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

Supporting Information

Chemical Modification of Dimethylpolysiloxane for Enhancement of CO_2 Binding Enthalpy

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Contents

Additional computational details

The DLPNO-CCSD(T) calculations were performed using ORCA 5.0.1. To speed up the two-electron integral calculations, the Coulomb integral and exact exchange term were obtained by applying the resolution of identity approximation and chain of spheres algorithm, respectively. The reference Gibbs free energy was estimated from the electron energy at the DLPNO-CCSD(T)/def2-TZVP level and the thermal correction at the M06-2X-D3/6-31G(d) level.

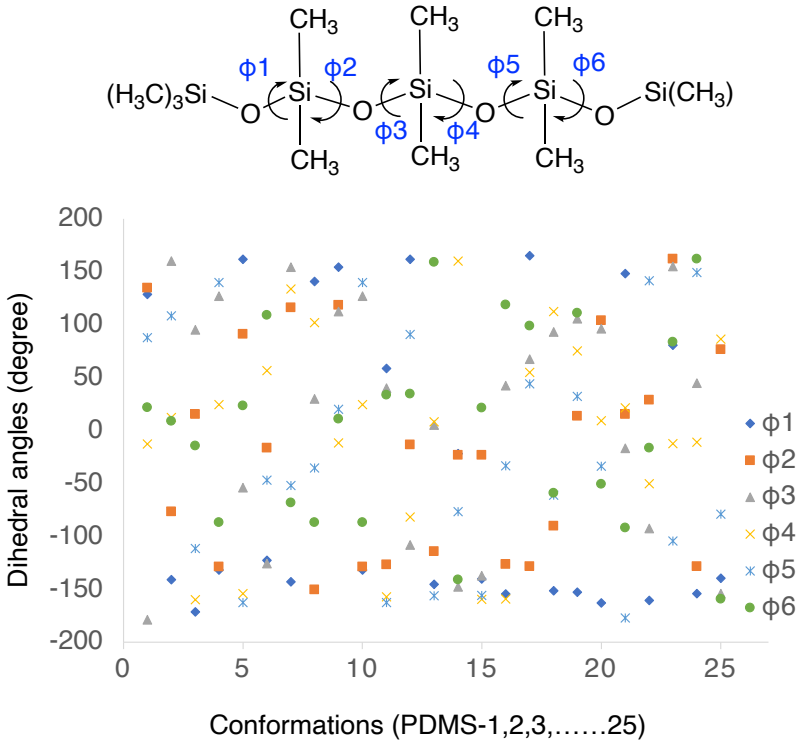

Figure S1. Distribution of dihedral angles of PDMS trimer.

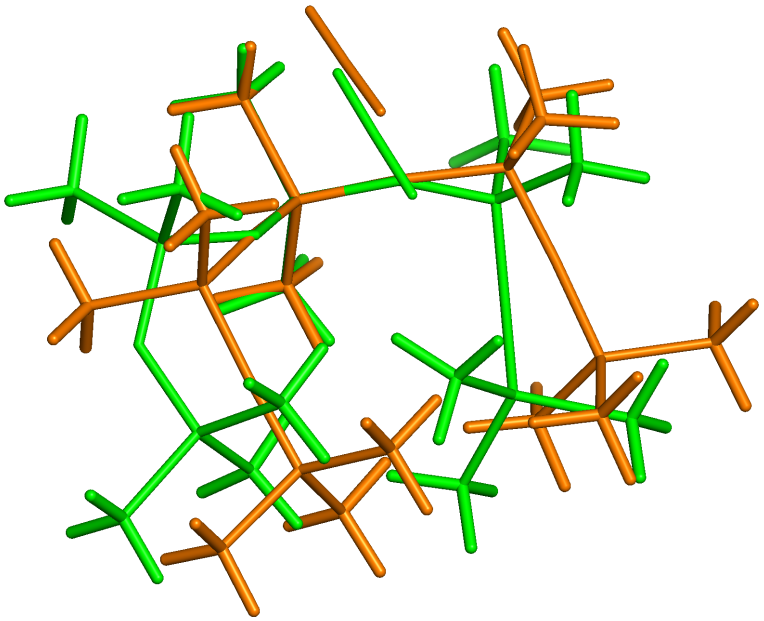

Figure S2. Structures optimized by M06-2X (green: PDMS-1 in Fig. 3) vs. structure optimized by PM6 (orange).

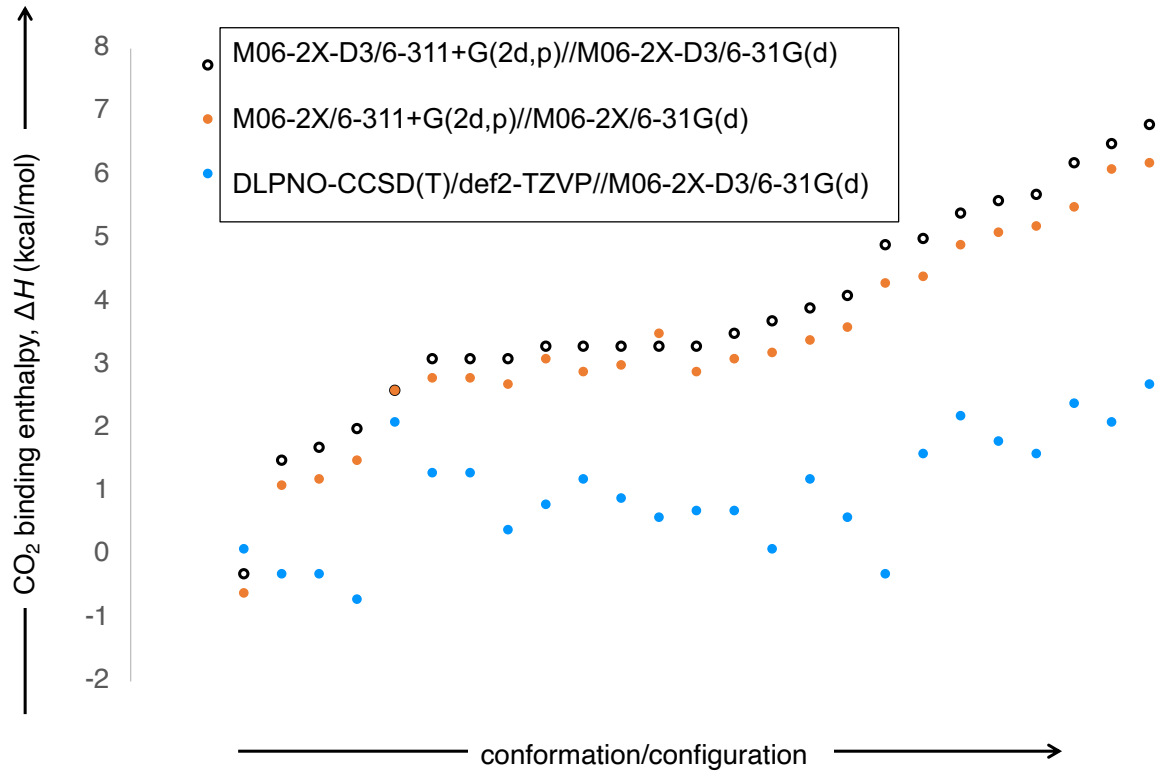

Figure S3. Plots of CO_2 binding enthalpies to PDMS trimers calculated at three theoretical levels.

Table S1. Mulliken and NBO charges of CO_2 bound to PDMS and chemically modified PDMS models[a]

				Mulliken charge			
	PDMS	**PDMS-C**	**PDMS-S**	**PDMS-CH_2F**	**PDMS-CN**	**PDMS-OH**	**PDMS-Ph**
C	0.74	0.75	0.74	0.73	0.75	0.76	0.74
O	-0.36	-0.36	-0.35	-0.35	-0.36	-0.33	-0.36
O	-0.36	-0.36	-0.36	-0.36	-0.35	-0.39	-0.35
SUM	0.02	0.03	0.03	0.02	0.04	0.04	0.02

				NBO charge			
	PDMS	**PDMS-C**	**PDMS-S**	**PDMS-CH_2F**	**PDMS-CN**	**PDMS-OH**	**PDMS-Ph**
C	0.55	0.55	0.55	0.55	0.55	0.56	0.55
O	-0.28	-0.28	-0.27	-0.27	-0.28	-0.27	-0.28
O	-0.27	-0.27	-0.28	-0.28	-0.27	-0.29	-0.27
SUM	0.00	0.00	0.00	0.00	0.00	0.01	0.00

				Mulliken charge			
	PDMS-Mg-M1	**PDMS-Mg-M2**	**PDMS-Mg-M3**	**PDMS-Mg-M4**	**PDMS-Mg-M5**	**PDMS-$Mg(OH)_2$-M1**	**PDMS-$Mg(OH)_2$-M6**
C	0.78	0.78	0.80	0.85	0.78	0.74	0.78
O	-0.35	-0.51	-0.33	-0.51	-0.60	-0.34	-0.51
O	-0.41	-0.63	-0.38	-0.62	-0.58	-0.36	-0.61
SUM	0.03	-0.36	0.09	-0.27	-0.40	0.04	-0.34

				NBO charge			
	PDMS-Mg-M1	**PDMS-Mg-M2**	**PDMS-Mg-M3**	**PDMS-Mg-M4**	**PDMS-Mg-M5**	**PDMS-$Mg(OH)_2$-M1**	**PDMS-$Mg(OH)_2$-M6**
C	0.57	0.55	0.57	0.54	0.55	0.56	0.54
O	-0.27	-0.36	-0.26	-0.35	-0.39	-0.27	-0.36
O	-0.30	-0.41	-0.31	-0.46	-0.45	-0.28	-0.48
SUM	0.00	-0.22	0.00	-0.26	-0.29	0.01	-0.29

[a] See Fig. 4, 5, and 7 in the text for the optimized structures.

Table 1. (Continue)

	Mulliken charge	
	PDMS-Mg-PDMS-M1	**PDMS-Mg-PDMS-M6**
C	0.75	0.77
O	-0.38	-0.25
O	-0.31	-0.38
SUM	0.07	0.15

	NBO charge	
	PDMS-Mg-PDMS-M1	**PDMS-Mg-PDMS-M6**
C	0.56	0.54
O	-0.28	-0.26
O	-0.27	-0.34
SUM	0.01	-0.06

	Mulliken charge		
	PDMS-Ti(OH)$_2$-M1	**PDMS-Ti(OH)$_2$-M4**	**PDMS-Ti(OH)$_2$-M6**
C	0.77	0.86	0.82
O	-0.34	-0.59	-0.65
O	-0.38	-0.47	-0.45
SUM	0.05	-0.20	-0.29

	NBO charge		
	PDMS-Ti(OH)$_2$-M1	**PDMS-Ti(OH)$_2$-M4**	**PDMS-Ti(OH)$_2$-M6**
C	0.56	0.55	0.54
O	-0.27	-0.18	-0.18
O	-0.29	-0.32	-0.29
SUM	0.00	0.05	0.07

Table S2. Imaginary frequencies (cm^{-1}) of optimized transition states

label	frequency
(H-profile)**TS-M3M4**	-249.8
(H-profile)**TS-M4M5**	-106.7

Table S3. Total electronic energy (E_{SCF}), thermal correction to enthalpy (H_{corr}). All are given in a.u.

