Supporting information for the manuscript:

Structural properties of the chelating agent 2,6-bis(1-(3-hydroxypropyl)-1,2,3-triazol-4-yl)pyridine: a combined XRD and DFT structural study

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Content:

DSC measurements

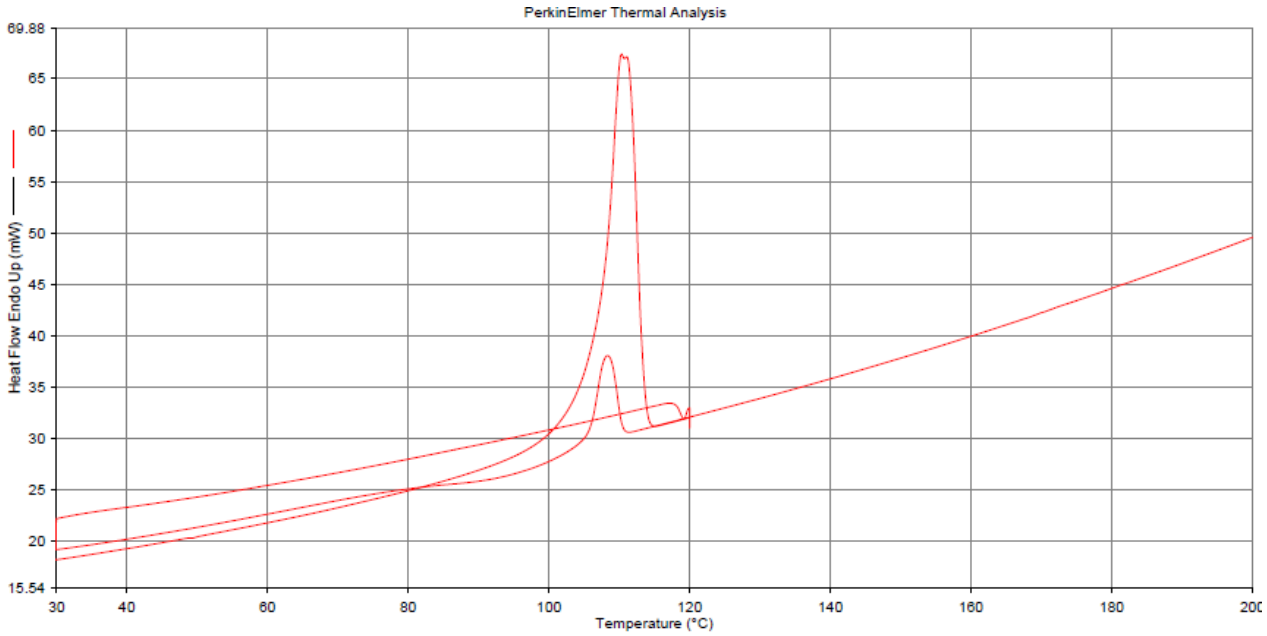


Figure S1. DSC patterns of a PTD sample.

NCI analysis technical details

Noncovalent interaction (NCI) analysis [E. R. Johnson, et al., *J. Am. Chem. Soc.*, 2010, **132**, 6498–6506] exploits the correlation between electron density ρ and its reduced gradient, s. The latter is a dimensionless quantity describing local inhomogeneity of ρ. Expanding on the concept of critical point within the quantum theory of atoms in molecules (QTAIM) [R. F. W. Bader, *Chem. Rev.*, 1991, **91**, 893–928], NCI also accounts for the topology of its immediate surroundings. As such, a wider range of interactions can be revealed by NCI analysis than it is possible with QTAIM.

Noncovalent interactions within the NCI framework appear in real space as s isosurfaces (values between 0.3 and 0.5 are usually recommended) separating two interacting atoms/moieties. The stronger and more obvious the interaction, the cleaner the isosurface shape: a hydrogen bond will be represented by a neat disk, while the isosurface representing a $\pi\cdots\pi$ interaction will be significantly more irregular.

Scatter plots of s against ρ show troughs departing from the usual $\rho^{-1/3}$ trend (imparted by non-overlapping Gaussian basis functions) for each separate noncovalent interaction. Such trough converges on a value of ρ for diminishing values of s. The value of $\rho(s_{min})$ can be used as a semi-quantitative index of the strength of the corresponding interaction. The sign of the second eigenvalue of the electron density Hessian matrix can be used to distinguish bonding ($\lambda_2<0$) from nonbonding ($\lambda_2>0$) interactions. The value of $\text{sign}(\lambda_2)\rho$ can be colour-mapped onto s-isosurfaces to obtain a comprehensive representation of noncovalent interactions in real space.

In this work, NCI analysis was carried out on cubic grids with spacing between 0.02 and 0.04 Bohr, starting from electron densities obtained at ωB97X-D/cc-pVTZ level of theory. Due to the range of interaction strengths detected, a colour-scale was not used. Instead, green surfaces were used to represent bonding interactions, while red was used for nonbonding ones. Furthermore, values of $\rho(s_{min})$ obtained from grid data were reported in specific labels (in 10^{-3} e) next to each bonding isosurface. It should be noted that, although reported, $\rho(s_{min})$ is not a reliable descriptor of the magnitude of interactions involving large isosurfaces.

NCI analysis of intermolecular interactions in PTD crystal

Noncovalent intermolecular interactions within a PTD stack:

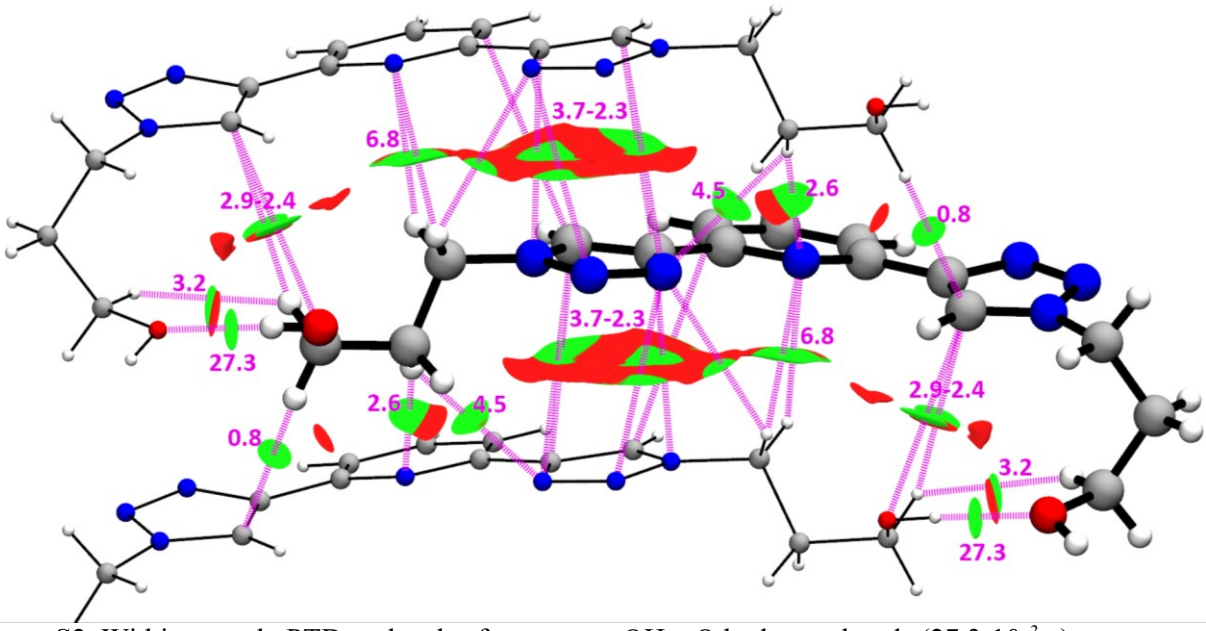


Figure S2. Within a stack, PTD molecules form strong OH···O hydrogen bonds ($27.3 \cdot 10^{-3}$ *e*) represented by small green disks. Large isosurfaces indicate effective π···π interactions between triazole units. The remaining isosurfaces represent weak CH···π interactions.

Noncovalent intermolecular interactions between front-facing stacks:

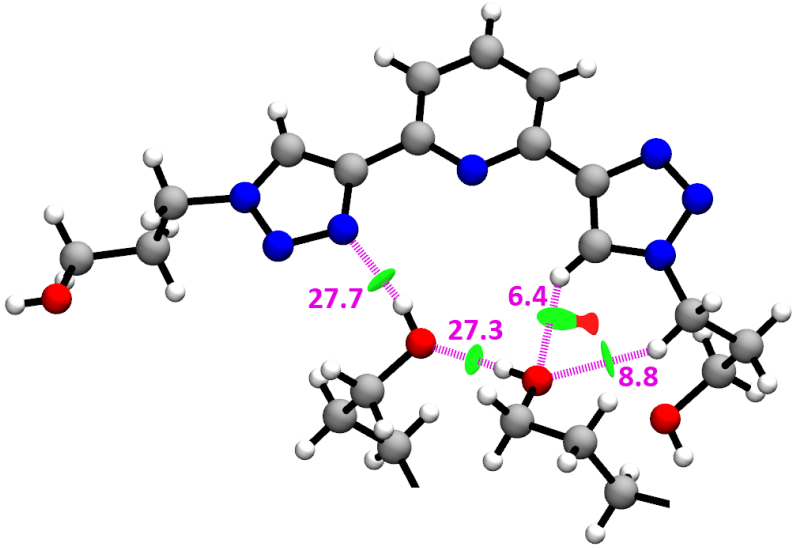


Figure S3. Detail of Figure 4c in the main text. The hydrogen bonds bridge locking front-facing stacks together is formed by a strong N···HO bond ($27.7 \cdot 10^{-3}$ *e*), a strong O···HO bond ($27.3 \cdot 10^{-3}$ *e*), and two weaker O···HC bonds ($6.4 \cdot 10^{-3}$ *e,* $8.8 \cdot 10^{-3}$ *e*) involving the proton on triazole and the aliphatic side chain.

