SUPPLEMENTARY INFORMATION

Dissociation of CH_3-O as a Driving Force for Methoxyacetophenone Adsorption on Si(001)

Kane M. ODonnell[1], Gareth Moore[2], Carly Byron[3], L. Thomsen[4], Oliver Warschkow[5], Andrew Teplyakov[3], and Steven R. Schofield[2,6,*]

[1]Department of Physics and Astronomy, Curtin University, Bentley, Western Australia 6102, Australia.
[2]Department of Physics and Astronomy, University College London, London WC1E 6BT, UK.
[3]Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware 19716, United States.
[4]Australian Synchrotron, ANSTO, Clayton, Victoria 3168, Australia.
[5]Centre for Quantum Computation and Communication Technology, School of Physics, University of Sydney, Sydney, New South Wales 2006, Australia.
[6]London Centre for Nanotechnology, University College London, London WC1H 0AH, UK.

*Correspondence: s.schofield@ucl.ac.uk.

May 23, 2019

1 Supplementary Figures

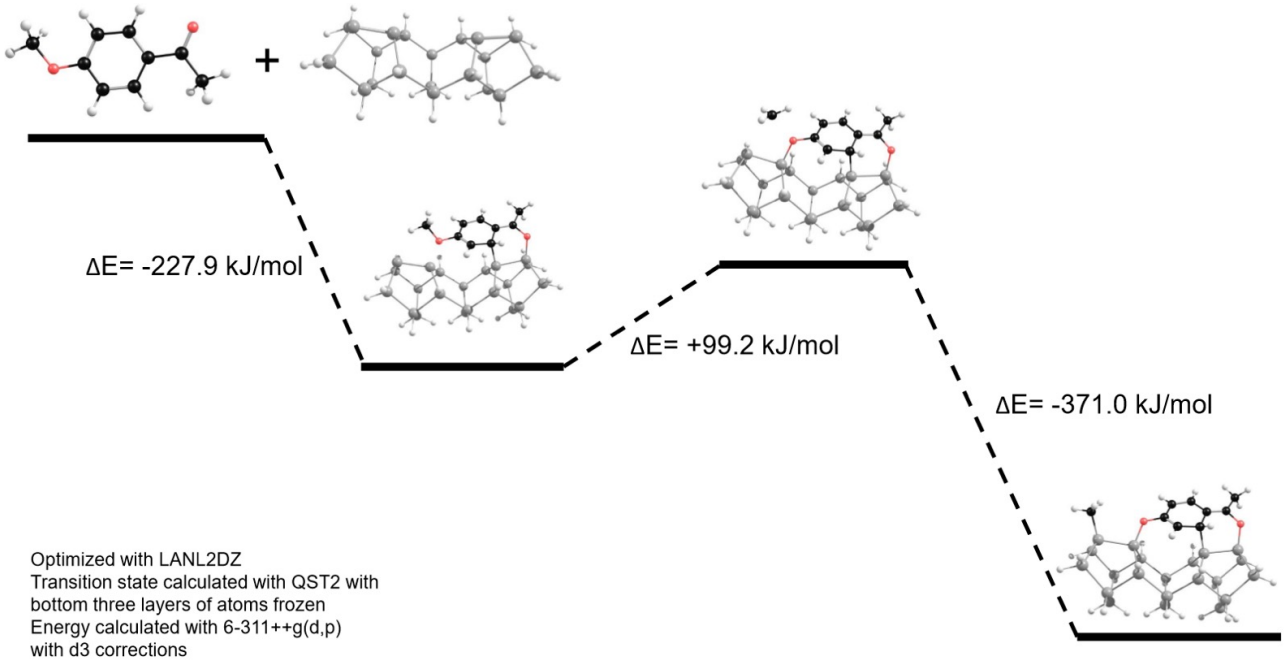

Figure S1: Computationally predicted reaction pathway for adsorption of methoxyacetophenone across the trough of the silicon dimers followed by dissociation of the methoxy group.

