Supporting Information for a Theoretical Insight into Excited-State Decay and Proton Transfer of *p*-Nitrophenylphenol in the Gas Phase and Methanol Solution

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1. UV-vis Absorption Spectra of NO$_2$-Bp-OH in Different Solvents

Figure S1. UV-vis absorption spectra of NO$_2$-Bp-OH in different solvents, where CHX, CAN, MeOH, IPA and TFEA denote cyclohexane, acetonitrile, methanol, isopropanol and 2,2,2-trifluroroethanol, respectively (a); the simulated absorption spectrum for the NO$_2$-Bp-OH system (b).

Table S1. The simulated absorption spectrum (nm) and fitted molar extinction coefficients (mol^{-1}s^{-1}) of NO$_2$-Bp-OH in the lowest excited singlet state.

States	Simulated spectrum	Experiment spectrum
S$_1$	356.3 [16461]	339.8 [15805]

2. Experimental and Theoretical Details for Choosing the Number of Methanol

Alcohol, like water, is an amphiprotic solvent, but with only one hydrogen bond donating site. In contrast to water, alcohol's hydrogen bond typically takes the form of a chain. To accurately describe the relationship between the pseudo-first-order decay rate constant and the methanol concentration (see Fig. S2), the following equations are used:

$$k = k_0 + k_M[MeOH]^n \qquad (1)$$

$$\log(k - k_0) = \log(k_M) + n \cdot \log[MeOH] \qquad (2)$$

where k and k_0 are the observation rate constants in the presence and absence of methanol, respectively. The rate constant for the reaction of $^3NO_2$-Bp-OH with methanol is given by k_M. Eq.(2) is obtained by performing the logarithm transformation on two sides of Eq.(1). The slope value of n=3.0±0.18 is obtained by fitting the plot of the logarithm of k-k_0 vs. the logarithm of methanol concentration with a linear function. The result of n=3 suggests that the methanol trimer is required to quench $^3NO_2$-Bp-OH.
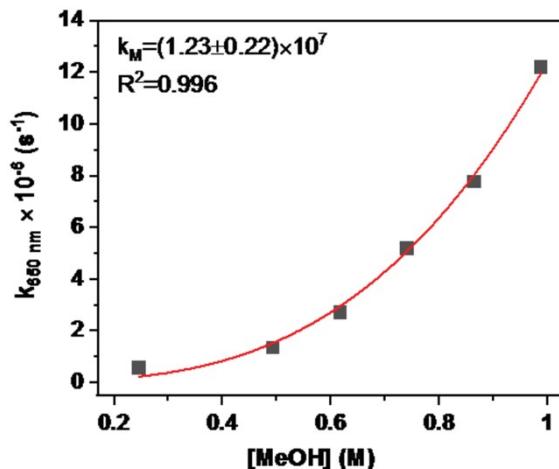
Figure S2. The pseudo-first-order decay time constants (solid squares) obtained by fitting the 650 nm kinetics with a single exponential function versus methanol concentrations, and the fitting curve (red curve) obtained with the equation $k = k_0 + k_M[MeOH]^3$.

Moreover, the potential energy surfaces of methanol oligomer assisted deprotonation in $^3NO_2$-Bp-OH are simulated using theoretical calculations, as shown in Fig. S3. The deprotonation barrier can be significantly reduced by increasing the number of methanol molecules around the hydroxyl group of $^3NO_2$-Bp-OH, and it is reduced to 3.7 kcal/mol in the methanol trimer structure. As the O-H distance in $^3NO_2$-Bp-OH increases, the energy surfaces of a single and two methanol molecules continue to grow, while the energy surface of three, four, and five methanol molecules exhibits minima. The energy barrier is slightly lower for four and five methanol molecules than that for three methanol molecules. This comes as no surprise given that the larger the cluster size, the more stable the structure. The greater the number of methanol molecules, the easier it is to deprotonate and stabilize the proton, but three-methanol is the critical size.
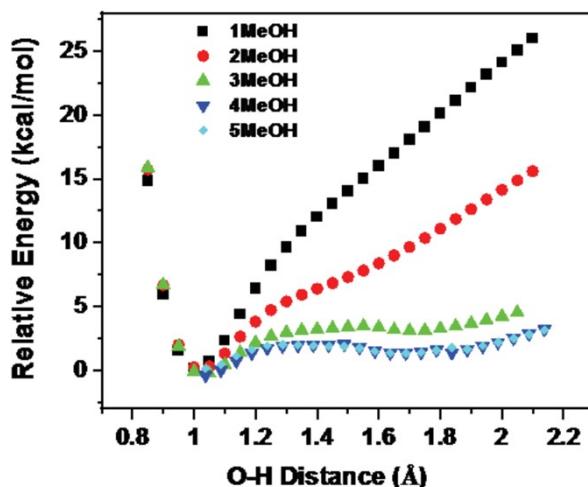
Figure S3. Potential energy curves of the T_1 state NO_2-Bp-OH⋯ $(MeOH)_n$ (n=1-5) hydrogen-bonded complexes in acetonitrile, obtained from the relaxed scans along the O-H (in NO_2-Bp-OH) stretching

