Supplementary Material (ESI) for Organic & Biomolecular Chemistry

What is the Mechanism of Amine Conjugate Additions to Pyrazol Crotonate Catalyzed by Thiourea Catalysts?

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Supporting information

Computational Details:

Calculations on model system:

Transition state and starting material structures were located using Gaussian03[1] in toluene with B3LYP[2] functional and 6-31G**[3-5] basis set. Solvent effects were included by PCM model [6-11]. The cavity for this PCM calculation was defined according to the UFF scheme. Vibrational contributions to Gibbs free energy were calculated at this level of theory. For each optimized structure, single point energy was calculated (MPWB1K[12-15]/6-31G**) with solvent (toluene) included implicitly by PCM model and UAKS[16,17] cavity definition. This energy was added to the Gibbs energy correction calculated previously. Energy barriers are relative to the corresponding starting materials, in all cases.

Calculations on real reactions:

Due to the relatively high size of the system hybrid QM/MM ONIOM calculations were performed. Transition state structures were located using Gaussian03. The high level layer was treated with B3LYP/6-31G** level of theory, and low level layer was studied using molecular mechanics UFF[18,19] method. Vibrational contributions to Gibbs free energy were calculated at this level of theory. On the optimized structures, single point energies were calculated using Jaguar 7.0[20] program at the M05X[15,21]/6-31G** level of theory. Solvent effects (trifluorotoluene) were included implicitly using a self-consistent reaction-field method as implemented in Jaguar 7.0[22,23] (dielectric constant: 7.58; probe radii: 2.525). To the value of the solvation free energy, Gibbs free energy corrections from previous calculation were added.

(1) Gaussian 03, R. D., 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.

(2) Becke, A. D. *J. Chem. Phys.* **1983**, *98*, 5648-5652.

(3) Gill, P. M. W.; Johnson, B. G.; Pople, J. A.; Frisch, M. J. *J. Chem. Phys.* **1992**, *197*, 499-505.

(4) R. Krishnam, R.; Binkley, J. S.; Seeger, R.; A., P. J. *J. Chem. Phys.* **1980**, *72*, 650-654.

(5) Clark, T.; Chandrasekhar, J.; Schleyer, P. v. R. *J. Comp. Chem.* **1983**, *4*, 294-301.

(6) Cammi, R.; Mennucci, B.; J., T. *J. Phys. Chem. A* **2000**, *104*, 5631-5637.

(7) Cammi, R.; Mennucci, B.; Tomasi, J. *J. Phys. Chem. A* **1999**, *103*, 9100-9108.

(8) Cossi, M.; Rega, N.; Scalmani, M.; V., B. *J. Chem. Phys.* **2001**, *114*, 5691-5701.

(9) Cossi, M.; Scalmani, G.; Rega, R.; Barone, V. *J. Chem. Phys.* **2002**, *117*, 43-54.

(10) Cossi, N.; Scalmani, G.; Rega, N.; Barone, V. *J. Comp. Chem.* **2003**, *24*, 669-681.

(11) Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999-3093.

(12) Zhao, Y.; Truhlar, D. G. *J. Chem. Theory Comput.* **2005**, *1*, 415-432.

(13) Zhao, Y.; Gonzalez-Garcia, N.; Truhlar, D. G. *J. Phys. Chem. A* **2005**, *109*, 2012-2018.

(14) Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2004**, *108*, 6908-6918.

(15) Rokob, T. A.; Hamza, A.; Papai, I. *Org. Lett.* **2007**.

(16) Barone, V.; Cossi, M.; Tomassi, J. *J. Chem. Phys.* **1997**, *107*, 3210-3221.

(17) Takano, Y.; Houk, K. N. *J. Chem. Theory Comput.* **2005**, *1*, 70-77.

(18) Rappé, A. K.; Casewit, C. J.; Colwell, K. S.; Goddard III, W. A.; M., S. W. *J. Am. Chem. Soc.* **1992**, *114*, 10024-10035.

(19) Rappi, A. K.; Casewit, C. J.; Colwell, K. S.; Goddard III, W. A.; Skid, W. M. *J. Am. Chem. Soc.* **1992**, *114*, 10024-10035.

(20) Jaguar 7.0, Schrodinger Inc. New York, NY, 2007.

(21) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**.

(22) D. J. Tannor; B. Marten; R. Murphy; R. A. Friesner; D. Sitkoff; A. Nicholls; M. Ringnalda; W. A. Goddard III; Honig, B. *J. Am. Chem. Soc.* **1994**, *116*, 11875-11882.

(23) Truhlar, D. G.; Cramer, C. J. *J. Comp. Aided Mol. Design* **1992**, *6*, 629-666.

(24) Glendening, E. D.; Weinhold, F. *J. Comp. Chem.* **1998**, *19*, 593-609.

***O*-methylhydroxylamine**

E(MPWB1K+solv) = -170.929527 Hartrees

O	-0.01156	0.57836	0.00345
N	-1.14859	-0.31565	-0.00387
H	-1.69745	0.00946	-0.80211
H	-1.68264	-0.02385	0.81747
C	1.17217	-0.20518	-0.00140
H	1.99972	0.51027	0.00188
H	1.24045	-0.84551	0.88734
H	1.23955	-0.83660	-0.89665

***s-cis* pyrazole-acrylate**

E(MPWB1K+solv) = -416.732373 Hartrees

C	-2.53255	0.46351	0.03023
C	-2.39964	-0.95130	-0.04488
C	-1.04870	-1.16914	-0.05514
N	-0.44079	0.07015	0.01062
N	-1.36355	1.07837	0.05962
H	-3.18186	-1.69423	-0.08690
C	0.94584	0.40138	0.00360
O	1.29884	1.56061	-0.06033
H	1.50781	-1.74625	0.24723
C	3.20318	-0.52894	-0.01848
C	1.88898	-0.74505	0.08601
H	3.58521	0.47529	-0.17140
H	3.91739	-1.34245	0.04799
H	-3.44308	1.04745	0.06573
H	-0.48844	-2.08701	-0.11961

***s-trans* pyrazole-acrylate**

E(MPWB1K+solv) = -416.742818 Hartrees

C	2.23549	-1.02980	-0.00009
C	2.62906	0.33889	0.00037
C	1.45225	1.04015	0.00020
N	0.44024	0.11011	-0.00012
N	0.92085	-1.17270	-0.00039
H	3.63105	0.74060	0.00075
C	-0.94654	0.40914	-0.00022
O	-1.29895	1.57645	-0.00034
H	-1.40924	-1.74426	0.00016
C	-3.17881	-0.56566	0.00034
C	-1.85638	-0.75851	0.00008
H	-3.59212	0.43823	0.00030
H	-3.87178	-1.40023	0.00066
H	2.86887	-1.90735	-0.00012
H	1.22673	2.09432	0.00048

1-(2-hydroxyethyl)thiourea

E(MPWB1K+solv) = -701.953584 Hartrees

H	2.40580	-2.05072	-0.15937
H	3.25400	-0.58611	-0.46240
N	2.37034	-1.06338	-0.37548
C	1.30711	-0.30245	0.00310

H	0.19876	-1.99712	0.15566
N	0.18440	-0.99631	0.30346
C	-1.09703	-0.41363	0.67397
H	-0.91175	0.51935	1.20823
H	-1.60495	-1.10710	1.35109
C	-1.99071	-0.14168	-0.53675
H	-1.51278	0.61786	-1.16919
H	-2.09740	-1.06208	-1.13374
O	-3.24346	0.29826	-0.02723
H	-3.76774	0.62847	-0.76767
S	1.42402	1.38848	0.05359

TS-1

E(MPWB1K+solv) = -1289.632501 Hartrees

C	5.13400	-0.96400	0.14200
C	4.51200	-2.14600	0.62800
C	3.16700	-1.91300	0.48200
N	3.03800	-0.66100	-0.06200
N	4.25000	-0.06800	-0.27300
H	4.98500	-3.03200	1.02600
H	6.19200	-0.73900	0.08200
H	2.29600	-2.50700	0.71100
C	1.80300	-0.02000	-0.37500
O	0.76400	-0.69500	-0.13900
H	2.83400	1.76400	-0.98500
H	-0.59200	-2.39900	-1.24300
H	-1.78400	-3.64000	-1.48800
N	-1.56600	-2.67600	-1.28200
C	-2.50300	-1.95200	-0.61700
H	-1.10900	-0.50600	-0.44300
N	-2.09600	-0.70700	-0.27700
C	-2.76500	0.18400	0.65800
H	-3.79800	-0.15300	0.77200
H	-2.77200	1.19800	0.24200
C	-2.05700	0.19700	2.01500
H	-2.54900	0.91300	2.68100
H	-2.11500	-0.79700	2.47700
O	-0.68600	0.61300	1.92000
H	-0.18500	-0.05800	1.41600
C	0.70600	1.95000	-1.30900
C	1.86700	1.28600	-0.90500
H	-0.19700	1.38000	-1.50800
H	0.81600	2.83800	-1.92300
O	-1.32200	3.56400	0.22300
N	-0.08000	2.86900	0.24500
H	-0.25400	2.09400	0.91300
H	0.64200	3.48900	0.64200
C	-1.28400	4.63700	-0.71600
H	-2.25400	5.12900	-0.62500
H	-0.49000	5.35500	-0.46900
H	-1.15100	4.27800	-1.74200
S	-4.05400	-2.58300	-0.31600

TS-2

E(MPWB1K+solv) = -1289.633041Hartrees

C	3.93200	0.68100	-1.06300

C	4.60100	-0.11900	-0.10700
C	3.65100	-1.01900	0.32000
N	2.50400	-0.75000	-0.37100
N	2.66600	0.30100	-1.22800
H	5.62700	-0.04600	0.21900
C	1.26300	-1.47700	-0.22000
O	1.16500	-2.15200	0.82200
H	0.54300	-0.71600	-2.10900
H	1.13200	1.62800	-1.52400
N	0.26400	2.16600	-1.47600
C	-0.52700	2.08800	-0.38100
H	1.08400	1.49200	0.67700
N	0.08200	1.63000	0.73800
O	-0.76000	-0.87100	2.27700
H	-0.07300	-1.43900	1.86900
C	-0.87700	-2.06200	-1.21100
C	0.31900	-1.36200	-1.27100
H	-0.98300	-2.86900	-0.49500
O	-3.63300	-1.53000	0.05400
N	-2.33800	-0.98400	-0.17500
H	-1.92100	-0.91500	0.76500
H	-2.44800	-0.01600	-0.52000
C	-4.37700	-1.54700	-1.15900
H	-4.50400	-0.53400	-1.56500
H	-3.90900	-2.18800	-1.91600
C	-0.49600	1.57000	2.07600
C	-0.13600	0.28500	2.82300
H	-1.57900	1.65400	1.97000
H	-0.47000	0.40800	3.86200
H	-0.15400	2.42900	2.67000
H	0.95400	0.15300	2.85000
H	-0.20000	2.39100	-2.34300
H	-5.35500	-1.95300	-0.89500
H	-1.48500	-2.14400	-2.10300
H	4.31700	1.51900	-1.62900
H	3.67800	-1.82600	1.03400
S	-2.17400	2.53900	-0.45600

