.489014
H	1.377960	-5.152906	5.237487
H	-2.077017	-3.754280	10.632340
H	-2.438217	-2.048348	11.020170
H	-5.036732	-4.949547	13.736537
H	-2.983372	-4.350611	16.526222
H	-1.457237	-3.892399	15.568535
H	-5.303960	-3.255576	14.124982
H	0.835707	-1.287894	16.769889
H	1.346816	-1.087642	18.437106
H	0.183419	-5.969896	15.855866
H	1.666438	-6.950478	15.979758
H	2.460191	-4.508218	18.882498
H	2.514153	-2.890656	19.603861
H	3.840805	-3.462480	18.593253
H	7.150615	-5.355217	11.158385
H	3.176348	2.818482	13.129021
H	3.776561	4.638114	11.621801
H	1.427639	4.225798	12.152188
H	2.826102	-4.501361	10.982611
H	8.509194	-4.423768	12.964163
H	9.159796	-4.061874	10.638729
H	9.697204	-3.054613	5.827061
H	7.527733	2.117226	5.510204
H	1.928880	1.985298	5.784370
H	2.823051	-5.553408	7.169726
H	8.511770	-5.018986	4.988585
H	7.848036	-2.783444	4.253074
H	9.262978	1.352729	12.654598
H	9.999691	1.486027	10.330573
H	9.548149	3.532476	11.591927
H	1.500637	-5.745769	14.677417
H	-0.761533	-0.506543	14.474043
H	-3.684211	-3.067045	10.227284
H	-5.137777	-4.441809	15.434123
H	2.989423	1.634175	16.405583
H	1.500824	0.839195	15.850990
H	1.687668	1.290464	17.554171
H	4.657358	0.400793	17.826639
H	3.383773	0.096262	19.018123
H	4.346856	-1.247455	18.385578
H	6.382568	-1.946201	14.854933
H	4.887614	-2.824370	14.395007
H	5.179231	-1.186467	13.762731

Jaa$_S$b$_S$

G = -2689,118923 u.a.

C	-1.794479	0.464771	13.891405
O	-1.876932	-0.536240	14.908608
C	-1.151880	-1.647176	14.739128
C	-1.285168	-2.615701	15.769950
C	-2.130805	-2.290197	16.975599
O	-0.441206	-1.768984	13.691424
La	1.718866	-2.019378	12.785482
O	5.147490	-2.333591	12.324648
Si	6.494548	-2.633045	13.324602
O	3.352914	-1.605799	10.623956
Si	2.165921	-1.766747	9.424720
O	2.659134	-2.854723	8.297467
Si	3.434178	-2.920811	6.828286
O	2.796475	-4.120802	5.925101
Si	1.970426	-5.564486	6.243109
B	2.429642	0.459630	13.545138
O	0.894414	-2.253805	10.332996
B	0.828460	-3.737500	10.785486
O	2.373119	-3.508956	14.443430
C	2.007087	-4.305031	15.389982
O	2.098747	-5.632591	15.167195
C	2.579253	-6.066836	13.897456

Si	5.006197	-1.774211	10.785622
O	5.572309	-2.884869	9.712079
Si	6.238278	-2.955037	8.192642
O	7.042523	-1.547059	7.870381
Si	6.780678	-0.076342	7.165759
O	5.615049	-0.181095	5.996198
Si	3.984038	-0.036190	5.806064
O	3.354095	1.044822	6.892242
Si	2.710009	1.110335	8.409060
O	1.672709	2.371334	8.436921
Si	0.598418	3.092399	9.523311
O	5.764799	-0.327953	10.585228
Si	5.528244	1.097860	9.757778
O	6.169651	2.337450	10.599036
Si	5.953574	3.122158	12.083359
O	6.299268	1.028849	8.301361
O	3.903497	1.312003	9.535752
O	8.219591	0.354014	6.500618
C	1.431923	-3.920012	16.607073
C	1.567882	-2.489577	17.057611
C	2.789008	-2.127181	17.956564
C	2.782042	-0.598184	18.164177
C	1.190538	-4.974894	17.660108
O	1.884680	-0.291192	8.751633
O	5.044720	-3.199273	7.079039
O	3.228456	-1.494326	6.025664
O	7.283945	-4.209369	8.167282
Si	8.813429	-4.479210	7.495755
C	-0.653069	-3.839374	15.610754
O	3.766739	0.504963	4.269834
C	2.678982	-2.771437	19.337498
O	1.507522	-2.471984	19.941585
C	1.355409	-2.999327	21.260667
C	4.110615	-2.557473	17.319381
O	3.533535	-3.442260	19.875076
H	2.742991	1.573308	13.867328
H	3.420568	-0.241248	13.295613
H	1.715783	0.470340	12.526254
H	1.969292	-4.055431	11.179586
H	0.080131	-3.746642	11.765572
H	0.541503	-5.264843	6.540030
H	2.079832	-6.383537	5.003631
H	-2.136199	0.070481	12.930730
H	-0.770948	0.834224	13.791181
H	-3.174915	-2.109180	16.694546
H	-0.927953	-4.662440	16.261700
H	-0.306876	-4.123942	14.622898
H	-1.786227	-1.392453	17.499768
H	1.627403	-1.835224	16.181377
H	0.660244	-2.194976	17.595598
H	1.915453	-5.756523	13.085399
H	2.602438	-7.155630	13.955357
H	0.842687	-5.912533	17.219711
H	0.437655	-4.628875	18.376376
H	2.099075	-5.206784	18.230598
H	6.373077	-4.028525	13.826810
H	-0.170139	2.046611	10.257395
H	1.354226	3.945074	10.483671
H	-0.323680	3.929849	8.706266
H	0.446955	-4.485366	9.927015
H	6.463155	-1.659865	14.448671
H	7.743070	-2.472996	12.525269
H	9.843639	-3.741490	8.281484
H	8.210196	1.176593	6.002212
H	2.850157	0.578368	3.987876
H	2.601285	-6.275747	7.391413
H	9.050575	-5.946813	7.586236
H	8.839436	-4.036704	6.072115
H	6.076344	2.141300	13.197681
H	7.039443	4.138928	12.166353
H	4.620390	3.785560	12.112865
H	3.584974	-5.684319	13.703557
H	1.788679	-0.113576	14.435748
H	-2.453177	1.267134	14.223779
H	-2.114508	-3.121689	17.685186
H	3.600885	-0.286395	18.821381
H	2.910543	-0.093653	17.201099
H	1.840500	-0.262828	18.607213
H	4.957364	-2.260619	17.943847
H	4.159761	-3.642047	17.193269
H	4.215911	-2.088352	16.336850
H	0.376215	-2.664146	21.603686