coordinate (step length=0.05 Å). The relative energy values are calculated in comparison to the

corresponding hydrogen-bonded complexes in the S_0 state.

3. Active Spaces for NO$_2$-Bp-OH in the Gas Phase and Methanol Solution

50

51

52

53

54

55

56(H)

57(L)

58

59

60
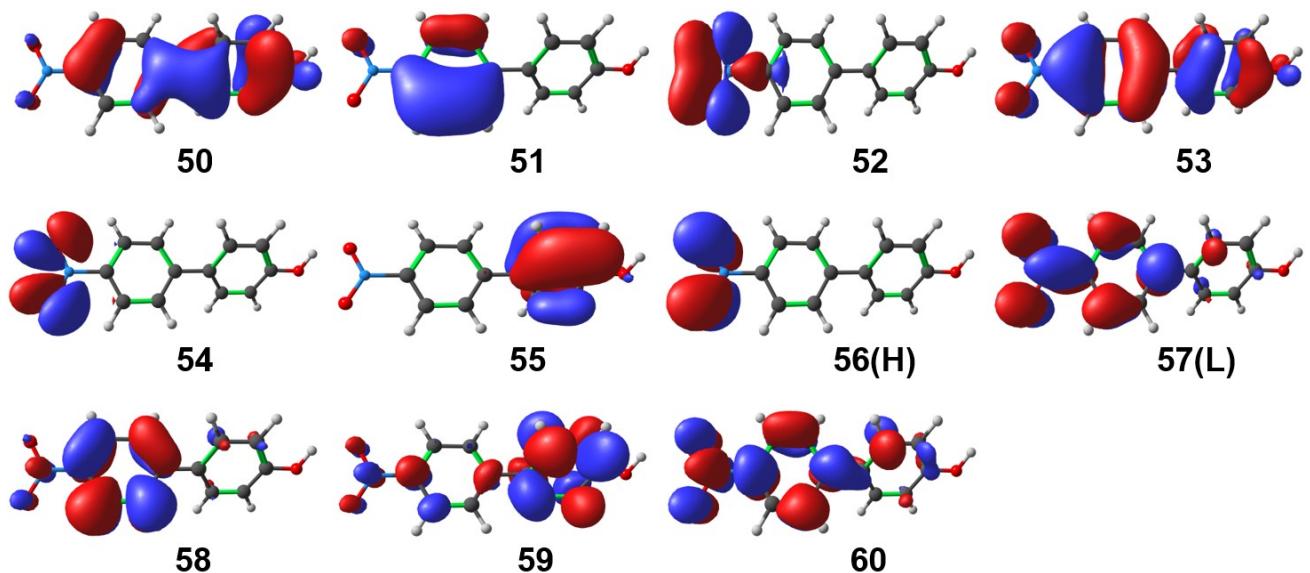
Figure S4. Molecular orbitals of NO$_2$-Bp-OH in the gas phase with the SA8-CASSCF and MS-CASPT2 computations.
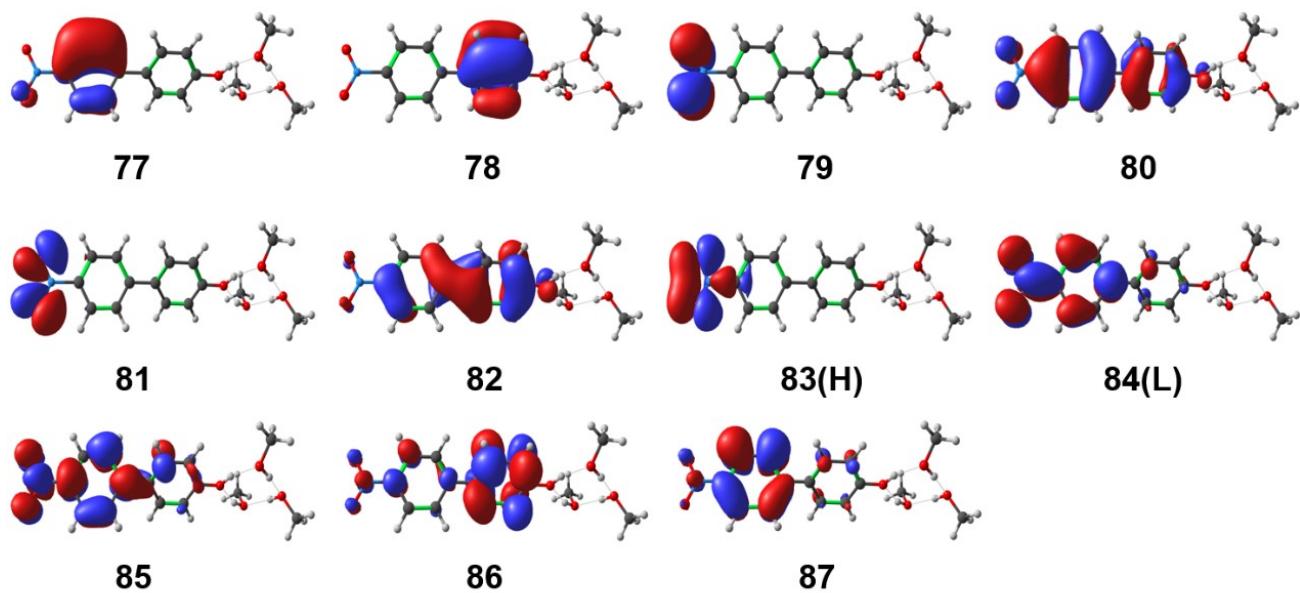
Figure S5. Molecular orbitals of NO$_2$-Bp-OH-methanol complex in methanol solution with the QM(SA8-CASSCF)/MM and QM(MS-CASPT2)/MM computations.