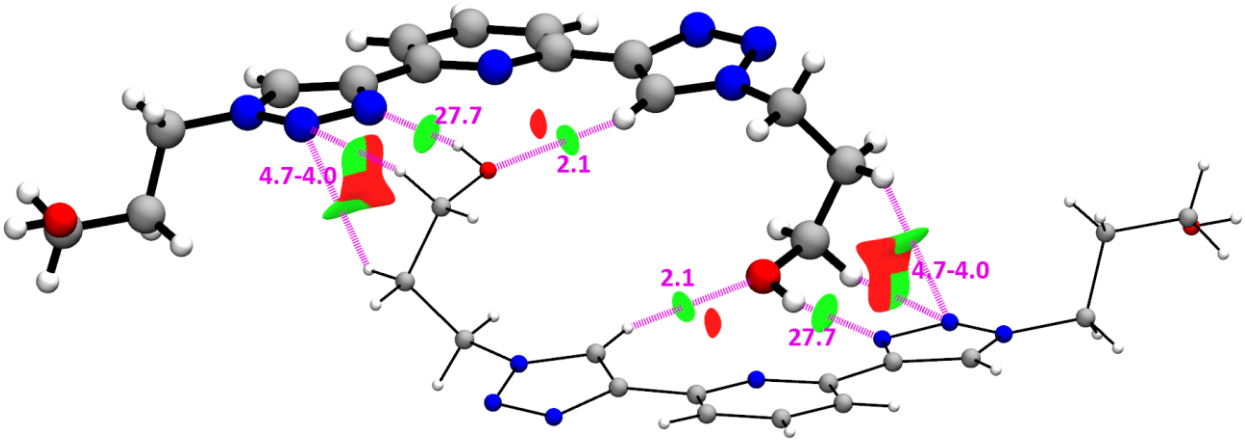


Figure S4. Front-facing stacks interact with each other with strong OH···N hydrogen bonds ($27.7 \cdot 10^{-3}$ *e*). Weaker interactions are detected between aliphatic fragments and triazole, and again between triazole and OH terminal groups.

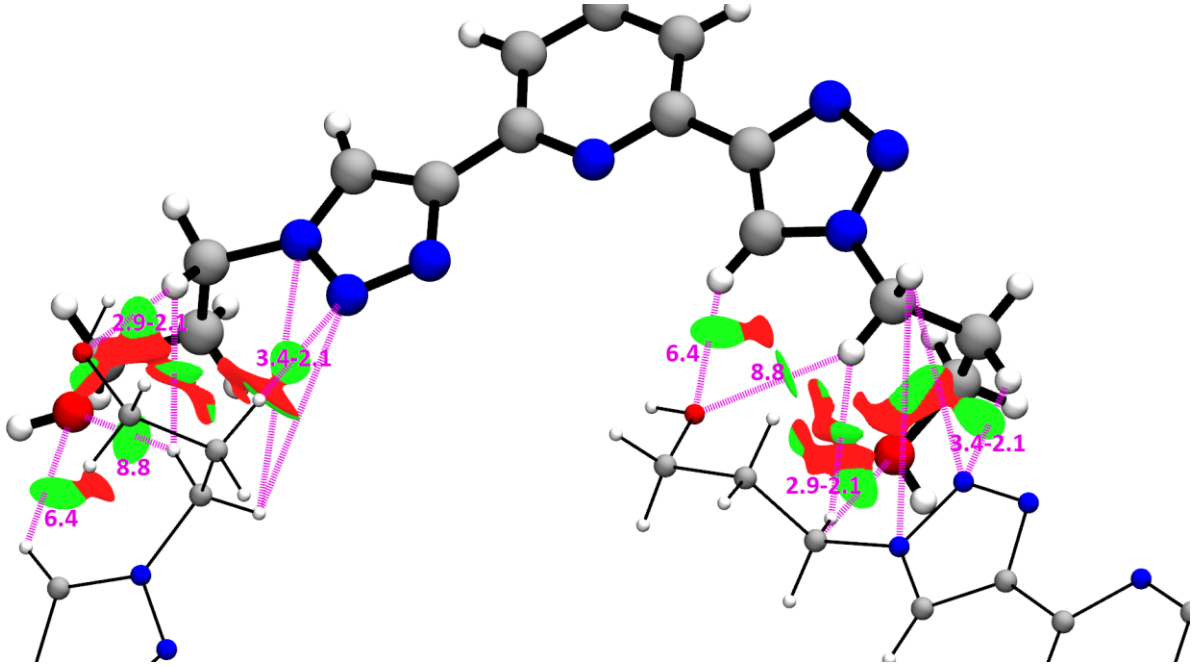


Figure S5. The weaker link in the hydrogen bond bridge consists of two CH···O interactions involving a proton on a triazole unit and one from a methylene on the aliphatic spacer. Additional weaker interactions include CH···π between triazole and aliphatic chains.

Noncovalent intermolecular interactions between back-to-back stacks:

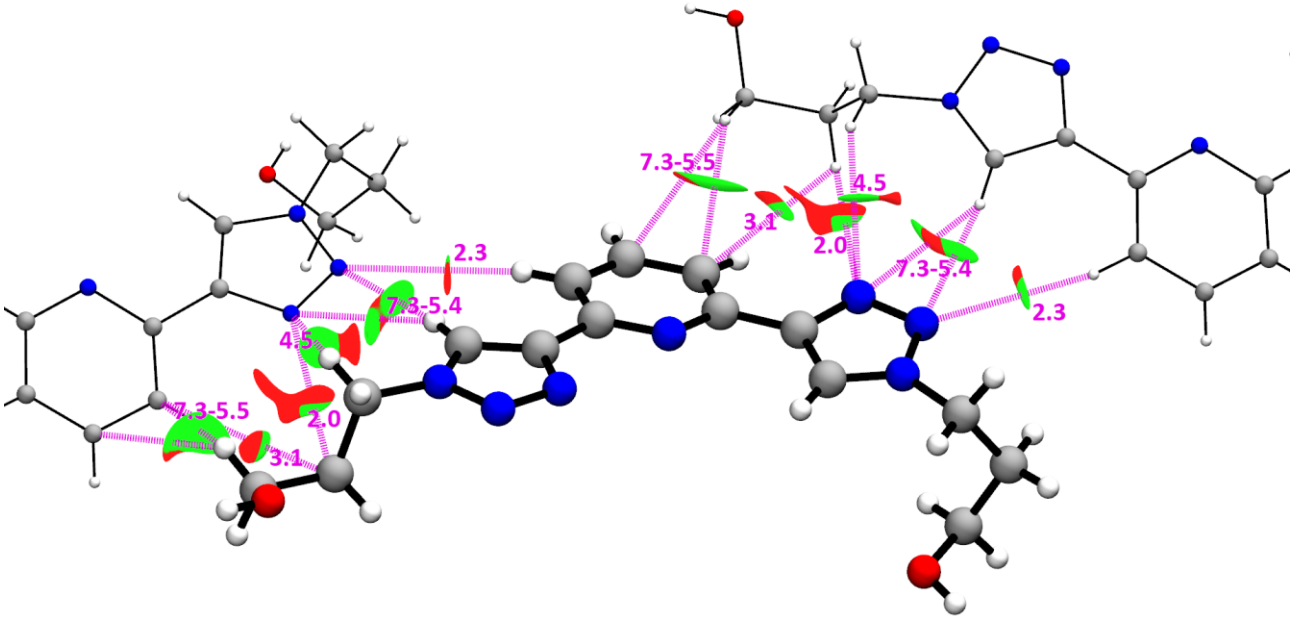


Figure S6. Extensive CH···π network between back-to-back PTD stacks.