TS-3

E(MPWB1K+solv) = -1289.630929 Hartrees

C	-1.68000	3.80900	-0.24400
C	-0.57500	4.69000	-0.31600
C	0.51700	3.89500	-0.06300
N	0.05100	2.62100	0.14200
N	-1.30700	2.56700	0.03900
H	-0.58000	5.75200	-0.51200
H	-2.72900	4.03200	-0.38900
H	1.56500	4.13100	0.02500
C	0.80100	1.44400	0.49400
O	0.18300	0.53300	1.08000
H	2.54900	2.20800	-0.53000
H	-2.55300	0.99200	-0.27200
H	-3.83600	0.44100	-1.32300
N	-3.20600	0.25900	-0.55900
C	-3.01900	-1.03700	-0.22600
S	-3.92000	-2.27700	-0.98000
H	-1.57700	-0.43600	1.06600
N	-2.10500	-1.24700	0.75200

C	-1.59400	-2.55100	1.14900
H	-2.35300	-3.29400	0.89600
H	-1.44700	-2.55400	2.23500
C	-0.27800	-2.91000	0.45600
H	-0.02600	-3.95300	0.67400
H	-0.40800	-2.81300	-0.63100
O	0.82600	-2.12300	0.91800
H	0.55200	-1.18100	0.99000
C	3.05300	0.49900	0.67100
C	2.17900	1.45700	0.15700
H	2.75300	-0.07100	1.54400
H	4.11900	0.67400	0.59100
O	4.14200	-2.06500	-0.52000
N	3.06600	-1.14100	-0.47900
H	2.26900	-1.68600	-0.09400
H	2.83800	-0.84700	-1.43700
C	5.28400	-1.47700	-1.13600
H	6.04100	-2.26200	-1.14400
H	5.06600	-1.17400	-2.17000
H	5.65500	-0.61500	-0.57200

TS-4

E(MPWB1K+solv) = -1289.622353 Hartrees

C	0.97700	3.54400	0.10300
C	0.10500	4.24300	-0.76600
C	-0.87700	3.33300	-1.07400
N	-0.57400	2.17100	-0.41200
N	0.57300	2.29800	0.31000
H	0.19100	5.25900	-1.12100
H	1.87700	3.90200	0.58600
H	-1.73400	3.39900	-1.72600
C	-1.29000	0.92800	-0.44500
O	-0.67700	-0.12400	-0.16400
H	-3.21200	1.92000	-0.71100
H	0.54200	-1.12200	-1.56500
H	1.54000	-2.05700	-2.65800
N	1.43900	-1.52700	-1.80900
C	2.40700	-1.65900	-0.86600
S	3.84200	-2.51800	-1.21500
H	1.22800	-0.60000	0.39200
N	2.13400	-1.05800	0.30700
C	2.99700	-1.01200	1.47500
H	3.99900	-1.32300	1.17100
H	2.63600	-1.71900	2.23400
C	3.01600	0.39400	2.07400
H	3.66600	0.38500	2.95800
H	3.45300	1.09400	1.34700
O	1.72600	0.81600	2.48900
H	1.29100	1.25100	1.72700
C	-3.33500	-0.21700	-1.02100
C	-2.66500	0.98900	-0.78000
H	-2.78200	-1.05100	-1.44300
H	-4.38200	-0.18100	-1.30500
O	-3.95500	-2.39300	0.97400
N	-3.46000	-1.09100	0.70000
H	-2.45300	-1.15000	0.87800
H	-3.86600	-0.42200	1.36500
C	-5.32800	-2.48300	0.59000

H	-5.63200	-3.49400	0.86400
H	-5.94400	-1.75800	1.13700
H	-5.45500	-2.34000	-0.48800

TS-5

E(MPWB1K+solv) = -1289.627198Hartrees

C	-5.35900	-0.65300	0.24200
C	-4.79500	-1.91400	-0.09100
C	-3.44300	-1.68300	-0.14800
N	-3.25500	-0.35600	0.13900
N	-4.43400	0.28700	0.38300
H	-5.30800	-2.84900	-0.25900
C	-1.99900	0.31300	0.20600
O	-0.97700	-0.37600	-0.07200
H	-2.90500	2.24200	0.55600
H	0.08000	-1.78000	-1.10500
H	1.12100	-2.86000	-2.01400
N	0.99700	-2.17500	-1.28700
C	2.00800	-2.01200	-0.39900
H	0.79300	-0.77400	0.64400
N	1.72800	-1.17600	0.62500
C	2.64100	-0.81500	1.69900
H	3.31500	-1.65500	1.89000
H	2.03700	-0.63900	2.59400
C	3.45900	0.44000	1.38500
H	4.06400	0.69800	2.26100
H	4.14100	0.23500	0.55100
O	2.63000	1.56900	1.10200
H	2.37600	1.52700	0.16800
C	-0.72800	2.30800	0.68200
C	-1.98300	1.68100	0.52300
H	0.10400	1.76000	1.12000
H	-0.72400	3.36500	0.93300
O	1.38800	2.55800	-1.35300
N	0.02300	2.30100	-1.02400
H	-0.09500	1.29800	-1.20300
H	-0.58600	2.82500	-1.66400
C	1.74300	3.90000	-0.98300
H	2.77300	4.01800	-1.32200
H	1.10300	4.62600	-1.49800
H	1.69100	4.03600	0.10000
H	-6.40200	-0.40200	0.38100
H	-2.60400	-2.32700	-0.35300
S	3.50100	-2.80700	-0.60900

TS-6

E(MPWB1K+solv) = -1289.622932 Hartrees

C	-0.56100	4.02700	-0.29700
C	0.60900	4.67000	0.17800
C	1.48200	3.64400	0.44700
N	0.83600	2.47400	0.13600
N	-0.42800	2.70800	-0.32000
H	0.77900	5.72700	0.31400
H	-1.49000	4.47600	-0.62200
H	2.47900	3.64500	0.85600
C	1.31500	1.13200	0.26100

O	0.46600	0.21100	0.22400
H	3.41200	1.70700	0.11400
H	-1.79700	1.28400	-0.97600
H	-3.05500	0.86500	-2.12600
N	-2.55000	0.66500	-1.27900
C	-2.98300	-0.37100	-0.52900
S	-4.28700	-1.34600	-1.05500
H	-1.48800	0.02700	0.75800
N	-2.32200	-0.54300	0.63800
C	-2.44600	-1.68600	1.53100
H	-3.33400	-2.24600	1.23000
H	-2.59200	-1.32300	2.55600
C	-1.20900	-2.58900	1.49600
H	-1.38900	-3.45600	2.14000
H	-1.05900	-2.95900	0.47100
O	-0.03900	-1.94800	1.99600
H	0.19300	-1.23200	1.37800
C	3.15400	-0.37600	0.64200
C	2.70800	0.92700	0.37400
H	2.53500	-1.04000	1.23900
H	4.22100	-0.54500	0.74800
O	2.87900	-2.76800	-1.16900
N	2.78000	-1.36800	-0.97400
H	1.77500	-1.17300	-0.99600
H	3.22300	-0.87700	-1.75900
C	4.23300	-3.19200	-0.99800
H	4.21800	-4.26600	-1.18400
H	4.89700	-2.70600	-1.72500
H	4.58900	-2.99800	0.01900

TS-7

E(MPWB1K+solv) = -1289.624501 Hartrees

C	-4.08800	-1.77300	-0.48000
C	-4.89500	-0.96000	0.35800
C	-4.08200	0.09300	0.70000
N	-2.87600	-0.11500	0.07900
N	-2.87400	-1.26800	-0.64700
H	-5.91400	-1.12900	0.67000
C	-1.68900	0.68100	0.14600
O	-0.62600	0.16700	-0.27600
H	-2.73000	2.52300	0.69000
H	-0.53300	-1.92300	-0.65500
H	-0.17900	-3.59300	-1.04000
N	0.11800	-2.70600	-0.67200
C	1.36600	-2.62900	-0.16300
S	2.41100	-3.98700	-0.20500
H	0.99900	-0.69400	0.32900
N	1.70300	-1.43000	0.35900
C	2.98600	-1.07700	0.93400
H	3.68900	-1.88400	0.72200
H	2.90000	-0.98000	2.02500
C	3.49700	0.23600	0.35900
H	4.49400	0.44700	0.77200
H	3.59000	0.14400	-0.73100
O	2.57300	1.27100	0.70800
H	2.65000	1.99800	0.07300
C	-0.57100	2.66900	0.91800
C	-1.78500	1.99800	0.64600

H	0.27000	2.09600	1.30100
H	-0.63100	3.68300	1.30300
O	1.54300	3.39300	-1.00000
N	0.22800	2.90500	-0.74300
H	0.26400	1.90100	-0.97200
H	-0.43500	3.36600	-1.37600
C	1.66400	4.75400	-0.56500
H	2.68300	5.04300	-0.82200
H	0.95700	5.39900	-1.09800
H	1.51300	4.84000	0.51500
H	-4.35200	-2.70400	-0.96400
H	-4.24600	0.94200	1.34500

Methanol

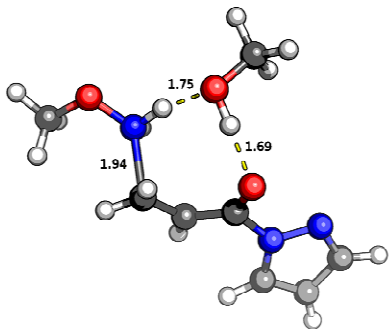
E(MPWB1K+solv) = -115.659975 Hartrees

C	0.66346	-0.01925	0.00000
H	1.08588	0.98882	-0.00071
H	1.03598	-0.54482	-0.89116
H	1.03609	-0.54361	0.89184
O	-0.75076	0.12246	0.00000
H	-1.13262	-0.76464	0.00002

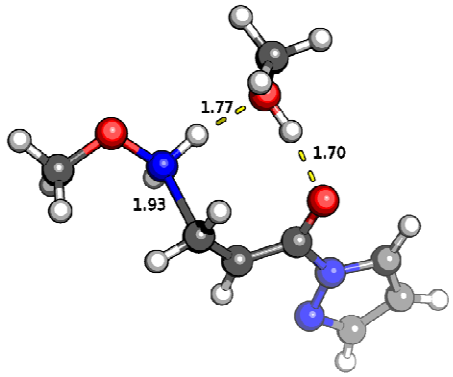
Proton switch addition to *s-cis*-pyrazole-acrylate catalyzed by methanol

E(MPWB1K+solv) = -703.322828 Hartrees

C	4.22359	0.31195	-0.53538
C	4.24422	-1.10423	-0.46496
C	2.97410	-1.44370	-0.06369
N	2.27379	-0.27294	0.08473
N	3.04257	0.81441	-0.19873
H	5.06844	-1.77251	-0.66549
H	5.02557	0.98038	-0.82127
H	2.52963	-2.39994	0.16110
C	0.90620	-0.09540	0.51463
O	0.61741	0.99503	1.03580
H	0.38076	-2.02973	-0.31608
C	-1.37878	3.21733	-0.52305
H	-2.31356	3.55503	-0.97872
H	-0.69555	2.89639	-1.32100
O	-1.68873	2.16179	0.38063
H	-0.83712	1.80794	0.74024
C	-1.23354	-1.24403	0.87008
C	0.04880	-1.20934	0.30817
H	-1.45443	-0.57291	1.69484
H	-1.74404	-2.19957	0.92434
O	-3.89517	-0.47772	-0.26385
N	-2.47814	-0.39552	-0.34555
H	-2.26855	0.61810	-0.20005
H	-2.17869	-0.66869	-1.28964
C	-4.33529	-1.81441	-0.48757
H	-5.42459	-1.76797	-0.44797
H	-4.02457	-2.17765	-1.47709
H	-3.97219	-2.50030	0.28523
H	-0.92249	4.06802	-0.00156