Kaa$_S$b$_S$

G = -2689,135973 u.a.

C	-2.071294	0.349161	14.113438
O	-2.023046	-0.641979	15.125394
C	-1.150541	-1.674446	14.950422
C	-1.243542	-2.762400	15.763477
C	-2.287432	-2.870432	16.839269
O	-0.251646	-1.529427	13.996101
La	1.669880	-1.768738	12.900033
O	5.520109	-2.317414	12.216822
Si	6.887549	-2.153233	13.208024
O	3.513177	-1.585695	10.680127
Si	2.283172	-1.699611	9.528691
O	2.667875	-2.821760	8.392819
Si	3.324987	-2.928762	6.869090
O	2.584228	-4.120241	6.034995
Si	1.577605	-5.425466	6.420209
B	2.869346	0.524881	13.613165
O	1.000633	-2.102409	10.470400
B	0.851295	-3.574500	10.956626
O	2.503100	-3.440911	14.519466
C	2.146073	-4.220111	15.422430
O	2.645720	-5.437305	15.487805
C	3.595734	-5.819146	14.474726
Si	5.171626	-1.774364	10.708131
O	5.601197	-2.904206	9.589416
Si	6.194105	-3.032997	8.048596
O	7.032711	-1.664596	7.648985
Si	6.769681	-0.198382	6.936675
O	5.530068	-0.286835	5.843463
Si	3.896475	-0.081330	5.762181
O	3.385536	1.045290	6.864950
Si	2.838251	1.158069	8.416545

O	1.817879	2.432126	8.479125
Si	0.805107	3.170003	9.612839
O	5.941075	-0.345349	10.418733
Si	5.722816	1.073903	9.580255
O	6.482977	2.291482	10.353675
Si	6.267107	3.275419	11.712819
O	6.388830	0.940042	8.077222
O	4.101094	1.378645	9.461560
O	8.176135	0.179413	6.176282
C	1.078165	-3.895188	16.434267
C	1.322453	-2.484085	17.020784
C	2.485621	-2.246570	18.018224
C	2.566673	-0.719878	18.254113
C	0.964734	-4.969928	17.520326
O	2.024714	-0.223536	8.846824
O	4.940235	-3.257420	6.996090
O	3.102699	-1.503812	6.066028
O	7.193751	-4.324887	8.003880
Si	8.593439	-4.726529	7.143895
C	-0.286347	-3.891387	15.560544
O	3.593505	0.439336	4.233061
C	2.217132	-2.875154	19.386990
O	0.993576	-2.557963	19.857473
C	0.701085	-3.047048	21.169301
C	3.841246	-2.743970	17.510258
O	3.009765	-3.537947	20.021160
H	3.398299	1.569638	13.877781
H	3.702775	-0.362510	13.381119
H	2.159956	0.630208	12.590649
H	1.945278	-3.907080	11.460561
H	0.013839	-3.532314	11.854723
H	0.235270	-4.923521	6.827777
H	1.469777	-6.238597	5.176585
H	-2.352375	-0.075166	13.142509
H	-1.115728	0.873274	14.010707
H	-3.019953	-2.065086	16.757452
H	-0.782802	-4.840722	15.793939
H	-0.025437	-3.944887	14.497521
H	-1.861551	-2.820812	17.853161
H	1.460346	-1.783310	16.190891
H	0.392280	-2.178647	17.503423
H	3.142667	-5.746597	13.484161
H	3.858765	-6.850183	14.705074
H	0.730230	-5.944237	17.084158
H	0.153134	-4.699620	18.200997
H	1.881727	-5.081130	18.104750
H	6.772087	-3.219752	14.242349
H	0.073136	2.135218	10.398321
H	1.614744	4.029009	10.522311
H	-0.155908	4.002573	8.836857
H	0.540127	-4.335460	10.081908
H	6.894611	-0.809625	13.847654
H	8.125308	-2.355426	12.400950
H	9.775105	-4.081007	7.784358
H	8.159627	0.997163	5.670191
H	2.663196	0.552904	4.017104
H	2.183074	-6.235642	7.515489
H	8.717179	-6.209267	7.217985
H	8.476206	-4.287547	5.723599
H	6.478741	2.473130	12.950034
H	7.299318	4.345197	11.610431
H	4.901480	3.869841	11.701843
H	4.475641	-5.175344	14.523447
H	2.134581	0.131664	14.524763
H	-2.839183	1.056400	14.433015
H	-2.826601	-3.825909	16.774488
H	3.329620	-0.480589	19.002249
H	2.835888	-0.214617	17.321157
H	1.608697	-0.321819	18.598423
H	4.631531	-2.491157	18.221265
H	3.863400	-3.831291	17.392407
H	4.075319	-2.275850	16.549773
H	-0.309746	-2.706586	21.393603
H	0.753127	-4.138576	21.195637
H	1.411270	-2.646025	21.896944