2 Supplementary Tables

Table S1: Calculated O(1s) binding energies for the structures shown in Fig. 3. The O(1s) binding energies in this table were predicted based on Koopmanns' theorem similarly to the approaches previously reported by our group for N 1s features and calibrated against experimental data to produce expected difference between computationally predicted and experimental values of +11.4 eV.

Structure	**O(1s) binding energies (eV) calibrated (+11.4 eV)**	
	Methoxy	**Ketone**
MA gas phase	531.3	533.1
Dative ketone	533.9	534.2
Intermediate	533.7	533.9
Allyl	530.3	531.5
Dative methoxy	532.2	535.1
Methyl cleavage	531.4	532.7
Across-trough dative	532.5	534.6
Across-trough methyl cleavage	532.1	532.2

Table S2: Calculated C(1s) binding energies for the structures shown in Fig. 3. The C(1s) binding energies in this table were predicted based on Koopmanns theorem similarly to the approaches previously reported by our group for N 1s features and calibrated against experimental data to produce expected difference between computationally predicted and experimental values of +7.67 eV.

Structure	**C 1s binding energies (eV), calibrated (+7.67 eV)**								
MA gas phase	284.6	285.0	285.0	285.1	285.1	285.3	286.4	286.9	287.1
Dative ketone	285.5	286.0	286.1	286.3	286.3	286.4	287.1	288.0	289.0
Intermediate	285.4	285.7	285.9	286.0	286.1	286.2	287.0	287.8	288.5
Allyl	284.9	285.6	285.9	286.0	286.3	286.3	286.7	286.8	287.3
Dative methoxy	285.2	286.0	286.1	286.1	286.1	286.1	287.3	287.8	287.8
Methyl cleavage	284.5	284.7	285.0	285.1	285.1	285.1	285.3	287.0	287.1
Across-trough dative	284.9	285.4	285.5	285.5	285.6	285.6	286.7	286.8	287.0
Across-trough methyl-cleavage	284.3	284.6	284.6	284.8	285.0	285.0	285.0	286.2	286.3

Table S3: Methoxyacetophenone gas phase coordinates. All coordinates listed in the tables below can be downloaded in XYZ format from https://doi.org/10.5281/zenodo.2650188.

Element	**X**	**Y**	**Z**
O	-3.063769	-1.452435	-0.00002
C	-2.598302	-0.284275	0.000009
C	-3.539808	0.914262	0.000013
H	-3.378608	1.54201	-0.886244
H	-4.571137	0.553491	-0.000005
H	-3.37863	1.541985	0.88629
C	1.685451	0.299418	-0.000003
C	-1.121999	-0.048937	0.000005
C	1.138794	-1.004457	-0.000021
C	-0.253627	-1.164291	-0.000017
C	0.83349	1.426443	0.000019
C	-0.553208	1.250136	0.000023
H	1.779627	-1.880261	-0.00004
H	-0.696103	-2.156532	-0.000031
H	1.282479	2.414755	0.000033
H	-1.19211	2.128626	0.00004
O	3.046735	0.58027	-0.000007
C	3.998882	-0.525078	0
H	3.884697	-1.146072	-0.89869
H	4.983358	-0.053909	0.000022
H	3.884664	-1.14609	0.898672

Table S4: Silicon dimer coordinates. All coordinates listed in the tables below can be downloaded in XYZ format from https://doi.org/10.5281/zenodo.2650188.