Proton switch addition to *s-trans*-pyrazole-acrylate catalyzed by methanol



E(MPWB1K+solv) = -703.332071 Hartrees

C	4.14728	-1.14311	-0.42655
C	4.45767	0.24130	-0.40766
C	3.27448	0.85493	-0.07026
N	2.34614	-0.13711	0.09296
N	2.87585	-1.37454	-0.12458
H	5.40655	0.71429	-0.61171
H	4.80359	-1.97488	-0.64868
H	2.99853	1.88701	0.07025
C	0.97034	0.07596	0.44987
O	0.64274	1.26972	0.64008
H	0.58102	-2.03446	0.29957
O	-1.56652	2.05897	-0.65785
H	-0.72294	1.88120	-0.17167
C	-1.15733	-0.97132	1.03162
C	0.15865	-1.07470	0.56209
H	-1.44322	-0.07215	1.56973
H	-1.64857	-1.87382	1.37950
O	-3.75062	-0.68948	-0.41454
N	-2.32963	-0.62586	-0.45777
H	-2.12613	0.37728	-0.66044
H	-1.98831	-1.20178	-1.23698
C	-4.18548	-2.02781	-0.18558
H	-5.27534	-1.98334	-0.20995
H	-3.83310	-2.70284	-0.97753
H	-3.85744	-2.40411	0.78927
C	-2.34190	2.97296	0.10977
H	-1.83731	3.94259	0.20816
H	-3.28903	3.12996	-0.41286
H	-2.56189	2.59463	1.11785

***s-cis* 3,5-dimethyl-pyrazole-acrylate**

E(MPWB1K+solv) = -495.325024 Hartrees

C	2.17468	-0.26291	0.06626
C	1.82935	1.11488	-0.03809
C	0.45809	1.16847	-0.06703
N	0.03336	-0.15499	0.02065
N	1.09561	-1.02587	0.08109
H	2.50118	1.95926	-0.10055
C	-1.26960	-0.73133	-0.04380
O	-1.40865	-1.88341	-0.40367
H	-2.19767	1.02130	0.96209
C	-3.66060	-0.24388	0.12421
C	-2.40428	0.12435	0.39214
H	-3.86238	-1.14974	-0.43848
H	-4.50709	0.34448	0.46171
C	-0.40856	2.37973	-0.22782
H	-1.19642	2.23535	-0.97184
H	-0.88481	2.68249	0.71146
H	0.21714	3.21205	-0.55729
C	3.54617	-0.86543	0.13043
H	3.59131	-1.64708	0.89346
H	3.81923	-1.32351	-0.82648
H	4.29440	-0.10455	0.36524

***s-trans* 3,5-dimethyl-pyrazole-acrylate**

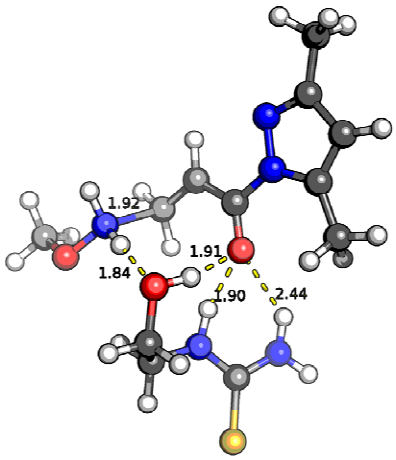
E(MPWB1K+solv) = -495.339539 Hartrees

C	-1.95216	-0.69852	-0.00020
C	-2.07636	0.72144	-0.00060
C	-0.79899	1.22426	-0.00085
N	0.03360	0.11179	-0.00007
N	-0.68216	-1.06622	-0.00064
H	-2.99012	1.29842	-0.00096
C	1.44645	0.09540	0.00099
O	2.07192	1.14489	0.00277
H	1.42476	-2.11204	-0.00538
C	3.40881	-1.35144	-0.00018
C	2.07677	-1.24895	-0.00201
H	4.03300	-0.46312	0.00326
H	3.90100	-2.31824	-0.00212
C	-3.05440	-1.71615	0.00142
H	-2.97621	-2.38153	-0.86388
H	-3.01269	-2.33946	0.90013
H	-4.03047	-1.22701	-0.02991
C	-0.33756	2.64495	-0.00116
H	0.26492	2.87281	0.88212
H	0.28650	2.86580	-0.87085
H	-1.21150	3.30038	-0.01401

3,5-dimethyl-pyrazole TS-1 analog

E(MPWB1K+solv) = -1368.2275 Hartrees

C	4.79000	-0.29400	0.04200
C	4.35100	-1.59600	0.41100
C	2.98200	-1.59100	0.29000
N	2.65100	-0.31500	-0.14200
N	3.76600	0.47500	-0.29100
H	4.95900	-2.43200	0.72900
C	1.36000	0.21700	-0.41700
O	0.37400	-0.54200	-0.18500
H	2.21100	2.09500	-1.02200
H	-0.93200	-2.19900	-1.40900
H	-2.05900	-3.48200	-1.72500
N	-1.89000	-2.52900	-1.44600
C	-2.83800	-1.93000	-0.67700
H	-1.51000	-0.44100	-0.39400
N	-2.48000	-0.70800	-0.22200
C	-3.17200	0.06500	0.79600
H	-4.15700	-0.38100	0.95200
H	-3.30600	1.09300	0.43900
C	-2.38100	0.08000	2.10600
H	-2.89300	0.71100	2.83800
H	-2.31500	-0.93600	2.51600
O	-1.06400	0.62800	1.95000
H	-0.53000	0.01900	1.40000
C	0.06400	2.10000	-1.28300
C	1.29400	1.53300	-0.92200
H	-0.78500	1.45000	-1.47600
H	0.08500	2.98800	-1.90600
O	-2.02000	3.51900	0.27400
N	-0.72600	2.92600	0.26400
H	-0.81700	2.14500	0.94300
H	-0.04600	3.60300	0.62900

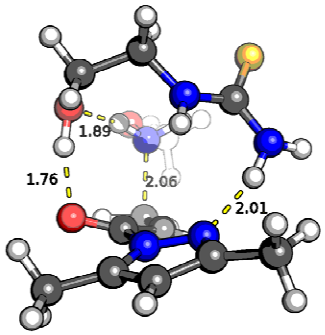


C	-2.10000	4.58300	-0.67600
H	-3.09800	5.00200	-0.54800
H	-1.35100	5.35900	-0.46900
H	-1.98500	4.22100	-1.70300
S	-4.34200	-2.67300	-0.39600
C	2.02500	-2.70900	0.55600
H	1.29600	-2.44800	1.32700
H	1.45800	-2.98100	-0.33800
H	2.59100	-3.58300	0.88700
C	6.19300	0.22800	-0.01100
H	6.73800	-0.19300	-0.86400
H	6.19000	1.31600	-0.11200
H	6.74800	-0.04100	0.89300

3,5-dimethyl-pyrazole TS-2 analog

E(MPWB1K+solv) = -1368.229484 Hartrees

C1	3.5098820	1.0257940	-0.6580340
C2	4.2545670	-0.0365370	-0.0892790
C3	3.3751610	-1.0896940	0.0578770
N4	2.1674980	-0.6445650	-0.4287260
N5	2.2488760	0.6540570	-0.8700480
H6	5.3018160	-0.0367850	0.1767890
C7	0.9241260	-1.3761640	-0.4792570
O8	0.7776090	-2.2748370	0.3743110
H9	0.2639860	-0.2022120	-2.1702540
H10	0.6868860	1.9047580	-1.0168790
N11	-0.1817800	2.4313440	-0.8798900
C12	-0.9990990	2.1099960	0.1484160
H13	0.5837110	1.2498970	1.0526150
N14	-0.4151200	1.4006590	1.1418370
O15	-1.2356200	-1.4053170	1.9949700
H16	-0.5176240	-1.8418430	1.4868910
C17	-1.1822670	-1.7110070	-1.6488240
C18	0.0137510	-1.0174540	-1.5058580
H19	-1.3009100	-2.6636430	-1.1444480
O20	-3.9652510	-1.5327340	-0.4654380
N21	-2.6811130	-0.9204770	-0.4780860
H22	-2.3127320	-1.0775220	0.4728570
H23	-2.8029520	0.0998250	-0.5850950
C24	-4.6645650	-1.2291570	-1.6679780
H25	-4.8099380	-0.1466760	-1.7840580
H26	-4.1488960	-1.6244980	-2.5510330
C27	-1.0244950	1.0145060	2.4085010
C28	-0.6615470	-0.4094280	2.8325090
H29	-2.1054820	1.1130050	2.2959470
H30	-1.0360240	-0.5496650	3.8545980
H31	-0.7114950	1.7068300	3.2029010
H32	0.4302160	-0.5280410	2.8713140
H33	-0.6260230	2.8452590	-1.6845770
H34	-5.6372870	-1.7137980	-1.5687370
H35	-1.7458140	-1.5984920	-2.5668500
S36	-2.6450740	2.5726700	0.1436440
C37	3.6237040	-2.4658900	0.5850270
H38	3.0816840	-2.6383330	1.5174580
H39	3.2870680	-3.2324880	-0.1181630
H40	4.6945190	-2.5946940	0.7590250
C41	3.9746980	2.4060020	-1.0055680
H42	4.7697130	2.3739470	-1.7583500

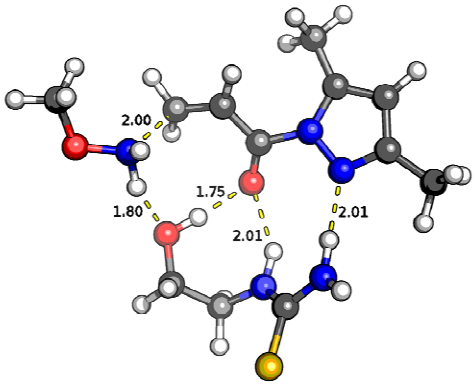


H43	3.1511430	3.0026030	-1.4042580
H44	4.3797010	2.9200300	-0.1275410

3,5-dimethyl-pyrazole TS-3 analog

E(MPWB1K+solv) = -1368.225474 Hartrees

C	3.49000	-1.39300	-0.20000
C	3.32900	-2.80200	-0.16100
C	1.98900	-3.02900	0.06100
N	1.39900	-1.78000	0.14000
N	2.32900	-0.78200	-0.00200
H	4.09600	-3.55600	-0.26000
C	0.05300	-1.40700	0.48600
O	-0.08600	-0.36400	1.15700
H	-0.77000	-2.99700	-0.72600
H	2.13400	1.13100	-0.58000
H	2.51400	2.42900	-1.69600
N	2.05700	2.11400	-0.85600
C	1.13800	2.94300	-0.31500
S	0.86000	4.49400	-0.97500
H	0.68000	1.48600	1.02400
N	0.50000	2.45700	0.77600
C	-0.65400	3.08400	1.40400
H	-0.57000	4.16300	1.25900
H	-0.62100	2.87000	2.47800
C	-1.98600	2.60000	0.82700
H	-2.79800	3.21900	1.22400
H	-1.96800	2.72900	-0.26400
O	-2.29300	1.24600	1.18100
H	-1.46900	0.70600	1.18700
C	-2.28900	-2.13000	0.52400
C	-0.98800	-2.25800	0.03400
H	-2.44700	-1.60100	1.45800
H	-2.99600	-2.92900	0.33400
O	-4.72500	-0.75700	-0.61400
N	-3.31100	-0.75400	-0.50400
H	-3.08800	0.11700	0.01900
H	-2.90000	-0.69600	-1.44300
C	-5.16100	-1.84500	-1.42400
H	-6.24700	-1.75600	-1.46700
H	-4.75100	-1.77400	-2.44200
H	-4.89000	-2.81300	-0.98900
C	4.74600	-0.60900	-0.42900
H	5.12100	-0.75100	-1.44900
H	4.56900	0.45700	-0.27000
H	5.53600	-0.93200	0.25500
C	1.29400	-4.34100	0.25400
H	0.57100	-4.30500	1.07200
H	0.75900	-4.66400	-0.64500
H	2.04200	-5.10400	0.48300