Iab_Sa_R

G = -2689,122204 u.a.

C	-2.506346	-1.340128	2.264487
O	-1.542920	-1.971532	1.409269
C	-0.275400	-2.224470	2.006735
C	-0.123381	-3.171156	2.959638
C	1.247511	-3.356896	3.556684
C	1.388742	-3.040247	5.090407
C	2.865415	-2.736810	5.326686
O	3.637112	-3.821567	5.129277
C	5.043358	-3.612695	5.282187
O	0.644810	-1.479516	1.438761
La	-0.137300	-0.541919	-0.530799
O	-0.595222	-2.836784	-1.397239
C	-0.700977	-4.025142	-1.713309
C	0.403451	-4.870874	-2.221972
C	0.137803	-6.333385	-2.440771
B	1.697903	-0.320521	-2.482062
B	-2.457298	0.760196	-1.361630
O	-2.021860	1.071401	0.087604
Si	-1.316325	2.402142	0.711836
O	-1.549277	3.785443	-0.145489
Si	-1.692263	5.425068	0.088199
O	-2.723313	6.046683	-1.014745
Si	-3.254363	5.597555	-2.558814
O	0.317277	1.955765	0.626148
Si	1.770886	2.797572	0.744204
O	2.104769	3.164854	2.306104
Si	1.647536	3.442654	3.873113
O	2.739918	2.831608	4.912291
Si	3.058516	1.175354	5.257257
O	2.894469	1.784144	0.140372
Si	4.276230	1.940576	-0.835572
O	1.658323	4.188818	-0.137186
Si	1.396851	5.805369	0.121104
O	2.254853	6.645023	-0.988394
Si	3.332855	7.945403	-0.927142
O	-1.785734	2.593682	2.273272
Si	-1.417380	3.049827	3.819472
O	-1.733690	4.659501	4.027547

Si	-1.799272	6.047875	3.135945
O	-2.305691	5.730958	1.591015
O	0.170054	2.728898	4.127658
O	-2.345646	2.171690	4.841415
Si	-3.409871	2.554634	6.098061
O	1.531271	5.078813	4.100054
Si	1.301378	6.430115	3.169538
O	-0.316235	6.777397	3.081905
O	-0.210095	6.138142	-0.068588
O	1.896616	6.228648	1.641195
C	1.574473	-4.270365	-2.477289
C	-1.243412	-4.092979	3.359515
C	0.988539	-4.247735	5.958273
C	0.567154	-1.812460	5.483966
O	3.339806	-1.659686	5.634796
O	2.124375	7.690385	3.832935
O	-2.894357	7.004524	3.904091
O	-1.853020	-4.669222	-1.631772
C	-2.983774	-3.921404	-1.145676
H	2.128022	-0.987204	-1.525338
H	0.673944	-0.875367	-2.901470
H	2.529928	-0.208372	-3.341389
H	3.909129	2.488909	-2.167999
H	1.353855	0.784125	-2.037960
H	4.865604	0.581101	-0.947095
H	5.235644	2.861200	-0.153967
H	-2.509239	-0.485954	-1.394095
H	-1.556113	1.117326	-2.125250
H	-3.528312	1.224459	-1.647078
H	-0.072019	-4.475933	5.827106
H	1.568432	-5.135909	5.695596
H	1.151295	-4.036540	7.021243
H	0.773933	-1.519648	6.517243
H	5.507817	-4.581583	5.098184
H	5.274760	-3.262415	6.291299
H	5.404473	-2.873152	4.562828
H	2.259422	7.618241	4.782554
H	2.720464	9.091004	-0.194609
H	3.604181	8.324333	-2.341903
H	-3.107631	7.823814	3.447694
H	-2.723038	3.390224	7.124621
H	-4.598487	3.277015	5.560749
H	-3.827344	1.253299	6.691940
H	4.517818	1.104791	5.533863
H	2.675765	0.413342	4.041622
H	2.248955	0.836625	6.454716
H	-2.110698	5.098442	-3.374366
H	-3.826113	6.829937	-3.171054
H	-4.304437	4.547760	-2.437908
H	4.597268	7.527795	-0.255599
H	2.415220	-4.839355	-2.862938
H	1.717019	-3.205528	-2.322952
H	1.038003	-6.832206	-2.806181
H	-0.178287	-6.823297	-1.514122
H	-2.750117	-3.478558	-0.175757
H	-3.792900	-4.645989	-1.067093
H	1.929583	-2.704122	3.003439
H	1.599234	-4.386251	3.399870
H	-3.294196	-0.951820	1.617392
H	-2.926921	-2.060147	2.972113
H	-2.055969	-0.510723	2.817137
H	-3.242576	-3.132576	-1.855614
H	-0.664074	-6.486023	-3.170122
H	0.789364	-0.960281	4.838780
H	-0.499693	-2.032422	5.394382
H	-0.869908	-5.120490	3.456056
H	-1.705007	-3.839992	4.325009
H	-2.040366	-4.107844	2.610823

