Hydrophobic Amplification of Noncovalent Organocatalysis

Christian M. Kleiner and Peter R. Schreiner*

Institut für Organische Chemie der Justus-Liebig-Universität, Heinrich-Buff-Ring 58, D-35392 Giessen, Germany; prs@org.chemie.uni-giesssen.de

Supporting Information

General

All ^{1}H NMR, ^{13}C NMR spectra were recorded using Bruker AC 200, AM 400 WB, Avance II 200 or Avance II 400 FT spectrometers at ambient temperature.

Chemicals

Propene oxide, cyclohexen oxide, and styrene oxide were purchased from Merck and fractionally distilled through a 10 cm Vigreux column and were stored under argon. All amines were freshly distilled prior to use and stored under argon. Thiophenol and phenol were purchased from Merck and were used as received. Allyl alcohol was freshly distilled prior to use. Dichloromethane was distilled from Sicapent® and stored over molecular sieves 4 Å under argon.

Reactions

All reactions were carried out in a carousel reaction station.

General procedure for the nucleophilic ring opening reaction

Epoxide (1 mmol) was dissolved in 2 mL of dist. H_2O and cooled to 0 °C. 10 mol% of thiourea catalyst was added to the solution; ultrasonication was used to homogenize the reaction mixtures. Amine (1 mmol) was added in one portion and the reaction mixture was allowed to warm to room temperature. The resulting emulsion was vigorously

stirred for the time indicated and then a saturated $NaHCO_3$ solution was added. The aqueous layer was extracted with Et_2O (3x 20 mL). The organic layer was dried over Na_2SO_4. Filtration and concentration under reduced pressure provided the desired products (which are all literature known), with spectral data identical to literature data (see below).

Spectroscopic data of the products can be found in the following references:

1-tert-Butylamino-propan-2-ol, 1-Morpholin-4-yl-propan-2-ol: Azizi, N.; Saidi, M.R. *Org. Lett.* **2005**, *7*, 3649–3651.

1-Butylamino-propan-2-ol, 1-Dipropylamino-propan-2-ol, 1-Piperidin-1-yl-propan-2-ol: Slipko, K.; Chlebicki, J. *Polish J. Chem.* **1979**, *53*, 2231–2237.

1-Dibutylamino-propan-2-ol: Froyen, P.; Juvvik, P. *Tetrahedron Lett.* **1995**, 36,9555–9558.

1-Diisopropylamino-propan-2-ol: Kojima, F.; Aida, T.; Inoue, S. *J. Am. Chem. Soc.* **1986**, *108*, 391–395.

1-Pyrrolidin-1-yl-propan-2-ol: Suzuki, K.; Okano, K.; Nakai, K.; Terao, Y.; Sekiya, M. *Synthesis* **1983**, 723–725.

1-Diallylamino-propan-2-ol: Dobrev, A.; Spassov, S.; Lattes, A. *J. Chem. Res*., *Synopses* **1993**, 251.

2-tert-Butylamino-cyclohexanol, 2-Butyamino-cyclohexanol, 2-Diisopropylamino-cyclohexanol, 2-Piperidin-1-yl-cylohexanol, 2-Morpholin-4-yl-cyclohexanol, 2-Diisopropylamino-2-phenyl-ethanol, 2-Morpholin-4-yl-2-phenyl-ethanol: Rampalli, S.; Chaudhari, S. S.; Akamanchi, K. G. *Synthesis* **2000**, 78–80.

2-Dipopylamino-cyclohexanol: Pachón, L.D.; Gamez, P.; van Brussel, J.J.M.; Reedijk, J. *Tetrahedron Lett.* **2003**, *44*, 6025–6027.

2-Pyrrolidin-1-yl-cyclohexanol: Periasamy, M.; Kumar, N.S.; Sivakumar, S.; Rao, V.D.; Ramanathan, C.R.; Venkatraman, L. *J. Org. Chem*. **2001**, *66*, 3828–3833.

2-tert-Butylamino-1-phenyl-ethanol, 2-tert-Butylamino-2-phenyl-ethanol, 2-Butylamino-2-phenyl-ethanol, 2-Diisopropylamino-1-phenyl-ethanol, 2-Phenyl-2-piperidin-1-yl-ethanol: Chini, M.; Crotti, P.; Macchia, F. *J. Org. Chem.* **1991**, *56*, 5939–5942.