TS-8*S* *s-trans*:

E(M05-X+solv) = -2813.131434 Hartrees

C	2.37164	-3.40486	1.80543
C	3.76027	-3.19526	1.97055
C	3.87501	-1.83059	2.14026
N	2.61731	-1.29375	2.09732

N	1.68050	-2.27138	1.88135
H	4.55642	-3.92437	1.96020
C	2.20859	0.10994	2.12301
O	3.08514	0.94495	1.83283
H	0.20255	-0.46091	2.69309
H	-0.03672	-1.78352	0.62582
N	-0.55546	-1.53900	-0.21635
C	0.14509	-0.88974	-1.20190
S	-0.51881	-0.04676	-2.51124
H	1.76489	-1.49580	-0.17672
N	1.48790	-0.95139	-0.98422
O	2.46333	1.72352	-0.70694
H	2.80132	1.43541	0.17030
C	0.38557	1.67840	2.39888
C	0.85922	0.36082	2.44474
H	1.15831	2.44136	2.38188
O	-0.63474	3.38387	0.16146
N	-0.12101	2.09466	0.47661
H	0.69802	1.89839	-0.13131
H	-0.86721	1.45842	0.19122
C	0.42808	4.34112	0.18821
H	0.85143	4.41225	1.19914
H	1.23679	4.04077	-0.49040
C	1.69385	-4.70547	1.53159
H	1.16506	-4.64941	0.55684
H	2.43821	-5.52857	1.49239
H	0.95917	-4.91908	2.33584
C	5.12925	-1.04903	2.35876
H	5.29422	-0.35513	1.50886
H	5.05197	-0.47308	3.30444
H	6.00106	-1.73363	2.42592
C	-0.90658	2.07816	3.05533
H	-1.32144	2.98159	2.60082
H	-1.65275	1.28025	2.99975
H	-0.72135	2.28538	4.11596
C	-4.75434	-1.84642	-0.02693
C	-4.09052	-2.22477	-1.20463
C	-2.69078	-2.11459	-1.26749
C	-1.96430	-1.61779	-0.17398
C	-2.63928	-1.27306	1.00420
C	-4.03834	-1.37381	1.08411
H	-5.83385	-1.92926	0.02856
H	-2.15716	-2.43062	-2.15441
H	-2.06630	-0.91997	1.85054
C	-4.78751	-0.99064	2.33613
F	-5.48299	-2.08818	2.81005
F	-3.93331	-0.54679	3.33109
F	-5.68535	0.01990	2.04371
C	-4.89503	-2.74944	-2.36790
F	-4.08952	-3.07054	-3.44703
F	-5.58162	-3.88478	-1.97735
F	-5.80503	-1.78814	-2.76874
C	-1.18387	8.11789	-1.08299
C	-1.14262	7.03851	-1.97003
C	-0.61934	5.80962	-1.55511
C	-0.13349	5.65271	-0.24597
C	-0.17664	6.74375	0.63969
C	-0.70134	7.97053	0.22043
H	-1.58905	9.06839	-1.40557
H	-1.51549	7.15430	-2.97962

H	-0.59094	4.98109	-2.25250
H	0.19262	6.64641	1.65328
H	-0.73355	8.80734	0.90638
C	2.50399	-0.52631	-1.92629
C	3.03480	0.97629	-1.76929
C	4.56480	0.88435	-1.63413
H	5.06822	1.33739	-2.51527
H	4.93392	1.37403	-0.70721
C	4.85336	-0.56600	-1.58608
C	6.10808	-1.15233	-1.39654
C	3.73050	-1.33587	-1.75828
C	6.20647	-2.55161	-1.38129
H	6.98917	-0.53905	-1.25858
C	3.81069	-2.73349	-1.76261
C	5.05889	-3.34148	-1.56582
H	7.16845	-3.02379	-1.23009
H	2.92311	-3.33776	-1.90079
H	5.13784	-4.42077	-1.55526
H	2.10954	-0.66096	-2.93576
H	2.78534	1.52803	-2.67965

TS-8*R s-trans*:

E(M05-X+solv) = -2813.12372 Hartrees

C	3.22183	3.04784	-0.92452
C	3.05046	3.51681	-2.25279
C	1.69066	3.46608	-2.45364
N	1.11651	3.00579	-1.29328
N	2.07074	2.74575	-0.34372
H	3.80478	3.84099	-2.95390
C	-0.28305	2.80987	-0.98385
O	-1.08183	2.80401	-1.94249
H	0.19556	2.63571	1.11962
H	1.07142	0.47319	-0.00644
N	1.50389	-0.40124	-0.27988
C	0.69651	-1.37379	-0.80377
S	1.11403	-2.98663	-1.06823
H	-0.66927	0.11603	-1.08415
N	-0.56015	-0.88993	-1.08104
O	-2.62898	0.62814	-2.04201
H	-2.02169	1.34666	-2.32565
C	-1.94407	2.74251	0.81230
C	-0.60298	2.66058	0.38981
H	-2.64027	3.11094	0.06181
O	-3.95955	0.56546	1.29188
N	-2.68996	0.93962	0.76186
H	-2.66967	0.69513	-0.24753
H	-2.02464	0.34837	1.26067
C	-4.99354	1.19474	0.52724
H	-4.98267	2.28321	0.67260
H	-4.84228	0.99638	-0.54175
C	4.52186	2.88409	-0.20878
H	4.68554	1.81335	0.02672
H	5.35965	3.24075	-0.84420
H	4.50737	3.47060	0.73372
C	0.94073	3.87656	-3.67961
H	0.39938	3.00355	-4.10004
H	0.21860	4.68074	-3.42564
H	1.64290	4.26096	-4.44929

C	-2.26605	3.11801	2.23578
H	-3.26666	2.78920	2.52885
H	-1.54035	2.68979	2.93383
H	-2.22064	4.20802	2.33749
C	5.39978	-0.98949	1.22350
C	5.09101	-1.42538	-0.07535
C	3.79057	-1.23260	-0.57354
C	2.80181	-0.63677	0.22478
C	3.13307	-0.18574	1.50945
C	4.42765	-0.36008	2.02068
H	6.40462	-1.13389	1.60082
H	3.54524	-1.52464	-1.58612
H	2.37771	0.30472	2.11255
C	4.74611	0.14694	3.40501
F	4.53121	1.51247	3.45417
F	3.91905	-0.47289	4.32404
F	6.06147	-0.10512	3.75516
C	6.16651	-2.07917	-0.90720
F	5.69536	-2.45640	-2.15303
F	7.21485	-1.19406	-1.08164
F	6.63213	-3.20581	-0.25372
C	-8.75722	-0.35975	1.90028
C	-8.36404	-0.55975	0.57399
C	-7.14024	-0.05621	0.12178
C	-6.29844	0.64963	0.99857
C	-6.70275	0.84974	2.32930
C	-7.92738	0.34475	2.77704
H	-9.70558	-0.74861	2.24806
H	-9.00907	-1.10296	-0.10473
H	-6.85252	-0.21546	-0.91000
H	-6.06908	1.39591	3.01781
H	-8.23348	0.50075	3.80350
C	-4.76119	-3.49427	0.22373
C	-4.95042	-2.73560	-0.94064
C	-3.84034	-2.13141	-1.53483
C	-2.58017	-2.27977	-1.01049
C	-2.36801	-3.04797	0.13970
C	-3.47190	-3.64993	0.76329
H	-5.60888	-3.96461	0.70481
H	-5.93860	-2.61786	-1.36584
H	-1.37590	-3.17488	0.55034
H	-3.32949	-4.24124	1.65841
C	-1.56425	-1.60037	-1.84994
C	-2.45563	-0.62609	-2.71433
C	-3.82838	-1.29527	-2.75607
H	-1.07046	-2.35460	-2.46987
H	-2.06944	-0.46271	-3.72579
H	-3.92555	-1.94517	-3.65243
H	-4.65301	-0.54921	-2.73925

TS-8*R s-cis*:

E(M05-X+solv) = -2813.128127 Hartrees

C	2.58663	3.51978	-0.89737
C	2.05694	4.82828	-1.01039
C	0.70022	4.62690	-1.14326
N	0.47374	3.27478	-1.10963
N	1.64467	2.58886	-0.96869
H	2.58447	5.77019	-1.00604

C	-0.73154	2.50788	-1.39028
O	-0.59198	1.54411	-2.17401
H	-1.83016	3.59487	0.11292
H	1.61710	0.46265	-0.93495
N	2.03172	-0.46333	-0.82446
C	1.24601	-1.56983	-0.96376
S	1.75550	-3.16784	-0.69968
H	-0.25000	-0.29210	-1.51772
N	-0.03582	-1.27048	-1.34428
O	-2.36580	-0.44329	-2.78912
H	-1.60215	0.16055	-2.87680
C	-3.17264	2.45248	-1.14073
C	-1.90396	2.92928	-0.73964
H	-3.22719	2.08955	-2.16570
O	-4.65714	0.16144	-0.08438
N	-3.38870	0.66841	-0.46321
H	-3.08805	0.10317	-1.28762
H	-2.70831	0.52956	0.29257
C	-4.87491	0.34813	1.31656
H	-4.29300	-0.38491	1.89585
H	-4.55366	1.35264	1.61715
C	4.02779	3.16328	-0.73769
H	4.33482	2.47114	-1.54978
H	4.65871	4.07574	-0.78296
H	4.18467	2.67273	0.24312
C	-0.34888	5.66048	-1.39985
H	-0.90618	5.40809	-2.32614
H	-1.05107	5.71103	-0.54334
H	0.12012	6.65897	-1.52576
C	-4.42365	3.14805	-0.66967
H	-5.29724	2.49576	-0.74145
H	-4.32446	3.50817	0.35875
H	-4.60300	4.01903	-1.30940
C	5.65814	-0.52956	1.31556
C	5.57833	-1.17958	0.07219
C	4.36460	-1.15803	-0.63668
C	3.24353	-0.50614	-0.10510
C	3.33967	0.14709	1.12945
C	4.54228	0.13888	1.85149
H	6.59549	-0.54700	1.85773
H	4.28160	-1.63879	-1.60332
H	2.47313	0.66276	1.52759
C	4.60725	0.85031	3.18052
F	4.31603	2.19071	3.00050
F	3.67674	0.29954	4.04328
F	5.86056	0.74541	3.75879
C	6.79768	-1.88189	-0.47214
F	6.54630	-2.47273	-1.69877
F	7.82463	-0.96817	-0.62544
F	7.19717	-2.86442	0.41594
C	-9.06671	-0.20702	2.09560
C	-8.47514	1.03821	2.32336
C	-7.11210	1.22379	2.07084
C	-6.32993	0.16019	1.58677
C	-6.93336	-1.08776	1.36036
C	-8.29633	-1.26901	1.61419
H	-10.12167	-0.34886	2.29181
H	-9.07302	1.86026	2.69568
H	-6.67022	2.19595	2.25093
H	-6.34995	-1.91803	0.98711