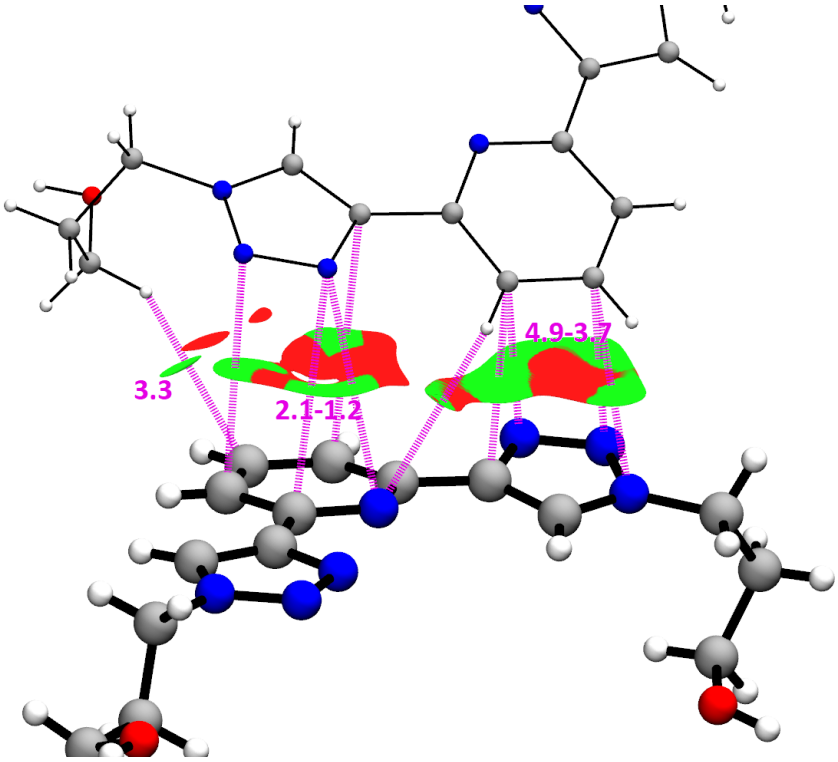


Figure S7. The reduced degree of superposition as well as the tilt angle between these periodic images prevents affective π···π interactions.

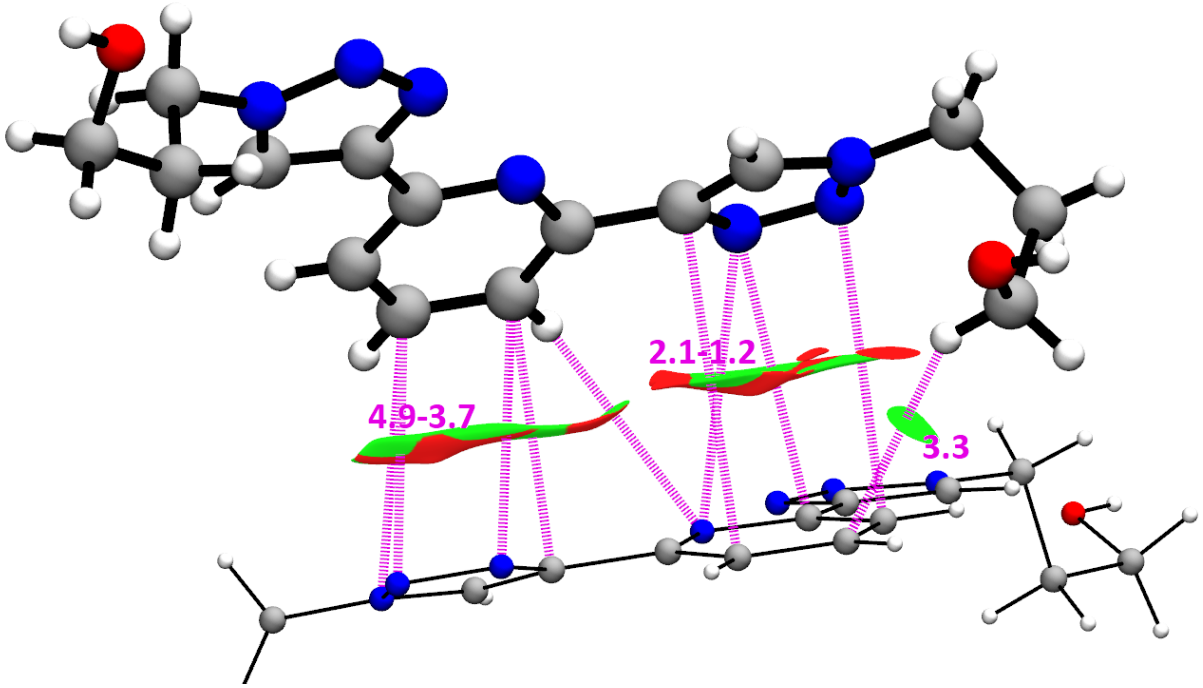


Figure S8. These interactions mirror those depicted in Figure S6 due to symmetry.

Survey of 2,6-bis(1,2,3-triazol-4-yl)pyridine subunit-containing crystal structures on the Cambridge structural database

Table S1. CSD entries featuring a 2,6-bis(1,2,3-triazol-4-yl)pyridine subunit not directly involved in metal ion complexation. Cyclic molecules were included for completeness, while entries featuring cationic triazole rings were excluded due to the obviously different character in the context of noncovalent intramolecular interactions. Notes include possible explanations for the specific arrangement. This investigation is based on CSD updated to November 2019.

CSD entry	*Arrangement*	*Notes*
ALEHAB	*anti/anti*	-
BULQOP	*anti/anti*	Protons on both triazoles interact with another triazole's nitrogen
CAQPIW	*anti/anti*	-
IJOJAU	*anti/anti*	Protons on both triazoles interact with another pyridine's nitrogen
IJOJEY	*anti/anti*	Protons on both triazoles interact with another pyridine's nitrogen
IPEYAE	*anti/anti*	-
IPEYEI	*anti/anti*	-
IPEYUY	*anti/anti*	-
IPEZAF	*anti/anti*	Protons on both triazoles interact with an acetone's oxygen
IPEZEJ	*anti/anti*	Protons on both triazoles interact with a nitro group
IVOWAT	*anti/anti* (cyclic)	Protons on both triazoles interact with another pyridine's nitrogen
IVOWEX	*anti/anti* (cyclic)	Protons on both triazoles interact with solvent molecules
JUDGOG	*anti/anti*	Protons on both triazoles interact with another triazole's nitrogen
LITHAY	*anti/anti*	Protons on triazoles interact with an ether's oxygen and a triazole
LITHEC	*anti/anti*	Protons on both triazoles interact with an ether's oxygen
LITHIG	*anti/anti*	Protons on both triazoles interact with dichloromethane
LITHOM	*anti/anti*	-
LITHUS	*anti/anti*	Protons on both triazoles interact with an ether's oxygen
LITJAA	*anti/anti*	Protons on both triazoles interact with another triazole's nitrogen
LITJEE	*anti/anti*	Protons on both triazoles interact with a DMSO molecule
LITJUU	*anti/anti*	Protons on both triazoles interact with an ether's oxygen
MIRGAX	*anti/anti*	-
NICKES	*anti/anti* (cyclic)	-
NICKIW	*anti/anti* (cyclic)	-
NOCNAX	*anti/anti*	Protons on both triazoles interact with a pyridine's nitrogen
OHACIL	*anti/anti* (cyclic)	Protons on both triazoles interact with another triazole's nitrogen
PEQGEA	*syn/anti*	A carboxylic group bridges a triazole's nitrogen to another's proton
SIDDOA	*anti/anti*	-
SOBHID	*anti/anti*	Protons on both triazoles interact with a pyridine's nitrogen
TEJHEY	*anti/anti*	Protons on both triazoles interact with another pyridine's nitrogen
UJIYUI	*anti/anti*	-
XUYBAV	*anti/anti*	Protons on both triazoles interact with an acetonitrile's nitrogen
XUYBEZ	*anti/anti*	-
XUYCAW	*anti/anti*	Protons on both triazoles interact with an acetone's oxygen
ZARYUP	*anti/anti*	-

Cartesian coordinates for truncated-PTD conformers A–D

```
Conformer A
Total energy: -808.987971586 Ea (wB97XD/cc-pVTZ)
 N    0.395495    0.162553    0.136583
 C    0.322248    0.263596    1.463180
 C    1.412214    0.608441    2.255330
 C    2.621278    0.855890    1.632554
 C    2.709987    0.754439    0.256780
 C    1.566168    0.403491   -0.452397
 C   -0.984209   -0.009726    2.065540
 N   -1.212025    0.054384    3.402705
 N   -2.446652   -0.234062    3.638229
 N   -3.036172   -0.488169    2.465008
 C   -2.160071   -0.360120    1.454083
 C   -4.435181   -0.842787    2.418422
 C    1.598289    0.280489   -1.911244
 N    2.717552    0.496988   -2.649050
 N    2.446171    0.316488   -3.896776
 N    1.154572   -0.018045   -3.988011
 C    0.584352   -0.052613   -2.771619
 C    0.563780   -0.283113   -5.278688
 H    3.631280    0.937937   -0.275347
 H    3.490378    1.126575    2.216698
 H    1.292524    0.674825    3.326254
 H   -2.414483   -0.517370    0.423101
 H   -0.447355   -0.298075   -2.605182
 H   -4.801844   -0.842922    3.440253
 H   -4.992059   -0.114454    1.831733
 H   -4.561411   -1.833660    1.985989
 H    1.343510   -0.153606   -6.022877
 H    0.185774   -1.302969   -5.320874
 H   -0.247289    0.415596   -5.475559
```

Conformer B
Total energy: -808.981043943 Ea (wB97XD/cc-pVTZ)