label	E_{SCF}	H_{corr}
PDMS	-2416.342136	0.528609
PDMS-C	-2164.819085	0.535628
PDMS-S	-2739.261171	0.527134
PDMS-CH_2F	-2614.796321	0.516685
PDMS-CN	-2522.210210	0.472200
PDMS-OH	-2488.281210	0.482107
PDMS-Ph	-2799.772832	0.643416
PDMS-Mg-M1	-2552.914991	0.560957
PDMS-Mg-M2	-2552.915424	0.562036
PDMS-Mg-M3	-2552.907484	0.561804
PDMS-Mg-M4	-2552.917037	0.562451
PDMS-Mg-M5	-2552.932390	0.562776
PDMS-MgOH2-M1	-2768.190369	0.562415
PDMS-MgOH2-M6	-2768.208692	0.564121
PDMS-Mg-PDMS-M1	-4843.813554	1.045274
PDMS-Mg-PDMS-M3	-4843.821357	1.045577
PDMS-TiOH-M1	-2257.028878	0.478656
PDMS-TiOH-M4	-2257.022933	0.479138
PDMS-TiOH-M6	-2257.025247	0.481234
(H-profile) **PDMS-Mg**	-2364.321350	0.544065
(H-profile) **PDMS-Mg'**	-2364.318958	0.544120
(H-profile) **PDMS-Mg-M3**	-2552.913100	0.560807
(H-profile) **TS-M3M4**	-2552.907021	0.559553
(H-profile) **PDMS-Mg-M4**	-2552.920793	0.561954
(H-profile) **TS-M4M5**	-2552.909667	0.561201
(H-profile) **PDMS-Mg-M5**	-2552.919219	0.562426

XYZ coordinates

PDMS

Si	2.979904	1.937667	-0.018573
O	3.424862	0.380784	-0.434705
Si	2.776667	-1.099962	-0.109930
O	1.122371	-0.974681	-0.196524
Si	-0.173896	-1.533674	-1.061295
O	-1.455050	-1.420711	-0.022098
Si	-3.023519	-0.880644	-0.027497
O	-3.079637	0.665363	-0.602279
Si	-2.552935	2.150017	-0.042602
C	-4.032266	-1.944839	-1.178830
H	-5.081534	-1.635018	-1.191849
H	-3.651328	-1.865113	-2.202801
H	-3.988824	-2.997336	-0.881466
C	-3.601672	-0.950237	1.745445
H	-2.950623	-0.343293	2.384378
H	-4.625954	-0.577951	1.847704
H	-3.574858	-1.976834	2.125798
C	-0.464192	-0.457068	-2.559494
H	-1.216715	-0.902086	-3.220070
H	-0.829043	0.533425	-2.270687
H	0.457534	-0.326984	-3.137249
C	0.059272	-3.323669	-1.532703
H	0.338672	-3.918767	-0.657693
H	-0.879474	-3.727877	-1.927348
H	0.828123	-3.450127	-2.301338
C	3.415049	-2.294466	-1.392934
H	3.082293	-3.317856	-1.192770
H	3.075870	-2.013048	-2.395920
H	4.509548	-2.288880	-1.401698
C	3.219995	-1.624741	1.626350
H	2.747404	-0.966832	2.364326
H	2.894687	-2.650749	1.825384
H	4.302551	-1.573568	1.780037
C	-2.126601	3.198924	-1.535676
H	-1.276635	2.795255	-2.094857
H	-2.979817	3.263329	-2.218492
H	-1.864415	4.217192	-1.226872
C	-3.948811	2.947376	0.924147
H	-4.836208	3.083594	0.297996
H	-4.232971	2.325560	1.780158
H	-3.652804	3.929116	1.309493
C	1.605795	2.484804	-1.172605
H	1.966413	2.552132	-2.204654
H	0.790902	1.754434	-1.147965
H	1.193854	3.460336	-0.890588
C	4.492449	3.019435	-0.238077
H	5.304449	2.697120	0.421176
H	4.858048	2.972652	-1.268659
H	4.265811	4.065966	-0.007791
C	-1.060185	1.894241	1.066378
H	-0.465526	2.811502	1.148268
H	-1.353461	1.594223	2.078333
H	-0.405228	1.103869	0.680386
C	2.416445	1.947259	1.772487
H	3.242115	1.665884	2.435764
H	2.068384	2.940970	2.075939
H	1.591727	1.244480	1.938367
C	0.009422	-1.861587	2.248826
O	0.197195	-2.950585	1.882544
O	-0.165772	-0.790041	2.666303

PDMS-C

Si	-3.502962	-1.387493	0.380420
O	-2.439251	-0.322408	-0.336756
Si	-2.054000	1.262690	-0.554035
O	-0.469430	1.336402	-0.062620
C	0.545625	2.307411	-0.223228
O	1.519341	2.051278	0.757602
Si	1.798080	0.544874	1.424266
O	2.125091	-0.551665	0.221934
Si	3.497995	-1.136740	-0.524344
C	3.304719	0.830339	2.493968
H	3.585312	-0.075589	3.040835
H	4.167129	1.153565	1.901235
H	3.096853	1.616361	3.227074
C	0.367018	-0.097016	2.431089
H	-0.441866	-0.419805	1.772120
H	0.674854	-0.949535	3.046147
H	-0.019512	0.683354	3.095414
C	1.174057	2.161286	-1.604299
H	2.046209	2.816110	-1.683203
H	1.483302	1.122763	-1.741633
H	0.457528	2.422420	-2.388619
C	0.013271	3.711657	0.030735
H	-0.437603	3.753366	1.025834
H	0.836477	4.428538	-0.014293
H	-0.733447	3.989728	-0.721098
C	-2.246712	1.693855	-2.360026
H	-1.984544	2.735320	-2.575132
H	-1.613098	1.043341	-2.970471
H	-3.286724	1.543127	-2.669360
C	-3.140045	2.327877	0.535655
H	-3.041807	2.025426	1.584615
H	-2.875664	3.387456	0.467206
H	-4.192929	2.228104	0.251238
C	4.615786	-1.950295	0.746911
H	5.083412	-1.216877	1.411055
H	4.052110	-2.656269	1.366027
H	5.417750	-2.507905	0.250468
C	2.939763	-2.410001	-1.780481
H	2.333782	-3.187262	-1.301627
H	2.342689	-1.951689	-2.574678
H	3.802293	-2.899187	-2.245627
C	-3.580855	-2.905911	-0.712741
H	-3.874828	-2.640370	-1.733309
H	-2.607944	-3.404602	-0.756150
H	-4.310572	-3.626922	-0.328846
C	-5.200039	-0.586722	0.492804
H	-5.214553	0.227575	1.224533
H	-5.515418	-0.179457	-0.474283
H	-5.950382	-1.322421	0.802860
C	4.408562	0.274137	-1.365092
H	5.391579	-0.051570	-1.722532
H	3.847884	0.656756	-2.223586
H	4.563531	1.109487	-0.672745

C	-2.899620	-1.830092	2.097144
H	-2.791984	-0.937319	2.722921
H	-3.608265	-2.503640	2.592029
H	-1.926687	-2.328910	2.053832
C	-0.125128	-1.586849	-1.010951
O	-0.251662	-2.291451	-0.093029
O	-0.004197	-0.933178	-1.966566

PDMS-S

Si	-3.941678	0.964311	-0.706925
O	-3.146913	-0.145835	0.270676
Si	-2.163054	-1.448141	0.015169
S	-0.188005	-0.615646	-0.270909
Si	1.209846	-2.001990	0.634403
O	2.694601	-1.356879	0.327486
Si	3.481544	-0.547389	-0.895408
O	2.974323	1.013802	-0.940305
Si	2.512673	2.278738	0.040997
C	5.297823	-0.613597	-0.477869
H	5.889787	-0.050844	-1.206187
H	5.473077	-0.174958	0.510337
H	5.667629	-1.643295	-0.456745
C	3.063873	-1.336705	-2.532626
H	1.982718	-1.288112	-2.704025
H	3.555526	-0.812682	-3.358021
H	3.373161	-2.386696	-2.563300
C	1.034937	-2.119490	2.489155
H	1.958113	-2.549798	2.893266
H	0.894166	-1.132340	2.938105
H	0.200099	-2.756107	2.792577
C	1.055926	-3.670256	-0.201501
H	1.215898	-3.567177	-1.279560
H	1.806042	-4.364956	0.191957
H	0.068499	-4.118845	-0.048282
C	-2.301295	-2.560102	1.508358
H	-1.668322	-3.449777	1.434100
H	-2.044282	-2.015969	2.420789
H	-3.341641	-2.894349	1.590693
C	-2.639021	-2.356023	-1.551007
H	-2.550202	-1.702961	-2.425426
H	-1.972007	-3.210266	-1.710244
H	-3.668247	-2.727661	-1.497885
C	3.951838	3.479366	0.144664
H	4.830002	3.001474	0.592199
H	4.236033	3.835509	-0.850631
H	3.697673	4.352552	0.755250
C	1.021154	3.081268	-0.748872
H	1.280904	3.527029	-1.714379
H	0.252678	2.320933	-0.919193
H	0.591551	3.861569	-0.111906
C	-4.741088	2.216938	0.429921
H	-5.396482	1.722545	1.154114
H	-3.988669	2.787982	0.980875
H	-5.348794	2.925613	-0.142992
C	-5.267904	0.066371	-1.689261
H	-4.840746	-0.606113	-2.439811
H	-5.910448	-0.526877	-1.030037
H	-5.904851	0.786165	-2.215324
C	2.112232	1.637322	1.761276
H	1.847528	2.462277	2.432706
H	1.270659	0.938397	1.726782
H	2.965285	1.105551	2.197447
C	-2.701978	1.762317	-1.861181
H	-2.151170	1.010898	-2.439290
H	-3.198096	2.432932	-2.571336
H	-1.969962	2.345910	-1.294569
C	-1.410302	1.323915	2.012964
O	-1.472076	2.240207	1.298646
O	-1.342789	0.437134	2.763879

PDMS-CH2F

Si	2.865709	2.238101	-0.066487
O	3.452605	0.702381	-0.361531
Si	2.860876	-0.817318	-0.120099
O	1.190850	-0.669036	-0.044327
Si	-0.093502	-1.439428	-0.710328
O	-1.369643	-1.325027	0.310748
Si	-2.967691	-0.842888	0.276603
O	-3.061159	0.600595	-0.516130
Si	-2.650345	2.177737	-0.138447
C	-3.969950	-2.096644	-0.660691
H	-5.026026	-1.812449	-0.693556
H	-3.602837	-2.166649	-1.688522
H	-3.895873	-3.085626	-0.197335
C	-3.478506	-0.663497	2.061842
H	-2.834888	0.054465	2.581210
H	-4.515066	-0.321471	2.145717
H	-3.397112	-1.621445	2.586457
C	-0.574059	-0.665611	-2.364360
F	-1.578848	-1.497045	-2.883074
H	-0.992298	0.342260	-2.264936
H	0.246842	-0.629752	-3.091292
C	0.351184	-3.262200	-0.986656
F	1.363850	-3.628409	-0.095773
H	-0.508015	-3.919340	-0.813184
H	0.716601	-3.446410	-2.005101
C	3.364202	-1.846708	-1.592705
H	3.156752	-2.907452	-1.433738
H	2.842816	-1.516515	-2.499006
H	4.436318	-1.724890	-1.776345
C	3.445460	-1.487731	1.513408
H	3.122455	-0.830026	2.328848
H	3.032698	-2.485280	1.688231
H	4.537629	-1.546789	1.546168
C	-2.276156	3.055225	-1.751108
H	-1.377922	2.662043	-2.237987
H	-3.112263	2.950998	-2.449860
H	-2.112791	4.124857	-1.577662
C	-4.110078	2.988729	0.713905
H	-4.997317	2.978654	0.073021
H	-4.359432	2.465270	1.643301
H	-3.888693	4.030847	0.968622
C	1.469067	2.568798	-1.280000
H	1.848739	2.579774	-2.307586
H	0.714113	1.779079	-1.204170
H	0.972116	3.526980	-1.091715
C	4.275477	3.433036	-0.365571
H	5.110368	3.230569	0.312495