H	-8.75522	-2.23308	1.43751
C	-3.94858	-3.60126	1.01658
C	-4.21625	-3.39153	-0.34502
C	-3.18954	-2.91877	-1.16473
C	-1.93502	-2.67345	-0.66635
C	-1.64315	-2.89067	0.68501
C	-2.66492	-3.34764	1.53142
H	-4.73175	-3.96007	1.67182
H	-5.20126	-3.58624	-0.74901
H	-0.65157	-2.71048	1.07739
H	-2.46185	-3.51421	2.58143
C	-1.00282	-2.26968	-1.74660
C	-1.99151	-1.82789	-2.88572
C	-3.26294	-2.63375	-2.61635
H	-0.44817	-3.16229	-2.05250
H	-1.60741	-2.03016	-3.89256
H	-3.25413	-3.58978	-3.18339
H	-4.18144	-2.05735	-2.86431

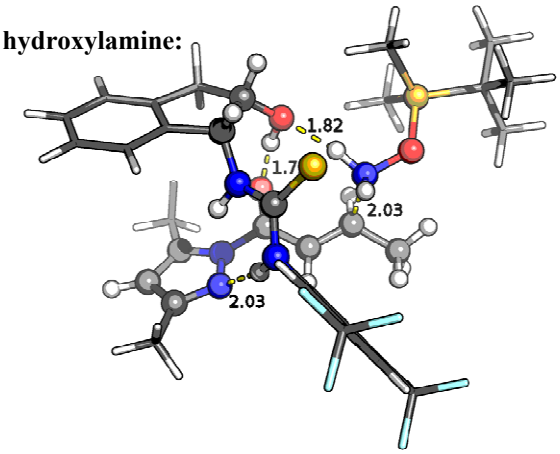
TS-8*S* *s-cis*:

E(M05-X+solv) = -2813.12362 Hartrees

C	2.70999	0.32268	3.47544
C	2.48193	-0.39193	4.67457
C	1.13129	-0.67683	4.63909
N	0.62294	-0.14313	3.48786
N	1.59601	0.48700	2.77321
H	3.18751	-0.64842	5.45021
C	-0.73326	-0.10460	2.94536
O	-1.11598	1.00686	2.53398
H	-0.85789	-2.24375	3.13305
H	1.31666	0.73452	0.83009
N	1.36274	0.64126	-0.18800
C	0.36075	1.15450	-0.95521
S	0.09573	0.79321	-2.59667
H	-0.25981	2.08071	0.74833
N	-0.45951	1.98104	-0.24160
O	-3.05335	1.29337	0.67983
H	-2.36703	1.30408	1.38941
C	-2.76615	-1.43735	2.55290
C	-1.41575	-1.33716	2.92767
H	-3.34234	-0.51478	2.56942
O	-3.99103	-2.03350	0.01221
N	-2.82980	-1.46214	0.56353
H	-2.79116	-0.45155	0.32558
H	-2.00082	-1.95822	0.22129
C	-4.12321	-1.71551	-1.38094
H	-4.10882	-0.62676	-1.51788
H	-3.28951	-2.13822	-1.95930
C	4.01927	0.84208	2.98198
H	3.95917	1.94307	2.85495
H	4.82695	0.60418	3.70569
H	4.26140	0.37391	2.00495
C	0.30801	-1.31669	5.70990
H	-0.52463	-0.64052	5.99553
H	-0.10333	-2.28149	5.35152
H	0.93251	-1.51397	6.60652
C	-3.55075	-2.68195	2.86832
H	-4.43355	-2.77484	2.23372

H	-2.93704	-3.58137	2.76258
H	-3.88355	-2.62439	3.91150
C	4.71085	-1.49830	-1.58436
C	4.37043	-0.28078	-2.19477
C	3.23749	0.41761	-1.74380
C	2.44914	-0.09759	-0.70262
C	2.81654	-1.30108	-0.08693
C	3.94355	-2.01513	-0.52815
H	5.58521	-2.04094	-1.92548
H	2.97766	1.37534	-2.17622
H	2.21743	-1.67117	0.73594
C	4.35508	-3.31642	0.11387
F	5.62714	-3.18674	0.64119
F	3.49108	-3.68333	1.13150
F	4.36256	-4.31784	-0.84019
C	5.24010	0.25655	-3.30445
F	4.76475	1.46161	-3.79286
F	6.52455	0.45023	-2.82907
F	5.27694	-0.65561	-4.34340
C	-7.82709	-3.42395	-2.73860
C	-6.79976	-4.25200	-2.27802
C	-5.59436	-3.69535	-1.83925
C	-5.40961	-2.30241	-1.85662
C	-6.44694	-1.47636	-2.32331
C	-7.65056	-2.03773	-2.76177
H	-8.75973	-3.85629	-3.07726
H	-6.93769	-5.32543	-2.26022
H	-4.80605	-4.34783	-1.48381
H	-6.32748	-0.40017	-2.34535
H	-8.44726	-1.39769	-3.11851
C	-1.55626	2.74683	-0.79223
C	-2.97219	2.45516	-0.12754
C	-3.36316	3.71803	0.65205
H	-4.37922	4.06471	0.36376
H	-3.31836	3.55182	1.75017
C	-2.34617	4.72028	0.26348
C	-2.31776	6.06421	0.64617
C	-1.36127	4.18895	-0.53160
C	-1.26453	6.87393	0.19459
H	-3.09369	6.47504	1.27922
C	-0.30145	4.97833	-0.98998
C	-0.25783	6.33166	-0.62340
H	-1.22596	7.91761	0.47829
H	0.47493	4.55282	-1.61313
H	0.55447	6.95831	-0.96806
H	-1.57544	2.55365	-1.86490
H	-3.70060	2.30967	-0.93339

TS-8S *s-trans* analog with O-(tert-butyldimethylsilyl) hydroxylamine:



E(M05-X+solv) = -3069.390151 Hartrees

C	0.11685	-3.89617	2.39907
C	1.38265	-4.39085	2.78884
C	2.19094	-3.27178	2.79832
N	1.42230	-2.19469	2.45306
N	0.13355	-2.58242	2.19972
H	1.66425	-5.40606	3.02424
C	1.81030	-0.79424	2.28315
O	3.01225	-0.58203	2.03724

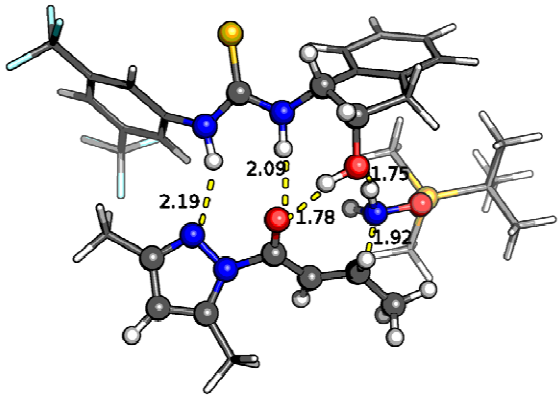
H	-0.22625	-0.19025	2.64009
H	-0.90094	-1.61571	0.74055
N	-1.24273	-1.21356	-0.13505
C	-0.31781	-0.94621	-1.10395
S	-0.54131	0.11586	-2.41231
H	0.88151	-2.21499	-0.08896
N	0.86563	-1.59105	-0.88665
O	3.10871	0.23859	-0.52455
H	3.15515	-0.12438	0.39006
C	1.03777	1.51269	2.22966
C	0.77186	0.14940	2.40606
H	2.08665	1.79434	2.26154
O	1.12565	3.32176	-0.09284
N	0.98396	1.94826	0.24326
H	1.71504	1.36945	-0.21270
H	0.08990	1.67222	-0.17369
C	-1.12762	-4.69270	2.18947
H	-1.46751	-4.58033	1.13858
H	-0.93884	-5.76715	2.39636
H	-1.92288	-4.32684	2.87214
C	3.64260	-3.20502	3.14406
H	4.22582	-2.88253	2.25672
H	3.79711	-2.48745	3.97653
H	4.00776	-4.20466	3.46085
C	0.06910	2.55547	2.71303
H	0.20413	3.50206	2.18571
H	-0.96744	2.22584	2.59459
H	0.24309	2.73342	3.78092
C	-5.19576	0.24605	-0.14855
C	-4.72236	-0.46992	-1.25946
C	-3.39971	-0.94466	-1.25507
C	-2.55762	-0.70027	-0.15934
C	-3.05403	-0.00881	0.95321
C	-4.37102	0.48040	0.96289
H	-6.21458	0.61636	-0.14569
H	-3.02102	-1.51955	-2.09051
H	-2.40535	0.15248	1.80229
C	-4.91964	1.24755	2.14024
F	-6.01180	0.57581	2.65840
F	-3.97621	1.39510	3.14258
F	-5.31949	2.50437	1.72418
C	-5.64773	-0.72020	-2.42404
F	-5.02406	-1.43568	-3.43183
F	-6.74815	-1.43730	-1.99091
F	-6.07350	0.48944	-2.94163
C	1.95993	-1.65217	-1.83947
C	3.24498	-0.75650	-1.52053
C	4.39768	-1.72951	-1.22400
H	5.27628	-1.51017	-1.86872
H	4.70478	-1.70621	-0.15638
C	3.84673	-3.06484	-1.54410
C	4.54145	-4.27700	-1.50354
C	2.51882	-3.02060	-1.88923
C	3.86088	-5.45867	-1.83399
H	5.58680	-4.30546	-1.22412
C	1.82254	-4.18751	-2.22259
C	2.50295	-5.41373	-2.19453
H	4.38247	-6.40668	-1.81139
H	0.77480	-4.14740	-2.49227
H	1.98049	-6.32696	-2.44863

H	1.55640	-1.37488	-2.81351
H	3.48313	-0.21760	-2.44391
Si	2.61419	3.99765	-0.53010
C	3.13918	3.39559	-2.23235
H	4.06769	3.91580	-2.54301
H	3.32964	2.30573	-2.19804
H	2.33390	3.59959	-2.96661
C	3.93989	3.53858	0.72457
H	4.89840	4.02344	0.44984
H	3.63047	3.87227	1.73566
H	4.08051	2.43938	0.73082
C	2.32506	5.88032	-0.54160
C	3.64493	6.60770	-0.85019
H	4.04644	6.29751	-1.83832
H	3.48615	7.70748	-0.87332
H	4.40853	6.38849	-0.07387
C	1.80388	6.32287	0.83691
H	1.62037	7.41895	0.85032
H	0.84827	5.81079	1.08081
H	2.54193	6.08897	1.63345
C	1.28205	6.22811	-1.61785
H	1.07160	7.31942	-1.61840
H	1.64921	5.95085	-2.62895
H	0.32711	5.69137	-1.42975