4. The Minima and Intersection Structures of NO$_2$-Bp-OH in the Gas Phase
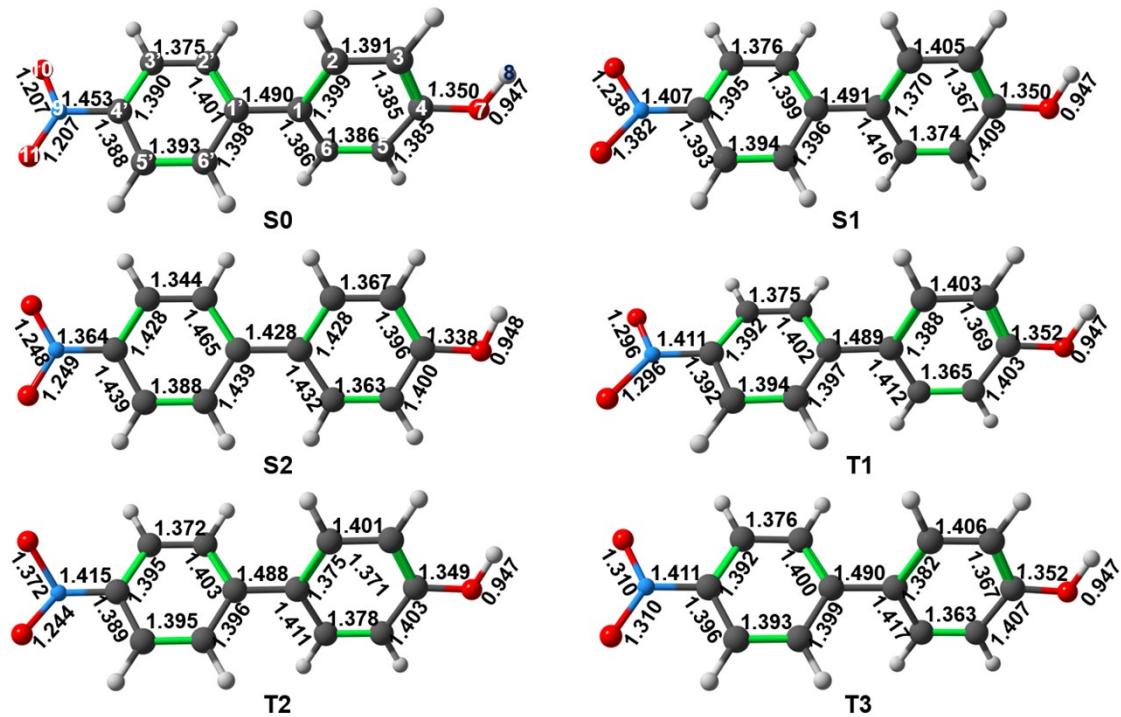
Figure S6. CASSCF optimized minimum-energy structures in the lowest six electronically singlet and triplet states in the gas phase together with the key