2-Butylamino-1-phenyl-ethanol: Ahlbrecht, H.; Kornetzky, D. *Synthesis* **1988**, 775

2-Dibutylamino-1-phenyl-ethanol, 1-Phenyl-2-piperidin-1-yl-ethanol, 2-Morpholin-4-yl-1-phenyl-ethanol, 2-Dibutylamino-cyclohexanol: Harris, C.E.; Fisher, G.B.; Beardsley, D.; Lee, L.; Goralski, C.T.; Nicholson, L.W.; Singaram, B. *J. Org. Chem.* **1994**, *59*, 7746–7751.

2-Dipropylamiono-1-phenyl-ethanol, 2-Dipropylamino-2-phenyl-ethanol: Duran Pachon, Laura; Gamez, Patrick; van Brussel, Jos J. M.; Reedijk, Jan. *Tetrahedron Lett*. **2003**, *44*, 6025–6027.

1-Phenyl-2-pyrrolidin-1-yl-ethanol: Miyano, S.; Lu, L.D.-L.;Viti, S.; Sharpless, K.B. *J. Org. Chem.* **1983**, *48*, 3608–3611.

2-Phenyl-2-pyrrolidin-1-yl-ethanol: Chakraborti, A.K.; Kondaskar, A. *Tetrahedron Lett.* **2003**, *44*, 8315–8319.

2-Diallylamino-1-phenyl-ethanol: Saravanan, P.; Bisai, A.; Baktharaman, S.; Chandrasekhar, M.; Singh, V.K. *Tetrahedron* **2002**, *58*, 4693–4706.

2-Diallylamino-2-phenyl-ethanol: Fiaux, H.; Popowyzc, F.; Favre, S.; Schütz, C.; Vogel, P.; Gerber-Lemaire, S.; Juillerat-Jeanneret, L. *J. Med. Chem.* **2005**, *48*, 4237–4246.

1-Phenyl-2-phenylsulfanyl-ethanol, 2-Phenyl-2-phenylsulfanyl-ethanol: Amantini, D.; Fringuelli, F.; Pizzo, F.; Tortoioli, S.; Vaccaro, L. *Synlett* **2003**, 2292–2296.

2-Phenoxy-1-phenyl-ethanol: Surendra, K.; Krishnaveni, N.S.; Nageswar, Y.V.D.; Rao, K.R. *J. Org. Chem.* **2003**, *68*, 4994–4995.

2-Phenoxy-2-phenyl-ethanol: Fringuelli, F.; Pizzo, F.; Vittoriani, C.; Vaccaro, L. *Chem. Comm.* **2004**, *23*, 2756–2757.

2-Allyloxy-2-phenyl-ethanol: Salehi, P.; Khodaei, M.M.; Zolfigol, M.A.; Keyvan, A. *Synthetic Communications* **2003**, *33*, 3041–3048.

Theoretical methods

All structures were optimized at the B3LYP[1]/6-31G(d)[2] level of theory; single-point energies were computed at the B3LYP/6-311++G(d,p) level. Solvent effects were modeled using the Self-Consistent-Isodensity Polarized Continuum Model (SCI-PCM),[3] and all gas-phase structures were reoptimized at the PCM-B3LYP/6-31G* level for methylene chloride and water as the solvents. We utilized Gaussian03[4] for all computations. Single-point energies were computed at the SCI-PCM/B3LYP/6-311++G(d,p) level as well. Harmonic frequencies were computed on all optimized structures in order to verify the nature of stationary points.

[1] a) A. D. Becke, *J. Chem. Phys*. 1993, *98*, 5648. b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*. **1988**, *37*, 785.

[2] W. Hehre, L. Radom, P. v. R. Schleyer, J. A. Pople. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.

[3] J. B. Foresman, T. A. Keith, K. B. Wiberg, J. Snoonian, and M. J. Frisch, *J. Phys. Chem.* **100**, 16098 (1996).

[4] Gaussian 03, Revision B.05, 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.