N	-0.041175	0.174672	0.133225
C	0.033544	0.422123	1.439122
C	1.094790	1.107847	2.021572
C	2.106049	1.559352	1.195680
C	2.029450	1.317338	-0.163927
C	0.934108	0.611276	-0.656253
C	-1.081813	-0.076419	2.243528
N	-1.156526	0.058903	3.591738
N	-2.253952	-0.475221	4.010010
N	-2.901987	-0.960660	2.943785
C	-2.206588	-0.734367	1.817717
C	-4.176223	-1.620162	3.108249
C	0.814112	0.312583	-2.090202
N	-0.359188	-0.034099	-2.683250
N	-0.156155	-0.234937	-3.939954
N	1.141682	-0.028393	-4.187149
C	1.786253	0.316784	-3.059553
C	1.664615	-0.193917	-5.522826
H	2.795492	1.681748	-0.833688
H	2.945188	2.104355	1.606436
H	1.103946	1.274579	3.088295
H	-2.530756	-1.032071	0.837828
H	2.842825	0.512073	-3.035419
H	-4.412176	-1.606958	4.167828
H	-4.950148	-1.091627	2.554945
H	-4.117667	-2.649548	2.759774
H	0.832044	-0.473536	-6.160992
H	2.099436	0.738046	-5.879464
H	2.417641	-0.979762	-5.542242

Conformer C
Total energy: -808.968799476 Ea (wB97XD/cc-pVTZ)

N	-0.093077	0.038257	-0.057961
C	-0.072855	-0.035750	1.269140
C	1.108843	0.002245	2.006790
C	2.305733	0.140806	1.330576
C	2.288747	0.227473	-0.048255
C	1.061402	0.162511	-0.705098
C	-1.367442	-0.164118	1.953398
N	-2.432354	-0.820229	1.421936
N	-3.416988	-0.767997	2.251755
N	-3.017651	-0.078592	3.325730
C	-1.739524	0.314568	3.184029
C	-3.929775	0.161155	4.418794
C	1.003780	0.232936	-2.172201
N	-0.026408	0.799313	-2.854065
N	0.207806	0.715061	-4.118564
N	1.380281	0.093290	-4.282274
C	1.916064	-0.222430	-3.090041
C	1.890196	-0.163820	-5.608224
H	3.203070	0.361457	-0.608884
H	3.241177	0.180745	1.872080
H	1.085379	-0.093742	3.083118
H	-1.226209	0.900172	3.924896
H	2.849597	-0.746235	-2.992926
H	-4.868521	-0.321800	4.165189
H	-3.538945	-0.264499	5.341370
H	-4.094670	1.229220	4.549820
H	1.176125	0.251525	-6.312769
H	2.857432	0.316841	-5.744095
H	1.986855	-1.234791	-5.778036

Conformer D
Total energy: -808.968217241 Ea (wB97XD/cc-pVTZ)

N	0.059827	-0.211778	0.009228
C	-0.053885	0.170589	1.277443
C	0.794166	1.112451	1.857290
C	1.791379	1.670574	1.081141
C	1.919642	1.267952	-0.233974
C	1.027051	0.320181	-0.731654
C	-1.136929	-0.431958	2.067767
N	-1.648999	-1.666198	1.820389
N	-2.576411	-1.918576	2.677725
N	-2.689330	-0.860995	3.490150
C	-1.805723	0.091337	3.146268
C	-3.672424	-0.856788	4.547221
C	1.122017	-0.118460	-2.131349
N	0.702122	-1.335434	-2.566760
N	0.919088	-1.429256	-3.832832
N	1.474899	-0.283525	-4.244487
C	1.622712	0.563959	-3.212033
C	1.813631	-0.097251	-5.635343
H	2.708892	1.659919	-0.859743
H	2.473612	2.396560	1.502210
H	0.686058	1.380303	2.898784
H	-1.740911	1.033817	3.658993
H	2.033287	1.550661	-3.326912
H	-4.190261	-1.810171	4.506846
H	-3.189528	-0.745834	5.516501
H	-4.387074	-0.048832	4.400161
H	1.546333	-1.011975	-6.155479
H	1.253897	0.736464	-6.055768
H	2.880927	0.085833	-5.746554

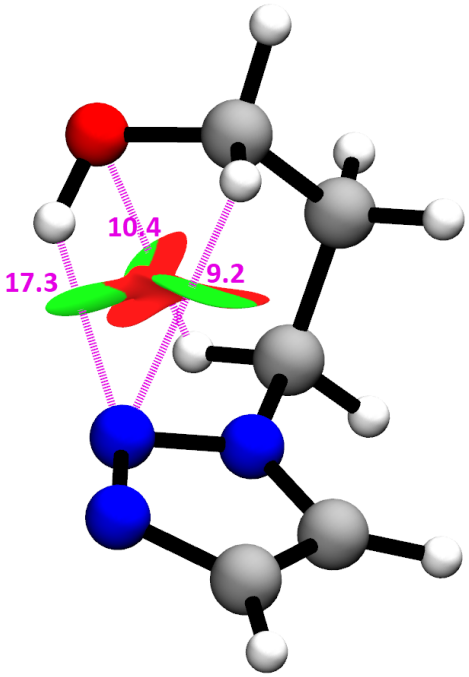
Sequences of dihedral angles for conformational isomers of 1-(3-hydroxypropyl)-1,2,3-triazole

Table S2. Dihedral angles (deg) identifying conformational isomers of (hydroxypropyl)triazole.

Isomer	N=N–$C_{(1)}$–$C_{(2)}$	N–$C_{(1)}$–$C_{(2)}$–$C_{(3)}$	$C_{(1)}$–$C_{(2)}$–$C_{(3)}$–O	$C_{(2)}$–$C_{(3)}$–O–H
$g^-g^-g^+$	85.3	–53.2	–50.6	83.3
$g^-g^+g^-$	79.6	–72.6	75.9	–69.5
g^+g^+a	78.6	57.1	55.3	179.6
$g^+g^+g^+$	83.7	59.7	53.2	69.1
ag^-a	82.0	179.4	–61.9	177.9
$g^+g^-g^-$	81.6	84.0	–55.4	–57.9
ag^-g^-	76.3	176.9	–60.8	–70.6
g^-aa	101.3	–61.5	–178.0	–175.6
ag^+g^+	82.9	–176.1	58.6	63.8
g^+ag^+	66.2	62.0	177.0	68.2
ag^+a	90.9	178.3	60.5	–179.8
$g^-g^-g^-$	100.3	–71.3	–64.0	–70.3
g^-ag^-	100.5	–64.1	–177.1	–74.0
g^-ag^+	104.5	–61.1	178.3	67.7
$g^+g^-g^+$	77.9	58.1	–84.6	64.6
g^+aa	72.0	60.3	174.5	170.9
g^+ag^-	77.7	64.3	179.9	–61.6
g^+g^-a	115.3	103.8	–60.8	176.7
aag^-	89.4	–177.3	–176.8	–64.1
aaa	98.5	–177.8	–177.9	–177.5
ag^+g^-	101.2	179.8	65.3	–81.1
aag^+	89.9	–179.9	177.2	62.8
$g^-g^+g^+$	111.0	–61.3	70.3	61.9

Cartesian coordinates, structures, and NCI analysis of 1-(3-hydroxypropyl)-1,2,3-triazole conformers

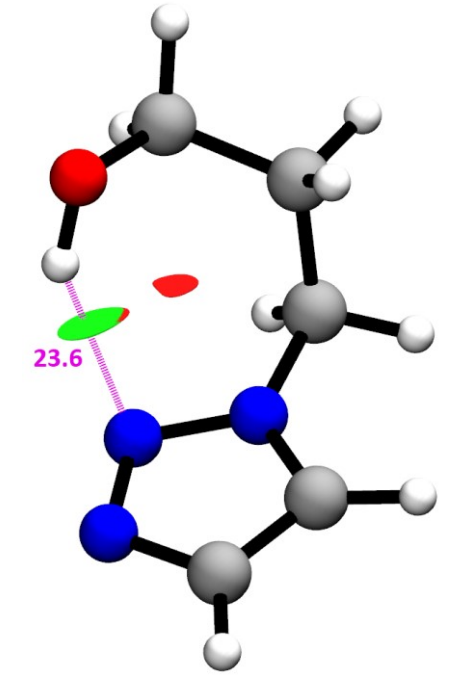
$g^-g^-g^+$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.400008524 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.368892
N	1.302563	0.000000	1.701784
N	2.063023	0.009597	0.603980
N	1.282939	0.007974	-0.427824
H	-0.826841	-0.010877	-0.686782
H	-0.784823	-0.009006	2.102826
C	1.925524	0.081200	3.012197
C	2.197634	1.516788	3.449524
H	1.279358	-0.431432	3.722047
H	2.860314	-0.470327	2.943281
C	2.993883	2.314823	2.416443
H	1.257453	2.034515	3.654847
H	2.756242	1.467601	4.385794
O	4.157180	1.644709	1.993304
H	2.352357	2.556828	1.562919
H	3.306153	3.259544	2.862087
H	3.894279	1.030999	1.298645