bond lengths in (Å) and an atom-labeling scheme in S0.
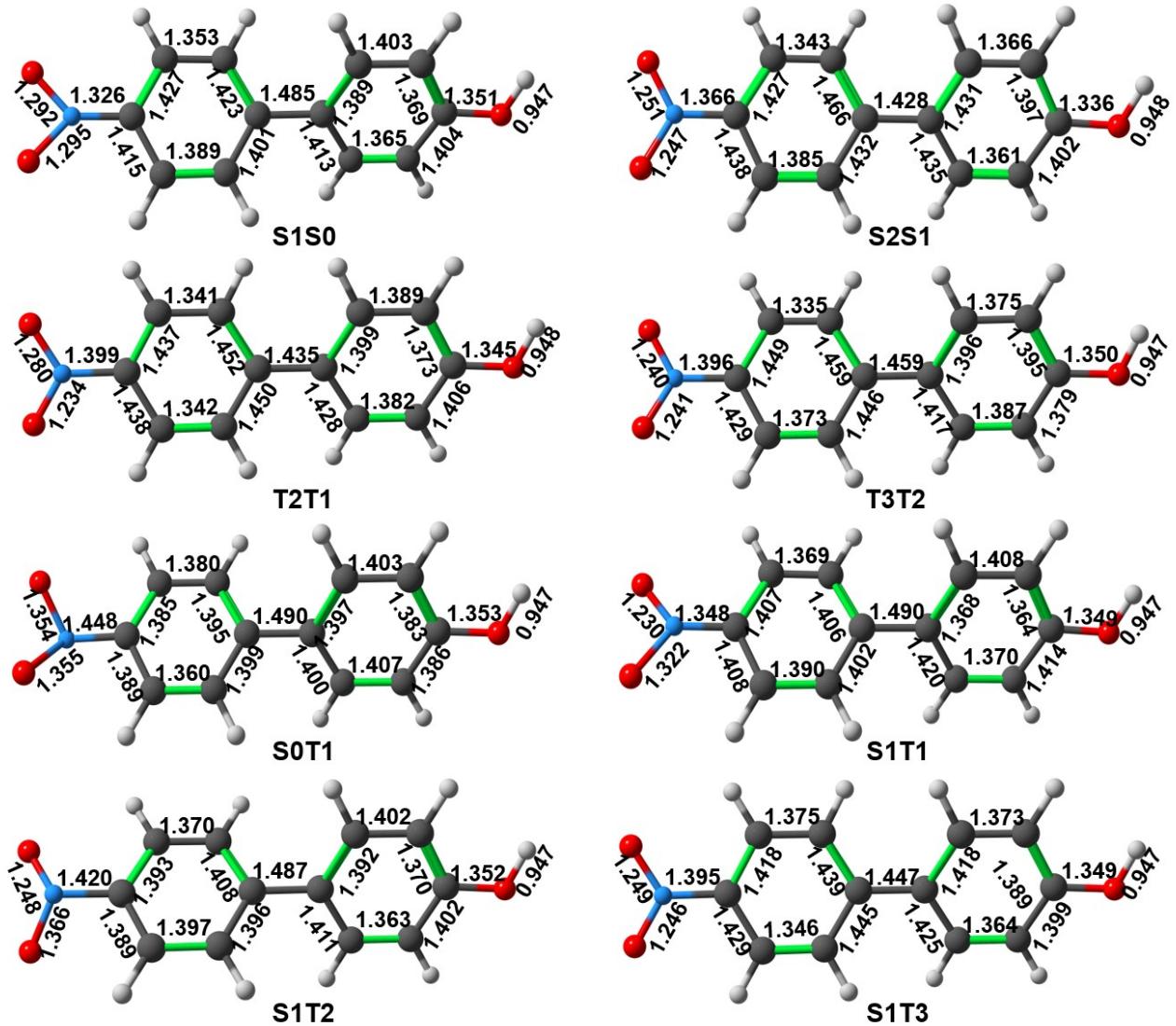
Figure S7. CASSCF optimized intersection structures in the gas phase in the lowest six electronically singlet and triplet states. Also shown are the selected bond lengths.