Jab_Sa_R

G = -2689,109703 u.a.

C	-2.777848	-1.601076	1.666650
O	-1.984118	-2.690070	2.117189
C	-0.640218	-2.533766	2.158877
C	0.070726	-3.621788	2.665780
C	1.536355	-3.446513	2.971875
C	1.918035	-3.206096	4.476609
C	3.330633	-2.625461	4.492279
O	4.212319	-3.447640	3.898768
C	5.563657	-2.978893	3.851381
O	-0.131399	-1.452582	1.660592
La	0.105443	-0.528257	-0.487676
O	-0.961210	-2.538478	-1.166021
C	-1.411056	-3.716522	-1.048622
C	-0.875274	-4.740326	-0.213789
C	-1.582728	-6.069605	-0.143754
B	2.422403	-1.071531	-1.680746
B	-1.591327	1.129985	-1.900717
O	-1.792828	1.187372	-0.362716
Si	-1.237245	2.457920	0.509510
O	-1.370640	3.902980	-0.256886
Si	-1.652461	5.515135	0.022563
O	-2.590816	6.135853	-1.159503
Si	-2.770932	5.890958	-2.825350
O	0.398471	2.045426	0.687472
Si	1.804043	2.945345	0.914741
O	2.048042	3.235186	2.510474
Si	1.326204	3.382961	3.998014
O	2.282632	2.738010	5.145661
Si	2.880128	1.122982	5.184775
O	2.997223	2.007601	0.318369
Si	4.374674	2.257664	-0.645377
O	1.684666	4.374205	0.098284
Si	1.379797	5.973846	0.418666
O	2.349638	6.875766	-0.538832
Si	3.327219	8.236168	-0.307880
O	-1.975170	2.489298	1.978631
Si	-1.712890	2.878665	3.569085
O	-2.093722	4.464216	3.847555
Si	-2.129257	5.916936	3.063964
O	-2.454326	5.710177	1.452728
O	-0.133178	2.594431	3.947658
O	-2.675040	1.915861	4.475465
Si	-3.745007	2.171811	5.759870
O	1.088259	4.987730	4.321410
Si	0.927641	6.396478	3.465232

O	-0.682053	6.702964	3.222801
O	-0.201012	6.306578	0.067942
O	1.699506	6.314216	2.006351
C	0.286270	-4.475398	0.480133
C	-0.690968	-4.774278	3.270591
C	1.961041	-4.522169	5.279921
C	0.966606	-2.213325	5.144234
O	3.667921	-1.561047	4.976033
O	1.635701	7.630668	4.289248
O	-3.339978	6.768948	3.779135
O	-2.473602	-4.079733	-1.772927
C	-3.004106	-3.118479	-2.689827
H	2.382140	-1.548479	-0.531991
H	1.468833	-1.547169	-2.313572
H	3.474796	-1.290387	-2.212689
H	3.967723	2.485067	-2.058457
H	2.211422	0.148348	-1.580254
H	5.210181	1.036315	-0.511960
H	5.111138	3.449057	-0.128043
H	-1.739479	-0.062830	-2.190147
H	-0.409865	1.433422	-2.140949
H	-2.359792	1.821372	-2.511054
H	0.961364	-4.951954	5.368611
H	2.616002	-5.257146	4.804826
H	2.332109	-4.341101	6.294944
H	1.306096	-1.967210	6.153751
H	6.129048	-3.761358	3.345612
H	5.950922	-2.816146	4.860275
H	5.626545	-2.041300	3.293585
H	1.579814	7.556458	5.246637
H	2.562836	9.310324	0.389205
H	3.730979	8.690076	-1.667831
H	-3.553517	7.605223	3.354753
H	-3.079048	2.953233	6.841553
H	-4.955964	2.894818	5.276408
H	-4.119637	0.818986	6.258690
H	4.359057	1.233852	5.282934
H	2.436044	0.500596	3.911997
H	2.280756	0.504795	6.393680
H	-1.467515	5.502808	-3.435737
H	-3.240699	7.187531	-3.389896
H	-3.790810	4.829917	-3.055618
H	4.531531	7.865550	0.489381
H	0.801479	-5.293339	0.973224
H	0.903810	-3.621328	0.221740
H	-1.048214	-6.747208	0.526741
H	-2.610670	-5.974080	0.222284
H	-3.324958	-2.212702	-2.170354
H	-3.857208	-3.607870	-3.159276
H	1.899075	-2.591785	2.391186
H	2.108337	-4.318797	2.628729
H	-3.810976	-1.891325	1.862787
H	-2.544809	-0.679986	2.206027
H	-2.664123	-1.433485	0.589167
H	-2.259201	-2.850805	-3.443287
H	-1.640766	-6.545021	-1.129370
H	0.895841	-1.284320	4.574224
H	-0.035933	-2.643176	5.213064
H	-0.064542	-5.672658	3.304604
H	-1.026793	-4.574950	4.297421
H	-1.584699	-5.006618	2.687142