H	4.647914	3.348905	-1.391291
H	3.955380	4.468383	-0.206614
C	-1.154736	2.166438	0.996931
H	-0.617927	3.121107	0.952994
H	-1.434089	1.989210	2.041046
H	-0.446829	1.375683	0.720627
C	2.290706	2.328350	1.716426
H	3.140927	2.185537	2.392886
H	1.837925	3.298335	1.949485
H	1.547360	1.554574	1.938108
C	0.154292	-1.358565	2.594693
O	0.397530	-2.465089	2.332742
O	-0.078269	-0.257440	2.893024

PDMS-CN

Si	3.888145	-1.297318	-0.455385
O	2.652935	-0.184148	-0.241016
Si	2.418015	1.065966	0.805486
O	1.217119	2.026422	0.131463
Si	-0.382726	2.132155	0.038108
O	-1.098895	0.807833	-0.523582
Si	-2.550687	0.290109	-1.214235
O	-2.717766	-1.263232	-0.712289
Si	-3.184413	-1.954197	0.749485
C	-3.889945	1.410299	-0.553945
H	-4.877304	1.101803	-0.912702
H	-3.914845	1.414948	0.541523
H	-3.726278	2.442026	-0.887691
C	-2.379536	0.369655	-3.058453
H	-1.551464	-0.260242	-3.393133
H	-3.295600	0.028753	-3.550310
H	-2.183818	1.398390	-3.379516
C	-1.079758	2.513196	1.715911
N	-1.522355	2.720634	2.765255
C	-0.833658	3.565485	-1.043563
N	-1.181370	4.419157	-1.743333
C	1.795397	0.444104	2.446024
H	1.458079	1.265072	3.087186
H	0.955151	-0.242704	2.296622
H	2.577553	-0.104538	2.981299
C	3.935563	2.136572	0.921393
H	4.210822	2.515236	-0.067918
H	3.758230	2.995537	1.575761
H	4.789317	1.579766	1.322887
C	-5.057274	-1.909189	0.842390
H	-5.431421	-0.879965	0.859293
H	-5.506245	-2.417543	-0.016885
H	-5.414657	-2.405385	1.751196
C	-2.566319	-3.718879	0.738840
H	-2.929232	-4.252365	-0.145323
H	-1.473072	-3.750430	0.733798
H	-2.915945	-4.258855	1.625193
C	3.182701	-2.772719	-1.364107
H	2.433221	-3.291856	-0.756822
H	2.716666	-2.477243	-2.308693
H	3.977038	-3.492383	-1.589895
C	4.515143	-1.818792	1.236356
H	4.927151	-0.974047	1.800741
H	3.705513	-2.257706	1.829717
H	5.308089	-2.569015	1.146565
C	-2.440744	-0.971100	2.162723
H	-2.653653	-1.452154	3.123699
H	-1.353828	-0.903466	2.054497
H	-2.836782	0.048913	2.215017
C	5.254413	-0.492105	-1.452692
H	5.692867	0.358131	-0.919693
H	6.059539	-1.204048	-1.663647
H	4.869636	-0.125446	-2.409646
C	0.266545	-1.565628	-0.808042
O	0.250791	-1.820266	0.329535
O	0.283255	-1.350001	-1.949365

PDMS-OH

Si	3.224277	1.613918	0.335284
O	2.943626	-0.038894	0.415836
Si	2.510847	-1.167676	-0.713259
O	0.866028	-1.073681	-0.897443
Si	-0.544867	-1.834579	-0.609418
O	-1.363747	-0.867979	0.422964
Si	-2.981342	-0.639907	0.779781
O	-3.534716	0.616005	-0.126377
Si	-2.776770	1.954296	-0.789303
C	-3.944227	-2.174974	0.350373
H	-4.996648	-2.076478	0.632928
H	-3.895202	-2.348177	-0.728784
H	-3.532862	-3.054707	0.856427
C	-3.031959	-0.216035	2.595687
H	-2.395113	0.650524	2.803304
H	-4.048083	0.027145	2.920409
H	-2.673568	-1.054084	3.203277
O	-1.420954	-2.054103	-1.979907
H	-1.469813	-2.973572	-2.273142
O	-0.302006	-3.341078	0.011261
H	0.158424	-3.350587	0.862400
C	3.266990	-0.782273	-2.375095
H	2.983818	-1.547229	-3.105412
H	2.912551	0.181286	-2.756421
H	4.359920	-0.750138	-2.323166
C	3.008616	-2.849074	-0.079339
H	2.731092	-2.964440	0.972488
H	2.531331	-3.649119	-0.653692
H	4.093565	-2.975962	-0.151250
C	-4.122001	2.985540	-1.585077
H	-4.622927	2.424535	-2.380166
H	-4.879215	3.273805	-0.849283
H	-3.711114	3.900595	-2.024655
C	-1.939233	2.898489	0.600761
H	-2.671293	3.261802	1.330013
H	-1.230672	2.249935	1.129353
H	-1.379561	3.761086	0.222484
C	1.757104	2.427188	-0.501167
H	1.646168	2.078709	-1.534462
H	0.830673	2.184321	0.029056
H	1.861638	3.517500	-0.524385
C	4.792906	1.930855	-0.649136
H	5.626294	1.335476	-0.261389
H	4.671054	1.691484	-1.710000
H	5.077508	2.986674	-0.578899

C	-1.515114	1.400335	-2.059031
H	-1.142375	2.252758	-2.638708
H	-0.654104	0.923544	-1.578928
H	-1.950400	0.675067	-2.754319
C	3.464785	2.227045	2.087089
H	4.264447	1.668437	2.584323
H	3.747439	3.285345	2.086327
H	2.553075	2.122378	2.680827
C	0.690719	-0.437022	2.135998
O	0.499739	0.705436	2.204380
O	0.884831	-1.587340	2.117270

PDMS-Ph

Si	-4.135558	-0.201803	-0.004926
O	-3.110802	-1.476520	0.339427
Si	-1.808076	-2.229199	-0.337116
O	-0.585390	-1.114887	-0.486062
Si	0.876791	-0.680445	0.136173
O	1.557443	0.283280	-1.009069
Si	2.432389	1.682984	-1.190511
O	1.815628	2.840361	-0.195511
Si	0.330124	3.605767	-0.091203
C	4.204534	1.360821	-0.711759
H	4.815203	2.261736	-0.825254
H	4.284366	1.031616	0.329115
H	4.633834	0.573793	-1.340216
C	2.266350	2.178231	-2.983178
H	1.217834	2.347825	-3.249978
H	2.823077	3.098186	-3.188914
H	2.655381	1.394958	-3.643062
C	-1.285059	-3.597640	0.812502
H	-0.393585	-4.112881	0.440574
H	-1.047874	-3.192512	1.802897
H	-2.087028	-4.332097	0.935798
C	-2.212246	-2.817183	-2.061975
H	-2.420466	-1.965356	-2.719290
H	-1.373585	-3.377420	-2.487661
H	-3.093985	-3.465820	-2.064599
C	-0.030281	3.960532	1.707743
H	-0.294243	3.039554	2.237563
H	0.838105	4.400316	2.208355
H	-0.868652	4.659700	1.802780
C	0.443971	5.196916	-1.080813
H	1.234043	5.846324	-0.690434
H	0.671410	4.987724	-2.131866
H	-0.498566	5.753918	-1.047321
C	-3.893569	1.131863	1.292955
H	-4.038944	0.719130	2.297740
H	-2.895002	1.578458	1.255016
H	-4.626491	1.934869	1.154377
C	-5.889044	-0.856406	0.097089
H	-6.047812	-1.660487	-0.628920
H	-6.099531	-1.258379	1.093245
H	-6.619785	-0.067244	-0.110208
C	-1.006026	2.503748	-0.815375
H	-1.988225	2.983150	-0.720475
H	-0.841060	2.290258	-1.876817
H	-1.056307	1.539026	-0.295834
C	-3.775863	0.447818	-1.728421
H	-4.174232	-0.225187	-2.495657
H	-4.233465	1.431925	-1.879625
H	-2.698145	0.554757	-1.895665
C	0.586380	0.181655	1.766516
C	1.642524	0.794559	2.457855
C	-0.670699	0.138203	2.385059
C	1.452839	1.344468	3.721753
H	2.630726	0.843080	2.004909
C	-0.867543	0.688907	3.651535
H	-1.511415	-0.327124	1.874065
C	0.195285	1.288833	4.321736
H	2.282033	1.818327	4.237889
H	-1.850555	0.649014	4.111485
H	0.044582	1.717374	5.307939
C	2.001792	-2.144158	0.400338
C	2.089181	-2.767306	1.653384
C	2.774193	-2.656750	-0.652615
C	2.906933	-3.877646	1.847422
H	1.514108	-2.376320	2.490588
C	3.594994	-3.765204	-0.462565
H	2.728130	-2.183476	-1.629650
C	3.659291	-4.377953	0.787271
H	2.961481	-4.348635	2.824145
H	4.185853	-4.150842	-1.287909
H	4.299562	-5.242322	0.936191
C	0.124428	-0.724880	-3.157896
O	0.783141	-1.683219	-3.110728
O	-0.544315	0.221017	-3.263123

PDMS-Mg-M1

Si	2.920075	-2.079914	-1.062536
O	2.252461	-1.439621	0.325913
Si	2.549375	-0.187462	1.444739
O	1.559015	1.034633	1.131196
Mg	0.022595	1.129700	-0.040421
O	-1.491243	1.474368	-1.326219
Si	-2.980819	0.868375	-1.236086
O	-3.123050	0.101999	0.268156
Si	-3.746988	-1.267514	0.979462
C	-4.328056	2.168937	-1.277558
H	-5.319638	1.716119	-1.168577
H	-4.196088	2.880145	-0.455105
H	-4.315067	2.733374	-2.215355
C	-3.309250	-0.437568	-2.550748
H	-2.548723	-1.228082	-2.543998
H	-4.287356	-0.915785	-2.421263
H	-3.293388	0.016057	-3.547465
C	2.200368	-0.993266	3.103603
H	2.318721	-0.278877	3.924697
H	1.171280	-1.371091	3.132583
H	2.867185	-1.841355	3.290713
C	4.366595	0.272944	1.324249
H	4.588472	0.795516	0.388502
H	4.638056	0.939618	2.150554
H	5.016658	-0.607745	1.384328
C	-5.617563	-1.136119	1.009750
H	-5.936412	-0.227759	1.530914
H	-6.021213	-1.094561	-0.008300
H	-6.073995	-1.994732	1.513515