5. Excited-State Decay Paths of NO_2-Bp-OH in the Gas Phase
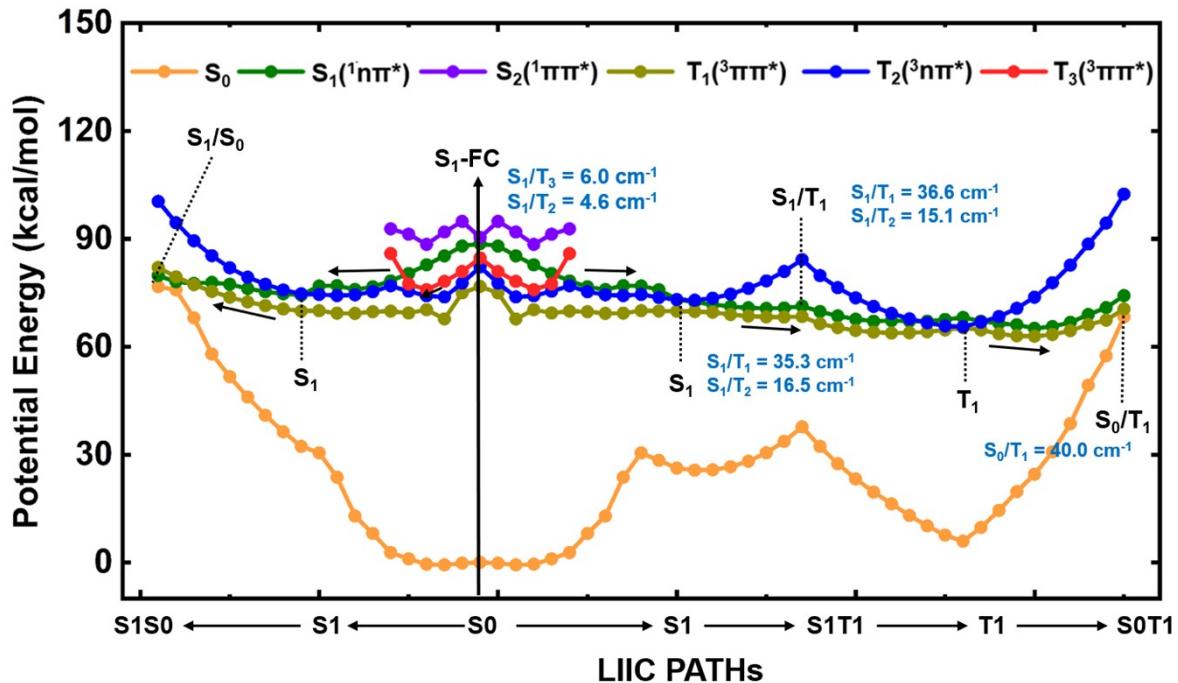
Figure S8. MS-CASPT2 computed LIIC paths of NO_2-Bp-OH connecting the minima and surface-crossing intersections in the gas phase.