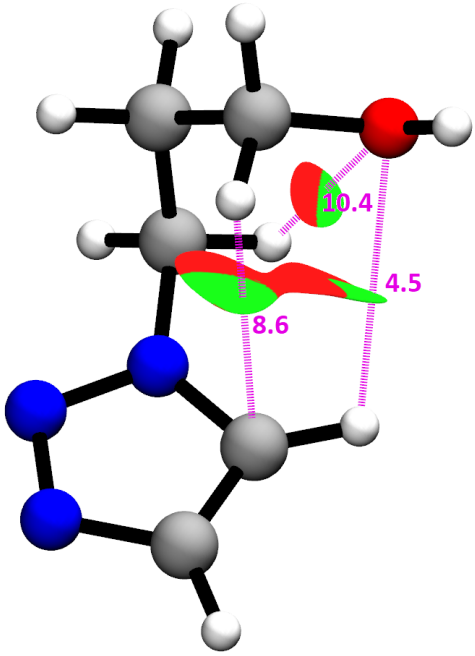
$g^-g^+g^-$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.397380823 Ea

C	-0.199542	-0.278239	0.018313
C	-0.139700	-0.278490	1.385800
N	1.162861	-0.096368	1.662862
N	1.867374	0.012372	0.535475
N	1.049919	-0.095021	-0.462975
H	-1.046335	-0.399731	-0.632445
H	-0.883474	-0.395173	2.152438
C	1.812990	0.015527	2.958896
C	2.097768	1.447970	3.401478
H	1.159693	-0.479346	3.675539
H	2.738406	-0.557238	2.900485
C	3.231127	2.155109	2.658298
H	1.188599	2.047449	3.324226
H	2.365717	1.400528	4.460085
O	2.897668	2.588692	1.366238
H	3.501610	3.050975	3.218127
H	4.115603	1.503731	2.646832
H	2.789792	1.813595	0.803877

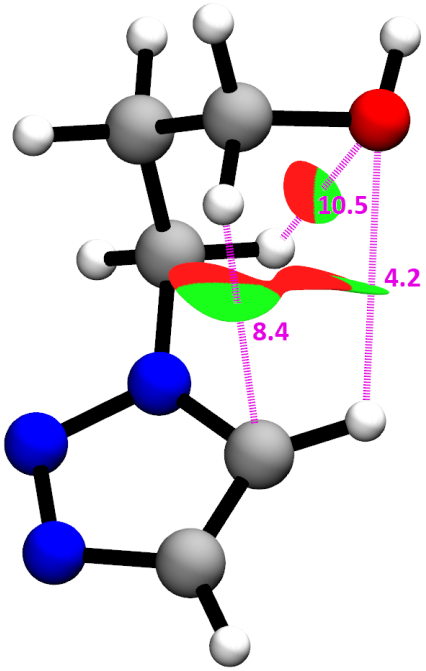
g^+g^+a



Optimized at wB97XD/cc-pVTZ
Total energy: -435.397186564 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367519
N	1.305865	0.000000	1.696039
N	2.068824	0.008343	0.602103
N	1.285342	0.004542	-0.428171
H	-0.826589	-0.008191	-0.687373
H	-0.774846	0.013373	2.111696
C	1.909543	0.075114	3.012400
C	2.328727	1.495037	3.377255
H	1.179986	-0.299844	3.725890
H	2.772066	-0.587439	3.013266
C	1.183745	2.486342	3.327386
H	2.748732	1.472834	4.384179
H	3.112668	1.827642	2.696024
O	0.145524	2.009247	4.168064
H	1.539482	3.465908	3.660768
H	0.829173	2.591403	2.296126
H	-0.579302	2.632686	4.147001

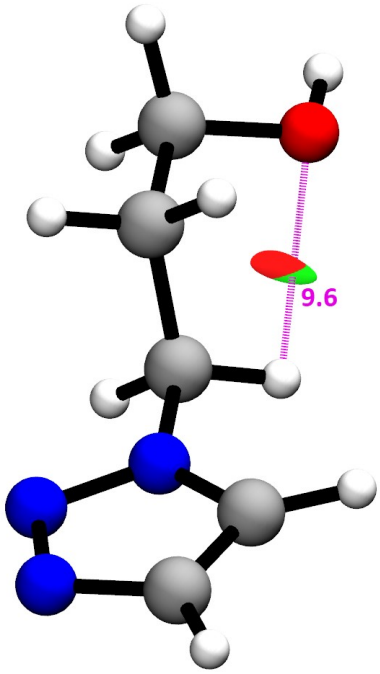
$g^+g^+g^+$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.396658825 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367282
N	1.306736	0.000000	1.694896
N	2.069659	0.007746	0.599669
N	1.285307	0.003871	-0.429039
H	-0.827214	-0.006717	-0.686531
H	-0.775549	0.016181	2.111263
C	1.913611	0.070888	3.008785
C	2.224760	1.502958	3.429762
H	1.222845	-0.389492	3.711919
H	2.823670	-0.523320	2.973667
C	0.991845	2.394059	3.484668
H	2.703247	1.467706	4.412384
H	2.947363	1.936060	2.735923
O	-0.045880	1.850423	4.281990
H	1.272635	3.393146	3.830512
H	0.567693	2.506221	2.487040
H	0.228030	1.869863	5.199224

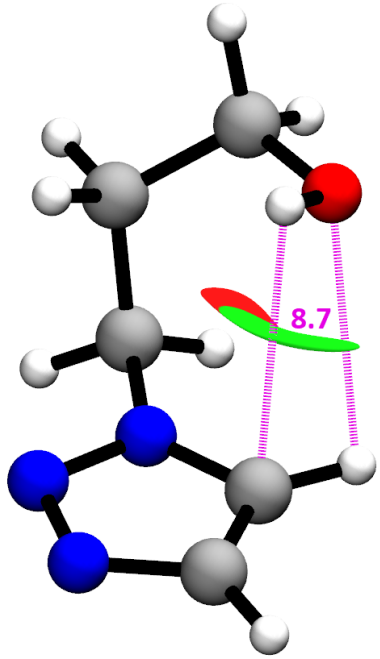
ag^-a



Optimized at wB97XD/cc-pVTZ
Total energy: -435.394925494 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367417
N	1.305608	0.000000	1.697019
N	2.068077	0.008054	0.602676
N	1.285074	0.003976	-0.427632
H	-0.826989	-0.009071	-0.686824
H	-0.782108	-0.004993	2.104323
C	1.914579	0.073147	3.009465
C	2.258220	1.505410	3.398593
H	1.224913	-0.362453	3.728667
H	2.812976	-0.541996	2.980856
C	2.878095	1.580183	4.777733
H	2.952006	1.918593	2.665601
H	1.353155	2.115316	3.378987
O	1.927665	1.102461	5.713308
H	3.792238	0.974602	4.807001
H	3.156314	2.616176	4.995273
H	2.317206	1.112321	6.586505

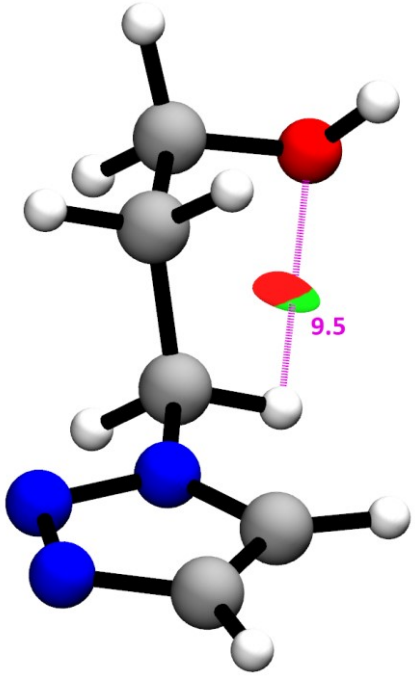
$g^+g^-g^-$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.39440391 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367100
N	1.305276	0.000000	1.695861
N	2.068640	0.001102	0.599124
N	1.285572	0.001927	-0.429606
H	-0.827680	-0.005837	-0.686067
H	-0.779010	0.029028	2.105168
C	1.938230	0.035515	3.001798
C	2.354372	1.439472	3.438663
H	1.247719	-0.408729	3.718116
H	2.812705	-0.607064	2.929506
C	1.246615	2.256953	4.086569
H	3.168076	1.349328	4.161451
H	2.766926	1.962904	2.573021
O	0.084614	2.384031	3.292954
H	0.916834	1.765693	5.003692
H	1.638595	3.240029	4.369131
H	0.322193	2.784579	2.455227

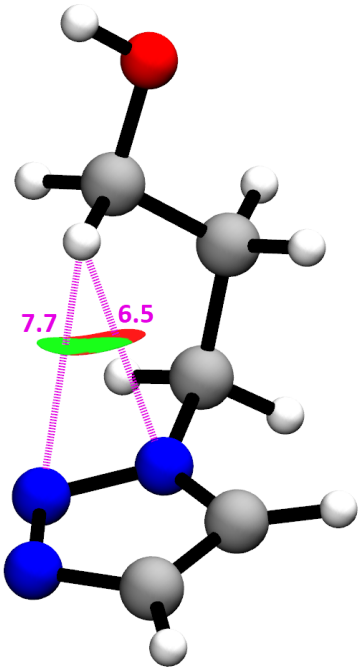
ag⁻g⁻



Optimized at wB97XD/cc-pVTZ
Total energy: -435.394400705 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367411
N	1.305737	0.000000	1.697300
N	2.068029	0.006566	0.603142
N	1.285081	0.003164	-0.427257
H	-0.826845	-0.008531	-0.686993
H	-0.782877	-0.007958	2.103435
C	1.916254	0.064981	3.009752
C	2.394297	1.469527	3.351879
H	1.184258	-0.276305	3.738632
H	2.751981	-0.633565	3.017281
C	2.965551	1.540175	4.759332
H	3.153722	1.776219	2.630970
H	1.560054	2.170489	3.256382
O	2.017490	1.196864	5.753380
H	3.780439	0.822921	4.868415
H	3.383234	2.535051	4.940239
H	1.367695	1.897889	5.808251