Element	**X**	**Y**	**Z**
H	2.047445	3.301094	-1.196917
H	2.047323	3.300335	1.197927
H	-2.047323	3.300336	-1.197926
H	-2.047445	3.301094	1.196918
H	5.19063	2.050221	-0.000134
H	-5.19063	2.050221	0.000134
H	-0.000114	-0.071009	-3.129122
H	0.000114	-0.071008	3.129122
H	3.73369	0.208728	-3.135822
H	3.733024	0.20893	3.135792
H	-3.733024	0.20893	-3.135792
H	-3.73369	0.208728	3.135822
H	5.166228	-1.267609	-1.86706
H	5.166271	-1.267366	1.867631
H	-5.166271	-1.267366	-1.867631
H	-5.166228	-1.267609	1.86706
Si	2.021525	2.415429	0.000222
Si	-2.021525	2.415429	-0.000222
Si	0	1.146443	0
Si	4.022377	1.118927	-0.000024
Si	-4.022377	1.118927	0.000023
Si	0.000095	-0.56002	-1.725093
Si	-0.000095	-0.56002	1.725093
Si	3.942796	-0.427865	-1.810494
Si	3.942796	-0.42774	1.810606
Si	-3.942796	-0.42774	-1.810606
Si	-3.942796	-0.427865	1.810494
Si	-2.017444	-1.576554	-1.104688
Si	-2.017477	-1.577065	1.105067
Si	2.017476	-1.577065	-1.105067
Si	2.017444	-1.576555	1.104688

Table S5: Dative ketone coordinates (https://doi.org/10.5281/zenodo.2650188).

Element	X	Y	Z
H	-5.86516	0.37164	-0.89923
H	-4.725008	-0.217991	-2.916874
H	-3.947614	3.837749	-0.806997
H	-2.802526	3.237845	-2.826667
H	-6.037473	-3.192379	-1.357833
H	-0.76317	5.650285	-0.990809
H	-3.386259	1.118293	2.572887
H	-0.362532	-0.416816	-2.656589
H	-5.509729	-2.006818	2.317985
H	-2.477345	-3.507343	-2.962485
H	-1.889758	4.273106	2.476939
H	1.108848	2.734541	-2.742185
H	-4.484848	-4.174964	1.994752
H	-2.753894	-5.101597	-1.181784
H	0.447384	4.75942	2.329077
H	2.361201	3.694701	-0.916054
Si	-4.65222	-0.310817	-1.431338
Si	-2.738667	3.151362	-1.340429
Si	-2.735911	0.87499	-0.662081
Si	-4.768956	-2.60847	-0.825602
Si	-0.796145	4.231614	-0.532293
Si	-2.271561	0.632273	1.71162
Si	-0.731362	-0.327723	-1.217087
Si	-4.499419	-2.761722	1.534823
Si	-2.7457	-3.650168	-1.506714
Si	-0.62438	3.865924	1.802229
Si	1.085265	3.020051	-1.282806
Si	-2.405255	-1.703189	1.533554
Si	-1.211516	-2.404792	-0.216501
Si	0.723176	1.077071	0.01678
Si	-0.09924	1.544414	2.238571
C	7.146858	-1.258522	-0.178337
C	4.420575	-0.867989	0.4703
C	6.539099	-2.042867	0.833815
C	5.19828	-1.849524	1.152277
C	6.392504	-0.276532	-0.869883
C	5.048807	-0.092565	-0.544086
H	7.142814	-2.787037	1.342455
H	4.755123	-2.46566	1.927124
H	6.844519	0.331128	-1.646354
H	4.457341	0.653317	-1.0647
C	9.199275	-0.779119	-1.445575
H	9.221717	0.2912	-1.205499
H	10.211224	-1.185157	-1.428774
H	8.748722	-0.938196	-2.43323
C	2.249751	-1.362129	1.836935
H	1.73167	-0.62303	2.471917
H	1.455828	-1.968873	1.375226
H	2.86991	-2.006716	2.458223
O	8.474691	-1.528609	-0.416329
C	3.014067	-0.639522	0.770268
O	2.400335	0.256173	0.05346

Table S6: Intermediate coordinates. (https://doi.org/10.5281/zenodo.2650188).