C	-3.238470	-2.830894	0.070259
H	-3.596086	-2.851828	-0.963606
H	-2.150117	-2.950383	0.068181
H	-3.659258	-3.704168	0.581915
C	1.469656	-2.501583	-2.182363
H	0.750200	-3.156877	-1.676445
H	0.961852	-1.581733	-2.492711
H	1.804131	-3.021978	-3.085896
C	3.867597	-3.633172	-0.607716
H	4.682557	-3.400628	0.086221
H	3.214169	-4.364271	-0.121220
H	4.306639	-4.106428	-1.492659
C	-3.023368	-1.299921	2.709662
H	-3.395826	-2.151907	3.287496
H	-1.932298	-1.389957	2.650666
H	-3.266560	-0.388557	3.266921
C	4.061749	-0.858280	-1.912268
H	5.021118	-0.770822	-1.393340
H	4.264025	-1.181858	-2.939481
H	3.607936	0.136523	-1.956572
O	1.030613	0.884799	-1.876579
H	0.241236	1.221017	-2.347639
H	1.715027	1.576555	-1.888362
O	-1.191962	1.494525	1.627168
H	-0.646477	1.041161	2.291707
H	-1.964217	0.923465	1.412776
O	0.095763	3.268283	-0.288787
H	-0.121427	3.584213	0.603482
H	-0.761165	3.125081	-0.753269
O	-0.375015	-0.930869	0.124766
H	0.535801	-1.322547	0.135733
H	-0.823168	-1.256911	-0.670478
C	2.756421	3.182290	0.158656
O	2.565098	3.782219	1.131599
O	3.017721	2.660488	-0.855387

PDMS-Mg-M2

Si	4.199732	-1.455745	-0.413330
O	3.132505	-0.322777	0.206727
Si	3.171772	1.154503	1.077436
O	1.676131	1.727627	1.007018
Mg	0.161824	1.043228	-0.060928
O	-1.522240	0.430859	-1.221906
Si	-3.098633	1.026061	-0.856303
O	-3.478902	0.357687	0.615847
Si	-4.023053	-1.125432	1.219419
C	-2.902214	2.860419	-0.610332
H	-3.883636	3.286281	-0.372815
H	-2.207042	3.123614	0.188466
H	-2.544071	3.334421	-1.529758
C	-4.330844	0.727945	-2.219114
H	-4.734081	-0.284068	-2.209863
H	-5.149548	1.451382	-2.143875
H	-3.839914	0.880988	-3.186704
C	3.745183	0.726121	2.808752
H	3.702793	1.604910	3.460106
H	3.096431	-0.041186	3.245411
H	4.772303	0.346592	2.822868
C	4.448237	2.207488	0.189592
H	4.170175	2.344898	-0.862262
H	4.536507	3.199817	0.643288
H	5.441888	1.743956	0.213289
C	-4.778876	-0.682083	2.879969
H	-4.039285	-0.224274	3.546123
H	-5.602283	0.028937	2.759259
H	-5.172209	-1.571217	3.384241
C	-5.309417	-1.879552	0.092160
H	-6.102801	-1.163903	-0.148183
H	-4.843400	-2.218140	-0.836974
H	-5.776181	-2.742911	0.579434
C	3.155342	-2.982305	-0.711677
H	2.741346	-3.368189	0.226462
H	2.315571	-2.760265	-1.381934
H	3.737614	-3.786742	-1.172602
C	5.581845	-1.776037	0.810071
H	6.178515	-0.872648	0.978676
H	5.186473	-2.103372	1.777158
H	6.257547	-2.554895	0.440857
C	-2.558536	-2.265557	1.476110
H	-2.815819	-3.069282	2.175033
H	-2.257469	-2.716079	0.526048
H	-1.692368	-1.732419	1.884899
C	4.880670	-0.797188	-2.031864
H	5.479114	0.106554	-1.876423
H	5.518741	-1.540356	-2.521964
H	4.072291	-0.547198	-2.728556
O	1.296227	0.637724	-1.776731
H	2.116376	0.284593	-1.381990
H	0.759221	-0.152488	-2.079700
O	-1.084334	1.441474	1.534822
H	-0.546162	1.226117	2.312301
H	-1.940798	0.967318	1.579351
O	0.198733	3.029003	-0.781237
H	0.635240	2.873080	-1.636055
H	0.933721	3.155152	-0.140669
O	0.470732	-0.926748	0.600193
H	1.450466	-0.948281	0.653036
H	0.236307	-1.488272	-0.170858
C	-1.508958	-0.955863	-1.643452
O	-2.596405	-1.511545	-1.612865
O	-0.363132	-1.373666	-1.935167

PDMS-Mg-M3

Si	3.950251	-1.833794	-0.666637
O	3.776491	-0.176558	-0.590541
Si	3.528499	0.849667	0.754059
O	1.973416	0.835245	1.151832
Mg	0.328561	0.777237	0.138579
O	-1.197918	1.023169	-1.055079
Si	-2.769750	0.765807	-0.911912
O	-2.948777	-0.623948	0.089312
Si	-4.163583	-1.754154	0.338594
C	-3.691357	2.130010	-0.012945
H	-4.731070	1.857288	0.198836
H	-3.202339	2.378327	0.936507
H	-3.697670	3.045883	-0.612108
C	-3.621832	0.361473	-2.533631
H	-3.157841	-0.507947	-3.011463

H	-4.689150	0.148412	-2.400641
H	-3.539550	1.205463	-3.226281
C	4.614032	0.218746	2.152165
H	4.564275	0.910699	2.999858
H	4.274194	-0.758131	2.514815
H	5.664097	0.127979	1.854605
C	4.153460	2.514815	0.163500
H	3.584233	2.858003	-0.706561
H	4.046886	3.272157	0.947060
H	5.209607	2.465573	-0.120829
C	-5.791800	-0.869587	0.620503
H	-5.724803	-0.189227	1.476370
H	-6.089105	-0.281089	-0.254269
H	-6.593577	-1.587100	0.825762
C	-4.273439	-2.911178	-1.132341
H	-4.628085	-2.394094	-2.029114
H	-3.295680	-3.348027	-1.361636
H	-4.965721	-3.734226	-0.923818
C	2.489251	-2.627291	0.227057
H	2.320746	-2.126912	1.188901
H	1.603173	-2.505853	-0.408380
H	2.638586	-3.695760	0.410804
C	5.572983	-2.397468	0.086971
H	6.405604	-1.801512	-0.301082
H	5.579434	-2.313718	1.177203
H	5.762906	-3.445387	-0.171080
C	-3.648128	-2.693548	1.877548
H	-4.382937	-3.462297	2.138313
H	-2.684231	-3.194824	1.733163
H	-3.549951	-2.017809	2.734006
C	3.898148	-2.298673	-2.482143
H	4.714132	-1.821301	-3.033816
H	3.990707	-3.381895	-2.615234
H	2.952071	-1.986773	-2.937153
O	1.209395	-0.149833	-1.506134
H	0.758144	0.288202	-2.245516
H	2.174223	0.034850	-1.521073
O	-2.160878	0.364506	2.695286
H	-1.509813	-0.354571	2.616569
H	-2.699420	0.238219	1.892804
O	-0.332333	2.076613	1.636730
H	0.524420	1.968928	2.096309
H	-1.027558	1.631452	2.179506
O	-0.424544	-0.998001	0.968392
H	0.199150	-1.715002	0.767988
H	-1.262264	-1.136484	0.465116
C	-0.223861	3.442028	-0.860473
O	-1.206251	4.052266	-0.874604
O	0.814007	2.896585	-0.861709

PDMS-Mg-M4

Si	-3.888119	1.491247	-0.920708
O	-3.228502	1.083647	0.565513
Si	-2.826423	-0.116773	1.587929
O	-1.766997	-1.209328	0.805642
Mg	0.253153	-1.463904	0.215202
O	1.984574	-1.880732	-0.648956
Si	3.343451	-1.018992	-0.592549
O	2.962647	0.399133	0.305282
Si	3.681237	1.907263	0.490336
C	4.730584	-1.866866	0.333979
H	5.643256	-1.262440	0.358495
H	4.430346	-2.069861	1.367826
H	4.976503	-2.825244	-0.134520
C	3.895945	-0.424106	-2.281789
H	3.085832	0.112520	-2.789458
H	4.766520	0.240028	-2.227693
H	4.169457	-1.272977	-2.917358
C	-1.747614	0.608756	2.932912
H	-1.287997	-0.173391	3.548623
H	-0.975916	1.243688	2.480642
H	-2.332476	1.248273	3.600559
C	-4.296955	-1.033983	2.256749
H	-4.855790	-1.481183	1.431038
H	-3.984070	-1.834539	2.934751
H	-4.960024	-0.359278	2.807386
C	5.533181	1.719033	0.695764
H	5.772548	1.085706	1.556202
H	5.992085	1.269348	-0.191485
H	6.005913	2.694371	0.853528
C	3.261263	2.956543	-1.003740
H	3.719344	2.561931	-1.916139
H	2.177745	2.995771	-1.164431
H	3.612333	3.985536	-0.870874
C	-2.670385	1.079032	-2.283913
H	-1.696459	1.531912	-2.072904
H	-2.540213	-0.002643	-2.387163
H	-3.024359	1.467112	-3.245550
C	-4.142857	3.349046	-0.849750
H	-4.822577	3.622694	-0.036450
H	-3.193147	3.867332	-0.683001
H	-4.570874	3.723520	-1.785882
C	2.889795	2.623506	2.032552
H	3.274690	3.624243	2.253512
H	1.804138	2.713263	1.906099
H	3.082523	1.994278	2.908492
C	-5.526030	0.615080	-1.147256
H	-6.197601	0.816924	-0.305610
H	-6.025577	0.952865	-2.061984
H	-5.367664	-0.464316	-1.216952
O	0.537887	-0.929476	-2.873074
H	1.164132	-1.467032	-2.341080
H	-0.298154	-1.421207	-2.779568
O	1.094575	-0.702254	1.942470
H	0.549862	-0.127342	2.500274
H	1.858643	-0.176324	1.612124
O	0.430201	-3.474855	0.850213
H	1.298692	-3.501758	0.398355
H	-0.193796	-3.884979	0.226758
O	0.244360	0.464107	-0.621360
H	0.266925	0.178018	-1.579255
H	1.157843	0.752548	-0.435074
C	-2.189713	-1.772195	-0.433833
O	-3.371489	-1.751859	-0.705603
O	-1.172981	-2.197386	-1.070729

PDMS-Mg-M5

Si	-4.014514	1.142870	-1.170996

O	-3.023564	0.312023	-0.106968
Si	-3.167544	-0.454568	1.426135
O	-1.827913	-1.307850	1.615362
Mg	-0.238093	-1.437979	0.463131
O	2.889434	-0.500552	-1.924878
Si	3.947657	-0.710506	-0.615102
O	3.305255	0.145613	0.670282
Si	3.126513	1.812481	0.875445
C	4.210165	-2.476123	-0.102017
H	5.146623	-2.582077	0.454997
H	3.381386	-2.825457	0.517572
H	4.264125	-3.122791	-0.983523
C	5.523811	0.091876	-1.208230
H	5.356399	1.119643	-1.545128
H	6.280464	0.107589	-0.417143
H	5.933123	-0.467775	-2.055554
C	-3.358495	0.939221	2.666164
H	-3.363715	0.548885	3.688890
H	-2.515651	1.635191	2.583585
H	-4.282097	1.508656	2.518197
C	-4.737421	-1.478226	1.319505
H	-4.665271	-2.206096	0.503210
H	-4.913010	-2.033717	2.246268
H	-5.620370	-0.854258	1.135750
C	4.765804	2.523140	1.444281
H	5.117296	2.014887	2.348053
H	5.540572	2.421597	0.677699
H	4.665386	3.589034	1.676377
C	2.584810	2.585416	-0.742375
H	3.356969	2.507161	-1.514313
H	1.686947	2.097528	-1.133002
H	2.357959	3.647882	-0.600262
C	-2.836709	2.101346	-2.271030
H	-2.249482	2.819402	-1.687778
H	-2.133532	1.430345	-2.779338
H	-3.371178	2.661613	-3.045054
C	-5.162565	2.290016	-0.233951
H	-5.833604	1.731227	0.427606
H	-4.598151	2.999013	0.380467
H	-5.785146	2.866100	-0.926983
C	1.825357	2.040483	2.204392
H	1.734842	3.099143	2.470130
H	0.850619	1.700738	1.839239
H	2.088333	1.497510	3.119667
C	-4.988384	-0.106566	-2.173057
H	-5.674024	-0.677661	-1.538499
H	-5.582117	0.385425	-2.950839
H	-4.319077	-0.819503	-2.667747
O	-1.388052	-1.704613	-1.317122
H	-2.124482	-1.083753	-1.156537
H	-0.774044	-1.275532	-1.963206
O	1.138374	-1.142628	1.964467
H	0.793634	-0.538297	2.637862
H	1.936717	-0.725515	1.569324
O	-0.563025	-3.497449	0.776466
H	-0.933937	-3.758283	-0.082357
H	-1.331845	-3.225111	1.321428
O	-0.295540	0.648124	-0.040864
H	-1.258369	0.835194	-0.039661
H	-0.024563	0.646094	-0.984741
C	1.591323	-0.822006	-1.700024
O	0.718543	-0.305108	-2.424800
O	1.386943	-1.599264	-0.717061