Kab_Sa_R

G = -2689,130254 u.a.

C	-2.556333	-1.285646	2.418695
O	-1.759691	-2.479704	2.527647
C	-0.509911	-2.437252	2.123724
C	0.228043	-3.761213	2.216529
C	1.625494	-3.533086	2.856572
C	1.778797	-3.297557	4.391529
C	3.189611	-2.735983	4.603977
O	4.129190	-3.552803	4.102501
C	5.483382	-3.114487	4.261596
O	0.002262	-1.393372	1.683575
La	0.001887	-0.459441	-0.667233
O	-1.070035	-2.396728	-0.856854
C	-1.359397	-3.685873	-0.831460
C	-0.674299	-4.620152	-0.121909
C	-0.992218	-6.086013	-0.253219
B	2.180329	-0.883263	-2.141989
B	-1.809967	1.211290	-1.881601
O	-1.944745	1.205176	-0.333047
Si	-1.362042	2.464092	0.535760
O	-1.470907	3.911602	-0.229762
Si	-1.683078	5.537114	0.021139
O	-2.613227	6.177918	-1.154989
Si	-2.826505	5.924846	-2.817054
O	0.266141	2.032351	0.707199
Si	1.709836	2.869255	0.891050
O	2.017711	3.157270	2.478995
Si	1.300692	3.355293	3.962999
O	2.236914	2.702238	5.124791
Si	2.768127	1.075436	5.251652
O	2.822590	1.853116	0.261000
Si	4.256838	2.045088	-0.637517
O	1.645475	4.295644	0.066286
Si	1.376683	5.906316	0.365867
O	2.351560	6.773073	-0.617063
Si	3.402621	8.082981	-0.417415
O	-2.080793	2.514981	2.017496
Si	-1.758716	2.935371	3.588371
O	-2.084457	4.533252	3.852392
Si	-2.098209	5.985822	3.064093
O	-2.455739	5.787126	1.460443
O	-0.178342	2.601722	3.925103
O	-2.714813	2.014027	4.547221
Si	-3.813366	2.357895	5.788886
O	1.104979	4.966530	4.271146
Si	0.977099	6.377786	3.411919
O	-0.627783	6.731540	3.203128
O	-0.200854	6.270712	0.037019
O	1.726123	6.257199	1.945441
C	0.500571	-4.208538	0.721435
C	-0.615872	-4.834920	2.905556
C	1.717609	-4.609884	5.204451
C	0.774228	-2.286498	4.948691

O	3.467302	-1.697003	5.170039
O	1.741463	7.595376	4.208712
O	-3.275149	6.868010	3.798189
O	-2.449865	-4.069592	-1.556240
C	-2.775912	-3.278881	-2.689930
H	2.300329	-1.348785	-0.991426
H	1.175926	-1.410689	-2.641878
H	3.163116	-1.076874	-2.801886
H	3.931045	2.459469	-2.027856
H	1.944743	0.329194	-2.024892
H	4.949300	0.731511	-0.604084
H	5.092544	3.090369	0.025666
H	-1.954517	0.032545	-2.217959
H	-0.642469	1.546987	-2.155063
H	-2.606405	1.920810	-2.431073
H	0.712231	-5.033037	5.197836
H	2.410679	-5.354446	4.804807
H	1.986817	-4.421357	6.249614
H	0.980215	-2.081643	6.002116
H	6.099011	-3.893050	3.811970
H	5.726699	-2.994907	5.320102
H	5.640891	-2.160671	3.752293
H	1.610451	7.601297	5.161570
H	2.711467	9.194853	0.296467
H	3.792202	8.512388	-1.789154
H	-3.517981	7.679719	3.342904
H	-3.152619	3.164351	6.854715
H	-4.990003	3.090847	5.241368
H	-4.237159	1.036751	6.332290
H	4.225648	1.136860	5.536040
H	2.474586	0.438263	3.941644
H	2.005768	0.473711	6.375510
H	-1.548593	5.475751	-3.438938
H	-3.246750	7.236155	-3.386470
H	-3.894671	4.907469	-3.021123
H	4.607048	7.652918	0.349392
H	1.184185	-5.063159	0.805505
H	1.078514	-3.409558	0.237087
H	-0.086512	-6.661711	-0.491593
H	-1.408816	-6.528687	0.662241
H	-3.021780	-2.249478	-2.414626
H	-3.649513	-3.754341	-3.140090
H	2.070733	-2.679996	2.331301
H	2.241455	-4.399321	2.595238
H	-3.518018	-1.545366	2.857794
H	-2.094262	-0.466051	2.970061
H	-2.687147	-1.012970	1.369860
H	-1.956857	-3.266635	-3.419725
H	-1.716545	-6.254237	-1.052125
H	0.823350	-1.334797	4.414578
H	-0.244714	-2.676094	4.876483
H	-0.048374	-5.769030	2.955805
H	-0.913566	-4.554769	3.917665
H	-1.526709	-5.018057	2.333319

