Supplementary Information

Unusual Complexes of Trapped Methanol with Azacryptands

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Synthesis. Compound **L1**[1] and **L2**[2] were prepared as reported earlier. Sulfate salts of these compounds were obtained by dissolving the respective ligand (50 mg) in MeOH (5 mL) and adding a few drops of H_2SO_4. The white solid was immediately formed that was filtered, washed by Et_2O and dried under vacuum.

X-ray crystallography. The sulfate salts were redissolved in the mixture of CH_3OH (5 mL) and H_2O (1 mL), and the solutions were kept in a desiccator under the saturated vapour pressure of methanol at room temperature. X-ray quality crystals were grown in two days for the salt of **L1** (**1**) while the crystals of **L2** (**2**) were grown after a week. Both samples gave colourless prism-shaped crystals that were selected for structural analysis.

Data collection: Intensity data were collected using a diffractometer with a Bruker APEX ccd area detector [3] and graphite-monochromated CuK_α radiation (λ = 1.54178 Å). Both samples were colloed to 100(2) K. For **1**, cell parameters were determined from a non-linear least squares fit of 1199 peaks in the range $34.5 < \theta < 68.8°$. A total of 35685 data were measured and corrected for absorption by the semi-empirical method (4) giving minimum and maximum transmission factors of 0.417 and 0.508. The data were merged to form a set of 9417 independent data with R(int) = 0.0794 and a coverage of 97.4 %. While for **2**, cell parameters were determined from a non-linear least squares fit of 2035 peaks in the range $2.98 < \theta < 54.13°$. A total of 11543 data were measured and corrected for absorption by the semi-empirical method (2) giving minimum and maximum transmission factors of 0.484 and 0.778. The data were merged to form a set of 1749 independent data with R(int) = 0.0719 and a coverage of 99.7 %.

Both structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 [5] Hydrogen atom positions were initially determined by geometry and refined by a riding model.

References

[1] M. A. Saeed, F. R. Fronczek and M. A. Hossain, *Chem. Commun.* **2009**, 6409–6411.

[2] M. A. Hossain, J. M. Llinares, S. Mason, P. Morehouse, D. Powell and K. Bowman- James, *Angew. Chem. Int. Ed*. **2002**, *41*, 2335–2338;

[3]. Data Collection: SMART Software Reference Manual, Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373 USA, **1998**. Data Reduction: SAINT Software Reference Manual, Bruker-AXS, 5465 E. Cheryl Parkway, Madison, WI 53711-5373 USA, **1998**.

[4]. G. M. Sheldrick, SADABS. Program for Empirical Absorption Correction of Area Detector Data. University of Göttingen, Germany, **2007**.

[5]. G. M. Sheldrick, *Acta Cryst.* **2008**, *A64*, 112-122. *International Tables for Crystallography, Vol C,* Tables 6.1.1.4, 4.2.6.8, and 4.2.4.2, Kluwer: Boston, **1995**.

Full list of the authors in Ref 12.

[12] Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M.

Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.

DFT calculations

Cartesian coordinates for M052x/6-31+G(d) geometries of the reagents and formed complexes

Water (fully optimized geometry)

8	0	0.000000	0.000000	0.115719
1	0	0.000000	0.770058	-0.462875
1	0	0.000000	-0.770058	-0.462875

Methanol (fully optimized geometry)

6	0	0.666933	-0.020964	0.000000
8	0	-0.746119	0.122569	0.000000
1	0	1.020963	-0.545176	0.892363
1	0	1.020963	-0.545177	-0.892362
1	0	1.079416	0.985301	0.000000
1	0	-1.153984	-0.749718	0.000000

L1 (geometry is modeled from the crystallographic coordinates with corrected lengths of bonds that involve hydrogen atoms)

6	0	0.266419	-2.953347	-2.756563
6	0	0.050490	3.043890	-2.483261
6	0	-0.517524	0.852028	3.847504
7	0	-4.708878	-0.027562	-0.333764
1	0	-3.688455	-0.020319	-0.223036
6	0	-5.174256	-1.407717	-0.511916
1	0	-6.234537	-1.388519	-0.778341
1	0	-5.084399	-1.931648	0.443525
6	0	-4.421412	-2.202887	-1.573185
1	0	-4.876230	-3.192470	-1.674527
1	0	-4.509338	-1.693480	-2.536263
7	0	-2.972021	-2.359102	-1.229867
1	0	-2.874105	-2.507532	-0.217903
1	0	-2.467978	-1.498109	-1.472176
6	0	-2.359820	-3.520145	-1.966042
1	0	-2.859413	-4.441464	-1.656451
1	0	-2.530211	-3.391862	-3.038541
6	0	-0.884950	-3.654706	-1.717312
6	0	-0.266553	-4.399740	-0.739657
1	0	-0.805418	-4.926115	0.045135
6	0	1.138901	-4.410723	-0.859405
1	0	1.798676	-4.961962	-0.193263