PDMS-MgOH2-M1

Si	-3.338495	2.050635	0.171570
O	-3.094141	0.534529	0.845848
Si	-3.131338	-1.066575	0.531431
O	-1.562237	-1.651183	0.265489
Si	-0.094440	-1.424881	1.063935
O	0.855018	-1.572079	-0.313102
Si	2.355469	-1.064741	-0.891751
O	2.749258	0.325274	-0.099000
Si	2.866936	1.974026	-0.428702
C	3.597910	-2.389456	-0.477747
H	4.619943	-2.045449	-0.667452
H	3.524302	-2.691523	0.571133
H	3.418709	-3.275576	-1.094741
C	2.120650	-0.834202	-2.722745
H	1.351952	-0.080875	-2.926721
H	3.047238	-0.514064	-3.211956
H	1.789873	-1.773889	-3.181379
C	-0.011588	0.287666	1.755995
H	0.956371	0.492224	2.219674
H	-0.160468	0.966809	0.908486
H	-0.809795	0.474020	2.481737
C	0.198910	-2.839477	2.228732
H	0.118914	-3.789070	1.691249
H	1.190422	-2.777062	2.684887
H	-0.546206	-2.838160	3.031297
C	-3.739118	-1.938161	2.064043
H	-3.675435	-3.025258	1.954754
H	-3.136143	-1.646612	2.931721
H	-4.777595	-1.674769	2.286229
C	-4.066343	-1.513634	-1.014877
H	-3.631872	-1.021139	-1.891802
H	-4.036268	-2.595342	-1.183533
H	-5.116149	-1.210002	-0.948713
C	2.423265	2.906514	1.135537
H	1.355134	2.824636	1.359317
H	2.990350	2.554765	2.003233
H	2.653168	3.969963	1.003763
C	4.643659	2.311437	-0.919326
H	5.332411	2.029395	-0.117200
H	4.913786	1.740655	-1.814834
H	4.796219	3.372562	-1.143692
C	-1.745895	3.032173	0.191372
H	-1.332603	3.104150	1.203373
H	-1.017635	2.542505	-0.461501
H	-1.921461	4.050685	-0.173243
C	-4.600060	2.887275	1.284948
H	-5.543350	2.331332	1.302353
H	-4.232378	2.953446	2.314137
H	-4.817264	3.904215	0.940277
C	1.676818	2.430725	-1.799911
H	1.430923	3.497507	-1.750410
H	2.096800	2.228590	-2.790985
H	0.746164	1.856614	-1.696059

C	-4.031819	1.901580	-1.562388
H	-5.001220	1.391992	-1.572323
H	-4.173306	2.894500	-2.003698
H	-3.331767	1.338215	-2.184303
Mg	-0.780036	-1.440516	-1.689136
O	-1.079273	0.414473	-1.696850
H	-1.133198	0.894711	-2.532139
O	-0.750440	-2.765063	-2.959361
H	-0.958530	-3.693397	-2.823367
C	3.877179	-0.258188	2.254704
O	4.741684	0.496627	2.077324
O	3.028274	-1.024964	2.478561

PDMS-MgOH2-M6

Si	-3.395555	1.892515	0.185915
O	-2.571012	0.465266	0.484819
Si	-2.662668	-1.156075	0.278706
O	-1.061484	-1.706497	0.379687
Si	0.185516	-1.405537	1.474943
O	1.411817	-1.566223	0.341987
Si	2.947358	-0.935024	0.017575
O	2.985787	0.594275	0.602259
Si	3.247062	2.193079	0.195166
C	4.164400	-1.983399	0.955371
H	5.194568	-1.667976	0.763079
H	3.988997	-1.907070	2.033636
H	4.065493	-3.034335	0.666651
C	3.110607	-1.054157	-1.831172
H	2.342729	-0.455384	-2.333770
H	4.092167	-0.714911	-2.177265
H	2.991378	-2.098835	-2.146543
C	0.099311	0.274765	2.250922
H	0.993998	0.461724	2.853863
H	0.037854	1.036535	1.471641
H	-0.783483	0.363806	2.892752
C	0.281617	-2.812421	2.681120
H	0.345364	-3.756795	2.131339
H	1.164915	-2.727015	3.322312
H	-0.602258	-2.846605	3.326463
C	-3.578967	-1.924557	1.709846
H	-3.527860	-3.017217	1.672405
H	-3.152794	-1.594552	2.664283
H	-4.634563	-1.633531	1.705144
C	-3.285646	-1.667077	-1.394314
H	-2.825657	-1.060886	-2.182026
H	-3.056133	-2.721903	-1.585910
H	-4.372135	-1.546521	-1.459162
C	1.915988	3.240637	1.001741
H	0.948175	3.138974	0.500780
H	1.781004	2.972996	2.054603
H	2.192093	4.299938	0.957022
C	4.921333	2.668128	0.893053
H	4.947051	2.535138	1.979331
H	5.715333	2.048761	0.462617
H	5.159737	3.714745	0.675675
C	-2.119474	3.248229	-0.029038
H	-1.359741	3.190327	0.760494
H	-1.645974	3.167540	-1.012719
H	-2.582562	4.238220	0.041577
C	-4.425838	2.239746	1.718195
H	-5.142818	1.432238	1.902866
H	-3.790718	2.330867	2.605765
H	-4.993530	3.170699	1.614596
C	3.222841	2.421846	-1.663280
H	3.346861	3.481363	-1.913977
H	4.030666	1.869763	-2.154510
H	2.271697	2.081463	-2.083843
C	-4.492312	1.699531	-1.314958
H	-5.267886	0.942841	-1.150260
H	-4.997595	2.642953	-1.549343
H	-3.887552	1.407076	-2.178407
Mg	0.196131	-2.188495	-1.242896
O	0.238274	0.852182	-1.019124
H	-0.133087	1.706047	-0.740430
O	0.595578	-3.945081	-1.543980
H	0.367677	-4.432191	-2.340868
C	-0.591626	0.407054	-2.037544
O	-1.495943	1.128596	-2.423262
O	-0.279562	-0.766479	-2.435766

PDMS-Mg-PDMS-M1

Si	5.311287	-1.966226	0.586692
O	3.696850	-1.924926	0.035499
Si	2.605563	-3.002705	-0.515121
O	1.422435	-2.006724	-1.289530
Si	1.523609	-0.925684	-2.617004
O	0.255193	0.022028	-1.975099
Si	-0.329758	1.625114	-2.231038
O	0.955214	2.566928	-1.923163
Si	1.490630	4.169257	-2.147238
C	-0.926066	1.717563	-3.983578
H	-1.414432	2.676868	-4.185932
H	-0.086153	1.628565	-4.682230
H	-1.646617	0.925488	-4.214295
C	-1.618929	1.741199	-0.888963
H	-1.127020	1.705146	0.092979
H	-2.160697	2.693086	-0.930715
H	-2.366282	0.937360	-0.938116
C	3.124300	-0.009960	-2.679590
H	3.120712	0.689078	-3.523225
H	3.295438	0.560972	-1.763257
H	3.962978	-0.700330	-2.822098
C	0.996083	-1.763078	-4.175927
H	0.020814	-2.246614	-4.066807
H	0.929556	-1.044091	-4.999466
H	1.724265	-2.526701	-4.470299
C	3.276972	-4.162534	-1.794510
H	2.483073	-4.763967	-2.248780
H	3.796486	-3.617796	-2.591587
H	4.001957	-4.855522	-1.353752
C	1.619333	-3.769153	0.864755
H	1.214415	-2.989999	1.525576
H	0.790515	-4.380826	0.490517
H	2.245712	-4.414146	1.490200
C	2.809210	4.433743	-0.851495
H	2.400680	4.380601	0.163412
H	3.598611	3.679438	-0.943136
H	3.277336	5.416511	-0.968296

C	2.178188	4.284270	-3.879123
H	3.009150	3.586668	-4.027015
H	1.412256	4.068474	-4.632030
H	2.557015	5.291441	-4.081871
C	5.625254	-0.285642	1.335971
H	5.518432	0.506251	0.586657
H	4.934819	-0.074456	2.159584
H	6.643344	-0.226842	1.734411
C	6.410560	-2.281943	-0.890010
H	6.216807	-3.257691	-1.348058
H	6.282255	-1.511455	-1.657786
H	7.464343	-2.269678	-0.591794
C	-0.003010	5.271495	-1.917561
H	0.268639	6.328340	-2.008078
H	-0.766689	5.072836	-2.679290
H	-0.458530	5.131669	-0.931086
C	5.413537	-3.352389	1.837746
H	5.176124	-4.322492	1.383954
H	6.424337	-3.434578	2.250557
H	4.729299	-3.194056	2.678631
Mg	-0.054541	-1.062476	-0.331186
Si	-5.366316	-0.143532	-1.230389
O	-4.241478	-1.036984	-0.306748
Si	-3.092274	-2.184503	-0.403257
O	-1.768873	-1.605154	0.540228
Si	-1.463244	-0.870567	2.065839
O	0.111171	-0.421617	1.527226
Si	1.373333	0.467714	2.315474
O	0.569305	1.583309	3.182857
Si	0.503745	3.273549	3.343623
C	2.296675	-0.740518	3.376522
H	3.067431	-0.225124	3.959597
H	1.641014	-1.254523	4.086300
H	2.795976	-1.492113	2.753309
C	2.371874	1.115833	0.889537
H	1.771669	1.666173	0.153017
H	3.169645	1.785678	1.230282
H	2.863094	0.266730	0.394750
C	-2.526552	0.623274	2.337885
H	-1.913019	1.528478	2.344078
H	-3.281378	0.708652	1.548246
H	-3.036452	0.554055	3.303204
C	-1.287809	-2.103098	3.428798
H	-0.577281	-2.893200	3.166700
H	-0.921788	-1.600143	4.331584
H	-2.246265	-2.565112	3.677314
C	-3.594427	-3.853083	0.220048
H	-2.821587	-4.595169	-0.006727
H	-3.766597	-3.861457	1.298792
H	-4.517013	-4.180824	-0.270975
C	-2.283978	-2.277177	-2.091904
H	-2.017880	-1.291188	-2.494254
H	-1.382386	-2.907807	-2.062067
H	-2.953651	-2.745737	-2.821378
C	-0.638979	3.618025	4.771412
H	-1.632694	3.191788	4.598744
H	-0.247393	3.194772	5.701276
H	-0.762111	4.695391	4.922142
C	2.241437	3.898089	3.626681
H	2.703370	3.410353	4.491245
H	2.887612	3.733624	2.757145
H	2.235376	4.975203	3.824788
C	-5.618360	1.460597	-0.309428
H	-6.055460	1.299961	0.680233
H	-4.675160	2.005292	-0.187039
H	-6.301263	2.111702	-0.865593
C	-6.913300	-1.165533	-1.404687
H	-6.706984	-2.120255	-1.900981
H	-7.372648	-1.375833	-0.435020
H	-7.653639	-0.636235	-2.013910
C	-0.180054	3.942210	1.723472
H	-0.045485	5.028845	1.671470
H	0.342480	3.506254	0.861485
H	-1.251773	3.740981	1.610831
C	-4.599918	0.188234	-2.912241
H	-4.409192	-0.730338	-3.476940
H	-5.291170	0.792822	-3.509962
H	-3.663286	0.752926	-2.837328
C	-5.349505	-1.361318	2.227313
O	-4.304735	-1.781521	2.542542
O	-6.385062	-0.942954	1.926127