Iab$_S$b$_R$

G = -2689,123887 u.a.

C	-3.854605	-3.681767	17.594336
C	-3.102488	-2.964576	16.456884
C	-1.549903	-2.998033	16.672648
C	-0.834957	-4.262796	16.276535
C	-0.010993	-4.262683	15.203546
O	0.230783	-3.227367	14.404474
La	0.776103	-1.538354	13.084291
B	-0.263881	0.743397	13.979611
C	-3.491081	-3.562635	15.104262
C	-3.524371	-1.496222	16.472442
O	-3.203509	-0.897238	17.641200
C	-3.538133	0.489972	17.718263
O	-4.077142	-0.906642	15.569921
C	-0.991771	-5.497444	17.123293
O	0.734781	-5.386071	14.913428
C	0.531766	-5.903881	13.607269
B	-0.360198	-2.239510	10.658593
O	0.544844	-0.990624	10.531878
Si	2.057361	-1.079014	9.944858
O	2.245539	-2.016949	8.607798
Si	3.117332	-2.099210	7.198724
O	2.164131	-2.598989	5.973533
Si	0.664253	-3.381519	5.847715
O	2.899300	-1.769697	11.252718
Si	4.250685	-2.746071	11.402956
O	5.602344	-1.827743	11.636260
Si	6.223643	-0.344622	11.234335
O	7.157775	0.175007	12.473648
Si	8.810132	0.475269	12.674330
O	2.827695	-0.975993	14.426802
C	3.421107	-0.650703	15.462964
O	3.973218	0.538211	15.609973
C	3.814755	1.486005	14.535395
O	2.655810	0.434361	9.680854
Si	4.038657	1.335349	9.823982
O	3.663100	2.874730	10.212485
Si	2.371312	3.916733	9.860873
O	4.976658	0.723984	11.044987
O	4.880098	1.284262	8.404312
Si	5.050243	0.335833	7.064414
O	6.384036	-0.630951	7.262845
Si	7.240420	-1.363776	8.473049
O	8.812220	-1.529266	8.020708
O	7.128600	-0.450032	9.855751
O	6.684511	-2.886828	8.782318
Si	5.284900	-3.760718	8.642479
O	5.640026	-5.330107	8.365412
Si	6.933447	-6.171775	7.672871
O	4.372642	-3.157889	7.403994
O	4.421606	-3.673198	10.053432
O	3.712965	-0.605440	6.807455
O	5.264504	1.335075	5.777202
O	3.944732	-3.672855	12.715701
Si	4.774390	-4.901776	13.546186
C	3.602263	-1.520461	16.649614
C	4.458347	-1.014855	17.776228
C	2.968233	-2.702036	16.659585
H	-1.064567	0.079536	13.300595
H	0.119920	0.017266	14.911326

H	-0.768472	1.752589	14.388111
H	0.719741	0.978181	13.259179
H	-1.192779	-1.944017	11.525553
H	0.340446	-3.166245	11.112254
H	-0.891662	-2.556259	9.629888
H	3.802960	-5.487251	14.504185
H	5.250617	-5.923883	12.570281
H	5.938983	-4.306755	14.263363
H	-0.426081	-2.423967	6.182385
H	0.625640	-4.560558	6.758257
H	0.554954	-3.818566	4.427782
H	8.065475	-6.230745	8.641350
H	6.430722	-7.542918	7.382364
H	7.371998	-5.502585	6.414088
H	4.884646	1.012111	4.954688
H	1.910088	3.703318	8.458736
H	1.260750	3.662676	10.819129
H	8.977197	0.922194	14.085288
H	9.592334	-0.771174	12.432010
H	9.254004	1.547327	11.737623
H	-3.227314	0.815320	18.711759
H	-3.011601	1.058196	16.947072
H	-2.972835	-3.059922	14.283845
H	-3.227279	-4.623327	15.074852
H	-1.116783	-2.169877	16.103048
H	-0.924694	-5.249079	18.190836
H	-0.220466	-6.234149	16.892110
H	-1.963977	-5.988421	16.979902
H	2.899982	5.299268	10.026185
H	-1.361768	-2.776100	17.732074
H	-3.629292	-4.750769	17.592707
H	-4.938111	-3.572765	17.471111
H	-4.565309	-3.459636	14.928431
H	-3.580725	-3.271068	18.569786
H	-4.613591	0.637126	17.587469
H	9.175117	-0.778434	7.541462
H	2.754302	1.653340	14.337626
H	4.312619	1.123913	13.634842
H	4.053030	-0.088607	18.195550
H	3.052548	-3.369379	17.511836
H	2.337813	-3.024286	15.837778
H	5.474449	-0.791273	17.435554
H	4.290215	2.398406	14.891334
H	4.515222	-1.759607	18.572973
H	1.147039	-6.802911	13.527851
H	-0.521096	-6.172268	13.449378
H	0.834415	-5.191757	12.831021

$Jab_S b_R$

G = -2689,112003 u.a.