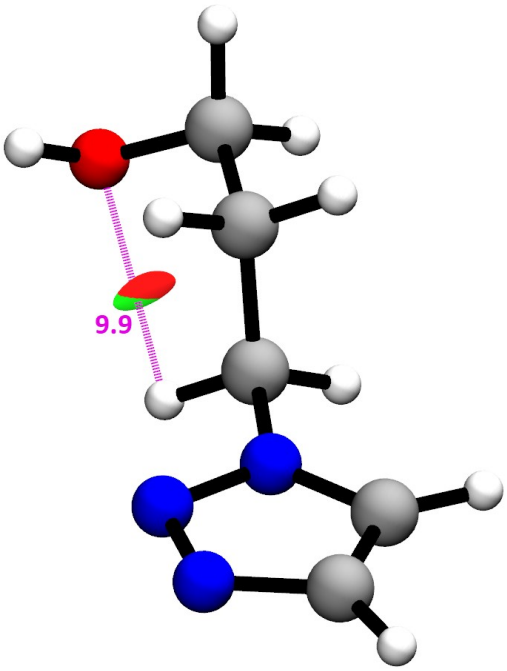
g⁻aa



Optimized at wB97XD/cc-pVTZ
Total energy: -435.394278346 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367278
N	1.305330	0.000000	1.697725
N	2.068113	0.008372	0.601523
N	1.284990	0.005571	-0.427911
H	-0.827133	-0.009237	-0.686701
H	-0.784466	-0.003063	2.101796
C	1.913419	0.079539	3.012873
C	1.828261	1.474737	3.615775
H	1.424499	-0.647461	3.659837
H	2.949086	-0.227795	2.879414
C	2.548930	2.522836	2.790861
H	0.783902	1.769909	3.734605
H	2.266818	1.446049	4.614514
O	2.435390	3.753040	3.478029
H	3.599039	2.232735	2.664940
H	2.105497	2.584281	1.791844
H	2.823667	4.441420	2.939504

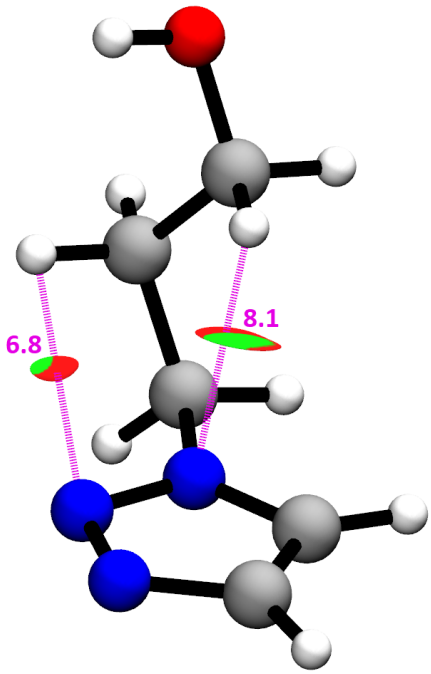
ag$^+$g$^+$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.394270536 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367364
N	1.305658	0.000000	1.697508
N	2.067999	0.009025	0.602942
N	1.285023	0.005730	-0.427258
H	-0.826943	-0.010491	-0.686854
H	-0.783660	-0.008054	2.102653
C	1.918742	0.077078	3.008168
C	2.239064	1.511811	3.406160
H	1.238328	-0.383525	3.724327
H	2.828641	-0.516875	2.978551
C	2.969143	1.583114	4.739050
H	2.851563	1.962755	2.621536
H	1.318473	2.096827	3.467831
O	4.184438	0.862202	4.740468
H	3.130119	2.630776	5.012861
H	2.361128	1.133440	5.526005
H	4.780303	1.265309	4.107875

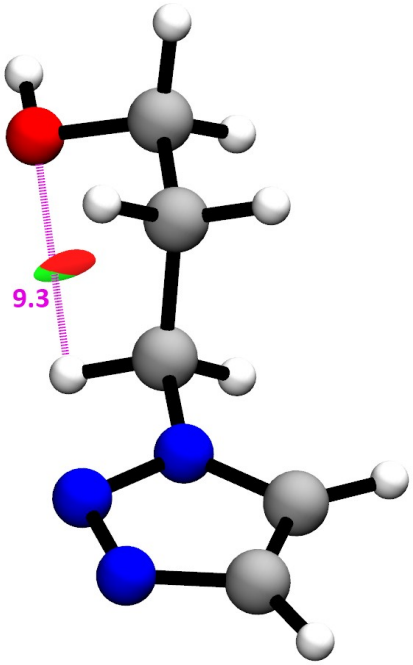
g$^+$ag$^+$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.393544323 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367460
N	1.305686	0.000000	1.697231
N	2.068068	0.004303	0.603575
N	1.284807	0.002341	-0.427098
H	-0.826890	-0.004642	-0.686880
H	-0.783275	-0.000880	2.103011
C	1.921183	0.053021	3.012542
C	2.631565	1.375513	3.264689
H	1.127656	-0.110322	3.741477
H	2.622503	-0.775933	3.086494
C	1.695768	2.575411	3.229910
H	3.115259	1.329444	4.241401
H	3.416352	1.497548	2.515581
O	2.360451	3.782836	3.531388
H	1.193623	2.634389	2.258047
H	0.919624	2.463653	3.989927
H	2.962965	3.984156	2.814917

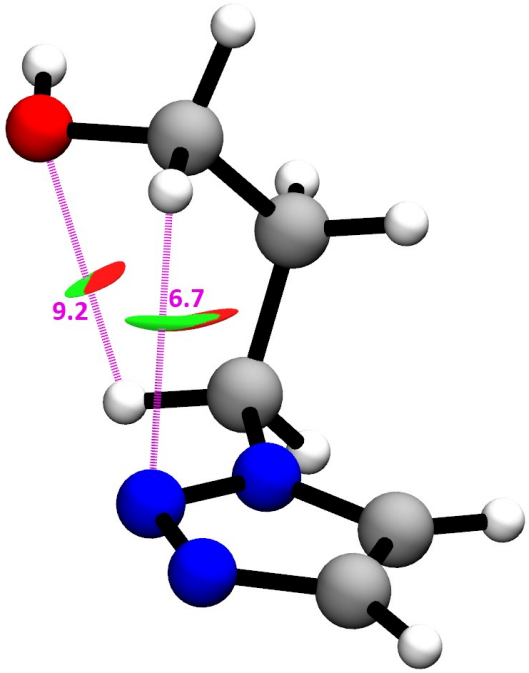
ag^+a



Optimized at wB97XD/cc-pVTZ
Total energy: -435.393489052 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.366963
N	1.306008	0.000000	1.697688
N	2.068306	0.008382	0.602878
N	1.285475	0.005080	-0.427067
H	-0.826784	-0.010435	-0.687131
H	-0.783949	-0.007183	2.102058
C	1.911931	0.073237	3.011844
C	2.054609	1.511110	3.495929
H	1.296704	-0.508511	3.699448
H	2.886563	-0.401440	2.942536
C	2.651197	1.584820	4.886363
H	2.688245	2.057947	2.796710
H	1.076713	1.996963	3.505129
O	3.935828	0.995352	4.847700
H	2.706623	2.632224	5.200362
H	2.001245	1.057634	5.596971
H	4.323911	1.031949	5.720806

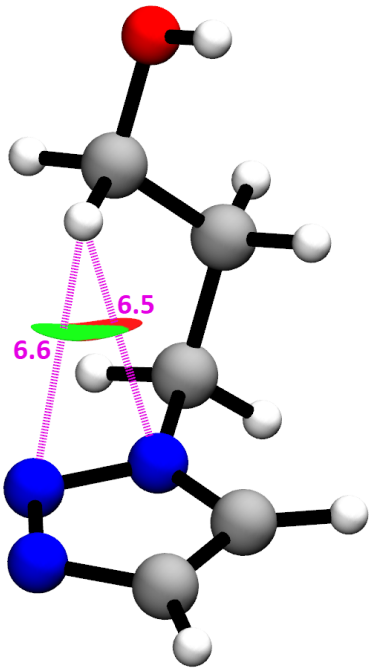
$g^-g^-g^-$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.393456719 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.366579
N	1.306230	0.000000	1.698423
N	2.068755	0.005672	0.601762
N	1.285507	0.004169	-0.427289
H	-0.826811	-0.008904	-0.687162
H	-0.784866	-0.007457	2.100742
C	1.904227	0.058232	3.018550
C	1.854147	1.461534	3.614285
H	1.384133	-0.655457	3.656141
H	2.936874	-0.264170	2.904642
C	2.809428	2.428431	2.926370
H	0.834522	1.850450	3.559826
H	2.110121	1.395015	4.675172
O	4.161818	2.054343	3.095221
H	2.633280	2.428289	1.850670
H	2.631300	3.445179	3.290746
H	4.406849	2.198121	4.009453