6. Cartesian Coordinates for Critical Structures (Unit: Angstrom)

GAS

S0

C	2.148340651	1.145221679	0.403836225
C	0.755559318	1.139238166	0.401752870
C	0.759713048	-1.122839900	-0.403130081
C	2.134501803	-1.137366948	-0.403031580
C	2.822986789	0.000626123	0.001403711
H	2.694136521	2.010815316	0.719827874
H	0.229335101	2.014053087	0.735885895
H	0.229524403	-1.995806928	-0.736632230
H	2.674919841	-2.007193997	-0.717408428
C	-1.451559409	0.006111172	-0.004675620
C	-2.170691505	-1.076033379	0.513518212
C	-2.170945351	1.073114447	-0.520577013
C	-3.561560237	-1.077555335	0.511300779
H	-1.648677887	-1.914218919	0.938064238
C	-3.556853655	1.080872895	-0.530514125
H	-1.647723347	1.912741472	-0.942352416
C	-4.254029800	0.002286956	-0.011927962
H	-4.098026522	-1.916006560	0.922619698

H	-4.103975448	1.908599168	-0.941161581
C	0.037993323	0.009296390	-0.002224201
O	-5.602788713	0.055386829	-0.042118360
H	-5.979518638	-0.729042114	0.331491515
N	4.276199528	-0.007936108	0.003153367
O	4.836424950	-1.018948266	-0.343524619
O	4.847689874	0.996638206	0.351519143
S1			
C	2.146490679	1.141430082	0.369042202
C	0.752974309	1.125279852	0.381156043
C	0.759872182	-1.115068837	-0.460948077
C	2.135767865	-1.128288092	-0.471500458
C	2.832989085	0.003302913	-0.046594210
H	2.676057990	2.018851444	0.689132773
H	0.227753856	1.995023042	0.731187468
H	0.230821607	-1.986080105	-0.802567351
H	2.676772612	-1.992767165	-0.802802866
C	-1.456242072	-0.009174833	-0.013059163
C	-2.160610800	-1.051357965	0.529992166
C	-2.192429879	1.070317142	-0.559617503
C	-3.565855754	-1.061551739	0.548633424

H	-1.636593945	-1.880706945	0.970905867
C	-3.566418878	1.075515753	-0.546537808
H	-1.668265637	1.894114402	-1.009729776
C	-4.262499552	-0.011613895	0.018597172
H	-4.086447907	-1.895425248	0.988569656
H	-4.129146319	1.887442926	-0.967756527
C	0.034718033	0.001256134	-0.031245429
O	-5.610168365	0.058132931	-0.002190265
H	-5.992054678	-0.712916242	0.394135020
N	4.238787294	0.002139564	-0.114640001
O	4.935959629	-1.013768542	-0.232306881
O	4.878746731	0.937966965	0.675239743

S2

C	2.157437324	1.242071742	0.044984315
C	0.769597354	1.228431436	0.036619103
C	0.779693124	-1.229988270	-0.053416834
C	2.124036863	-1.229032481	-0.055594806
C	2.865107409	-0.009846988	0.000338822
H	2.707234007	2.156921588	0.089800326
H	0.267476191	2.173072935	0.092742605
H	0.277310511	-2.173527546	-0.121632269

H	2.664179802	-2.153513803	-0.106467319
C	-1.425719351	0.010335049	0.003465259
C	-2.186253068	-1.188451883	0.160061909
C	-2.194054501	1.210299760	-0.141968572
C	-3.553634437	-1.186172426	0.169152370
H	-1.687367343	-2.125703951	0.297518822
C	-3.556562396	1.207006065	-0.135184409
H	-1.697081783	2.147989203	-0.283133011
C	-4.260847429	0.007758590	0.021151051
H	-4.088506665	-2.111681495	0.298190210
H	-4.113156334	2.117530263	-0.254810969
C	0.002652829	0.011562750	-0.006171741
O	-5.597472461	0.069151184	0.020810922
H	-5.986145382	-0.788768525	0.128216398
N	4.229481485	-0.009327098	0.007839332
O	4.846439577	-1.093561078	-0.027533039
O	4.857131799	1.069505935	0.050122542

T1

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C	0.762812195	-1.127423162	-0.400292727

C	2.137522723	-1.135499995	-0.399050918
C	2.832790596	0.001787788	0.002356791
H	2.676629522	2.017210047	0.717105040
H	0.223158856	2.008051354	0.725723861
H	0.240110240	-2.005710348	-0.732780852
H	2.674115602	-2.008963285	-0.714010332
C	-1.457998126	-0.008400250	-0.001956188
C	-2.178768570	-1.079068797	0.508902198
C	-2.190980187	1.080472440	-0.523356119
C	-3.581826487	-1.078920400	0.508154159
H	-1.661329478	-1.920558728	0.932907110
C	-3.555934818	1.086169647	-0.525846819
H	-1.663488230	1.917581079	-0.944458250
C	-4.263662049	-0.006948632	-0.002631000
H	-4.116070926	-1.920199030	0.916847337
H	-4.110363739	1.912381129	-0.930728598
C	0.030764100	0.000596859	-0.002477269
O	-5.613021779	0.069516486	-0.038267474
H	-6.001908207	-0.711289900	0.330678455
N	4.243741806	-0.002850641	0.003258700
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O	4.944216160	1.028558432	0.356126647