TS-8R *s-cis* analog with O-(tert-butyldimethylsilyl) hydroxylamine:

E(M05-X+solv) = -3069.384523 Hartrees

C	2.80293	3.49868	-0.95574
C	2.36254	4.83485	-1.12507
C	0.99902	4.71790	-1.28001
N	0.68366	3.38434	-1.20500
N	1.80459	2.62868	-1.01503
H	2.95049	5.74019	-1.14147
C	-0.55588	2.68166	-1.49296
O	-0.44590	1.67144	-2.22003
H	-1.63633	3.91496	-0.09231
H	1.61234	0.44511	-0.98317
N	2.03621	-0.47831	-0.90493
C	1.26880	-1.58440	-1.14027
S	1.81761	-3.18714	-1.08833
H	-0.25914	-0.28750	-1.50635
N	-0.03291	-1.27388	-1.43737
O	-2.30381	-0.19908	-2.69132
H	-1.54416	0.40679	-2.82105
C	-3.00815	2.75276	-1.28680
C	-1.72423	3.20261	-0.90468
H	-3.07851	2.30276	-2.27571
O	-4.52676	0.57125	-0.03065
N	-3.25121	1.05289	-0.43066
H	-2.91054	0.39107	-1.16161
H	-2.58629	1.07770	0.34813
C	4.21431	3.05514	-0.75509
H	4.48975	2.31686	-1.53727
H	4.90435	3.92259	-0.81845
H	4.32085	2.58948	0.24446
C	0.02561	5.80877	-1.59186
H	-0.53561	5.55884	-2.51630
H	-0.68192	5.93987	-0.74845



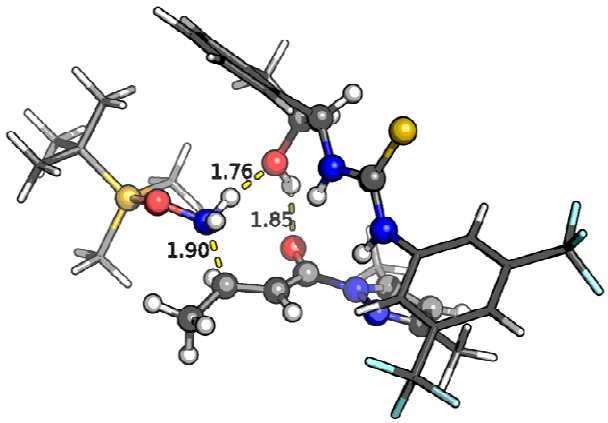
H	0.56242	6.76811	-1.74801
C	-4.23161	3.52290	-0.86718
H	-5.12784	2.89861	-0.89215
H	-4.11633	3.94873	0.13385
H	-4.38012	4.35338	-1.56614
C	5.58387	-0.60796	1.36478
C	5.54080	-1.25040	0.11619
C	4.35697	-1.20186	-0.64041
C	3.22342	-0.54176	-0.14546
C	3.28508	0.10548	1.09479
C	4.46038	0.07775	1.86014
H	6.49913	-0.64439	1.94263
H	4.30848	-1.66864	-1.61578
H	2.41269	0.63246	1.46376
C	4.48890	0.78760	3.19104
F	4.22487	2.13209	3.00197
F	3.52001	0.25105	4.01941
F	5.71919	0.66371	3.81343
C	6.76615	-1.97635	-0.38122
F	6.55193	-2.55855	-1.61878
F	7.81752	-1.08431	-0.48944
F	7.10869	-2.96955	0.51846
C	-3.82237	-4.21978	0.42857
C	-4.14862	-3.64606	-0.80856
C	-3.15731	-2.95828	-1.51231
C	-1.88098	-2.84285	-1.01952
C	-1.53375	-3.41841	0.20836
C	-2.51665	-4.10552	0.93665
H	-4.57661	-4.75368	0.99161
H	-5.14793	-3.74284	-1.21273
H	-0.52711	-3.34633	0.59433
H	-2.26773	-4.55230	1.89007
C	-0.97708	-2.21156	-2.01203
C	-1.99216	-1.55750	-3.02498
C	-3.28477	-2.35570	-2.85790
H	-0.40827	-3.01040	-2.49745
H	-1.64252	-1.60216	-4.06306
H	-3.35219	-3.16222	-3.61962
H	-4.18685	-1.70757	-2.91735
Si	-4.88177	0.38830	1.61668
C	-3.64096	-0.79007	2.39748
H	-3.90610	-0.96635	3.45967
H	-3.65593	-1.74935	1.84812
H	-2.62306	-0.35389	2.34281
C	-4.75395	2.04959	2.49036
H	-3.72250	2.44245	2.37962
H	-5.46907	2.76748	2.04052
H	-4.98247	1.92225	3.56808
C	-6.64814	-0.30764	1.70425
C	-7.05025	-0.51558	3.17414
H	-8.08387	-0.91853	3.24088
H	-6.36773	-1.23667	3.67261
H	-7.01812	0.44428	3.73246
C	-7.61805	0.68380	1.03857
H	-7.61739	1.65748	1.57312
H	-7.33333	0.86316	-0.02080
H	-8.65531	0.28494	1.05556
C	-6.70008	-1.65305	0.96015
H	-6.02653	-2.39497	1.43911
H	-7.73117	-2.06747	0.97523

H	-6.39218	-1.52971	-0.10073

TS-8R *s-trans* analog with O-(tert-butyldimethylsilyl) hydroxylamine:

E(M05-X+solv) = -3069.386578Hartrees

C	-2.68500	-3.11100	1.49600
C	-2.26400	-3.57000	2.77000
C	-0.89600	-3.42000	2.74500
N	-0.55500	-2.91000	1.51700
N	-1.66900	-2.72000	0.74100
H	-2.86800	-3.95200	3.57900
C	0.76000	-2.62900	0.97900
O	1.71700	-2.62500	1.77800
H	-0.07400	-2.36600	-1.00800
H	-1.43200	-0.51300	0.13800
N	-1.91400	0.36700	0.29100
C	-1.20400	1.44200	0.74400
S	-1.82800	2.98600	1.04200
H	0.44100	0.20400	0.77300
N	0.12300	1.15300	0.93300
O	2.44500	-0.03500	1.76800
H	2.14600	-0.87300	2.17400
C	2.09100	-2.40900	-1.05200
C	0.83100	-2.39400	-0.41600
H	2.89000	-2.86100	-0.46800
O	4.10400	-0.27600	-1.42500
N	2.82000	-0.65900	-0.93300
H	2.75000	-0.38200	0.06800
H	2.17000	-0.07500	-1.46300
C	-4.09200	-3.05300	0.99900
H	-4.37100	-2.00300	0.78200
H	-4.78800	-3.45600	1.76500
H	-4.18600	-3.65600	0.07200
C	0.07200	-3.77500	3.82700
H	0.61700	-2.86600	4.15700
H	0.79300	-4.53100	3.45200
H	-0.46600	-4.20200	4.70000
C	2.15900	-2.65400	-2.54000
H	3.09500	-2.29900	-2.97700
H	1.32500	-2.16900	-3.05800
H	2.08400	-3.73000	-2.72900
C	-5.84800	0.49100	-1.21500
C	-5.59300	0.96800	0.08100
C	-4.27900	0.93500	0.57900
C	-3.22800	0.45000	-0.21500
C	-3.50400	-0.04900	-1.49400
C	-4.80800	-0.02500	-2.00900
H	-6.86200	0.51800	-1.59500
H	-4.06900	1.26100	1.58900
H	-2.69500	-0.45200	-2.09300
C	-5.06200	-0.55800	-3.39700
F	-4.68900	-1.88900	-3.45300
F	-4.31000	0.16000	-4.30900
F	-6.39700	-0.45900	-3.75000
C	-6.73900	1.49400	0.91000
F	-6.31700	1.92500	2.15600
F	-7.67800	0.49300	1.08500
F	-7.33100	2.55800	0.25400
C	3.78400	4.49600	-0.38200

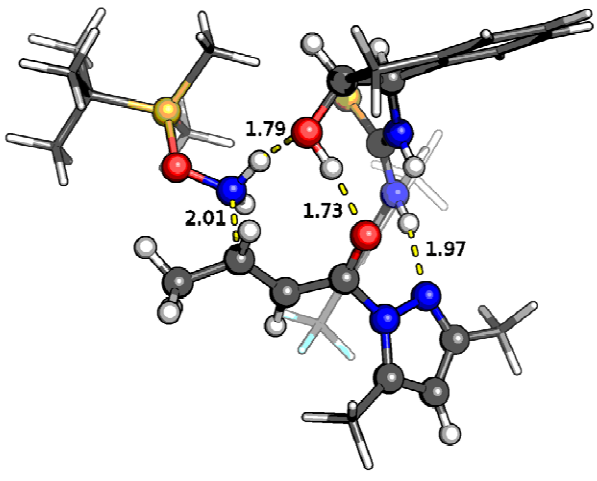


C	4.13700	3.74400	0.74900
C	3.17500	2.91500	1.32900
C	1.89700	2.84700	0.83200
C	1.52000	3.60500	-0.28300
C	2.47800	4.42500	-0.89800
H	4.51800	5.13600	-0.85500
H	5.13800	3.80000	1.15600
H	0.51100	3.56300	-0.67100
H	2.20800	5.01100	-1.76700
C	1.03800	1.98700	1.68000
C	2.10300	1.15800	2.49000
C	3.34200	2.05200	2.52000
H	0.45600	2.63800	2.33900
H	1.78000	0.90100	3.50300
H	3.35400	2.68200	3.43600
H	4.28100	1.46200	2.45800
S	5.52500	-1.02600	-0.87100
C	6.92700	0.21700	-1.20600
C	7.06900	0.42900	-2.72300
H	7.85900	1.18000	-2.93900
H	6.11500	0.79400	-3.16100
H	7.35000	-0.51800	-3.23100
C	8.24900	-0.32300	-0.63400
H	8.17600	-0.46600	0.46500
H	9.07800	0.39000	-0.83200
H	8.51400	-1.29600	-1.10100
C	6.58400	1.55600	-0.53400
H	7.38800	2.30200	-0.71500
H	6.47100	1.43200	0.56500
H	5.63600	1.96600	-0.94200
C	5.40400	-1.42100	0.96400
H	4.53900	-2.08900	1.14900
H	5.27500	-0.48600	1.54200
H	6.33100	-1.93200	1.29500
C	5.82800	-2.62800	-1.81200
H	5.79700	-2.43200	-2.90300
H	5.04600	-3.36800	-1.55000
H	6.82000	-3.04000	-1.53700

TS-8S *s-cis* analog with O-(tert-butyldimethylsilyl) hydroxylamine:

E(M05-X+solv) = -3069.386578Hartrees

C	2.68000	2.62800	2.75600
C	2.67400	2.35000	4.14300
C	1.44100	1.76400	4.35800
N	0.78400	1.72600	3.16100
N	1.54300	2.27200	2.17000
H	3.44000	2.55600	4.87400
C	-0.53200	1.21600	2.78100
O	-1.22100	1.97500	2.07500
H	-0.02700	-0.68100	3.65900
H	1.14200	1.63500	0.35400
N	1.13500	1.08900	-0.51200
C	0.01800	1.08400	-1.29100
S	-0.27700	0.00600	-2.57600
H	-0.67700	2.53600	-0.05100
N	-0.87600	2.04400	-0.91600
O	-3.16300	1.06100	0.42800
H	-2.51200	1.49900	1.02600

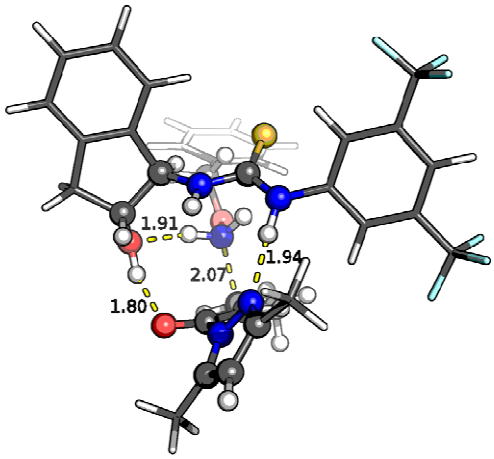


C	-2.08100	-0.68200	3.02500
C	-0.82500	-0.08900	3.22700
H	-2.90500	-0.01200	2.79000
O	-2.94600	-2.49000	0.90300
N	-2.10100	-1.38000	1.13500
H	-2.43000	-0.56000	0.58800
H	-1.13200	-1.61700	0.90600
C	3.80100	3.22000	1.96900
H	3.46400	4.16200	1.48800
H	4.66500	3.44000	2.63100
H	4.12200	2.50200	1.18400
C	0.83600	1.36900	5.66500
H	-0.13100	1.89600	5.80300
H	0.66900	0.27300	5.69500
H	1.51500	1.64300	6.50000
C	-2.46500	-1.93000	3.76900
H	-3.24100	-2.48900	3.24500
H	-1.60200	-2.58300	3.93000
H	-2.85600	-1.64100	4.75200
C	4.47800	-1.41400	-1.05500
C	4.03900	-0.61200	-2.12000
C	2.91400	0.21000	-1.94000
C	2.22900	0.22200	-0.71500
C	2.69300	-0.56500	0.34700
C	3.81400	-1.39600	0.18300
H	5.34600	-2.05000	-1.18700
H	2.57500	0.85800	-2.73800
H	2.16900	-0.52700	1.29400
C	4.32500	-2.26300	1.30600
F	5.62800	-1.90900	1.60500
F	3.55700	-2.12700	2.45000
F	4.29700	-3.58900	0.91200
C	4.79400	-0.64200	-3.42600
F	4.23000	0.20400	-4.36600
F	6.10300	-0.25000	-3.21000
F	4.78700	-1.92900	-3.93300
C	-2.14700	2.29500	-1.55900
C	-3.42600	1.86200	-0.71200
C	-4.16600	3.15200	-0.33600
H	-5.23000	3.10800	-0.65700
H	-4.11100	3.35500	0.75500
C	-3.45200	4.21800	-1.07300
C	-3.79500	5.57200	-1.10900
C	-2.35100	3.74700	-1.74500
C	-2.99700	6.45200	-1.85500
H	-4.66100	5.93700	-0.57300
C	-1.54200	4.60900	-2.49400
C	-1.87300	5.97100	-2.54800
H	-3.24800	7.50400	-1.89700
H	-0.67400	4.23300	-3.02000
H	-1.25800	6.65300	-3.12100
H	-2.13000	1.78600	-2.52200
H	-4.07800	1.26200	-1.35500
S	-3.05600	-3.14600	-0.66400
C	-3.68600	-1.84900	-1.86900
H	-3.80300	-2.29800	-2.87600
H	-4.66200	-1.45400	-1.51900
H	-2.95800	-1.01600	-1.92300
C	-1.35600	-3.74000	-1.21000
H	-0.96700	-4.48000	-0.48100

H	-1.42700	-4.20700	-2.21300
H	-0.66200	-2.87700	-1.25900
C	-4.28000	-4.59900	-0.52200
C	-5.66800	-4.05800	-0.13800
H	-6.39100	-4.89300	-0.01200
H	-5.62100	-3.49300	0.81800
H	-6.06200	-3.38200	-0.92700
C	-4.36800	-5.33400	-1.87000
H	-3.38100	-5.75600	-2.15600
H	-5.09400	-6.17300	-1.80800
H	-4.70400	-4.64600	-2.67500
C	-3.79100	-5.57200	0.56600
H	-4.49800	-6.42300	0.67200
H	-2.79200	-5.98400	0.30800
H	-3.71800	-5.05900	1.54900

TS-9*R s-trans*:

E(M05-X+solv) = -2813.126451 Hartrees



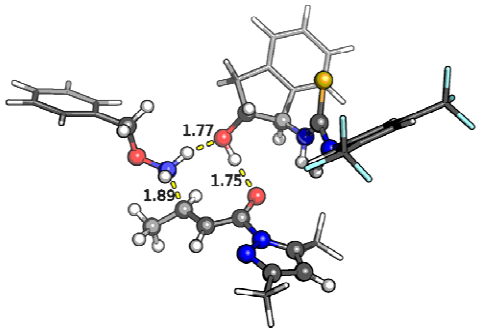
C	-2.54114	3.94698	-0.10899
C	-2.28130	5.25319	-0.57622
C	-1.06299	5.13903	-1.21962
N	-0.66735	3.83864	-1.13848
N	-1.57858	3.09284	-0.45207
H	-2.88934	6.13835	-0.46790
C	0.55262	3.21336	-1.67059
O	1.61929	3.80218	-1.43759
H	-0.67529	1.64839	-2.50242
H	-1.41836	1.35304	0.38149
N	-1.36998	0.41563	0.79743
C	-0.11437	-0.03030	1.09777
S	0.43333	-1.63380	0.94315
H	0.25300	1.87677	1.67132
N	0.69868	0.98216	1.50982
C	1.38367	1.43198	-3.11289
C	0.33189	2.04003	-2.42781
H	2.31228	1.99589	-3.15684
O	3.18122	-0.85454	-2.29755
N	2.26529	0.09709	-1.79458
H	2.74945	0.72360	-1.13125
H	1.50863	-0.40098	-1.30923
C	3.74560	-1.61470	-1.21537
H	4.39453	-0.96793	-0.60690
H	2.94796	-2.00174	-0.56827
C	-3.72598	3.51720	0.69207
H	-3.66064	2.43699	0.94110
H	-3.76727	4.10069	1.63516
H	-4.65320	3.69590	0.10928
C	-0.31980	6.19431	-1.97096
H	0.67295	6.36046	-1.50449
H	-0.18529	5.87453	-3.02555
H	-0.88807	7.14839	-1.95619
C	1.14373	0.49121	-4.25836
H	1.99075	-0.18184	-4.40591
H	0.23622	-0.10060	-4.11101
H	1.01475	1.08213	-5.17398
C	-4.65648	-2.12636	0.10310
C	-3.93038	-2.24880	1.29842
C	-2.82313	-1.41152	1.51504

C	-2.44564	-0.46448	0.55100
C	-3.19430	-0.33737	-0.62664
C	-4.29725	-1.17496	-0.86520
H	-5.51088	-2.77041	-0.07135
H	-2.25977	-1.47405	2.43754
H	-2.90428	0.41107	-1.35349
C	-5.10685	-1.07260	-2.13364
F	-4.61338	-0.09523	-2.98086
F	-5.07739	-2.28590	-2.79702
F	-6.41747	-0.76274	-1.81899
C	-4.36497	-3.26500	2.32523
F	-3.54393	-3.25321	3.43987
F	-5.65841	-2.98659	2.72848
F	-4.32965	-4.52922	1.76572
C	5.90495	-4.97338	-2.80247
C	6.56693	-4.03318	-2.00791
C	5.87298	-2.92960	-1.50200
C	4.50717	-2.76179	-1.78768
C	3.84803	-3.71313	-2.58425
C	4.54710	-4.81241	-3.09195
H	6.44319	-5.82826	-3.19069
H	7.61698	-4.16221	-1.77920
H	6.39824	-2.21502	-0.88025
H	2.79333	-3.60460	-2.80709
H	4.03466	-5.54232	-3.70523
C	3.76437	0.59006	5.59320
C	4.22083	1.53051	4.65716
C	3.59285	1.59764	3.41056
C	2.55526	0.75882	3.09139
C	2.10038	-0.20111	4.00235
C	2.70505	-0.27454	5.26609
H	4.23777	0.52043	6.56391
H	5.05121	2.18301	4.89405
H	1.30406	-0.88416	3.73900
H	2.36551	-1.00914	5.98475
C	2.13897	0.91708	1.67995
C	2.86851	2.22972	1.23912
C	3.97481	2.46326	2.27213
H	2.50692	0.05249	1.12586
H	4.01074	3.52966	2.58362
H	4.96655	2.14560	1.88290
O	3.39344	2.18934	-0.08028
H	2.92316	2.86471	-0.61454
H	2.15337	3.06259	1.32290

TS-9*S* *s-trans*:

E(M05-X+solv) = -2813.123653 Hartrees

C	-0.77678	-4.72826	-1.68364
C	-1.52536	-4.03719	-2.66900
C	-0.75431	-2.93175	-2.95953
N	0.37580	-3.00081	-2.18179
N	0.36292	-4.11693	-1.39340
H	-2.47171	-4.31168	-3.11069
C	1.51549	-2.10282	-2.12299
O	1.29293	-0.89239	-2.38316
H	2.73080	-3.77670	-1.58689
H	-1.71850	-0.58256	-0.98314
N	-2.20335	0.23824	-0.64337