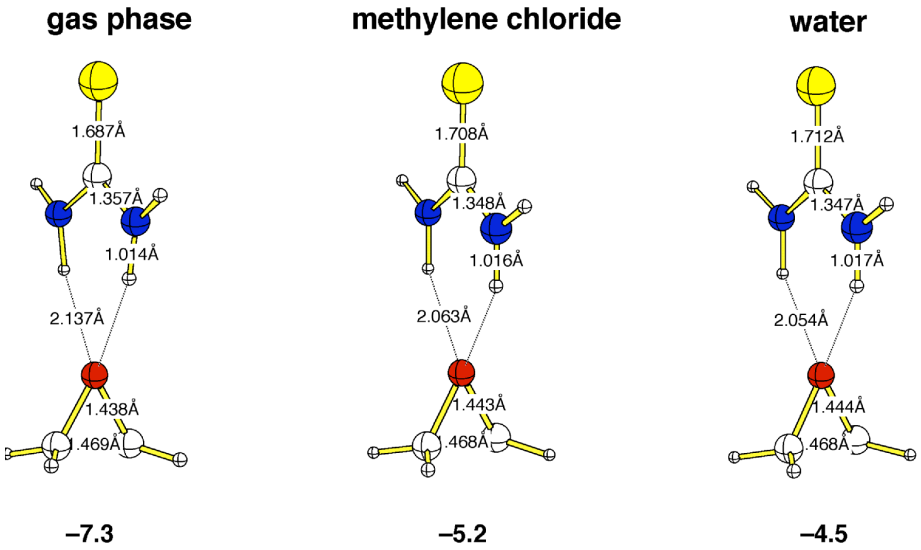

Figure S1. Complexes of epoxide (**S1**) and thiourea (**S2**) in the gase phase, methylene chloride, and water; complexation energies in kcal mol^{-1} at B3LYP/6-311++G(d,p)//B3LYP/6-31G(d).

Table S1. Absolute energies (in –au), zero-point vibrational energies (ZPVEs, in kcal mol^{-1}) of all computed species. First entry: gas phase, second entry: methylene chloride, third entry: water.

Species	B3LYP/6-31G(d)	ZPVE	B3LYP/6-311++G(d,p) //B3LYP/6-31G(d)
Epoxide (**S1**)	153.78626 (gas)	36.2	153.83603
	153.78982 (CH_2Cl_2)	36.5	153.83987
	153.79047 (H_2O)	36.5	153.84057
Thiourea (**S2)**	548.21563	38.7	548.30231
	548.23041	38.6	548.31551
	548.23356	38.6	548.31831
S1•S2	702.01518	75.2	702.14992
	702.03126	76.4	702.16368
	702.03406	76.3	702.16610
NH_3 (**S3**)	56.54795	21.7	56.58248
	56.55294	21.9	56.58664
	56.55385	21.9	56.58739
TS	210.27228	59.5	210.36118
	210.30476	58.8	210.38930
	210.30889	58.8	210.39305
S2•TS	758.52800	99.9	758.69354
	758.56060	98.9	758.72327
	758.56521	98.9	758.72765
H_2O	76.40895	13.3	76.45840
S1•H_2O	230.20764	51.7	230.30251
S2•H_2O	624.64007	53.3	624.77294
H_2O•TS	286.71317	75.4	286.84256
H_2O•TS•S2	834.97525	115.6	835.18243
$(H_2O)_2$	152.83034	29.1	152.92261

XYZ-Coordinates of all optimized {B3LYP/6-31G(d)} species in Å

S1

C	-0.371918746	0.000000000	-0.734299625
C	-0.371918746	0.000000000	0.734299625
O	0.855242808	0.000000000	0.000000000
H	-0.594729379	-0.920211157	-1.275642607
H	-0.594729379	0.920211157	-1.275642607
H	-0.594729379	-0.920211157	1.275642607
H	-0.594729379	0.920211157	1.275642607

S1/CH_2Cl_2

C	-0.374695745	0.000000000	-0.733751434
C	-0.374695745	0.000000000	0.733751434
O	0.859731636	0.000000000	0.000000000
H	-0.595376035	-0.920459050	-1.273692349
H	-0.595376035	0.920459050	-1.273692349
H	-0.595376035	-0.920459050	1.273692349
H	-0.595376035	0.920459050	1.273692349