T2

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C	2.134571062	-1.114068522	-0.468536494
C	2.828982123	0.021996903	-0.052181952
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H	0.224005836	2.015291933	0.707695951
H	0.235522225	-1.985924045	-0.784634047
H	2.668717550	-1.979970262	-0.813008161
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C	-2.156568113	-1.072870576	0.483623777
C	-2.192623626	1.094859828	-0.508982755
C	-3.557102236	-1.087567130	0.503820726
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C	-3.570918155	1.094374847	-0.495195428
H	-1.673952922	1.940026021	-0.923947499
C	-4.260072846	-0.014406343	0.019693252
H	-4.075533361	-1.940679089	0.907979654
H	-4.135351378	1.922697196	-0.880565971

C	0.034148924	0.012737931	-0.032039703
O	-5.607896486	0.045374504	0.005716591
H	-5.983155451	-0.745103596	0.368602884
N	4.242385017	0.035202061	-0.114932097
O	4.849833238	-1.162753523	0.164037623
O	4.932775374	0.975472731	0.316445053

T3

C	2.146917545	1.137133554	0.422178429
C	0.753649465	1.123480411	0.416880810
C	0.766969888	-1.119692401	-0.417848199
C	2.142524114	-1.128254241	-0.418180628
C	2.840436197	0.000319131	0.001995030
H	2.677116233	2.007705494	0.753274696
H	0.228366966	1.996311165	0.759607763
H	0.245983530	-1.993728923	-0.764320165
H	2.673129523	-1.999151117	-0.749760642
C	-1.455769787	-0.011081929	0.001283181
C	-2.173631725	-1.067966860	0.527518739
C	-2.188532880	1.072374896	-0.542561322
C	-3.579919507	-1.071190560	0.525011587
H	-1.656085739	-1.902384156	0.965822739

C	-3.551259717	1.077243311	-0.546216301
H	-1.658654482	1.901503198	-0.976211573
C	-4.260319437	-0.009954253	-0.003941481
H	-4.112685769	-1.906686827	0.947009757
H	-4.106932167	1.895690265	-0.964935769
C	0.034331792	-0.001269422	-0.001084750
O	-5.609382638	0.068205714	-0.044223803
H	-6.000044815	-0.705292121	0.338069675
N	4.251723847	-0.002934870	0.001943059
O	4.894451193	-1.082610030	-0.369018304
O	4.898592984	1.074283998	0.372802768

S1S0

C	2.132844356	1.175346957	0.373277149
C	0.743668155	1.153014724	0.370725716
C	0.763249195	-1.142872815	-0.378312149
C	2.116038481	-1.166315965	-0.378327707
C	2.835921865	0.004892482	0.002410842
H	2.671492603	2.058038247	0.660739968
H	0.216448047	2.037084965	0.679258309
H	0.230845457	-2.023213938	-0.689048210
H	2.656221823	-2.047709897	-0.668883678

C	-1.463057256	-0.002493272	-0.001044241
C	-2.182065487	-1.089104199	0.480258183
C	-2.200943351	1.098419428	-0.491539845
C	-3.584712731	-1.093525010	0.479813563
H	-1.664373253	-1.941037601	0.882563075
C	-3.565550726	1.099935209	-0.492420026
H	-1.678190383	1.948047819	-0.892681114
C	-4.270409551	-0.009615992	0.000197309
H	-4.115602737	-1.947815251	0.864966985
H	-4.122546066	1.935242380	-0.874389282
C	0.021521342	0.011050613	-0.001302078
O	-5.619110286	0.064567356	-0.033292144
H	-6.007376725	-0.726520791	0.313751234
N	4.162010883	-0.010490812	0.006611853
O	5.055044778	-0.903552706	-0.264244247
O	5.069606175	0.870681522	0.286005872

S2S1

C	2.155482284	1.231799549	0.052982184
C	0.770279924	1.220337866	0.045677845
C	0.777072448	-1.234302319	-0.054153814
C	2.119964643	-1.237509149	-0.059473723

C	2.861310594	-0.019638710	-0.000202331
H	2.712587264	2.141331275	0.103179356
H	0.270051141	2.166093267	0.107558096
H	0.271910617	-2.176216745	-0.124374630
H	2.655472471	-2.164833455	-0.114720659
C	-1.422795615	0.010466422	0.003432969
C	-2.185479876	-1.189344574	0.164086800
C	-2.191800369	1.211886429	-0.149465103
C	-3.551750064	-1.186037337	0.173093952
H	-1.686515029	-2.125570053	0.305837234
C	-3.552527134	1.209221185	-0.142405540
H	-1.692713393	2.147333293	-0.296584173
C	-4.258372949	0.009043211	0.019794933
H	-4.087911494	-2.110222722	0.305480400
H	-4.109637205	2.118667074	-0.267324217
C	0.005089643	0.011373379	-0.003161210
O	-5.592668812	0.072342726	0.018925500
H	-5.984757673	-0.783441117	0.131957189
N	4.227185845	0.011755080	0.004109231
O	4.844595166	-1.075648767	-0.039467494
O	4.846905718	1.093175171	0.050316226