Element	X	Y	Z
H	-5.800018	-0.001886	0.921775
H	-5.680918	-0.165819	-1.465659
H	-3.982646	3.549081	1.016771
H	-3.770453	3.632613	-1.370838
H	-5.786278	-3.521849	-0.079093
H	-1.244921	5.739435	0.083523
H	-2.231459	0.291002	3.026021
H	-1.707211	0.266689	-3.195425
H	-3.658971	-2.778432	3.072043
H	-3.53958	-2.835514	-3.144634
H	-0.517934	3.682443	3.251237
H	-0.174355	3.759708	-3.043863
H	-3.021958	-4.77359	1.910533
H	-2.894187	-4.818365	-1.93618
H	1.507859	4.188418	2.031725
H	1.724482	4.193778	-1.594175
Si	-4.942489	-0.46012	-0.206112
Si	-3.125155	3.131295	-0.125532
Si	-2.918651	0.765327	-0.131746
Si	-4.491385	-2.782467	-0.042439
Si	-1.038825	4.264995	0.08127
Si	-1.631166	-0.027235	1.701202
Si	-1.366098	-0.024307	-1.777512
Si	-3.079326	-3.287698	1.797206
Si	-3.063523	-3.343563	-1.828997
Si	0.19354	3.493363	1.962651
Si	0.383136	3.560383	-1.683902
Si	-0.940916	-2.291682	1.325074
Si	-1.073025	-2.275006	-1.109632
Si	0.416436	1.301927	-1.028299
Si	0.314316	1.229324	1.321017
O	2.090623	0.553489	-1.023717
C	2.683077	0.144682	0.104294
C	1.887601	0.077202	1.364459
H	2.518083	0.178415	2.250442
H	1.401449	-0.942497	1.434389
C	6.760143	-1.086614	-0.30399
C	4.067094	-0.263115	-0.015539
C	6.08018	-0.490228	-1.396927
C	4.757092	-0.090512	-1.255851
C	6.094354	-1.27595	0.93179
C	4.764879	-0.866548	1.066831
H	6.617547	-0.363317	-2.331151
H	4.224861	0.358574	-2.087191
H	6.597937	-1.741382	1.772194
H	4.260747	-1.037388	2.012667
H	0.12991	-2.832467	-1.790835
O	8.067416	-1.451567	-0.54847
C	8.850594	-2.092131	0.50862
H	8.393063	-3.042091	0.813086
H	9.828589	-2.277713	0.062849
H	8.955781	-1.427455	1.375672

Table S7: Allyl coordinates (https://doi.org/10.5281/zenodo.2650188).

Element	X	Y	Z
H	-5.42996	2.85971	-1.58977
H	-1.69232	3.98569	-1.35333
H	2.37178	4.82139	-1.33002
H	-5.5106	3.10769	0.79184
H	-1.82702	3.99177	1.03872
H	2.36789	4.93099	1.06946
H	-8.24384	0.92024	-0.28015
H	5.67895	4.0779	-0.08277
H	-6.36567	0.00774	2.9953
H	-2.95032	0.54386	3.07531
H	0.98629	1.51821	3.14812
H	4.58068	2.27977	3.14465
H	6.23814	0.82046	-1.76002
H	-7.3997	-2.2801	-1.88867
H	-7.52224	-1.85174	2.00962
H	6.22112	1.00043	1.90616
Si	-5.28923	2.12296	-0.30296
Si	-1.52377	3.13654	-0.14114
Si	2.4774	4.00555	-0.09028
Si	-6.86421	0.36695	-0.16704
Si	-3.06776	1.31278	-0.13038
Si	0.72997	2.4042	-0.02222
Si	4.64192	3.009	-0.03701
Si	-6.41779	-0.8756	1.79783
Si	-6.3574	-1.2199	-1.8334
Si	-2.81186	-0.1475	1.76469
Si	-2.69198	-0.4311	-1.74594
Si	1.03819	0.8948	1.79913
Si	1.05998	0.76286	-1.70972
Si	4.85863	1.59366	1.85782
Si	4.88176	1.43111	-1.79581
Si	-4.32194	-1.9518	1.38924
Si	-4.28303	-2.03854	-1.02582
Si	-0.57921	-0.75132	1.32345
Si	-0.49796	-0.86737	-1.05008
Si	3.1871	0.03142	1.27118
Si	3.1854	-0.05551	-1.09736
O	0.35505	-2.46621	-1.02898
C	1.08644	-2.55144	0.19021
C	0.19205	-2.54133	1.41415
H	-0.6084	-3.28177	1.30058
H	0.72219	-2.74038	2.34771
C	5.29205	-2.73075	0.11774
C	2.4361	-2.35954	0.17058
C	4.61071	-2.52231	-1.0924
C	3.19973	-2.09504	-1.11175
C	4.64755	-2.49948	1.34584
C	3.25726	-2.02864	1.41236
H	5.12019	-2.63481	-2.04559
H	2.65685	-2.41989	-2.00059
H	5.22456	-2.62807	2.25877
H	2.78207	-2.29314	2.35791