6	0	1.572330	-3.659471	-1.892834
6	0	2.936175	-3.504785	-2.511966
1	0	3.231376	-4.468387	-2.935255
1	0	2.859127	-2.793671	-3.338812
7	0	4.021714	-3.043436	-1.597457
1	0	4.845298	-2.825438	-2.170818
1	0	4.276731	-3.830505	-0.987891
6	0	3.741796	-1.852918	-0.722039
1	0	3.566612	-2.182976	0.305356
1	0	2.841596	-1.341251	-1.072115
6	0	4.928294	-0.894632	-0.757808
1	0	5.844032	-1.439714	-0.516379
1	0	5.034190	-0.485428	-1.766254
7	0	4.745082	0.198938	0.194317
1	0	3.739363	0.396309	0.261353
6	0	5.419762	1.427389	-0.242809
1	0	6.426170	1.175954	-0.585811
1	0	5.517051	2.101518	0.611181
6	0	4.683678	2.150469	-1.360883
1	0	5.241298	3.048247	-1.642197
1	0	4.624840	1.500548	-2.237445
7	0	3.303559	2.539123	-0.936091
1	0	3.332328	2.920015	0.017789
1	0	2.699697	1.708639	-0.930774
6	0	2.732521	3.567797	-1.869389
1	0	2.836899	3.215673	-2.898803
1	0	3.303769	4.495330	-1.773420
6	0	1.285506	3.848252	-1.588330
6	0	0.747783	4.719904	-0.686634
1	0	1.342616	5.341079	-0.020877
6	0	-0.670002	4.726271	-0.713650
1	0	-1.276768	5.346529	-0.056560
6	0	-1.197529	3.886542	-1.636031
6	0	-2.639944	3.647296	-1.935311
1	0	-2.792276	3.681280	-3.017175
1	0	-3.235392	4.448150	-1.487899
7	0	-3.125302	2.319355	-1.411435
1	0	-2.662796	1.559027	-1.924223
1	0	-2.872768	2.231560	-0.419405
6	0	-4.612350	2.194580	-1.562975
1	0	-4.912789	2.642428	-2.513627
1	0	-5.101525	2.752500	-0.761001
6	0	-5.083172	0.754454	-1.525121
1	0	-6.172527	0.749172	-1.608158
1	0	-4.686955	0.243223	-2.406264
6	0	-5.338304	0.568370	0.860295

1	0	-6.423250	0.497580	0.751194
1	0	-5.081573	1.630769	0.893019
6	0	-4.944652	-0.062947	2.180318
1	0	-5.327370	0.552517	2.999276
1	0	-5.412147	-1.047928	2.257421
7	0	-3.463027	-0.210989	2.331470
1	0	-3.002232	0.617379	1.937045
1	0	-3.151886	-1.028826	1.793553
6	0	-3.031077	-0.375546	3.769679
1	0	-3.341761	0.498479	4.348165
1	0	-3.511315	-1.258013	4.199491
6	0	-1.546577	-0.524762	3.842733
6	0	-0.827818	-1.680168	3.806593
1	0	-1.278562	-2.669403	3.774630
6	0	0.569262	-1.455715	3.818877
1	0	1.308706	-2.253776	3.810330
6	0	0.888495	-0.129320	3.842340
6	0	2.260916	0.477115	3.837910
1	0	2.179177	1.566802	3.792758
1	0	2.781085	0.214752	4.763041
7	0	3.047368	-0.015324	2.663747
1	0	3.084220	-1.040548	2.693064
1	0	2.564687	0.257399	1.799496
6	0	4.438074	0.523685	2.635434
1	0	4.921728	0.350913	3.599360
1	0	4.414375	1.600876	2.451937
6	0	5.223388	-0.166814	1.535194
1	0	6.278729	0.100685	1.625932
1	0	5.139172	-1.248909	1.661846

L2 (geometry is modeled from the crystallographic coordinates with corrected lengths of bonds that involve hydrogen atoms)

7	0	-4.930670	0.491382	-0.255682
6	0	-5.515376	0.923543	1.038886
1	0	-6.603641	0.966891	0.946967
1	0	-5.156207	1.927634	1.278569
6	0	-5.137974	-0.040022	2.184653
1	0	-5.542802	0.348670	3.122566
1	0	-5.599250	-1.013178	1.997994
7	0	-3.685190	-0.217005	2.326077
1	0	-3.227794	0.667032	2.073101
1	0	-3.366796	-0.938924	1.668668
6	0	-3.264659	-0.584587	3.687258
1	0	-3.780544	-1.496156	3.999594
1	0	-3.534980	0.213683	4.383204
6	0	-1.760260	-0.812222	3.730951

6	0	-0.862882	0.156798	4.225614
1	0	-1.230526	1.096831	4.631717
6	0	0.489538	-0.109380	4.182513
1	0	1.172281	0.634309	4.588141
6	0	-1.248790	-1.984386	3.219509
1	0	-1.927611	-2.747201	2.843929
6	0	0.094033	-2.203502	3.173638
1	0	0.460368	-3.136817	2.751187
6	0	1.025168	-1.270276	3.654641
6	0	2.487456	-1.524884	3.583767
1	0	2.658314	-2.585430	3.382030
1	0	2.938740	-1.293148	4.551905
7	0	3.153837	-0.712655	2.529316
1	0	2.699405	-0.896745	1.612145
1	0	3.045083	0.285585	2.744765
6	0	4.583394	-1.045613	2.443420
1	0	4.695725	-2.094062	2.155692
1	0	5.047942	-0.912339	3.423768
6	0	5.295154	-0.162887	1.422776
1	0	5.156135	0.886093	1.696572
1	0	6.366515	-0.378082	1.445693
7	0	4.790496	-0.376606	0.068442
6	0	5.400552	-1.591240	-0.509646
1	0	5.427077	-2.365639	0.261231
1	0	6.434464	-1.363286	-0.781146
6	0	4.709423	-2.141356	-1.705296
1	0	5.200515	-3.069975	-2.007198
1	0	4.803616	-1.431699	-2.531228
7	0	3.260668	-2.414230	-1.458881
1	0	3.153993	-2.759275	-0.497480
1	0	2.740916	-1.516039	-1.527521
6	0	2.640037	-3.377758	-2.367570
1	0	2.981081	-4.384060	-2.111261
1	0	2.965684	-3.166579	-3.389336
6	0	1.171840	-3.338396	-2.315355
6	0	0.438076	-2.972766	-1.175296
1	0	0.967982	-2.775948	-0.245669
6	0	-0.948767	-2.852964	-1.201362
1	0	-1.486440	-2.565684	-0.300184
6	0	0.449706	-3.572750	-3.452510
1	0	0.996444	-3.805638	-4.363875
6	0	-0.952816	-3.530959	-3.519589
1	0	-1.485317	-3.819073	-4.423567
6	0	-1.638509	-3.099639	-2.368678
6	0	-3.136586	-2.929676	-2.474577
1	0	-3.413553	-2.766934	-3.519303