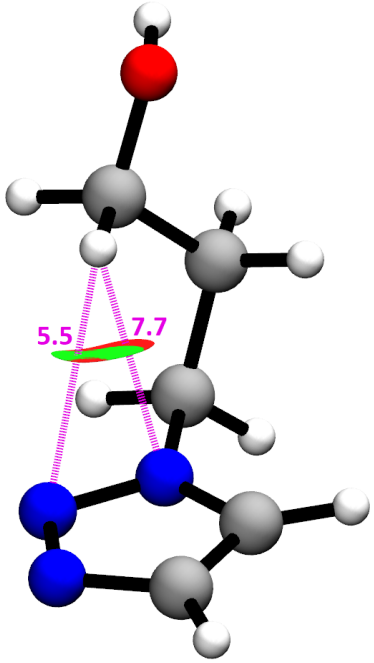
g⁻ag⁻



Optimized at wB97XD/cc-pVTZ
Total energy: -435.39339353 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367188
N	1.305663	0.000000	1.697965
N	2.068223	0.006840	0.601671
N	1.285203	0.004634	-0.427543
H	-0.826901	-0.009850	-0.686989
H	-0.784676	-0.006956	2.101538
C	1.911591	0.071021	3.014543
C	1.853344	1.470470	3.613737
H	1.406054	-0.645728	3.660274
H	2.942147	-0.255875	2.887204
C	2.655671	2.496669	2.823764
H	0.810600	1.793418	3.684198
H	2.241664	1.428382	4.632446
O	2.636797	3.768591	3.437802
H	3.702312	2.192218	2.785173
H	2.301677	2.547199	1.789736
H	1.775306	4.161855	3.300144

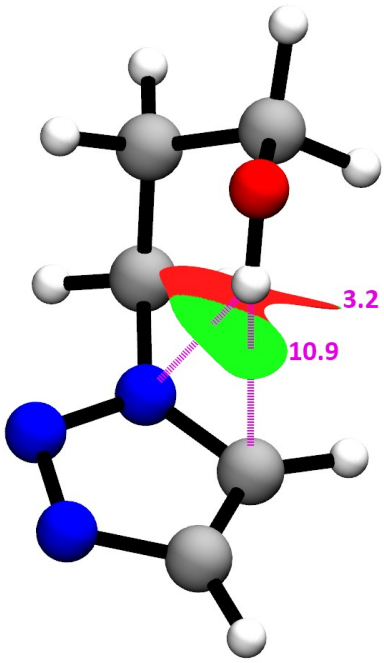
g⁻ag⁺



Optimized at wB97XD/cc-pVTZ
Total energy: -435.39337025 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367082
N	1.305709	0.000000	1.697353
N	2.068409	0.007469	0.600559
N	1.285069	0.004753	-0.428047
H	-0.827162	-0.007336	-0.686645
H	-0.784824	-0.001908	2.101179
C	1.915324	0.068294	3.011445
C	1.772166	1.443336	3.651643
H	1.464854	-0.698198	3.640966
H	2.962914	-0.187747	2.862870
C	2.439959	2.550976	2.847184
H	0.716942	1.689380	3.785492
H	2.216136	1.395237	4.649687
O	2.261764	3.820021	3.438720
H	3.502093	2.320203	2.703956
H	1.994152	2.615727	1.855241
H	2.748987	3.845911	4.262242

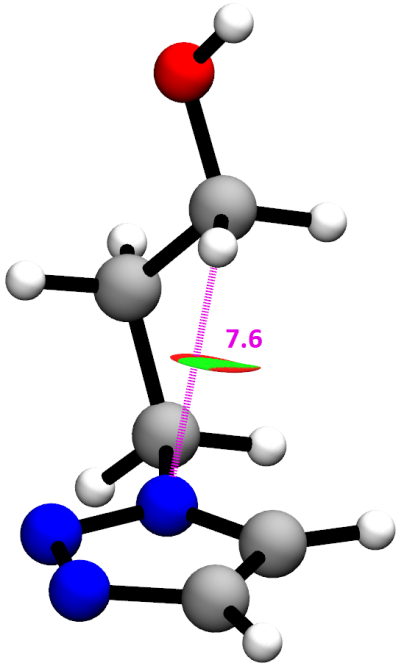
$g^+g^-g^+$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.393281025 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.368172
N	1.308359	0.000000	1.697526
N	2.069008	0.002468	0.602804
N	1.285764	-0.001452	-0.427038
H	-0.826848	-0.009212	-0.686931
H	-0.782831	-0.007902	2.104380
C	1.918048	0.105767	3.011546
C	2.338121	1.528889	3.362710
H	1.189686	-0.268563	3.730930
H	2.777434	-0.561396	3.020151
C	1.208527	2.557609	3.337885
H	2.769558	1.495782	4.365545
H	3.122753	1.857570	2.680490
O	0.940816	3.092055	2.061616
H	0.301531	2.128884	3.787609
H	1.492267	3.411091	3.952179
H	0.620471	2.400559	1.480406

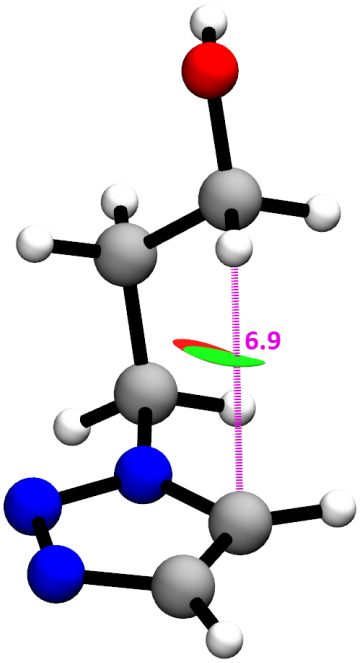
g^+aa



Optimized at wB97XD/cc-pVTZ
Total energy: -435.393012994 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367315
N	1.306029	0.000000	1.697191
N	2.068225	0.004787	0.603509
N	1.285113	0.002193	-0.426977
H	-0.826712	-0.007290	-0.687145
H	-0.782932	-0.003965	2.103296
C	1.918693	0.064824	3.012822
C	2.496519	1.437814	3.322663
H	1.150319	-0.209976	3.735346
H	2.700576	-0.690798	3.047665
C	1.457678	2.541507	3.301872
H	2.953421	1.402230	4.312930
H	3.284574	1.669514	2.606495
O	2.087909	3.731546	3.726386
H	1.051246	2.649188	2.290420
H	0.624845	2.278810	3.969280
H	1.491136	4.465416	3.585794

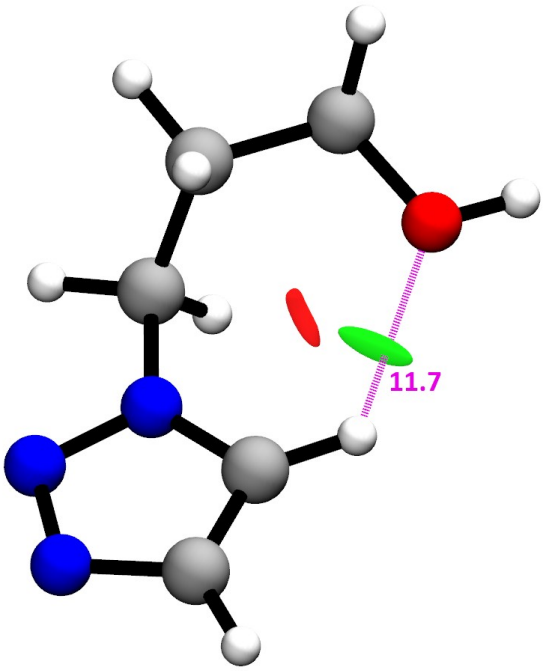
g^+ag^-



Optimized at wB97XD/cc-pVTZ
Total energy: -435.392609346 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367023
N	1.306467	0.000000	1.696795
N	2.068565	0.004042	0.601990
N	1.285276	0.001366	-0.427340
H	-0.826918	-0.006206	-0.686830
H	-0.783093	-0.002219	2.102902
C	1.923645	0.059804	3.008863
C	2.385019	1.464174	3.376545
H	1.194024	-0.314539	3.727302
H	2.768074	-0.625671	2.996991
C	1.240549	2.459149	3.505926
H	2.920231	1.399430	4.328175
H	3.093302	1.819723	2.628060
O	1.681454	3.753798	3.846483
H	0.726314	2.563772	2.550502
H	0.505172	2.087135	4.232893
H	2.117119	3.715920	4.698251