Table S8: Dative methoxy coordinates. (https://doi.org/10.5281/zenodo.2650188).

Element	X	Y	Z
H	-5.290169	2.378034	-0.648857
H	-4.660848	1.336015	-2.720003
H	-2.003218	4.505032	-0.63091
H	-1.394696	3.514764	-2.737945
H	-7.124084	-0.726217	-0.991678
H	1.666216	4.634919	-1.061906
H	-2.529699	1.787445	2.681476
H	-0.888861	-0.903535	-2.653962
H	-5.816509	0.08997	2.610818
H	-4.190027	-2.622209	-2.791394
H	0.30714	3.841233	2.518919
H	1.866369	1.169701	-2.885341
H	-5.928664	-2.315353	2.272807
H	-5.106839	-3.906451	-0.979257
H	2.559923	3.128748	2.134065
H	3.487738	1.429304	-1.108114
Si	-4.575431	1.207302	-1.236071
Si	-1.282207	3.360075	-1.257821
Si	-2.290213	1.312379	-0.583352
Si	-5.687576	-0.786941	-0.575914
Si	0.989511	3.389477	-0.587513
Si	-1.799871	0.872252	1.755134
Si	-1.151022	-0.699123	-1.198461
Si	-5.355334	-1.040212	1.762335
Si	-4.400974	-2.636024	-1.314813
Si	1.140409	2.888999	1.725755
Si	2.033612	1.445328	-1.431895
Si	-3.019538	-1.102798	1.48379
Si	-2.316193	-2.497207	-0.167933
Si	0.818219	-0.062266	-0.072976
Si	0.534221	0.606237	2.177189
C	6.096749	-1.031136	-0.16015
C	3.374703	-1.491619	-0.037291
C	5.415792	-1.550802	-1.269653
C	4.047857	-1.782028	-1.215514
C	5.383974	-0.750728	1.012082
C	4.013042	-0.983389	1.084117
H	5.978681	-1.760865	-2.170476
H	3.498701	-2.164931	-2.066572
H	5.885519	-0.341504	1.879424
H	3.446389	-0.751858	1.977724
C	8.315615	-0.173675	0.886052
H	8.235943	-0.807305	1.774489
H	9.364107	-0.057347	0.618253
H	7.891903	0.802758	1.138641
O	1.97059	-1.691843	-0.021727
C	1.524671	-2.830973	0.79519
H	1.663293	-2.594701	1.850124
H	0.470682	-2.978703	0.566197
H	2.112466	-3.696665	0.493729
C	7.578709	-0.792829	-0.283545
O	8.162571	-1.09214	-1.306062

Table S9: Methyl cleavage coordinates (https://doi.org/10.5281/zenodo.2650188).