S1/H_2O

C	-0.375216007	0.000000000	-0.733630889
C	-0.375216007	0.000000000	0.733630889
O	0.860631788	0.000000000	0.000000000
H	-0.595615556	-0.920518719	-1.273269900
H	-0.595615556	0.920518719	-1.273269900
H	-0.595615556	-0.920518719	1.273269900
H	-0.595615556	0.920518719	1.273269900

S2

C	0.000000000	0.000000000	-0.315754843
S	0.000000000	0.000000000	1.359051276
N	1.146346638	-0.087262731	-1.056572087
H	1.157703830	0.294080071	-1.995400562
H	2.004601829	0.016370551	-0.533740507
N	-1.146346638	0.087262731	-1.056572087
H	-1.157703830	-0.294080071	-1.995400562
H	-2.004601829	-0.016370551	-0.533740507

S2/CH_2Cl_2

C	0.000000000	0.000000000	-0.336000583
S	0.000000000	0.000000000	1.367298319
N	1.147706219	-0.008692539	-1.046855921
H	1.164201242	0.107359798	-2.051685486
H	2.021055414	0.081543103	-0.550707874
N	-1.147706219	0.008692539	-1.046855921
H	-1.164201242	-0.107359798	-2.051685486
H	-2.021055414	-0.081543103	-0.550707874

S2/H_2O

C	0.000000000	0.000000000	-0.339095030
S	0.000000000	0.000000000	1.368860093
N	1.147478639	-0.003005182	-1.046795836
H	1.164033236	0.095604839	-2.053631344
H	2.022096490	0.085115127	-0.552393454
N	-1.147478639	0.003005182	-1.046795836
H	-1.164033236	-0.095604839	-2.053631344
H	-2.022096490	-0.085115127	-0.552393454

S1•S2

C	0.682048672	-3.261554574	-0.734501077
C	0.681361086	-3.261698284	0.734501078
H	1.627067419	-3.280369073	-1.274348980
H	-0.175822212	-3.657187553	-1.275224621
H	1.625876796	-3.280618675	1.275224622
H	-0.177013137	-3.657435712	1.274348981
N	-1.267664831	0.473780753	-0.004560464
H	-2.225289158	0.785231370	-0.004720834
N	0.971788503	0.941843634	0.004560464
H	1.724506761	1.610768937	0.004720833
C	-0.296853484	1.420299605	-0.000000000
S	-0.642225518	3.072736880	-0.000000000
H	1.170601302	-0.051949667	0.001621117
H	-1.051801654	-0.516448889	-0.001621117
O	0.428659853	-2.050929002	0.000000000

S1•S2/CH_2Cl_2

C	0.673539052	-3.219579573	-0.734134780
C	0.672346569	-3.219828811	0.734134780
H	1.618929171	-3.235411129	-1.271910709
H	-0.185491749	-3.612561995	-1.273435209
H	1.616863500	-3.235855958	1.273435209
H	-0.187562662	-3.612981744	1.271910709
N	-1.260853286	0.447271254	-0.003872510
H	-2.223449841	0.745497421	-0.004069737
N	0.976164720	0.914825133	0.003872510
H	1.738735616	1.573624497	0.004069736
C	-0.288640934	1.381006544	-0.000000000
S	-0.638129800	3.053140861	-0.000000000
H	1.171860046	-0.082582487	0.001788316
H	-1.040686003	-0.545021540	-0.001788316
O	0.418778821	-2.003653063	0.000000000

S1•S2/H_2O

C	0.672360213	-3.213455648	-0.734077870
C	0.670973978	-3.213745382	0.734077871
H	1.617963805	-3.228946604	-1.271280719
H	-0.186862146	-3.606178858	-1.273055535
H	1.615562612	-3.229458293	1.273055536
H	-0.189267273	-3.606671727	1.271280719
N	-1.260041186	0.443456087	-0.003614606
H	-2.223552769	0.739355640	-0.003806405
N	0.976948648	0.911004078	0.003614606
H	1.741289828	1.568038078	0.003806405
C	-0.287356928	1.374863201	-0.000000000
S	-0.637577967	3.050500608	-0.000000000
H	1.172838970	-0.086929180	0.001873616
H	-1.039842046	-0.549396442	-0.001873616
O	0.417362585	-1.996877065	0.000000000