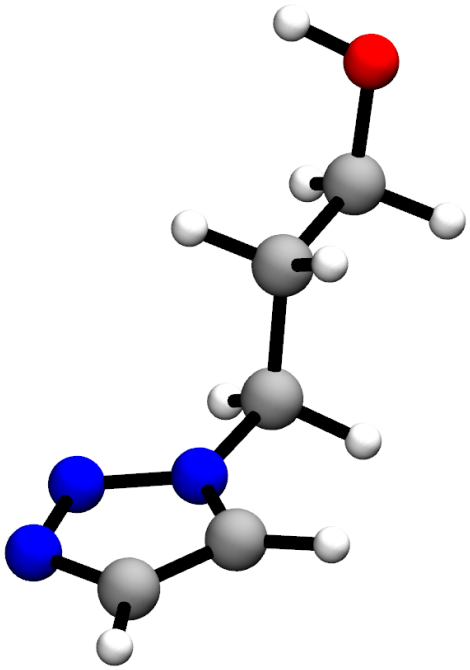
g^+g^-a



Optimized at wB97XD/cc-pVTZ
Total energy: -435.392607138 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367145
N	1.306732	0.000000	1.693725
N	2.069133	0.003065	0.594142
N	1.284374	0.001635	-0.432219
H	-0.828478	-0.000984	-0.685351
H	-0.769503	0.019648	2.115847
C	1.939187	0.009013	2.997947
C	1.669434	1.281587	3.813120
H	1.613947	-0.874594	3.548476
H	2.999760	-0.097892	2.786669
C	0.650666	1.103308	4.920421
H	2.600371	1.612953	4.274923
H	1.349406	2.078793	3.141576
O	-0.589237	0.715512	4.355737
H	1.006755	0.339840	5.622741
H	0.548257	2.043229	5.472120
H	-1.215766	0.554210	5.060010

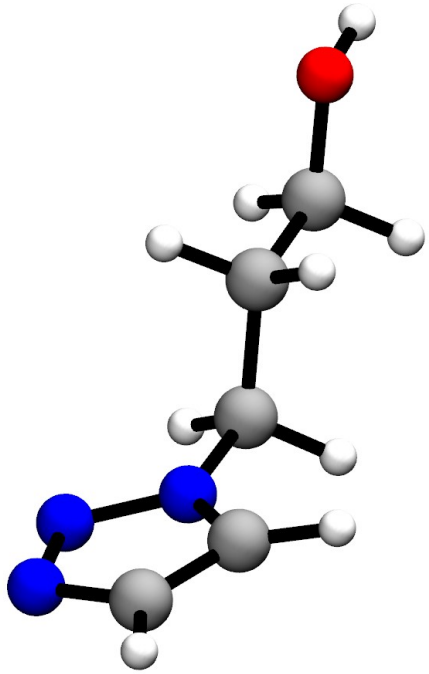
aag⁻



Optimized at wB97XD/cc-pVTZ
Total energy: -435.392580888 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.367127
N	1.306053	0.000000	1.696432
N	2.068544	0.008706	0.601106
N	1.285218	0.004951	-0.427875
H	-0.827105	-0.009795	-0.686637
H	-0.783646	-0.004112	2.102518
C	1.919056	0.077350	3.006138
C	2.096078	1.515055	3.475344
H	1.299110	-0.487562	3.702617
H	2.881432	-0.425822	2.927433
C	2.799634	1.584981	4.822682
H	2.676267	2.056170	2.724069
H	1.124648	2.006076	3.553353
O	2.909852	2.903176	5.309703
H	2.225748	1.038820	5.573303
H	3.783105	1.103497	4.755418
H	3.466080	3.404094	4.712502

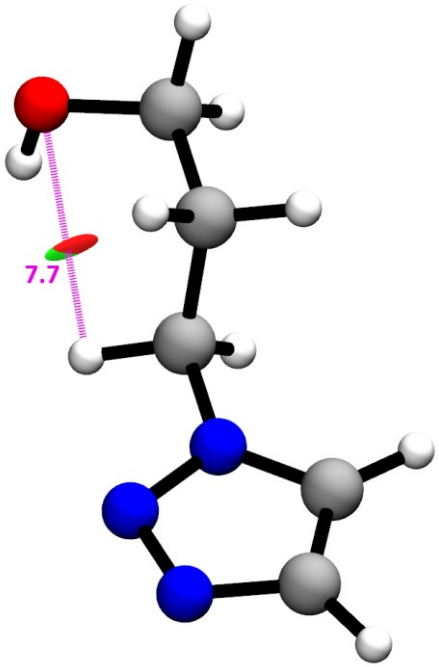
aaa



Optimized at wB97XD/cc-pVTZ
Total energy: -435.392152863 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.366939
N	1.306086	0.000000	1.696492
N	2.068517	0.007088	0.600749
N	1.285288	0.004001	-0.427946
H	-0.827160	-0.007748	-0.686648
H	-0.783926	-0.002493	2.102023
C	1.916710	0.061902	3.008015
C	1.906642	1.471303	3.582623
H	1.389418	-0.632437	3.663447
H	2.935551	-0.300412	2.882402
C	2.595971	1.528003	4.930764
H	2.408158	2.147334	2.889636
H	0.879368	1.822312	3.695119
O	2.498473	2.851935	5.409621
H	2.116788	0.823205	5.622851
H	3.643795	1.222557	4.821471
H	2.963337	2.915772	6.243038

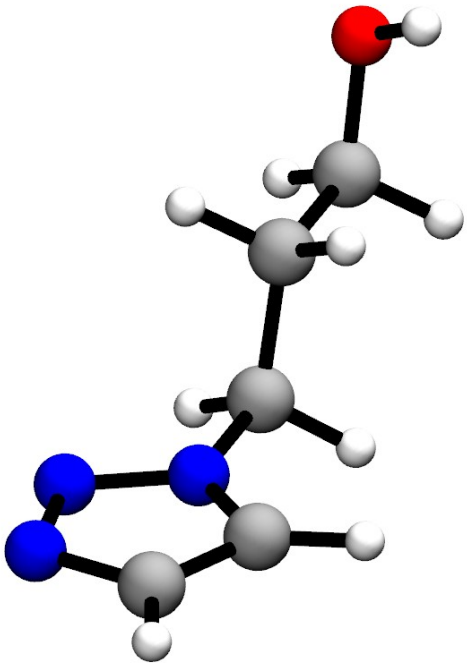
ag$^+$g$^-$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.391987382 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.366810
N	1.306298	0.000000	1.696840
N	2.068618	0.006350	0.600695
N	1.285460	0.003989	-0.427734
H	-0.827105	-0.007693	-0.686746
H	-0.784644	-0.005001	2.101161
C	1.915340	0.056163	3.009177
C	1.854609	1.447843	3.623692
H	1.417570	-0.673619	3.650862
H	2.948086	-0.256648	2.867760
C	2.490208	1.499236	5.006109
H	2.365535	2.150147	2.963984
H	0.812751	1.767638	3.704140
O	3.881401	1.250722	4.987382
H	2.367651	2.500340	5.417861
H	1.976582	0.806540	5.683994
H	4.036510	0.308027	4.948273

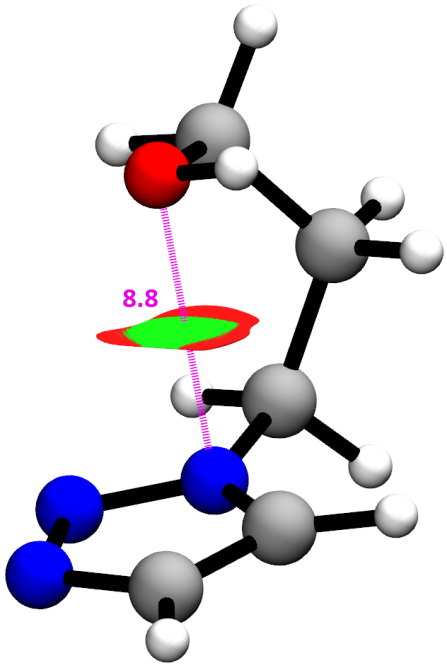
aag$^+$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.391914104 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.366988
N	1.306286	0.000000	1.696565
N	2.068629	0.007679	0.601256
N	1.285406	0.004056	-0.427608
H	-0.826944	-0.009822	-0.686850
H	-0.783932	-0.005925	2.102095
C	1.917506	0.073136	3.007328
C	2.088058	1.508292	3.487185
H	1.300347	-0.501733	3.698476
H	2.883575	-0.422293	2.926853
C	2.734375	1.566150	4.863580
H	2.703298	2.056660	2.773558
H	1.110070	1.997480	3.518934
O	2.961227	2.885311	5.304743
H	2.127534	1.006396	5.587213
H	3.715627	1.090541	4.832320
H	2.117645	3.329779	5.391489

$g^-g^+g^+$



Optimized at wB97XD/cc-pVTZ
Total energy: -435.390753814 Ea

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.366605
N	1.305382	0.000000	1.695849
N	2.067066	0.003410	0.600872
N	1.285198	-0.000046	-0.427828
H	-0.827034	-0.007302	-0.686953
H	-0.785311	-0.004083	2.100236
C	1.916436	0.063210	3.007015
C	1.666066	1.375480	3.742431
H	1.551285	-0.775570	3.600600
H	2.981732	-0.082433	2.837572
C	2.210013	2.618915	3.047276
H	0.594801	1.501113	3.927979
H	2.137902	1.291720	4.724282
O	1.515323	2.968914	1.871536
H	2.216165	3.450919	3.760688
H	3.242147	2.447481	2.738417
H	0.606580	3.170359	2.095465