C	-2.822322	-2.878095	18.375772
C	-2.414813	-2.366550	16.978911
C	-0.898380	-2.628756	16.687616
C	-0.508938	-4.014087	16.243520
C	-0.510418	-4.300155	14.873802
O	-0.502028	-3.434612	13.921797
La	0.591067	-1.790163	12.701375
B	-0.383750	0.584903	13.349827
C	-3.323388	-2.979586	15.911762
C	-2.632875	-0.852187	16.979634
O	-1.759754	-0.222561	17.795714
C	-1.896233	1.200679	17.839800
O	-3.484992	-0.261482	16.354287
C	-0.624523	-5.164132	17.214287
O	-0.425950	-5.606645	14.538436
C	-0.383909	-5.934712	13.152044
B	-0.283992	-2.704411	10.232087
O	0.511499	-1.378960	10.161036
Si	2.066083	-1.317666	9.676385
O	2.422634	-2.216699	8.348703
Si	3.383053	-2.184268	6.993415
O	2.554560	-2.746813	5.705644
Si	1.134859	-3.644221	5.475266
O	2.863270	-1.943797	11.044738
Si	4.296530	-2.786627	11.266000
O	5.532707	-1.749787	11.614181
Si	6.035430	-0.209860	11.255840
O	6.843207	0.363945	12.557326
Si	8.345960	1.101111	12.799195
O	2.358220	-1.696665	14.300921
C	2.547238	-1.555900	15.551411
O	3.090268	-0.424482	16.009817
C	3.416925	0.594177	15.059822
O	2.526676	0.247777	9.462370
Si	3.800234	1.281355	9.712909
O	3.254465	2.770489	10.084537
Si	1.863980	3.682393	9.751852
O	4.707855	0.733402	10.982899
O	4.729807	1.336370	8.348196
Si	5.076061	0.427209	7.016880
O	6.478379	-0.414992	7.294098
Si	7.324046	-1.081285	8.549657
O	8.930856	-1.083066	8.202241
O	7.029291	-0.214362	9.934208
O	6.903874	-2.659523	8.792635
Si	5.597465	-3.648926	8.555487
O	6.109796	-5.178234	8.299290
Si	7.560381	-5.897620	7.810467
O	4.718307	-3.125299	7.257262
O	4.629098	-3.637875	9.897299
O	3.853057	-0.633137	6.663227
O	5.277099	1.460149	5.754164
O	4.030816	-3.808925	12.515868
Si	5.068108	-4.587136	13.611872
C	2.268037	-2.527107	16.554399
C	2.508918	-2.169918	17.999860
C	1.813212	-3.776774	16.168174
H	-1.142410	-0.053596	12.600858
H	-0.185128	-0.113760	14.356584
H	-0.844473	1.654841	13.632306
H	0.707106	0.691843	12.762111
H	-1.241121	-2.461119	10.972476
H	0.440268	-3.540626	10.813867
H	-0.633385	-3.114451	9.158963
H	4.254750	-5.646020	14.268516
H	6.210904	-5.196229	12.870680

H	5.571593	-3.609250	14.615231
H	-0.048825	-2.790970	5.773949
H	1.144770	-4.850573	6.350509
H	1.137549	-4.045206	4.040599
H	8.545599	-5.852127	8.928844
H	7.229775	-7.309867	7.473014
H	8.110024	-5.194315	6.615752
H	5.005818	1.105736	4.902207
H	1.467788	3.499713	8.325076
H	0.762826	3.256645	10.657330
H	8.372766	1.525828	14.226207
H	9.439897	0.124120	12.529925
H	8.489414	2.286019	11.904516
H	-1.133523	1.549708	18.536571
H	-1.736970	1.632523	16.848678
H	-3.054384	-2.632728	14.911082
H	-3.245574	-4.070740	15.931377
H	-0.578712	-1.916976	15.919624
H	-0.339083	-4.843840	18.222060
H	0.016786	-6.002225	16.926085
H	-1.645598	-5.563705	17.276436
H	2.234905	5.102680	10.003579
H	-0.335656	-2.362271	17.588326
H	-2.749773	-3.966979	18.426105
H	-3.860656	-2.606429	18.595820
H	-4.364986	-2.700819	16.089156
H	-2.185762	-2.450718	19.155636
H	-2.892475	1.482896	18.190464
H	9.254443	-0.280309	7.782783
H	2.527234	0.919522	14.515690
H	4.173420	0.241714	14.354942
H	1.909004	-1.312330	18.322170
H	1.834678	-4.589887	16.885522
H	1.895431	-4.069328	15.127476
H	3.557816	-1.906800	18.178536
H	3.815393	1.418772	15.650674
H	2.260530	-3.016778	18.645361
H	-0.426316	-7.023808	13.111164
H	-1.233620	-5.505057	12.615986
H	0.542354	-5.589966	12.682040

Kab$_S$b$_R$

G = -2689,127317 u.a.