1	0	-3.633404	-3.839620	-2.128423
7	0	-3.590724	-1.765262	-1.649482
1	0	-3.005060	-0.947867	-1.858268
1	0	-3.462419	-2.003197	-0.658698
6	0	-4.993761	-1.407018	-1.906711
1	0	-5.550155	-2.319021	-2.137635
1	0	-5.041179	-0.754537	-2.782307
6	0	-5.680943	-0.704039	-0.717988
1	0	-6.686904	-0.400314	-1.018728
1	0	-5.776308	-1.410334	0.110686
6	0	-5.061387	1.482121	-1.352808
1	0	-6.120861	1.690486	-1.522363
1	0	-4.653520	1.053340	-2.271742
6	0	-4.331894	2.803441	-1.049976
1	0	-4.504944	3.497606	-1.876316
1	0	-4.723985	3.203628	-0.234921
7	0	-2.881902	2.652384	-0.853099
1	0	-2.548014	1.830711	-1.370884
1	0	-2.693427	2.507145	0.145956
6	0	-2.155719	3.897635	-1.314818
1	0	-2.374824	4.048779	-2.374911
1	0	-2.560953	4.754634	-0.770771
6	0	-0.682499	3.886470	-1.140884
6	0	0.174380	3.574120	-2.207007
1	0	-0.272869	3.259221	-3.147513
6	0	1.551020	3.640802	-2.133070
1	0	2.152029	3.366094	-2.997401
6	0	-0.065037	4.266359	0.059528
1	0	-0.670534	4.521411	0.926745
6	0	1.334880	4.316513	0.145745
1	0	1.788594	4.562738	1.103483
6	0	2.178704	4.060722	-0.948015
6	0	3.631400	4.325910	-0.819329
1	0	3.855498	4.600972	0.214484
1	0	3.899031	5.171738	-1.457763
7	0	4.454205	3.139135	-1.201573
1	0	4.298864	2.941437	-2.197321
1	0	5.445949	3.377885	-1.082531
6	0	4.166482	1.906511	-0.423936
1	0	4.251126	2.131303	0.642344
1	0	3.137473	1.593532	-0.618444
6	0	5.084510	0.785000	-0.754365
1	0	4.972815	0.521832	-1.809313
1	0	6.118748	1.097817	-0.589601

L1 + CH_3OH (geometry is modeled from the crystallographic coordinates with corrected lengths of bonds that involve hydrogen atoms)

6	0	0.196590	-3.020830	-2.737425
6	0	0.025071	2.981071	-2.547862
6	0	-0.534847	0.882653	3.815204
7	0	-4.748226	-0.025099	-0.337813
1	0	-3.727366	-0.023732	-0.230951
6	0	-5.224242	-1.404196	-0.494788
1	0	-6.285357	-1.381024	-0.757555
1	0	-5.134567	-1.915280	0.467604
6	0	-4.481185	-2.219675	-1.547509
1	0	-4.943527	-3.207246	-1.633223
1	0	-4.569064	-1.723236	-2.517338
7	0	-3.031674	-2.381600	-1.207355
1	0	-2.931011	-2.516493	-0.193768
1	0	-2.522338	-1.527795	-1.463624
6	0	-2.430673	-3.557310	-1.929345
1	0	-2.935741	-4.470521	-1.604967
1	0	-2.604183	-3.442885	-3.002910
6	0	-0.955884	-3.699099	-1.684168
6	0	-0.339201	-4.434795	-0.698393
1	0	-0.878889	-4.946142	0.095715
6	0	1.065674	-4.457698	-0.823142
1	0	1.723958	-5.004306	-0.151729
6	0	1.500616	-3.724231	-1.868641
6	0	2.863194	-3.588206	-2.494902
1	0	3.149817	-4.559790	-2.905654
1	0	2.788166	-2.888248	-3.331397
7	0	3.955489	-3.121961	-1.590982
1	0	4.778456	-2.918053	-2.170383
1	0	4.207110	-3.902216	-0.971329
6	0	3.687499	-1.917242	-0.731404
1	0	3.513817	-2.231534	0.301178
1	0	2.789706	-1.404005	-1.085341
6	0	4.880752	-0.968222	-0.785034
1	0	5.793431	-1.516511	-0.539318
1	0	4.985792	-0.574023	-1.799529
7	0	4.709053	0.139936	0.152255
1	0	3.692484	0.348794	0.220998
6	0	5.390942	1.357171	-0.304616
1	0	6.394202	1.093613	-0.647739
1	0	5.496331	2.042517	0.539427
6	0	4.655886	2.069798	-1.430053
1	0	5.218916	2.959445	-1.726037

1	0	4.589037	1.408059	-2.297148
7	0	3.280229	2.474430	-1.005707
1	0	3.315357	2.868480	-0.057400
1	0	2.662850	1.638330	-0.986238
6	0	2.713122	3.494009	-1.951301
1	0	2.811059	3.126692	-2.976028
1	0	3.291421	4.418614	-1.870511
6	0	1.269245	3.788922	-1.668901
6	0	0.741252	4.677062	-0.777606
1	0	1.343073	5.303189	-0.122859
6	0	-0.676542	4.693376	-0.799495
1	0	-1.276320	5.327217	-0.148983
6	0	-1.213611	3.844623	-1.708006
6	0	-2.658839	3.611704	-1.998579
1	0	-2.815009	3.631580	-3.080246
1	0	-3.246785	4.423088	-1.560309
7	0	-3.151804	2.294834	-1.454263
1	0	-2.696750	1.524020	-1.957983
1	0	-2.896164	2.219161	-0.462029
6	0	-4.640277	2.178774	-1.598560
1	0	-4.941061	2.615385	-2.554316
1	0	-5.122370	2.751466	-0.802733
6	0	-5.121356	0.742791	-1.538686
1	0	-6.211026	0.744277	-1.617634
1	0	-4.732179	0.216346	-2.413989
6	0	-5.368809	0.592136	0.850037
1	0	-6.454643	0.527723	0.745935
1	0	-5.104280	1.652992	0.866843
6	0	-4.974746	-0.023405	2.177368
1	0	-5.349905	0.606287	2.988975
1	0	-5.449057	-1.003773	2.270061
7	0	-3.493670	-0.180095	2.325142
1	0	-3.028391	0.639266	1.917392
1	0	-3.190486	-1.007662	1.797661
6	0	-3.057488	-0.327552	3.763929
1	0	-3.359654	0.556762	4.331180
1	0	-3.542467	-1.200366	4.207895
6	0	-1.573841	-0.486535	3.833618
6	0	-0.863597	-1.647540	3.811119
1	0	-1.321601	-2.633817	3.794755
6	0	0.535105	-1.433119	3.815101
1	0	1.268722	-2.236586	3.815081
6	0	0.864008	-0.108885	3.818698
6	0	2.240752	0.487414	3.800677
1	0	2.166726	1.576925	3.740476
1	0	2.762504	0.234305	4.727494