Element	X	Y	Z
H	-5.734233	1.296057	0.090794
H	-5.219482	0.719458	-2.174732
H	-3.113533	4.294032	-0.058819
H	-2.585248	3.727446	-2.33618
H	-6.78949	-2.080315	-0.563713
H	0.297478	5.4039	-0.827368
H	-2.494646	1.164452	2.90258
H	-1.124557	-0.358048	-2.999481
H	-5.21562	-1.45556	2.964405
H	-3.830229	-2.97355	-2.965174
H	-0.301535	3.956094	2.699516
H	1.015468	2.447784	-3.215038
H	-4.835663	-3.743712	2.280426
H	-4.020911	-4.642004	-1.225107
H	2.000756	3.836436	1.982717
H	2.822071	2.937294	-1.682366
Si	-4.855373	0.444524	-0.757393
Si	-2.24577	3.44224	-0.915971
Si	-2.608892	1.149868	-0.421232
Si	-5.341118	-1.839984	-0.286851
Si	0.024573	3.973702	-0.523373
Si	-1.812928	0.505818	1.756082
Si	-1.071916	-0.344398	-1.51442
Si	-4.603173	-2.320834	1.924673
Si	-3.805814	-3.198336	-1.497618
Si	0.616714	3.377218	1.684674
Si	1.399076	2.521512	-1.782588
Si	-2.348429	-1.767989	1.565287
Si	-1.860636	-2.311781	-0.523741
Si	0.974675	0.467465	-0.666697
Si	0.499666	1.009459	1.625385
C	6.275879	-1.249292	-0.114051
C	3.511447	-0.89083	-0.611725
C	5.633033	-0.033047	0.21774
C	4.267094	0.152381	-0.025319
C	5.505412	-2.282664	-0.702559
C	4.138635	-2.110025	-0.950577
H	6.230305	0.755781	0.666289
H	3.793062	1.097231	0.228655
H	5.969596	-3.227899	-0.96951
H	3.536564	-2.893395	-1.399668
C	8.439623	-2.693768	-0.196506
H	8.36304	-2.894347	-1.273248
H	9.494126	-2.615249	0.078617
H	7.992824	-3.545412	0.333283
O	2.16247	-0.78702	-0.877987
C	7.736816	-1.391747	0.168811
O	8.383321	-0.453339	0.70065
C	1.581142	0.085038	2.895909
H	1.325514	0.390201	3.917797
H	1.428641	-0.997722	2.813848
H	2.645744	0.2889	2.73282

Table S10: Silicon Double Dimer Coordinates (https://doi.org/10.5281/zenodo.2650188). Fixed atoms = −1.

Element	X	Y	Z	Fixed
H	-0.121448	2.898801	2.607478	-1
H	-0.121448	2.898801	-2.607478	-1
H	-0.121606	2.910247	-5.087972	-1
H	-0.121606	2.910247	5.087972	-1
H	-0.107461	2.904604	-1.240254	-1
H	-0.107461	2.904604	1.240254	-1
H	-3.220612	1.512644	-3.838004	-1
H	-3.220612	1.512644	3.838004	-1
H	3.135482	1.69286	-3.83877	-1
H	3.135482	1.69286	3.83877	-1
H	-3.220322	1.514442	0	-1
H	3.1351	1.694604	0	-1
H	-1.948518	-0.036555	-6.912954	-1
H	1.97616	0.049722	-6.912953	-1
H	-1.948518	-0.036555	6.912954	-1
H	1.97616	0.049722	6.912953	-1
H	3.222137	-1.395041	1.911436	0
H	3.222137	-1.395041	-1.911436	0
H	3.232267	-1.518292	-5.561402	0
H	-3.127789	-1.540386	1.909958	0
H	-3.127789	-1.540386	-1.909958	0
H	-3.132734	-1.663371	-5.564401	0
H	-3.132734	-1.663371	5.564401	0
H	3.232267	-1.518292	5.561402	0
Si	-0.110905	2.12751	-3.851331	-1
Si	-0.110905	2.12751	3.851331	-1
Si	-0.110905	2.127482	0	-1
Si	-1.975022	0.752267	-3.792949	-1
Si	1.952322	0.838624	-3.792942	-1
Si	-1.975022	0.752267	3.792949	-1
Si	1.952322	0.838624	3.792942	-1
Si	-1.974976	0.752256	0	-1
Si	1.952276	0.838608	0	-1
Si	-1.942865	-0.641203	-1.921383	0
Si	-1.951942	-0.763767	-5.598076	0
Si	1.996809	-0.551039	-1.920103	0
Si	2.010835	-0.674514	-5.597969	0
Si	-1.951942	-0.763767	5.598076	0
Si	-1.942865	-0.641203	1.921383	0
Si	2.010835	-0.674514	5.597969	0
Si	1.996809	-0.551039	1.920103	0
Si	0.052589	-1.706638	-2.610937	0
Si	0.053321	-1.770394	-4.856916	0
Si	0.053321	-1.770394	4.856916	0
Si	0.052589	-1.706638	2.610937	0