TS

C	0.499370565	-0.828661011	0.000000000
C	-0.029286832	0.613967989	0.000000000
O	1.799896787	-0.658852250	0.000000000
H	0.014906623	-1.352873157	0.894131998
H	0.014906623	-1.352873157	-0.894131998
H	0.270811269	1.150239699	0.900144449
H	0.270811269	1.150239699	-0.900144449
H	-1.999767216	0.195313021	-0.824107333
N	-1.672089179	0.704664631	0.000000000
H	-2.086953793	1.640964594	0.000000000
H	-1.999767216	0.195313021	0.824107333

TS/CH_2Cl_2

O	-1.388451086	0.584788502	1.143961859
C	-0.035843431	0.491568184	0.961604614
H	0.530536041	1.443836442	0.859169659
H	0.530535957	-0.149148267	1.673496656
C	-0.321293094	-0.168652692	-0.329918065
H	-0.729859270	0.465506927	-1.105873642
H	-0.729859356	-1.169009131	-0.270315998
N	1.275815914	-0.693137500	-1.355913946
H	1.035978717	-1.144083674	-2.238053902
H	1.841192136	-1.340110554	-0.808874733
H	1.841192213	0.129169792	-1.559964586

TS/H_2O

O	-1.886991665	0.038768468	0.000000000
C	-0.771115318	-0.763946997	0.000000000
H	-0.604697209	-1.399366627	0.895460828
H	-0.604697209	-1.399366627	-0.895460828
C	-0.000884941	0.491315878	0.000000000
H	0.002185850	1.058937699	0.920523478
H	0.002185850	1.058937699	-0.920523478
N	1.986539572	0.218049215	0.000000000
H	2.495402778	1.101021372	0.000000000
H	2.265888907	-0.310434525	-0.824693850
H	2.265888907	-0.310434525	0.824693850

S2•TS

S	-3.818253562	-0.003282517	-0.195868514
C	-2.122680221	-0.004211822	-0.251298322
N	-1.387243597	1.134369612	-0.275938945
N	-1.387243899	-1.142979667	-0.237767450
H	-1.889307730	-2.010127916	-0.341905686
H	-0.381986533	-1.080280204	-0.432268772
H	-1.889307198	1.997540874	-0.409079707
H	-0.381986248	1.065186716	-0.468229738
O	1.180721825	-0.009116699	-0.543901972
C	1.885379838	0.010546436	0.629225775
H	1.765524365	-0.871442736	1.292328752
H	1.765524602	0.914262986	1.262397877
C	3.173197295	-0.002113581	-0.126073172
H	3.363830895	-0.922327672	-0.668605860
H	3.363831137	0.899401474	-0.699140537
N	4.689674506	0.015704767	0.936999183
H	4.673663526	0.851590770	1.521392327
H	4.673663306	-0.800126731	1.549077376
H	5.561141727	0.006787126	0.404970768

S2•TS/CH_2Cl_2

S	0.374420000	-3.838331000	0.000000000
C	0.064486000	-2.152491000	0.000000000
N	-0.064520000	-1.442960000	1.137220000
N	-0.064520000	-1.442960000	-1.137220000
H	0.014073000	-1.917821000	-2.022065000
H	-0.260721000	-0.436236000	-1.081167000
H	0.014073000	-1.917821000	2.022065000
H	-0.260721000	-0.436236000	1.081167000
O	-0.485363000	1.080004000	0.000000000
C	0.523944000	2.049743000	0.000000000
H	1.155617000	2.086422000	-0.899955000
H	1.155617000	2.086422000	0.899955000
C	-0.644367000	2.932096000	0.000000000
H	-1.186982000	3.057766000	-0.925289000
H	-1.186982000	3.057766000	0.925289000
N	-0.064520000	4.937679000	0.000000000
H	0.499590000	5.140278000	0.823774000
H	0.499590000	5.140278000	-0.823774000
H	-0.860428000	5.574033000	0.000000000

S2•TS/H_2O

S	0.332986138	-3.849659061	0.000000000
C	0.031699816	-2.159445729	0.000000000
N	-0.101170629	-1.452619685	1.137504353
N	-0.101170629	-1.452619685	-1.137504353
H	0.023440860	-1.917298084	-2.022758104
H	-0.234391979	-0.435026641	-1.081349175
H	0.023440860	-1.917298084	2.022758104
H	-0.234391979	-0.435026641	1.081349175
O	-0.402740827	1.083311717	0.000000000
C	0.592076448	2.072196215	0.000000000
H	1.220297541	2.119610026	-0.900714320
H	1.220297541	2.119610026	0.900714320
C	-0.602392763	2.916437177	0.000000000
H	-1.142808784	3.039498540	-0.926449674
H	-1.142808784	3.039498540	0.926449674
N	-0.083593078	4.961676952	0.000000000
H	0.470440420	5.190952141	0.823156790
H	0.470440420	5.190952141	-0.823156790
H	-0.906568362	5.562390229	0.000000000