7	0	3.019179	-0.027204	2.630685
1	0	3.048727	-1.052156	2.674309
1	0	2.528005	0.240339	1.751938
6	0	4.413630	0.501209	2.589665
1	0	4.899662	0.338491	3.554145
1	0	4.397029	1.575857	2.391098
6	0	5.189766	-0.210397	1.496384
1	0	6.247349	0.050657	1.579462
1	0	5.098206	-1.289962	1.638579
8	0	1.322402	0.941366	0.574954
1	0	1.021200	1.748405	1.105549
6	0	0.243035	0.068573	0.220460
1	0	0.632188	-0.781181	-0.345826
1	0	-0.479950	0.614636	-0.390890
1	0	-0.248564	-0.291010	1.128568

L2 + CH_3OH (geometry is modeled from the crystallographic coordinates with corrected lengths of bonds that involve hydrogen atoms)

7	0	-4.972989	0.478047	-0.271843
6	0	-5.556972	0.916490	1.021198
1	0	-6.645661	0.958461	0.929869
1	0	-5.198412	1.922553	1.255446
6	0	-5.177910	-0.040576	2.171537
1	0	-5.581883	0.352218	3.107716
1	0	-5.638470	-1.015409	1.989736
7	0	-3.724080	-0.215669	2.312132
1	0	-3.268366	0.667286	2.054329
1	0	-3.406574	-0.941106	1.658712
6	0	-3.302588	-0.575593	3.675373
1	0	-3.817877	-1.486595	3.992727
1	0	-3.572911	0.225727	4.366864
6	0	-1.798027	-0.802011	3.718469
6	0	-0.901001	0.169615	4.207584
1	0	-1.269008	1.111669	4.608555
6	0	0.451429	-0.095815	4.164192
1	0	1.134077	0.650767	4.566184
6	0	-1.286557	-1.976593	3.213069
1	0	-1.964578	-2.742367	2.841496
6	0	0.057240	-2.195068	3.167084
1	0	0.423366	-3.129726	2.748973
6	0	0.987860	-1.258372	3.641871
6	0	2.450539	-1.512213	3.570841
1	0	2.621971	-2.573996	3.375495
1	0	2.902071	-1.275357	4.537422
7	0	3.115114	-0.705314	2.512094

1	0	2.660180	-0.894601	1.596754
1	0	3.005912	0.294104	2.722238
6	0	4.544794	-1.037154	2.426194
1	0	4.657715	-2.087391	2.144233
1	0	5.010410	-0.898815	3.406126
6	0	5.254663	-0.158958	1.400479
1	0	5.115655	0.891074	1.669579
1	0	6.326645	-0.374145	1.423558
7	0	4.749260	-0.380691	0.048418
6	0	5.360003	-1.597216	-0.524254
1	0	5.387121	-2.368034	0.250088
1	0	6.392952	-1.370235	-0.798509
6	0	4.668497	-2.154989	-1.716646
1	0	5.159012	-3.084308	-2.013778
1	0	4.760930	-1.448799	-2.546004
7	0	3.219620	-2.426707	-1.466918
1	0	3.113881	-2.767704	-0.504402
1	0	2.699146	-1.529416	-1.539963
6	0	2.599250	-3.395728	-2.370594
1	0	2.940902	-4.400572	-2.109856
1	0	2.923531	-3.189538	-3.394272
6	0	1.130631	-3.357877	-2.317441
6	0	0.397892	-2.986761	-1.177856
1	0	0.928327	-2.784813	-0.249937
6	0	-0.988972	-2.867519	-1.203808
1	0	-1.526436	-2.576906	-0.303607
6	0	0.408098	-3.597958	-3.452409
1	0	0.954127	-3.835765	-4.363202
6	0	-0.995343	-3.558292	-3.518584
1	0	-1.527631	-3.850554	-4.420162
6	0	-1.680040	-3.121201	-2.369337
6	0	-3.177959	-2.953284	-2.474583
1	0	-3.456037	-2.795584	-3.519581
1	0	-3.674225	-3.861274	-2.123244
7	0	-3.632657	-1.784798	-1.655511
1	0	-3.047451	-0.967855	-1.869199
1	0	-3.503260	-2.017561	-0.663695
6	0	-5.035813	-1.428822	-1.912649
1	0	-5.591712	-2.342991	-2.138555
1	0	-5.084848	-0.781356	-2.791730
6	0	-5.722689	-0.720413	-0.727758
1	0	-6.729528	-0.419265	-1.028489
1	0	-5.816904	-1.422268	0.105068
6	0	-5.105255	1.463395	-1.374287
1	0	-6.165109	1.669149	-1.543731
1	0	-4.698224	1.030335	-2.290838