C	-2.127756	-2.966006	18.613563
C	-1.987693	-2.386400	17.188135
C	-0.587490	-2.669905	16.565020
C	-0.275483	-4.034415	15.898871
C	-1.007545	-4.116482	14.582619
O	-0.966528	-3.226210	13.717747
La	0.434149	-1.515158	12.581212
B	-0.792389	0.794999	12.965124
C	-3.163060	-2.842823	16.318043
C	-2.107650	-0.863538	17.350927
O	-1.018925	-0.338772	17.944542
C	-1.055006	1.079605	18.135833
O	-3.066859	-0.200043	17.026789
C	-0.564109	-5.242767	16.795204
O	-1.657930	-5.239988	14.353139
C	-2.314608	-5.368805	13.076492
B	-0.254472	-2.709430	10.174371
O	0.518757	-1.387160	10.006926
Si	2.098607	-1.316481	9.606592
O	2.557980	-2.348541	8.413176
Si	3.601203	-2.431126	7.121778
O	2.876334	-3.188341	5.870212
Si	1.467430	-4.104881	5.661731
O	2.829934	-1.736530	11.081801
Si	4.288664	-2.467205	11.486889
O	5.441818	-1.319796	11.772468
Si	5.909720	0.180298	11.244818
O	6.622301	0.947296	12.500404
Si	8.025587	1.866727	12.704145
O	1.866335	-1.553729	14.322645
C	2.428968	-1.900330	15.456658
O	3.274838	-0.996115	16.026494
C	3.562016	0.187838	15.299279
O	2.499727	0.234037	9.227116
Si	3.706798	1.359692	9.404450
O	3.064885	2.850097	9.552500
Si	1.586975	3.584135	9.164600
O	4.569693	1.022649	10.773290
O	4.702412	1.303484	8.086819
Si	5.173284	0.248537	6.911139
O	6.590979	-0.481016	7.368263
Si	7.394702	-0.951471	8.735566
O	9.017541	-0.907772	8.475264
O	6.978784	0.052194	9.988832
O	7.042526	-2.515025	9.131712
Si	5.785498	-3.579581	8.963120
O	6.368981	-5.105019	8.928221
Si	7.875515	-5.806839	8.616211
O	4.957536	-3.265689	7.566303
O	4.741835	-3.437833	10.235971
O	4.020882	-0.909047	6.630828
O	5.403448	1.125054	5.539204
O	4.004822	-3.355949	12.824260
Si	5.013519	-4.010045	14.028729
C	2.219881	-3.089602	16.094711
C	2.870446	-3.420112	17.408835
C	1.287981	-4.079170	15.476176
H	-1.386724	0.118848	12.113209
H	-0.733090	0.127775	14.010929
H	-1.323350	1.854605	13.142885
H	0.384180	0.933139	12.571161
H	-1.262219	-2.411299	10.823384
H	0.439640	-3.469734	10.886967
H	-0.533935	-3.244575	9.135673
H	4.277216	-5.150120	14.635762
H	6.259570	-4.515456	13.373522
H	5.358470	-2.969448	15.031049
H	0.270255	-3.234103	5.828047
H	1.435590	-5.226451	6.643219
H	1.531936	-4.637520	4.271912
H	8.796917	-5.555409	9.761119
H	7.628366	-7.267886	8.465921
H	8.456115	-5.249536	7.360479

H	5.266490	0.632213	4.724739
H	1.253678	3.320632	7.734173
H	0.515258	3.058474	10.052905
H	7.950224	2.443920	14.074608
H	9.227457	0.992914	12.576969
H	8.081824	2.956855	11.686959
H	-0.113290	1.335095	18.621473
H	-1.143229	1.592673	17.175228
H	-3.118936	-2.399075	15.319530
H	-3.182827	-3.932749	16.225067
H	-0.380558	-1.897875	15.817515
H	-0.014660	-5.135153	17.734674
H	-0.234271	-6.168684	16.316152
H	-1.625033	-5.357457	17.026363
H	1.786818	5.043544	9.383194
H	0.167295	-2.514496	17.338333
H	-2.164405	-4.057070	18.602347
H	-3.056019	-2.611962	19.074944
H	-4.107913	-2.524453	16.764399
H	-1.292649	-2.654357	19.246879
H	-1.902062	1.361810	18.766388
H	9.336826	-0.110904	8.041631
H	2.654762	0.751889	15.062786
H	4.103224	-0.025344	14.371806
H	2.152847	-3.453383	18.243255
H	1.623698	-5.095801	15.713802
H	1.354912	-3.990709	14.385893
H	3.630311	-2.680962	17.669441
H	4.200410	0.783952	15.954072
H	3.353235	-4.407497	17.378911
H	-2.753871	-6.365000	13.081124
H	-3.087682	-4.604926	12.974762
H	-1.592285	-5.264611	12.265073