PDMS-Mg-PDMS-M3

Si	5.540996	0.099249	0.368096
O	3.988562	-0.607196	0.337913
Si	3.322747	-2.068012	0.601328
O	1.760029	-1.971394	-0.129107
Si	1.330071	-1.779889	-1.780896
O	-0.179015	-1.097711	-1.352029
Si	-1.217005	-0.079030	-2.305346
O	-0.162299	0.516728	-3.390156
Si	0.036391	1.832117	-4.452506
C	-2.519132	-1.173683	-3.045406
H	-3.088854	-0.626797	-3.805113
H	-2.089142	-2.056302	-3.530079
H	-3.227492	-1.505927	-2.277283
C	-1.912489	1.171884	-1.123098
H	-1.141222	1.701103	-0.552389
H	-2.487560	1.925249	-1.673684
H	-2.607895	0.681671	-0.432393
C	2.529050	-0.698378	-2.673245
H	2.295544	-0.691494	-3.742030
H	2.500272	0.331823	-2.311054
H	3.546375	-1.085688	-2.543233
C	1.038618	-3.444158	-2.537429
H	0.292063	-4.024121	-1.983247
H	0.676286	-3.340447	-3.566132
H	1.964194	-4.028631	-2.577164
C	4.247068	-3.444477	-0.232623
H	3.719455	-4.401115	-0.165550
H	4.429179	-3.223867	-1.290940
H	5.227619	-3.581843	0.237407
C	2.944348	-2.346659	2.406441
H	2.143479	-1.687643	2.768300
H	2.682923	-3.384506	2.640118
H	3.832712	-2.111762	3.003883
C	1.676400	2.621515	-4.022257
H	1.724843	2.885089	-2.959124

H	2.521134	1.964404	-4.251945
H	1.816188	3.544590	-4.594790
C	0.017686	1.136817	-6.181145
H	0.807999	0.391712	-6.319285
H	-0.939916	0.657825	-6.409199
H	0.176816	1.927025	-6.922024
C	5.256690	1.937676	0.205885
H	4.795381	2.184605	-0.756429
H	4.611372	2.318388	1.005390
H	6.207388	2.477710	0.263820
C	6.507661	-0.579478	-1.078862
H	6.662366	-1.660943	-1.003179
H	6.007053	-0.369905	-2.030259
H	7.498553	-0.115096	-1.125695
C	-1.376849	3.021756	-4.146486
H	-1.353249	3.835178	-4.879400
H	-2.354637	2.534331	-4.242265
H	-1.314822	3.479022	-3.152430
C	6.313682	-0.369307	2.004820
H	6.415300	-1.456613	2.107529
H	7.319435	0.053541	2.097557
H	5.725582	-0.000039	2.852335
Mg	-0.040948	-1.349073	0.629065
Si	-5.706156	-0.372169	-0.184309
O	-4.139051	-0.742572	0.363313
Si	-3.352655	-1.899701	1.196748
O	-1.826388	-1.185263	1.552787
Si	-1.407554	0.129590	2.564985
O	0.121357	0.270520	1.791251
Si	1.150860	1.663225	1.728770
O	0.118273	2.848295	2.156963
Si	-0.040370	4.503519	1.789307
C	2.512556	1.396050	2.959231
H	3.083905	2.320828	3.097138
H	2.121334	1.102557	3.938832
H	3.206842	0.623112	2.610790
C	1.757395	1.767547	-0.027394
H	0.959027	1.658806	-0.770137
H	2.243167	2.734769	-0.205269
H	2.513638	0.993265	-0.195267
C	-2.591943	1.535054	2.384163
H	-2.419825	2.261392	3.183701
H	-2.490041	2.048900	1.425840
H	-3.618884	1.159210	2.466909
C	-1.134198	-0.453760	4.298401
H	-0.503295	-1.348396	4.328335
H	-0.646518	0.326960	4.892651
H	-2.082973	-0.690934	4.790994
C	-4.162086	-2.303925	2.816099
H	-3.532242	-2.951199	3.435233
H	-4.388582	-1.395490	3.386727
H	-5.111959	-2.825906	2.656003
C	-2.948060	-3.363754	0.118139
H	-2.219092	-3.101721	-0.661150
H	-2.560596	-4.207365	0.696627
H	-3.851513	-3.706481	-0.398021
C	-1.290305	5.195368	2.984098
H	-2.285106	4.768909	2.819430
H	-0.999834	5.000134	4.021088
H	-1.376606	6.280367	2.864688
C	1.653764	5.271128	1.986611
H	2.012362	5.175246	3.016849
H	2.396280	4.808033	1.325046
H	1.632811	6.338948	1.745601
C	-5.480519	1.018146	-1.411026
H	-5.045965	1.900850	-0.929643
H	-4.824832	0.719385	-2.236742
H	-6.441215	1.316326	-1.842902
C	-6.714926	0.155740	1.295884
H	-6.813763	-0.650828	2.030279
H	-6.269211	1.021222	1.797770
H	-7.727339	0.441735	0.991714
C	-0.640743	4.614284	0.015484
H	-0.746047	5.660628	-0.290395
H	0.057567	4.137995	-0.683501
H	-1.621501	4.139236	-0.102427
C	-6.389803	-1.922332	-0.976257
H	-6.458190	-2.746426	-0.255866
H	-7.400207	-1.752215	-1.362316
H	-5.771215	-2.254981	-1.817315
C	0.648139	-4.268545	1.117173
O	1.355006	-5.133533	0.850822
O	-0.083763	-3.386645	1.394520

PDMS-TiOH-M1

Si	3.659887	1.093536	-0.321134
O	2.305345	0.209758	0.100861
Si	1.595072	-0.120655	1.572861
O	-0.011706	-0.384059	1.269838
Ti	-0.861273	-1.263811	-0.059833
O	-2.485698	-2.070263	0.297342
Si	-3.632616	-0.876838	0.351867
O	-2.559950	0.397506	0.142519
Si	-2.449660	1.964590	-0.471415
C	-4.825545	-0.960722	-1.076832
H	-5.484466	-0.085295	-1.098561
H	-4.271555	-0.996529	-2.020634
H	-5.456106	-1.853327	-1.016325
C	-4.466517	-0.753471	2.010414
H	-3.713165	-0.666564	2.799259
H	-5.116085	0.127027	2.058685
H	-5.077807	-1.637463	2.216502
O	-0.695325	-0.461877	-1.677441
H	0.077276	-0.737902	-2.199475
O	0.221456	-2.708620	-0.257751
H	-0.151846	-3.582889	-0.441267
C	2.353527	-1.656090	2.308160
H	1.940387	-1.852027	3.303166
H	2.138644	-2.517189	1.668450
H	3.440897	-1.561019	2.399444
C	1.759115	1.352115	2.715655
H	1.353959	2.258519	2.255971
H	1.208028	1.167730	3.643701
H	2.804943	1.543868	2.981823
C	-3.731753	2.978075	0.454653
H	-4.742576	2.593900	0.273090
H	-3.549125	2.947355	1.533879
H	-3.718170	4.026842	0.139449

C	-0.717627	2.557064	-0.097976
H	-0.556038	2.562667	0.984683
H	0.020531	1.883717	-0.547024
H	-0.550871	3.570580	-0.479257
C	3.318670	2.922829	-0.075971
H	2.378254	3.207167	-0.560291
H	3.241390	3.183930	0.983997
H	4.120194	3.529520	-0.511512
C	4.028917	0.760027	-2.128956
H	4.409874	-0.253859	-2.291099
H	3.137641	0.891930	-2.750070
H	4.796176	1.455464	-2.486736
C	-2.832605	1.944484	-2.302140
H	-3.871870	1.654148	-2.490583
H	-2.676902	2.933961	-2.745890
H	-2.174620	1.227617	-2.801192
C	5.104310	0.531848	0.739374
H	5.266080	-0.544801	0.616728
H	6.028556	1.047448	0.456950
H	4.929440	0.725660	1.803742
C	2.535168	-2.049767	-1.545762
O	3.243938	-2.494208	-0.741066
O	1.881366	-1.619932	-2.411490

PDMS-TiOH-M4

Si	-4.180965	-0.653326	-0.134708
O	-3.038666	0.583734	-0.302168
Si	-1.944158	1.448919	0.577580
O	-0.542324	0.452810	0.574772
Ti	0.565515	-0.265472	-1.292808
O	1.234837	1.459733	-1.408430
Si	2.487154	1.536476	-0.340859
O	2.340679	-0.071069	0.176982
Si	3.426421	-1.208240	0.819448
C	4.124386	1.818904	-1.182875
H	4.971697	1.691646	-0.500470
H	4.235533	1.112174	-2.011543
H	4.174948	2.832500	-1.593730
C	2.172268	2.678979	1.096059
H	1.262528	2.362092	1.616637
H	3.000864	2.657791	1.811932
H	2.041206	3.713053	0.761240
O	1.597505	-1.311303	-2.329828
H	1.196465	-1.844929	-3.032018
O	-0.953863	-0.164600	-2.210729
H	-1.836462	0.051113	-1.856093
C	-1.442250	2.963477	-0.365282
H	-0.659193	3.511278	0.168895
H	-1.043675	2.694203	-1.347879
H	-2.298835	3.632073	-0.498095
C	-2.471335	1.769531	2.329174
H	-2.573129	0.829575	2.876130
H	-1.717004	2.381201	2.835804
H	-3.422668	2.309952	2.364733
C	4.376050	-0.303980	2.164995
H	4.931974	0.553640	1.768692
H	3.695794	0.062995	2.941108
H	5.101994	-0.969096	2.644870
C	2.453177	-2.628922	1.532817
H	1.715355	-2.282984	2.263806
H	1.909794	-3.168557	0.753071
H	3.132132	-3.326982	2.035815
C	-3.408131	-2.223475	-0.796017
H	-3.058261	-2.100853	-1.826882
H	-2.554839	-2.533065	-0.183803
H	-4.141351	-3.037955	-0.787639
C	-5.639783	-0.133465	-1.188069
H	-6.076020	0.802195	-0.824139
H	-5.336994	0.019904	-2.228914
H	-6.424149	-0.897669	-1.176024
C	4.558490	-1.765458	-0.561465
H	5.144145	-2.640878	-0.260959
H	3.955835	-2.033155	-1.435748
H	5.258685	-0.977436	-0.857138
C	-4.677021	-0.840732	1.659121
H	-5.057637	0.096192	2.079321
H	-5.470548	-1.591185	1.748084
H	-3.824253	-1.174968	2.257607
C	-0.681077	-0.906731	0.919765
O	-0.006415	-1.601635	0.073253
O	-1.369529	-1.247150	1.849313