6	0	-4.377237	2.786712	-1.078456
1	0	-4.551377	3.476222	-1.908856
1	0	-4.768416	3.190831	-0.265520
7	0	-2.926065	2.637389	-0.882337
1	0	-2.591914	1.813599	-1.396123
1	0	-2.736744	2.497683	0.117622
6	0	-2.201723	3.881234	-1.351356
1	0	-2.422117	4.026190	-2.411919
1	0	-2.607522	4.740984	-0.810918
6	0	-0.728184	3.872084	-1.178884
6	0	0.127789	3.555127	-2.243276
1	0	-0.320115	3.234349	-3.182059
6	0	1.505079	3.622782	-2.171324
1	0	2.105493	3.344754	-3.034729
6	0	-0.110568	4.258302	0.019932
1	0	-0.715034	4.517376	0.885637
6	0	1.289789	4.310429	0.104122
1	0	1.743810	4.561658	1.060063
6	0	2.132349	4.049490	-0.988768
6	0	3.585256	4.316684	-0.863042
1	0	3.810544	4.596904	0.169260
1	0	3.852289	5.159579	-1.506006
7	0	4.408891	3.128202	-1.239970
1	0	4.252464	2.925617	-2.234191
1	0	5.400746	3.368989	-1.122874
6	0	4.122723	1.899369	-0.455261
1	0	4.208959	2.129355	0.609368
1	0	3.094118	1.585103	-0.647878
6	0	5.040891	0.777290	-0.781003
1	0	4.929660	0.508310	-1.834511
1	0	6.075950	1.091199	-0.618656
8	0	1.440510	-0.191772	0.202357
1	0	1.571870	-0.191321	-0.689390
6	0	0.188039	0.433806	0.535132
1	0	0.043245	0.403310	1.618198
1	0	-0.630498	-0.095299	0.041668
1	0	0.202165	1.474159	0.199087

L1 + H_2O (partially optimized geometry – geometry of a cryptand is frozen and the position of the encapsulated small molecule inside it is optimized)

16	0	0.262623	-2.929330	-2.771471
16	0	0.043700	3.067076	-2.482763
16	0	-0.521838	0.858719	3.842488
7	0	-4.713642	-0.012294	-0.340124

1	0	-3.693199	-0.004815	-0.229597
6	0	-5.178356	-1.392224	-0.521712
1	0	-6.238704	-1.372884	-0.787859
1	0	-5.088028	-1.918556	0.432365
6	0	-4.425335	-2.184291	-1.585174
1	0	-4.879672	-3.173842	-1.688953
1	0	-4.513728	-1.672463	-2.546925
7	0	-2.975792	-2.340646	-1.242566
1	0	-2.877583	-2.491618	-0.231007
1	0	-2.472239	-1.478779	-1.482778
6	0	-2.363158	-3.499488	-1.981844
1	0	-2.862216	-4.421851	-1.674507
1	0	-2.533845	-3.368545	-3.053974
6	0	-0.888166	-3.633934	-1.733775
6	0	-0.269181	-4.381154	-0.758163
1	0	-0.807610	-4.909812	0.025394
6	0	1.136254	-4.391114	-0.878240
1	0	1.796451	-4.943723	-0.213651
6	0	1.569078	-3.636998	-1.909833
6	0	2.932711	-3.480033	-2.528859
1	0	3.228311	-4.442397	-2.954677
1	0	2.855124	-2.766842	-3.353864
7	0	4.018211	-3.020474	-1.613402
1	0	4.841562	-2.800589	-2.186379
1	0	4.273760	-3.808971	-1.005909
6	0	3.737876	-1.832345	-0.734879
1	0	3.563081	-2.165123	0.291706
1	0	2.837340	-1.320241	-1.083450
6	0	4.923878	-0.873366	-0.768447
1	0	5.839946	-1.418598	-0.528610
1	0	5.029350	-0.461527	-1.775864
7	0	4.740315	0.217668	0.186516
1	0	3.734509	0.414355	0.254271
6	0	5.414276	1.447579	-0.247606
1	0	6.420737	1.197535	-0.591466
1	0	5.511405	2.119567	0.608086
6	0	4.677583	2.173145	-1.363668
1	0	5.234686	3.071924	-1.642799
1	0	4.618887	1.525441	-2.241879
7	0	3.297358	2.560007	-0.937587
1	0	3.326138	2.938468	0.017260
1	0	2.693920	1.729204	-0.934268
6	0	2.725596	3.590777	-1.868125
1	0	2.829932	3.241343	-2.898460
1	0	3.296394	4.518351	-1.769902
6	0	1.278499	3.869773	-1.586039

6	0	0.740526	4.738839	-0.681999
1	0	1.335187	5.358610	-0.014780
6	0	-0.677267	4.744553	-0.708696
1	0	-1.284208	5.362817	-0.049889
6	0	-1.204566	3.906921	-1.633112
6	0	-2.646922	3.667707	-1.932696
1	0	-2.799505	3.704384	-3.014436
1	0	-3.242682	4.467109	-1.483107
7	0	-3.131493	2.338182	-1.412119
1	0	-2.668710	1.579405	-1.926951
1	0	-2.878701	2.247975	-0.420371
6	0	-4.618508	2.213037	-1.563660
1	0	-4.919381	2.663166	-2.513097
1	0	-5.107796	2.768652	-0.760156
6	0	-5.088590	0.772579	-1.529394
1	0	-6.177960	0.766956	-1.612212
1	0	-4.692303	0.263809	-2.411928
6	0	-5.343115	0.580257	0.855591
1	0	-6.428049	0.509195	0.746542
1	0	-5.086917	1.642700	0.890982
6	0	-4.948859	-0.054238	2.173910
1	0	-5.331713	0.558931	2.994523
1	0	-5.415836	-1.039651	2.248589
7	0	-3.467125	-0.201912	2.324365
1	0	-3.006837	0.627698	1.931964
1	0	-3.155684	-1.018211	1.784288
6	0	-3.034783	-0.369932	3.762056
1	0	-3.345786	0.502449	4.342845
1	0	-3.514479	-1.253742	4.189708
6	0	-1.550192	-0.518578	3.834410
6	0	-0.830852	-1.673522	3.795158
1	0	-1.281100	-2.662901	3.760757
6	0	0.566116	-1.448389	3.807717
1	0	1.305964	-2.246049	3.796968
6	0	0.884679	-0.121896	3.834510
6	0	2.256790	0.485247	3.831340
1	0	2.174487	1.575004	3.788996
1	0	2.777292	0.220780	4.755685
7	0	3.043241	-0.003782	2.655751
1	0	3.080620	-1.029059	2.682435
1	0	2.560235	0.270907	1.792305
6	0	4.433667	0.536007	2.628522
1	0	4.917615	0.361012	3.591899
1	0	4.409380	1.613652	2.447790
6	0	5.219095	-0.151274	1.526349
1	0	6.274319	0.116530	1.617547