S3

N	-0.056252176	0.097431647	-0.039776297
H	-0.025183700	0.043619629	0.977763369
H	0.913449519	0.043619495	-0.349664715
H	-0.494500590	-0.769260651	-0.349664575

S3/CH_2Cl_2

N	-0.057865453	0.100225925	-0.040917056
H	-0.020757381	0.035953016	0.976680267
H	0.913903800	0.035952882	-0.345130506
H	-0.488088249	-0.773487377	-0.345130366

S3/H_2O

N	-0.058162383	0.100740223	-0.041127018
H	-0.019940657	0.034538409	0.976469363
H	0.913977200	0.034538276	-0.344290190
H	-0.486899864	-0.774258247	-0.344290051

S1•H2O

C	0.141041524	-0.917813688	-0.845981167
C	0.056566528	-1.171111205	0.596468605
O	-0.925399687	-0.347211384	-0.061877931
H	0.866360767	-0.192550978	-1.208363638
H	-0.174393846	-1.684619344	-1.551729306
H	0.725095481	-0.635347105	1.267592980
H	-0.323399044	-2.124817115	0.959263586
H	-0.166179357	1.391682662	0.255729879
H	0.423443954	2.688023045	-0.314900979
O	0.608327653	1.983608659	0.323063288

H2O•TS

C	-0.744090510	-1.485721143	0.000000000
C	-0.715948553	0.015745029	0.000000000
O	0.599410876	-1.615337855	0.000000000
H	-1.288513101	-1.883242063	0.893241239
H	-1.288513101	-1.883242063	-0.893241239
H	-0.285755126	0.441438149	0.902027651
H	-0.285755126	0.441438149	-0.902027651
H	-2.844554869	0.566131747	-0.826740632
N	-2.321326870	0.853517705	0.000000000
H	-2.237811795	1.871403758	0.000000000
H	-2.844554869	0.566131747	0.826740632
H	3.198344374	0.254616464	0.000000000
O	2.281639670	0.565607483	0.000000000
H	1.746588896	-0.268676485	0.000000000

H2O•TS•S2

C	0.303503458	-1.038964197	-2.193832797
C	-0.796065544	-0.611336011	-1.310271156
O	0.139264338	0.201837659	-2.794190613
H	1.266507773	-1.215480458	-1.686380502
H	0.073175772	-1.902123159	-2.840242488
H	-0.574051089	0.166584942	-0.595270029
H	-1.789002313	-0.611030782	-1.740536855
H	-0.997719739	-2.881393812	-0.117741243
N	-1.209550300	-1.926843203	0.167960618
H	-2.178908265	-1.899218491	0.482957455
H	-0.607469921	-1.680738678	0.969197963
H	2.231078952	2.342809700	-2.188057472
O	1.792308757	1.760744974	-1.551469370
H	1.130756154	1.191566810	-2.098507991
C	1.381982545	0.397431718	1.383122679
S	0.837222299	-0.600887999	2.659908617
N	0.784836853	1.569982899	1.080262282
H	1.029671096	2.055784767	0.213261408
H	-0.004866642	1.856597021	1.636615667
N	2.428446721	0.064733338	0.601443703
H	2.591452919	0.586508395	-0.265616185
H	2.858969754	-0.833294558	0.755272663

H2O

H	-0.083623032	0.000000000	-0.895723567
O	-0.094992033	0.000000000	0.072889950
H	0.843559293	0.000000000	0.312603965

(H2O)2

H	1.769818921	-0.761250958	-0.019611717
O	1.351513982	0.108564504	0.070298765
H	0.664688164	0.108853976	-0.618962673
O	-1.414941752	-0.116015427	-0.040888667
H	-1.835741161	0.751868615	0.055393480
H	-0.718148875	-0.113572497	0.638443072