Table S11: Across-trough dative coordinates. (https://doi.org/10.5281/zenodo.2650188).

Element	X	Y	Z	Fixed
H	3.254699	-3.426719	0.785478	-1
H	-1.926335	-4.019176	0.747114	-1
H	-4.389488	-4.311974	0.731806	-1
H	5.720316	-3.155908	0.806647	-1
H	-0.567942	-3.865642	0.77221	-1
H	1.89648	-3.583853	0.790442	-1
H	-3.181067	-3.660145	-2.619967	-1
H	4.445053	-2.788102	-2.563509	-1
H	-3.4019	-2.135208	3.549194	-1
H	4.225766	-1.263001	3.605642	-1
H	0.632155	-3.22574	-2.591006	-1
H	0.412139	-1.700881	3.577519	-1
H	-6.433183	-1.63782	-1.718952	-1
H	-6.557075	-0.806312	1.592323	-1
H	7.143117	-0.085424	-1.618422	-1
H	7.027817	0.747035	1.692837	-1
H	1.966368	1.470326	2.863836	0
H	-1.840937	1.062533	2.732536	0
H	-5.267956	0.914835	2.692769	0
H	2.172042	-0.030889	-3.262672	0
H	-1.617339	-0.514305	-3.302859	0
H	-5.045604	-0.593419	-3.408682	0
H	5.565404	0.545977	-3.29406	0
H	5.368494	2.069955	2.784125	0
Si	-3.245352	-3.419531	0.54021	-1
Si	4.407229	-2.54452	0.596799	-1
Si	0.580902	-2.981994	0.568488	-1
Si	-3.264815	-2.594934	-1.625213	-1
Si	-3.403411	-1.628661	2.179892	-1
Si	4.271585	-1.732827	-1.569426	-1
Si	4.132946	-0.76675	2.235732	-1
Si	0.503452	-2.163953	-1.597306	-1
Si	0.364763	-1.197671	2.207886	-1
Si	-1.521248	-1.128144	-1.947873	0
Si	-5.092302	-1.088199	-2.009248	0
Si	-1.649839	-0.115117	1.841765	0
Si	-5.222035	-0.18751	1.696837	0
Si	5.695525	0.154375	-1.860557	0
Si	2.232572	-0.583993	-1.878234	0
Si	5.575519	1.051467	1.713993	0
Si	2.09941	0.349952	1.889349	0
Si	-2.171395	0.454934	-0.378445	0
Si	-4.508381	0.563487	-0.416079	0
Si	4.924828	1.891672	-0.419989	0
Si	2.683148	1.155236	-0.272811	0
O	1.724783	2.94193	-0.554554	0
C	2.401025	4.171098	-1.087395	0
H	2.046166	4.328048	-2.109942	0
H	2.132063	5.006136	-0.436329	0
H	3.475458	3.96849	-1.051776	0
C	-2.565298	3.250529	-0.175133	0
C	-1.925635	2.236913	-1.115062	0
C	-1.655717	4.044181	0.652129	0
C	-0.458355	2.375204	-1.343712	0
H	-2.473201	2.198229	-2.064811	0
C	-0.290985	3.923217	0.566368	0
H	-2.076721	4.714417	1.396813	0
C	0.291033	3.068331	-0.464312	0
H	-0.000249	1.804457	-2.14681	0
H	0.362985	4.46245	1.245751	0
O	-4.72044	2.30546	-0.737965	0
C	-4.782728	4.219672	0.74871	0
H	-4.19753	5.04224	1.16974	0
H	-5.555107	4.646115	0.095739	0
H	-5.30377	3.701645	1.566374	0
C	-3.938217	3.264198	-0.049878	0

Table S12: Across-trough methyl-cleavage coordinates. (https://doi.org/10.5281/zenodo.2650188).