PDMS-TiOH-M6

Si	-3.554918	-0.496015	-0.837586
O	-2.091931	-0.853139	-0.030457
Si	-1.485759	-1.792777	1.234832
O	-0.180388	-0.796920	1.499804
Ti	-0.300395	0.483939	0.175400
O	1.070474	1.592768	0.602435
Si	2.731033	1.371890	0.581135
O	3.022611	0.296730	-0.649898
Si	3.585199	-1.278324	-0.821620
C	3.527064	3.001808	0.170663
H	4.616758	2.907999	0.130034
H	3.182874	3.361459	-0.804034
H	3.279332	3.760727	0.919534
C	3.234965	0.663225	2.230399
H	4.256316	0.267277	2.220416
H	3.179117	1.431585	3.008355
H	2.549516	-0.144286	2.509095
O	0.268981	-0.123129	-1.413798
H	1.183582	0.118447	-1.654943
O	-0.629059	3.818511	0.102161
H	0.091732	3.227686	0.399582
C	-2.673810	-1.833879	2.664511
H	-2.248242	-2.375330	3.515183
H	-2.907045	-0.815518	2.990614
H	-3.610932	-2.329231	2.386745
C	-0.982350	-3.466507	0.601617
H	-0.370588	-3.346244	-0.298605
H	-0.395342	-4.014783	1.345318
H	-1.856681	-4.072998	0.343026
C	5.457609	-1.244951	-0.749823
H	5.869890	-0.611667	-1.541620
H	5.810620	-0.854307	0.210935
H	5.873881	-2.250769	-0.870708
C	2.879963	-2.357385	0.541469
H	3.425926	-2.239223	1.482964

H	1.828427	-2.109537	0.731085
H	2.933177	-3.413839	0.254460
C	-3.095362	0.440589	-2.383255
H	-2.981594	1.505702	-2.156137
H	-2.149683	0.067078	-2.790248
H	-3.867847	0.335378	-3.152397
C	-4.650836	0.498817	0.300215
H	-4.768183	0.021633	1.279055
H	-4.225222	1.497884	0.437808
H	-5.649108	0.613033	-0.136880
C	2.984544	-1.863420	-2.495258
H	3.395809	-2.850841	-2.730867
H	1.892067	-1.941604	-2.518274
H	3.293841	-1.175275	-3.288903
C	-4.299838	-2.179762	-1.207861
H	-5.253986	-2.085964	-1.736832
H	-3.625880	-2.775543	-1.832573
H	-4.491769	-2.741416	-0.285601
C	-1.741281	3.102412	-0.108224
O	-1.612311	1.794722	0.159580
O	-2.767608	3.589618	-0.495547

CO2

C	0.000000	-0.000081	0.000000
O	0.001302	0.000031	1.162812
O	-0.001302	0.000029	-1.162812

(H-profile)PDMS-Mg

Si	-3.407606	-1.201727	1.182063
O	-2.633360	-0.724698	-0.214875
Si	-2.757903	0.386594	-1.493649
O	-1.425672	1.290757	-1.498227
Mg	0.006132	1.339006	-0.129081
O	1.369360	1.356823	1.297822
Si	2.914374	0.925849	1.172112
O	3.093118	0.030716	-0.261850
Si	3.370136	-1.513731	-0.819956
C	4.081693	2.375689	0.961202
H	5.119552	2.043503	0.853313
H	3.817532	2.943295	0.062056
H	4.027752	3.058387	1.814991
C	3.477821	-0.168792	2.592022
H	2.766935	-0.981619	2.776084
H	4.461055	-0.614873	2.402391
H	3.551741	0.415271	3.515560
C	-2.921132	-0.675711	-3.029229
H	-2.989659	-0.064122	-3.934535
H	-2.047875	-1.329175	-3.132156
H	-3.810172	-1.313631	-2.981396
C	-4.327690	1.383526	-1.229344
H	-4.252907	2.013593	-0.336581
H	-4.506992	2.042279	-2.085861
H	-5.208819	0.741035	-1.117089
C	5.207709	-1.713661	-1.138776
H	5.565964	-0.961943	-1.849217
H	5.778632	-1.594055	-0.211510
H	5.437493	-2.703390	-1.547816
C	2.801849	-2.829932	0.392640
H	3.370239	-2.807036	1.327115
H	1.737832	-2.725277	0.626150
H	2.941176	-3.820476	-0.055756
C	-2.050617	-1.812293	2.331313
H	-1.427132	-2.578551	1.856043
H	-1.413781	-0.972999	2.634362
H	-2.471985	-2.251743	3.241455
C	-4.593287	-2.590779	0.753824
H	-5.353519	-2.244145	0.045055
H	-4.065084	-3.429819	0.289933
H	-5.111743	-2.965267	1.642929
C	2.392226	-1.666450	-2.415798
H	2.542664	-2.645678	-2.882140
H	1.322776	-1.555280	-2.204023
H	2.689374	-0.906346	-3.147645
C	-4.330070	0.201782	2.013224
H	-5.182813	0.552464	1.424886
H	-4.709628	-0.133283	2.985475
H	-3.653154	1.043048	2.189111
O	-1.179840	1.560012	1.655635
H	-0.292730	1.608299	2.084965
H	-1.478479	2.480839	1.575705
O	1.323459	1.479140	-1.735326
H	0.775615	0.998707	-2.379643
H	2.068046	0.894630	-1.461199
O	-0.464286	3.422430	-0.396373
H	-1.039597	3.037920	-1.103584
H	0.289262	3.837453	-0.842846
O	0.055789	-0.754618	-0.015627
H	-0.906743	-0.979696	-0.022922
H	0.380010	-0.862959	0.893458

(H-profile)PDMS-Mgd

Si	3.440304	-1.047923	0.929132
O	2.945132	0.541074	0.831000
Si	2.822016	1.593222	-0.508578
O	1.471003	1.256765	-1.310247
Mg	0.109155	-0.082609	-1.064120
O	-1.269070	-1.511329	-0.882169
Si	-2.857674	-1.155469	-0.845157
O	-3.062194	0.434711	-0.311802
Si	-3.233208	1.245236	1.143803
C	-3.593500	-1.164103	-2.569247
H	-4.660906	-0.922047	-2.549033
H	-3.098620	-0.418542	-3.202544
H	-3.480022	-2.144232	-3.044718
C	-3.797679	-2.303893	0.299564
H	-3.257006	-2.452823	1.239685
H	-4.795824	-1.915401	0.530550
H	-3.924785	-3.285815	-0.169514
C	2.821195	3.301477	0.260905
H	2.741849	4.079703	-0.504995
H	1.969569	3.414412	0.940811
H	3.734871	3.481921	0.836124
C	4.366168	1.345229	-1.549519
H	4.386713	0.344378	-1.996337
H	4.383959	2.065480	-2.374328
H	5.283017	1.478674	-0.965317
C	-4.985982	1.907782	1.228564
H	-5.200748	2.567674	0.381983

H	-5.712744	1.088704	1.206804
H	-5.150386	2.476518	2.150201
C	-2.909580	0.114468	2.602880
H	-3.753663	-0.560432	2.778145
H	-2.013918	-0.498277	2.460061
H	-2.766544	0.710816	3.511216
C	2.934665	-1.671610	2.625739
H	3.376554	-1.057171	3.416390
H	1.846928	-1.654762	2.758549
H	3.270172	-2.703608	2.777307
C	5.297820	-1.193972	0.722572
H	5.615960	-0.971397	-0.299996
H	5.814945	-0.500915	1.394121
H	5.631669	-2.208906	0.965156
C	-2.005519	2.665000	1.093843
H	-2.086168	3.285758	1.992630
H	-0.981755	2.278846	1.043430
H	-2.181585	3.320039	0.232163
C	2.549892	-2.054197	-0.393227
H	2.615292	-1.587918	-1.383280
H	2.969427	-3.063161	-0.477575
H	1.486106	-2.174493	-0.144136
O	-0.584905	-2.397681	1.514591
H	-0.876246	-2.284717	0.566200
H	-0.027825	-3.186920	1.549439
O	-1.116473	1.314173	-1.979066
H	-0.503814	2.054266	-1.808255
H	-1.922892	1.404805	-1.427784
O	0.456214	-1.147251	-2.846031
H	0.302734	-0.527836	-3.576208
H	-0.371256	-1.650407	-2.702719
O	0.212614	0.079092	0.984920
H	1.115202	0.374010	1.232119
H	0.028320	-0.789341	1.422280

(H-profile)PDMS-Mg-M3

Si	-3.393999	1.533677	-0.938080
O	-2.492897	1.095980	0.394624
Si	-2.530125	-0.151485	1.553439
O	-1.526501	-1.320764	1.112388
Mg	0.236084	-1.365431	0.326995
O	1.897424	-1.661041	-0.740673
Si	3.332594	-0.978428	-0.408634
O	3.089217	0.362446	0.597208
Si	2.963075	2.025521	0.437685
C	4.410671	-2.125033	0.610959
H	5.374617	-1.662949	0.846870
H	3.921899	-2.366789	1.562304
H	4.606226	-3.063890	0.082321
C	4.219267	-0.412126	-1.959285
H	3.532721	0.099809	-2.641345
H	5.050818	0.264140	-1.730784
H	4.631873	-1.275631	-2.492475
C	-1.979017	0.706292	3.135380
H	-1.833156	-0.011467	3.949918
H	-1.037896	1.250350	2.978677
H	-2.713158	1.446948	3.469027
C	-4.306449	-0.733409	1.700172
H	-4.668245	-1.140781	0.748844
H	-4.376964	-1.538430	2.438888
H	-4.982288	0.070787	2.009616
C	4.597553	2.771316	0.982030
H	4.833230	2.496518	2.015149
H	5.417444	2.417634	0.347409
H	4.575718	3.864811	0.919588
C	2.603345	2.544237	-1.328377
H	3.511830	2.526975	-1.938945
H	1.861930	1.898089	-1.806960
H	2.214839	3.569299	-1.340325
C	-2.502211	2.998453	-1.695978
H	-2.477804	3.841739	-0.998469
H	-1.464993	2.745203	-1.944177
H	-2.991523	3.334593	-2.616054
C	-5.143886	1.995959	-0.452338
H	-5.719381	1.122504	-0.131146
H	-5.141162	2.719895	0.369017
H	-5.669874	2.450959	-1.298801
C	1.604677	2.568166	1.617012
H	1.546298	3.660612	1.669201
H	0.632541	2.193537	1.282283
H	1.795852	2.207028	2.635170
C	-3.406175	0.098313	-2.153081
H	-3.898539	-0.780021	-1.719918
H	-3.938708	0.356030	-3.074733
H	-2.381501	-0.181217	-2.427133
O	0.873429	-0.335893	-2.827832
H	1.324973	-0.974162	-2.211316
H	0.284477	-0.874013	-3.374418
O	1.205876	-0.841240	2.083222
H	0.569353	-0.335794	2.613825
H	1.924807	-0.231761	1.785210
O	0.582364	-3.432130	0.704187
H	0.828479	-3.508249	1.638732
H	1.415532	-3.328676	0.196390
O	0.072063	0.533879	-0.462067
H	-0.825909	0.884871	-0.275352
H	0.199446	0.426438	-1.439479
C	-2.007019	-2.706933	-0.990197
O	-3.027294	-3.144674	-0.670136
O	-0.987802	-2.310459	-1.420930