1	0	5.135456	-1.233731	1.650247
1	0	0.002878	-1.396169	-0.088652
8	0	0.184135	-0.483855	0.178593
1	0	0.124514	-0.448970	1.140706

L1 + CH_3OH (partially optimized geometry – geometry of a cryptand is frozen and the position of the encapsulated small molecule inside it is optimized)

16	0	0.249389	-2.814165	-2.870140
16	0	-0.001993	3.171586	-2.427695
16	0	-0.538268	0.799221	3.840460
7	0	-4.736413	0.011840	-0.352359
1	0	-3.715733	0.022219	-0.244275
6	0	-5.193956	-1.365586	-0.567975
1	0	-6.255108	-1.345402	-0.830840
1	0	-5.098147	-1.915604	0.372103
6	0	-4.439420	-2.125988	-1.653252
1	0	-4.888541	-3.115099	-1.781133
1	0	-4.533234	-1.590263	-2.601376
7	0	-2.988115	-2.282911	-1.318445
1	0	-2.886351	-2.459121	-0.311329
1	0	-2.489996	-1.412377	-1.537829
6	0	-2.371058	-3.419033	-2.088661
1	0	-2.864166	-4.351733	-1.803730
1	0	-2.545350	-3.261704	-3.156655
6	0	-0.894681	-3.551495	-1.847865
6	0	-0.268941	-4.319911	-0.893252
1	0	-0.802322	-4.871426	-0.122096
6	0	1.136198	-4.318915	-1.017123
1	0	1.801234	-4.884608	-0.368561
6	0	1.562060	-3.536274	-2.030203
6	0	2.923132	-3.355898	-2.648484
1	0	3.222916	-4.305396	-3.099514
1	0	2.839374	-2.622311	-3.454790
7	0	4.008526	-2.913794	-1.724347
1	0	4.829101	-2.674727	-2.293612
1	0	4.270075	-3.716107	-1.137861
6	0	3.723973	-1.750087	-0.815031
1	0	3.553786	-2.109957	0.203154
1	0	2.819678	-1.234306	-1.148103
6	0	4.904546	-0.783925	-0.827094
1	0	5.824264	-1.329958	-0.603607
1	0	5.005023	-0.345899	-1.823921
7	0	4.717506	0.281311	0.155908
1	0	3.698205	0.473596	0.232148
6	0	5.383469	1.525672	-0.248350
1	0	6.390373	1.290145	-0.601051

1	0	5.479173	2.176116	0.623990
6	0	4.639767	2.275368	-1.343620
1	0	5.191126	3.184096	-1.601105
1	0	4.582301	1.649991	-2.237948
7	0	3.258569	2.643469	-0.904276
1	0	3.287819	2.997570	0.059857
1	0	2.652341	1.799187	-0.920867
6	0	2.678602	3.694450	-1.806704
1	0	2.782102	3.372044	-2.845896
1	0	3.244510	4.622401	-1.686257
6	0	1.230744	3.958027	-1.513893
6	0	0.690396	4.800682	-0.586567
1	0	1.283403	5.406531	0.094759
6	0	-0.727475	4.799122	-0.609498
1	0	-1.336060	5.396939	0.066440
6	0	-1.252606	3.982433	-1.553677
6	0	-2.694415	3.742862	-1.855603
1	0	-2.850107	3.806307	-2.935660
1	0	-3.293386	4.527164	-1.384212
7	0	-3.170206	2.397775	-1.367949
1	0	-2.704610	1.655006	-1.903184
1	0	-2.914252	2.283681	-0.379477
6	0	-4.656908	2.268202	-1.518852
1	0	-4.962822	2.740743	-2.455703
1	0	-5.147104	2.800355	-0.700163
6	0	-5.118904	0.824724	-1.520219
1	0	-6.208444	0.815106	-1.600379
1	0	-4.722176	0.340897	-2.416476
6	0	-5.365943	0.570111	0.859712
1	0	-6.450755	0.495771	0.751644
1	0	-5.115545	1.632724	0.921594
6	0	-4.964630	-0.095633	2.160372
1	0	-5.348670	0.494215	2.997363
1	0	-5.425935	-1.085237	2.211028
7	0	-3.481703	-0.238787	2.303230
1	0	-3.027078	0.603146	1.930992
1	0	-3.167194	-1.039263	1.741673
6	0	-3.044570	-0.441052	3.735051
1	0	-3.358842	0.414449	4.338738
1	0	-3.518208	-1.338176	4.141192
6	0	-1.558989	-0.583167	3.799800
6	0	-0.833366	-1.732677	3.729206
1	0	-1.278213	-2.723365	3.670674
6	0	0.562361	-1.500105	3.743959
1	0	1.306589	-2.293066	3.710941
6	0	0.873636	-0.172962	3.803838

6	0	2.242347	0.441751	3.812694
1	0	2.153892	1.531756	3.798429
1	0	2.766792	0.156681	4.728648
7	0	3.028332	-0.012666	2.622990
1	0	3.071467	-1.038064	2.623362
1	0	2.534239	0.285200	1.755710
6	0	4.415666	0.535434	2.606025
1	0	4.903167	0.338603	3.563379
1	0	4.384921	1.617191	2.452962
6	0	5.201926	-0.119046	1.484649
1	0	6.255890	0.152255	1.579974
1	0	5.124623	-1.204769	1.581050
8	0	1.264194	-1.141361	0.638526
1	0	1.538686	-0.268732	0.257814
6	0	-0.154070	-1.174601	0.578045
1	0	-0.492571	-2.123424	0.990858
1	0	-0.491235	-1.086493	-0.456998
1	0	-0.593336	-0.349424	1.146116

L2 + H_2O (partially optimized geometry – geometry of a cryptand is frozen and the position of the encapsulated small molecule inside it is optimized)