Element	X	Y	Z	Fixed
H	3.128326	-3.469457	0.788708	-1
H	-2.062979	-3.964026	0.752016	-1
H	-4.531224	-4.210286	0.737495	-1
H	5.598621	-3.24523	0.809074	-1
H	-0.701922	-3.836166	0.776672	-1
H	1.767385	-3.600939	0.794109	-1
H	-3.312014	-3.579112	-2.614324	-1
H	4.329223	-2.851153	-2.560327	-1
H	-3.501651	-2.054443	3.555941	-1
H	4.141135	-1.32635	3.609928	-1
H	0.508736	-3.216752	-2.586594	-1
H	0.319914	-1.692177	3.583034	-1
H	-6.525045	-1.496394	-1.710661	-1
H	-6.631946	-0.664931	1.601217	-1
H	7.078167	-0.200502	-1.614513	-1
H	6.979874	0.631749	1.697347	-1
H	1.955561	1.427956	2.860671	0
H	-1.865684	1.112832	2.741436	0
H	-5.311989	1.025644	2.71174	0
H	2.133137	-0.0696	-3.25035	0
H	-1.676482	-0.479224	-3.299635	0
H	-5.117029	-0.479072	-3.397235	0
H	5.512902	0.514151	-3.291784	0
H	5.349118	2.031086	2.773939	0
Si	-3.370527	-3.33946	0.546039	-1
Si	4.297223	-2.609034	0.600158	-1
Si	0.463312	-2.974215	0.573082	-1
Si	-3.375264	-2.513182	-1.618826	-1
Si	-3.494133	-1.547034	2.186978	-1
Si	4.176082	-1.793464	-1.565471	-1
Si	4.057166	-0.827511	2.240386	-1
Si	0.400474	-2.153397	-1.592135	-1
Si	0.281512	-1.187238	2.213756	-1
Si	-1.606262	-1.078364	-1.937177	0
Si	-5.173786	-0.963382	-1.994083	0
Si	-1.711544	-0.059414	1.836682	0
Si	-5.285729	-0.064154	1.701273	0
Si	5.644985	0.041419	-1.88671	0
Si	2.152958	-0.611811	-1.861186	0
Si	5.541361	0.956456	1.762534	0
Si	2.04437	0.306006	1.883613	0
Si	-2.224833	0.531796	-0.384126	0
Si	-4.55441	0.687778	-0.40888	0
Si	4.804119	1.647503	-0.370435	0
Si	2.469689	1.192817	-0.284427	0
O	1.750508	2.782627	-0.489204	0
C	-2.517337	3.341228	-0.262496	0
C	-1.913201	2.279517	-1.168527	0
C	-1.567573	4.16925	0.48787	0
C	-0.434039	2.332029	-1.383069	0
H	-2.463474	2.235402	-2.117259	0
C	-0.209576	3.987654	0.404837	0
H	-1.955202	4.928645	1.162549	0
C	0.363742	3.011531	-0.525492	0
H	-0.006099	1.68139	-2.142262	0
H	0.475541	4.578173	1.006964	0
O	-4.714078	2.425393	-0.755175	0
C	-4.69659	4.386133	0.671757	0
H	-4.08417	5.2072	1.055796	0
H	-5.473463	4.810547	0.022512	0
H	-5.210794	3.906728	1.517575	0
C	-3.886335	3.388478	-0.111173	0
C	5.147028	3.46736	-0.822298	0
H	4.788573	3.68747	-1.834391	0
H	4.621788	4.134644	-0.129853	0
H	6.220353	3.689362	-0.777611	0