(H-profile)TS-M3M4

Si	-3.387819	1.609850	-0.833053
O	-2.501837	0.961344	0.429020
Si	-2.550383	-0.379136	1.457109
O	-1.574145	-1.528585	0.857724
Mg	0.282295	-1.473923	0.189535
O	1.984893	-1.645437	-0.821909
Si	3.381175	-0.904612	-0.461069
O	3.063498	0.364039	0.618802
Si	2.884074	2.028613	0.549436
C	4.533278	-2.036920	0.491081
H	5.469235	-1.530347	0.747655
H	4.067900	-2.358965	1.430305
H	4.780718	-2.932606	-0.088052
C	4.224244	-0.202952	-1.980202
H	3.508428	0.310917	-2.630063
H	5.022262	0.501041	-1.718156

H	4.675965	-1.012475	-2.563903
C	-1.880731	0.264695	3.092339
H	-1.584949	-0.555099	3.756138
H	-1.018303	0.924897	2.929991
H	-2.628848	0.865160	3.620002
C	-4.325861	-0.941449	1.614655
H	-4.738642	-1.220488	0.639576
H	-4.387166	-1.827438	2.254633
H	-4.958064	-0.160553	2.050300
C	4.488745	2.796294	1.148005
H	4.726878	2.472225	2.166132
H	5.323657	2.504814	0.501445
H	4.431683	3.890274	1.145404
C	2.513586	2.638922	-1.185102
H	3.423094	2.692599	-1.791802
H	1.796747	1.996266	-1.703982
H	2.087183	3.647820	-1.136593
C	-2.450276	3.147507	-1.351294
H	-2.411460	3.873843	-0.533214
H	-1.417556	2.903912	-1.626776
H	-2.918160	3.633319	-2.213728
C	-5.124198	2.031694	-0.270857
H	-5.705131	1.132031	-0.045550
H	-5.102406	2.655352	0.628766
H	-5.657250	2.586686	-1.050483
C	1.498642	2.460416	1.744491
H	1.410796	3.545598	1.863683
H	0.540861	2.082987	1.372921
H	1.688031	2.041565	2.740720
C	-3.420034	0.364925	-2.237303
H	-3.963601	-0.543075	-1.955095
H	-3.901807	0.781118	-3.128479
H	-2.400434	0.072998	-2.519213
O	0.846911	-0.306033	-2.857641
H	1.359884	-0.931914	-2.280423
H	0.195587	-0.864157	-3.306758
O	1.156766	-0.930695	1.996676
H	0.544769	-0.424173	2.553328
H	1.882436	-0.321278	1.706629
O	0.754196	-3.494433	0.629981
H	1.058782	-3.502915	1.550672
H	1.555942	-3.374045	0.077949
O	0.084848	0.487263	-0.455143
H	-0.819656	0.814522	-0.267636
H	0.215774	0.404276	-1.437663
C	-2.028264	-2.407206	-0.913788
O	-3.141503	-2.745943	-0.825436
O	-0.960397	-2.255169	-1.434470

(H-profile)PDMS-Mg-M4

Si	-3.602591	1.465586	-0.825487
O	-2.708082	0.865497	0.479792
Si	-2.655779	-0.442115	1.490248
O	-1.665790	-1.575335	0.700240
Mg	0.368410	-1.518722	0.034977
O	2.054203	-1.603270	-0.964824
Si	3.454831	-0.863710	-0.645389
O	3.166017	0.292149	0.567431
Si	3.067483	1.960260	0.687737
C	4.713335	-2.027262	0.113994
H	5.648266	-1.506944	0.346305
H	4.334619	-2.452308	1.051048
H	4.946197	-2.856611	-0.561649
C	4.167452	0.001409	-2.146866
H	3.399938	0.568226	-2.684213
H	4.980775	0.687224	-1.883300
H	4.574152	-0.740272	-2.842872
C	-1.668660	0.065774	2.995639
H	-1.233547	-0.803833	3.501047
H	-0.876437	0.772746	2.720638
H	-2.307090	0.580002	3.720690
C	-4.315085	-1.137961	1.942836
H	-4.812586	-1.542173	1.059414
H	-4.190275	-1.947950	2.669321
H	-4.952054	-0.372221	2.397619
C	4.734973	2.599529	1.259589
H	5.021082	2.155020	2.218078
H	5.515320	2.352478	0.531448
H	4.724620	3.688173	1.379792
C	2.593817	2.763190	-0.937870
H	3.433330	2.797161	-1.638494
H	1.767020	2.231809	-1.418805
H	2.269088	3.794565	-0.757627
C	-3.704088	3.314501	-0.537159
H	-4.240839	3.541151	0.389573
H	-2.704573	3.755151	-0.462333
H	-4.228310	3.812018	-1.359972
C	-5.303556	0.693177	-0.869656
H	-5.224105	-0.375988	-1.084853
H	-5.835349	0.824652	0.078682
H	-5.906653	1.160308	-1.656167
C	1.751737	2.296508	1.987175
H	1.707955	3.360018	2.243496
H	0.773682	2.003661	1.590980
H	1.948406	1.745545	2.914971
C	-2.645343	1.102699	-2.395047
H	-2.557995	0.021700	-2.546973
H	-3.179333	1.516267	-3.258089
H	-1.643054	1.546004	-2.396919
O	0.600473	-0.174683	-2.793083
H	1.269032	-0.778993	-2.389205
H	-0.170563	-0.758696	-2.907629
O	1.232099	-1.030071	1.876878
H	0.695693	-0.461499	2.450082
H	1.989816	-0.469080	1.556513
O	0.871776	-3.505395	0.559263
H	1.324765	-3.409728	1.412605
H	1.582625	-3.470206	-0.113112
O	0.064484	0.528337	-0.318682
H	-0.852924	0.832774	-0.176651
H	0.213395	0.480877	-1.311124
C	-2.045809	-1.862310	-0.669156
O	-3.228919	-1.814357	-0.939880
O	-1.010369	-2.056896	-1.362438

(H-profile)TS-M4M5

Si	-3.287181	1.335143	-1.145649
O	-2.540503	0.830564	0.284005

Si	-2.792155	-0.296817	1.475566
O	-1.689803	-1.538167	1.140665
Mg	0.910380	-1.921943	-0.045741
O	2.681998	-1.648986	-0.808178
Si	3.621145	-0.374406	-0.471569
O	2.779850	0.636648	0.598311
Si	2.294854	2.235168	0.635402
C	5.172226	-0.873139	0.455859
H	5.785573	0.000711	0.700494
H	4.915312	-1.367244	1.399790
H	5.786343	-1.564311	-0.130287
C	4.066502	0.602618	-2.008378
H	3.174632	0.857361	-2.590253
H	4.599990	1.531327	-1.775556
H	4.718185	-0.000025	-2.650244
C	-2.185977	0.398455	3.098344
H	-2.205976	-0.373675	3.874773
H	-1.170675	0.801965	3.040041
H	-2.835418	1.216554	3.426496
C	-4.544969	-0.890903	1.654125
H	-4.876533	-1.428680	0.765058
H	-4.602094	-1.570323	2.511691
H	-5.228244	-0.057080	1.846826
C	3.707649	3.257437	1.327448
H	3.995049	2.909648	2.324785
H	4.590822	3.184560	0.682793
H	3.437033	4.316186	1.401369
C	1.786615	2.902126	-1.041976
H	2.639553	3.100436	-1.696917
H	1.117781	2.197844	-1.544935
H	1.244147	3.845274	-0.905538
C	-3.399507	3.201318	-1.015730
H	-4.036322	3.503807	-0.178279
H	-2.406770	3.635294	-0.855064
H	-3.814161	3.638791	-1.930006
C	-4.973808	0.555726	-1.352002
H	-4.870344	-0.529988	-1.438004
H	-5.651166	0.781946	-0.522772
H	-5.437370	0.930595	-2.271607
C	0.813458	2.293905	1.788761
H	0.538813	3.328219	2.022212
H	-0.059748	1.823888	1.321178
H	1.020640	1.790716	2.741048
C	-2.192487	0.856080	-2.590200
H	-2.031525	-0.227525	-2.610478
H	-2.687633	1.131357	-3.528125
H	-1.224923	1.369523	-2.575004
O	0.648688	-1.689621	-2.664573
H	1.578627	-1.857506	-2.404792
H	0.135402	-2.496788	-2.488586
O	1.100273	-1.158073	1.847491
H	0.188361	-0.898369	2.071194
H	1.621442	-0.346359	1.634389
O	1.864638	-3.713743	0.555581
H	1.924326	-3.785548	1.519695
H	2.709207	-3.331744	0.237584
O	0.129333	-0.026387	-0.631730
H	-0.769333	0.270940	-0.384516
H	0.102000	-0.279170	-1.582735
C	-1.814002	-2.147629	-0.117852
O	-2.832416	-1.930650	-0.759033
O	-0.787938	-2.825647	-0.439005

(H-profile)PDMS-Mg-M5

Si	-3.098504	1.409151	-1.118325
O	-2.392098	0.586177	0.168993
Si	-2.826093	-0.508857	1.344258
O	-1.679013	-1.744494	1.254960
Mg	1.169632	-2.088112	-0.301312
O	3.020799	-1.433022	-0.584611
Si	3.572017	0.016609	-0.150732
O	2.292801	0.870532	0.575839
Si	1.766925	2.451598	0.496988
C	4.897317	-0.069729	1.174764
H	5.223182	0.932233	1.475857
H	4.508963	-0.573237	2.067123
H	5.778208	-0.622394	0.832549
C	4.196019	1.007210	-1.619252
H	3.438248	1.053537	-2.408216
H	4.482310	2.032330	-1.357878
H	5.081239	0.516883	-2.038996
C	-2.503776	0.268859	3.007716
H	-2.733219	-0.430690	3.817635
H	-1.457207	0.573277	3.108818
H	-3.120233	1.162873	3.147262
C	-4.563783	-1.156847	1.206760
H	-4.733187	-1.602098	0.224364
H	-4.702510	-1.939508	1.960871
H	-5.311770	-0.379770	1.390548
C	3.086467	3.583047	1.206006
H	3.313606	3.314651	2.243019
H	4.018087	3.517153	0.633228
H	2.761625	4.629090	1.190991
C	1.372415	2.937515	-1.272761
H	2.278050	3.083558	-1.868452
H	0.774893	2.155760	-1.756370
H	0.804399	3.874323	-1.299586
C	-2.478686	3.170657	-0.988887
H	-2.805406	3.632611	-0.051239
H	-1.384438	3.195159	-1.009313
H	-2.844753	3.785719	-1.817785
C	-4.967021	1.365530	-0.980566
H	-5.364543	0.356172	-1.120405
H	-5.312499	1.738985	-0.010594
H	-5.404382	2.006353	-1.754486
C	0.215744	2.536126	1.548835
H	-0.175353	3.559182	1.588946
H	-0.585460	1.899903	1.153196
H	0.427069	2.223851	2.578240
C	-2.546740	0.603498	-2.716186
H	-2.694459	-0.481012	-2.653922
H	-3.136328	0.979633	-3.559135
H	-1.493125	0.808535	-2.935064
O	1.394215	-2.632370	-2.315729
H	2.321493	-2.317520	-2.259220
H	1.416176	-3.601158	-2.353698
O	1.035166	-1.334583	1.613129
H	0.077449	-1.375292	1.817040

H	1.321118	-0.399043	1.518609
O	2.313766	-3.772934	0.282692
H	2.079451	-4.000973	1.194907
H	3.078473	-3.157312	0.313528
O	0.019283	-0.474241	-1.096183
H	-0.637061	-0.018363	-0.529296
H	-0.532063	-0.923704	-1.764099
C	-1.561602	-2.428829	0.028695
O	-2.423159	-2.209110	-0.816523
O	-0.515583	-3.132653	-0.041895