7	0	-4.961374	0.479879	-0.280176
6	0	-5.536780	0.953313	1.004344
1	0	-6.625574	1.000123	0.916704
1	0	-5.170765	1.962410	1.212566
6	0	-5.158713	0.021969	2.175926
1	0	-5.555996	0.439952	3.104027
1	0	-5.626292	-0.953974	2.019816
7	0	-3.705418	-0.159096	2.314478
1	0	-3.245231	0.714376	2.033368
1	0	-3.395464	-0.902202	1.677494
6	0	-3.280163	-0.488600	3.684226
1	0	-3.799838	-1.388280	4.025805
1	0	-3.542282	0.330982	4.357225
6	0	-1.776901	-0.723666	3.726335
6	0	-0.871521	0.253687	4.187868
1	0	-1.231718	1.207552	4.567440
6	0	0.478980	-0.021487	4.145116
1	0	1.168164	0.730172	4.525934
6	0	-1.275196	-1.913447	3.247392
1	0	-1.959740	-2.683585	2.897427
6	0	0.066960	-2.141688	3.200944

1	0	0.425246	-3.088562	2.804066
6	0	1.005647	-1.199819	3.648856
6	0	2.466345	-1.464793	3.577719
1	0	2.630123	-2.532090	3.407460
1	0	2.923681	-1.207516	4.536318
7	0	3.131333	-0.688122	2.496857
1	0	2.671127	-0.896583	1.588344
1	0	3.029450	0.316782	2.683156
6	0	4.558469	-1.031218	2.412889
1	0	4.663426	-2.088691	2.156013
1	0	5.029320	-0.872193	3.387166
6	0	5.269352	-0.182766	1.363124
1	0	5.138251	0.874360	1.607261
1	0	6.340031	-0.404282	1.386809
7	0	4.756525	-0.433919	0.019027
6	0	5.356933	-1.667905	-0.526578
1	0	5.382580	-2.419889	0.266117
1	0	6.390079	-1.454346	-0.810698
6	0	4.656575	-2.249915	-1.702099
1	0	5.139820	-3.189325	-1.978700
1	0	4.749818	-1.564648	-2.548739
7	0	3.207120	-2.506092	-1.439626
1	0	3.103495	-2.822968	-0.468674
1	0	2.692065	-1.607475	-1.532184
6	0	2.576558	-3.492685	-2.316847
1	0	2.912946	-4.493109	-2.033273
1	0	2.897584	-3.313475	-3.346612
6	0	1.108461	-3.444026	-2.258314
6	0	0.383191	-3.040651	-1.124931
1	0	0.919034	-2.819720	-0.204474
6	0	-1.002985	-2.913076	-1.147806
1	0	-1.534568	-2.597248	-0.252619
6	0	0.379361	-3.706851	-3.384005
1	0	0.919798	-3.970202	-4.291098
6	0	-1.024078	-3.659694	-3.445089
1	0	-1.562233	-3.970262	-4.337013
6	0	-1.700845	-3.190443	-2.303855
6	0	-3.198116	-3.015408	-2.406703
1	0	-3.479834	-2.881282	-3.454014
1	0	-3.698597	-3.911377	-2.031304
7	0	-3.641691	-1.824488	-1.614278
1	0	-3.052240	-1.016779	-1.850240
1	0	-3.509366	-2.033979	-0.617672
6	0	-5.043679	-1.465751	-1.873943
1	0	-5.606403	-2.381500	-2.075208
1	0	-5.092496	-0.839476	-2.768258

6	0	-5.720733	-0.724389	-0.703649
1	0	-6.726959	-0.424091	-1.007268
1	0	-5.815714	-1.405226	0.146361
6	0	-5.092258	1.439055	-1.405627
1	0	-6.151521	1.647515	-1.575456
1	0	-4.692086	0.981276	-2.313141
6	0	-4.354496	2.764401	-1.145126
1	0	-4.527930	3.434698	-1.991256
1	0	-4.739462	3.190634	-0.340562
7	0	-2.903449	2.610460	-0.951682
1	0	-2.576855	1.772309	-1.446759
1	0	-2.710570	2.493807	0.050549
6	0	-2.173278	3.837845	-1.453856
1	0	-2.397465	3.958481	-2.516666
1	0	-2.571169	4.713057	-0.932699
6	0	-0.699074	3.823317	-1.287548
6	0	0.150108	3.475107	-2.347606
1	0	-0.304013	3.134583	-3.276395
6	0	1.528108	3.535546	-2.283238
1	0	2.122883	3.232782	-3.142217
6	0	-0.073670	4.234462	-0.101124
1	0	-0.672606	4.518358	0.760631
6	0	1.327353	4.279524	-0.024244
1	0	1.787222	4.550897	0.923358
6	0	2.163353	3.986711	-1.114092
6	0	3.618482	4.247440	-1.001135
1	0	3.850151	4.551129	0.023085
1	0	3.888021	5.072754	-1.665505
7	0	4.432826	3.044851	-1.352651
1	0	4.270680	2.819248	-2.340981
1	0	5.426709	3.281964	-1.245697
6	0	4.142319	1.837282	-0.537132
1	0	4.234762	2.092439	0.521222
1	0	3.110880	1.525121	-0.717642
6	0	5.051845	0.701702	-0.839495
1	0	4.934207	0.407994	-1.885678
1	0	6.089599	1.012729	-0.689263
8	0	1.135417	0.972930	1.148413
1	0	0.986011	1.850746	0.758993
1	0	0.617911	0.948872	1.968111

L2 + CH_3OH (partially optimized geometry – geometry of a cryptand is frozen and the position of the encapsulated small molecule inside it is optimized)

7	0	-4.954446	0.466389	-0.292549
6	0	-5.533914	0.931996	0.993005
1	0	-6.622474	0.978680	0.902431