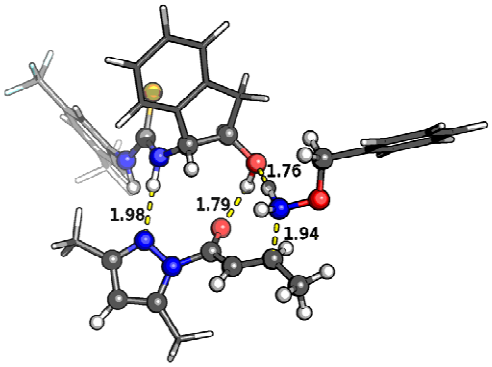
C	-1.46706	1.40312	-0.57127
S	-1.72419	2.63074	0.55915
H	-0.40167	0.58919	-2.07911
N	-0.50830	1.44317	-1.54370
C	3.96316	-2.01085	-1.79168
C	2.73645	-2.71683	-1.80451
H	3.96054	-1.03743	-2.27972
O	5.45571	-0.98521	0.38600
N	4.15262	-1.29549	-0.05473
H	3.57645	-0.42587	-0.09501
H	3.73374	-2.00500	0.55524
C	5.43413	-0.45024	1.71496
H	4.83108	0.46725	1.76098
H	4.98837	-1.18314	2.40468
C	-1.17362	-6.00627	-1.02114
H	-0.39746	-6.32679	-0.29395
H	-2.13494	-5.86409	-0.48486
H	-1.29642	-6.79875	-1.78881
C	-0.99261	-1.92234	-4.03537
H	-1.16649	-0.92532	-3.58918
H	-0.11531	-1.88152	-4.71421
H	-1.89003	-2.19881	-4.62784
C	5.25317	-2.77644	-1.95574
H	6.11824	-2.19075	-1.63933
H	5.23377	-3.71624	-1.39593
H	5.37314	-3.02309	-3.01616
C	-5.66776	-0.39891	1.66596
C	-5.64237	0.64924	0.73215
C	-4.47888	0.86108	-0.02638
C	-3.35909	0.03305	0.13967
C	-3.40695	-1.02585	1.05603
C	-4.55582	-1.23974	1.83801
H	-6.55938	-0.56294	2.26051
H	-4.43572	1.65927	-0.75682
H	-2.53830	-1.66318	1.16597
C	-4.62165	-2.34666	2.86071
F	-3.44152	-3.06843	2.91371
F	-4.86190	-1.80388	4.11027
F	-5.65301	-3.21004	2.53890
C	-6.86488	1.51718	0.56253
F	-6.67340	2.49216	-0.40157
F	-7.93837	0.73065	0.18520
F	-7.16014	2.13691	1.76331
C	9.49206	0.44544	2.81220
C	8.85427	1.18928	1.81525
C	7.53439	0.89589	1.45812
C	6.84144	-0.14370	2.10128
C	7.48901	-0.88617	3.10435
C	8.81048	-0.59198	3.45512
H	10.51425	0.67247	3.08619
H	9.38273	1.99331	1.31898
H	7.05073	1.47935	0.68384
H	6.97604	-1.69519	3.61019
H	9.30645	-1.16907	4.22517
C	0.67718	6.39752	-0.89501
C	1.57724	5.53764	-0.24673
C	1.50207	4.16674	-0.50548
C	0.57177	3.66043	-1.37988
C	-0.31360	4.50274	-2.05991
C	-0.26588	5.88090	-1.80160

H	0.71644	7.46225	-0.70533
H	2.31862	5.93142	0.43653
H	-1.02514	4.10072	-2.76963
H	-0.95012	6.54881	-2.30850
C	0.73184	2.20440	-1.55920
C	1.76126	1.80871	-0.45032
C	2.39573	3.11273	0.03326
H	1.18412	2.03118	-2.54027
H	3.41939	3.24695	-0.37908
H	2.42404	3.15264	1.14380
O	2.75382	0.90129	-0.93211
H	2.27959	0.27847	-1.53842
H	1.20024	1.36933	0.38746

TS-9*S* *s-cis*:

E(M05-X+solv) = -2813.117187 Hartrees

C	-0.98109	3.52806	-2.17864
C	-0.43355	4.82018	-2.34303
C	0.70850	4.79878	-1.56792
N	0.80214	3.56195	-0.98983
N	-0.24985	2.77680	-1.36377
H	-0.82216	5.64772	-2.91730
C	1.83626	2.93680	-0.15300
O	1.42758	2.23961	0.78689
H	3.35700	3.67201	-1.50217
H	-2.21087	1.22710	-0.01426
N	-2.54214	0.27984	-0.14600
C	-1.55097	-0.67886	-0.23625
S	-1.73144	-2.31041	0.18365
H	-0.40035	0.85849	-0.91779
N	-0.39714	-0.14188	-0.70530
C	4.25457	2.82455	0.26890
C	3.16829	3.18961	-0.54896
H	4.00676	2.58290	1.30113
O	5.91861	0.53127	0.42624
N	4.71178	0.98505	-0.14411
H	3.91242	0.41283	0.21358
H	4.77159	0.93213	-1.16632
C	6.10932	-0.86958	0.18773
H	5.25725	-1.44442	0.56849
H	6.19522	-1.05717	-0.89348
C	-2.22158	3.00887	-2.82746
H	-2.40343	1.95272	-2.53636
H	-3.08996	3.62479	-2.51394
H	-2.11347	3.06293	-3.93082
C	1.60907	5.95798	-1.28099
H	0.99784	6.83539	-0.98301
H	2.31044	5.73293	-0.45298
H	2.18642	6.21227	-2.19414
C	5.59696	3.48257	0.07583
H	6.40304	2.90367	0.53029
H	5.81862	3.63459	-0.98563
H	5.57143	4.46882	0.55314
C	-6.51261	-0.54557	1.00703
C	-5.78062	0.43848	1.69028
C	-4.45709	0.70444	1.29766

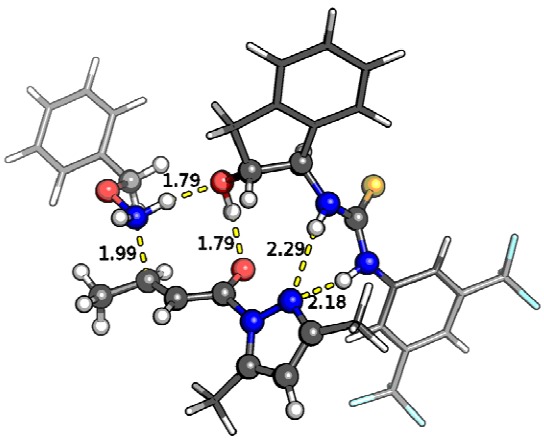


C	-3.86615	-0.01435	0.24908
C	-4.62023	-0.97571	-0.44208
C	-5.94392	-1.25511	-0.06222
H	-7.53334	-0.75636	1.30550
H	-3.87333	1.45916	1.80952
H	-4.17044	-1.49337	-1.27967
C	-6.76862	-2.29591	-0.77817
F	-6.05787	-2.90128	-1.80040
F	-7.16129	-3.27027	0.12151
F	-7.89451	-1.70020	-1.31698
C	-6.43315	1.18362	2.82819
F	-5.57728	2.11494	3.39075
F	-7.55655	1.84247	2.36253
F	-6.81228	0.28503	3.80893
C	9.65541	-2.11093	2.27549
C	8.53290	-1.68489	2.99087
C	7.38224	-1.27511	2.30995
C	7.34675	-1.29166	0.90511
C	8.47930	-1.72241	0.19258
C	9.62901	-2.12835	0.87785
H	10.54509	-2.42836	2.80395
H	8.55352	-1.67423	4.07328
H	6.51714	-0.95063	2.87557
H	8.47478	-1.74316	-0.89049
H	10.49924	-2.45819	0.32509
C	1.42139	-4.48437	-2.64457
C	1.86316	-4.24467	-1.33439
C	1.64411	-2.98518	-0.77029
C	1.01010	-1.99386	-1.47592
C	0.57793	-2.20535	-2.78892
C	0.78043	-3.46536	-3.37143
H	1.58083	-5.45349	-3.09910
H	2.36823	-5.02090	-0.77404
H	0.09466	-1.41321	-3.34643
H	0.44796	-3.65127	-4.38438
C	0.92750	-0.73427	-0.70896
C	1.51927	-1.11351	0.69956
C	2.06662	-2.53750	0.57699
H	1.58353	0.00220	-1.18239
H	1.62832	-3.19920	1.35539
H	3.17398	-2.56303	0.64583
O	2.55329	-0.22449	1.14041
H	2.13365	0.66128	1.23409
H	0.70309	-1.11850	1.42997

TS-9*R s-cis*:

E(M05-X+solv) = -2813.125322 Hartrees

C	-1.45969	-1.33523	3.54457
C	-1.34132	-2.69904	3.89229
C	-0.29412	-3.15074	3.11514
N	0.15876	-2.09848	2.36601
N	-0.57044	-0.97168	2.62600
H	-1.94388	-3.27332	4.57968
C	1.25585	-1.98091	1.40025
O	1.01600	-1.32192	0.37893
H	2.60744	-2.97541	2.77348
H	-1.83673	-0.05637	1.07811
N	-2.25483	0.60055	0.42542



C	-1.36892	1.54624	-0.03614
S	-1.44702	2.38388	-1.50311
H	-0.33497	1.11065	1.65491
N	-0.36236	1.75321	0.86719
C	3.47899	-2.80352	0.80289
C	2.46758	-2.62079	1.75793
H	3.16531	-2.66554	-0.22879
O	5.71940	-1.01923	-0.08207
N	4.59363	-1.15463	0.78179
H	3.94762	-0.35047	0.61985
H	4.99126	-1.08739	1.71867
C	5.25421	-0.83052	-1.42633
H	4.66269	-1.69373	-1.75914
H	4.61418	0.05906	-1.47689
C	-2.45460	-0.37035	4.09903
H	-2.31173	0.63684	3.65287
H	-3.48104	-0.72412	3.86861
H	-2.32937	-0.29902	5.19947
C	0.16328	-4.56900	2.98323
H	-0.71635	-5.22614	2.81971
H	0.84840	-4.69969	2.12243
H	0.67882	-4.87993	3.91531
C	4.57940	-3.80977	1.01424
H	5.46138	-3.57077	0.41411
H	4.87346	-3.86578	2.06737
H	4.22357	-4.80264	0.71662
C	-5.68181	-0.72528	-1.65279
C	-4.82632	-1.65948	-1.04855
C	-3.68374	-1.20304	-0.36896
C	-3.39793	0.16852	-0.28821
C	-4.29734	1.09176	-0.84852
C	-5.42701	0.65137	-1.55889
H	-6.55709	-1.07130	-2.19087
H	-3.00689	-1.90816	0.09778
H	-4.11869	2.15061	-0.71976
C	-6.37161	1.62293	-2.22288
F	-5.96556	2.93521	-2.05020
F	-6.42622	1.35576	-3.57913
F	-7.63685	1.47761	-1.68366
C	-5.15647	-3.12856	-1.14256
F	-4.22483	-3.90872	-0.47909
F	-6.40026	-3.35677	-0.58168
F	-5.18493	-3.50972	-2.47176
C	8.67988	-0.46923	-3.99533
C	8.47158	-1.64233	-3.26470
C	7.35926	-1.75692	-2.42519
C	6.44840	-0.69355	-2.30787
C	6.66414	0.48281	-3.04643
C	7.77681	0.59192	-3.88665
H	9.53967	-0.38324	-4.64707
H	9.17054	-2.46419	-3.35089
H	7.20547	-2.67332	-1.86818
H	5.97183	1.31280	-2.97646
H	7.93755	1.49860	-4.45566
C	1.79300	6.11683	2.45170
C	2.72506	5.07508	2.32652
C	2.31894	3.88110	1.72570
C	1.04199	3.72314	1.24677
C	0.10423	4.75645	1.34129
C	0.48349	5.95665	1.96240

H	2.08539	7.04906	2.91743
H	3.73927	5.19731	2.68524
H	-0.89463	4.63699	0.94128
H	-0.22960	6.76571	2.05354
C	0.88015	2.42712	0.54980
C	2.13890	1.63768	1.01399
C	3.15394	2.68757	1.46134
H	0.90702	2.61008	-0.52767
H	3.88513	2.91690	0.65543
H	3.68553	2.36112	2.38166
O	2.70546	0.77479	0.03274
H	2.04938	0.05005	-0.09303
H	1.86068	1.04718	1.90434