1	0	-5.169120	1.940076	1.208179
6	0	-5.158739	-0.005937	2.160253
1	0	-5.559002	0.406400	3.089597
1	0	-5.625270	-0.981227	1.997083
7	0	-3.705750	-0.186958	2.302029
1	0	-3.245261	0.688404	2.027370
1	0	-3.393476	-0.926160	1.661645
6	0	-3.284331	-0.524189	3.671083
1	0	-3.804468	-1.426147	4.005883
1	0	-3.548921	0.291304	4.348068
6	0	-1.781058	-0.758620	3.716251
6	0	-0.877627	0.216556	4.186135
1	0	-1.239512	1.167982	4.570193
6	0	0.473159	-0.057577	4.145761
1	0	1.160768	0.692253	4.532981
6	0	-1.277231	-1.945298	3.231867
1	0	-1.960280	-2.713783	2.875408
6	0	0.065193	-2.172482	3.188047
1	0	0.425214	-3.116818	2.786718
6	0	1.001992	-1.232690	3.644202
6	0	2.463051	-1.496394	3.575828
1	0	2.627971	-2.562584	3.399838
1	0	2.917410	-1.244438	4.537252
7	0	3.130752	-0.713051	2.501472
1	0	2.673347	-0.916484	1.590408
1	0	3.027718	0.290692	2.693319
6	0	4.558335	-1.054819	2.419713
1	0	4.664682	-2.110716	2.156992
1	0	5.026220	-0.901199	3.396282
6	0	5.271795	-0.199851	1.377007
1	0	5.139341	0.855758	1.626909
1	0	6.342533	-0.420877	1.402556
7	0	4.763078	-0.443468	0.029964
6	0	5.365830	-1.673904	-0.521046
1	0	5.389595	-2.430478	0.267327
1	0	6.399678	-1.458090	-0.800872
6	0	4.669285	-2.249464	-1.701998
1	0	5.153905	-3.186965	-1.982639
1	0	4.764608	-1.559222	-2.544353
7	0	3.219217	-2.508011	-1.445292
1	0	3.112926	-2.830598	-0.476511
1	0	2.703897	-1.609172	-1.534133
6	0	2.591832	-3.489844	-2.330099
1	0	2.927985	-4.491708	-2.051367
1	0	2.915780	-3.304451	-3.357852
6	0	1.123541	-3.442384	-2.275611

6	0	0.394695	-3.046042	-1.142039
1	0	0.927693	-2.830164	-0.218737
6	0	-0.991484	-2.919144	-1.168256
1	0	-1.525889	-2.608847	-0.272816
6	0	0.397915	-3.699071	-3.404958
1	0	0.941178	-3.956817	-4.311973
6	0	-1.005367	-3.652377	-3.469901
1	0	-1.540707	-3.958057	-4.365201
6	0	-1.685771	-3.190178	-2.327952
6	0	-3.182837	-3.015421	-2.434191
1	0	-3.461552	-2.875359	-3.481530
1	0	-3.683884	-3.913853	-2.065494
7	0	-3.629459	-1.829396	-1.636155
1	0	-3.039801	-1.019982	-1.865671
1	0	-3.499941	-2.044612	-0.640400
6	0	-5.030890	-1.469970	-1.897857
1	0	-5.592470	-2.384858	-2.106109
1	0	-5.077451	-0.838524	-2.788648
6	0	-5.711831	-0.735833	-0.725265
1	0	-6.717340	-0.434358	-1.030093
1	0	-5.808906	-1.421667	0.120481
6	0	-5.082592	1.432029	-1.412775
1	0	-6.141476	1.640858	-1.584508
1	0	-4.679477	0.979778	-2.321757
6	0	-4.346397	2.756265	-1.142387
1	0	-4.517741	3.431379	-1.985106
1	0	-4.733985	3.177580	-0.336491
7	0	-2.895832	2.602047	-0.945567
1	0	-2.567279	1.766985	-1.444553
1	0	-2.705834	2.479668	0.056532
6	0	-2.164924	3.832763	-1.438429
1	0	-2.386054	3.959458	-2.501175
1	0	-2.564872	4.704691	-0.913359
6	0	-0.691207	3.818125	-1.267866
6	0	0.161301	3.476592	-2.327427
1	0	-0.289880	3.141220	-3.259517
6	0	1.539069	3.537459	-2.258648
1	0	2.136551	3.240052	-3.117618
6	0	-0.069545	4.222714	-0.077229
1	0	-0.671186	4.501237	0.784396
6	0	1.331218	4.268146	0.004040
1	0	1.788133	4.534262	0.954558
6	0	2.170598	3.982175	-1.085027
6	0	3.625231	4.243090	-0.966265
1	0	3.853702	4.540942	0.060385
1	0	3.896230	5.072417	-1.625019

7	0	4.441328	3.043045	-1.322377
1	0	4.282228	2.823109	-2.312479
1	0	5.434750	3.280110	-1.211116
6	0	4.149147	1.830575	-0.514765
1	0	4.238322	2.079616	0.545325
1	0	3.118432	1.518870	-0.700129
6	0	5.060241	0.697307	-0.821055
1	0	4.945859	0.409631	-1.869273
1	0	6.097362	1.008060	-0.665958
8	0	1.214481	0.951417	0.663525
1	0	1.278580	1.900549	0.473252
6	0	-0.156448	0.598211	0.705094
1	0	-0.228853	-0.388383	1.159662
1	0	-0.576215	0.562754	-0.307613
1	0	-0.719488	1.301228	1.326726

Energies used in calculation

Table 1. HF energies of the reagents (Hartree)

Reagent	**Energy**
Water	-76.404808
Methanol	-115.696643
L1	-2808.228379
L2	-1843.193380

Table 2. Couterpoise corrected HF energies (E_{CORR}) and corresponding BSSE energies (E_{BSSE}) for investigated complexes (Hartree)

Complex	**E_{CORR}**	**E_{BSSE}**
Geometry is modeled from the crystallographic coordinates with corrected lengths of bonds that involve hydrogen atoms		
L1 + CH_3OH	-2923.925963	0.005291
L2 + CH_3OH	-1958.899439	0.006283
Partially optimized geometry – geometry of a cryptand is frozen and the position of the encapsulated small molecule inside it is optimized		
L1 + H_2O	-2884.634164	0.003804
L1 + CH_3OH	-2923.940858	0.004681
L2 + H_2O	-1919.619293	0.005897
L2 + CH_3OH	-1958.910385	0.006407