T2T1

C	2.090966200	1.257816352	0.590041904
C	0.750424283	1.213659289	0.551529130
C	0.827220078	-1.026896075	-0.450873711
C	2.168401517	-1.004824340	-0.437345983
C	2.850461544	0.143327102	0.092269716
H	2.607748345	2.104453161	0.993596903
H	0.209674944	2.048287679	0.952215719
H	0.343819307	-1.884580834	-0.875709336
H	2.742442318	-1.822119990	-0.822667662
C	-1.418077132	0.030811123	0.017965689
C	-2.128605583	-1.160769235	-0.162172353
C	-2.204530951	1.211547438	0.181777465
C	-3.516931063	-1.201717267	-0.180218001
H	-1.604684176	-2.090343258	-0.264690697
C	-3.585392539	1.173794176	0.160125352
H	-1.728751284	2.164851965	0.294221979
C	-4.250234626	-0.052047085	-0.021680064
H	-4.015509680	-2.147172243	-0.312668764
H	-4.167547998	2.068722489	0.271602488
C	0.016526840	0.073787327	0.037158281

O	-5.594658545	-0.019053350	-0.029706524
H	-5.954996639	-0.885656661	-0.160149652
N	4.248486346	0.182703525	0.125544551
O	4.906672944	-0.822564467	-0.315678841
O	4.834546699	1.171502262	0.573278421

T3T2

C	2.148217765	1.227079330	0.213191676
C	0.775568796	1.222898279	0.199625883
C	0.783922806	-1.210153426	-0.214787627
C	2.119064375	-1.229008488	-0.216561228
C	2.852218355	0.001303702	0.006054920
H	2.696704904	2.130515723	0.387633146
H	0.259194689	2.143585755	0.389189208
H	0.258960248	-2.125537424	-0.411122922
H	2.663485871	-2.134828702	-0.392967618
C	-1.445306736	0.009158561	-0.009078919
C	-2.178449349	-1.136878253	0.303099382
C	-2.192843849	1.172635352	-0.318985352
C	-3.553615567	-1.146333973	0.317185705
H	-1.667856879	-2.043451386	0.569827254
C	-3.579575600	1.165947065	-0.308853344

H	-1.689514162	2.078622982	-0.596605115
C	-4.265803820	0.012347012	0.008999781
H	-4.079966464	-2.049344896	0.576715919
H	-4.135717240	2.052044859	-0.553024410
C	0.013806711	0.010855172	-0.004842311
O	-5.614931606	0.054037586	0.007648262
H	-5.980032729	-0.789510675	0.235235088
N	4.248364106	-0.016521559	0.013310009
O	4.870861043	-1.072019940	-0.175241221
O	4.894222425	1.024610923	0.209449075

S0T1

C	2.129815394	1.158077845	0.406295090
C	0.740762591	1.137711913	0.398158831
C	0.757931186	-1.131448841	-0.399689158
C	2.122424396	-1.148851883	-0.402646799
C	2.829196207	0.002617999	0.003381231
H	2.668440462	2.031172680	0.722180511
H	0.211587364	2.014027236	0.725378705
H	0.229523498	-2.007209756	-0.729743353
H	2.661593395	-2.022132507	-0.719021254
C	-1.465680965	-0.007585079	0.001455380

C	-2.182899381	-1.075510509	0.508030395
C	-2.201006471	1.084552079	-0.522193019
C	-3.588513531	-1.080871429	0.505877966
H	-1.665548910	-1.917566939	0.931776470
C	-3.563507170	1.087351109	-0.524665039
H	-1.673799450	1.921884248	-0.942985370
C	-4.271041881	-0.010668981	-0.002538648
H	-4.119454470	-1.925131052	0.912253454
H	-4.120417667	1.912338668	-0.928614397
C	0.022180343	0.004831118	0.000222810
O	-5.619536909	0.066552543	-0.041096863
H	-6.010262355	-0.713921314	0.326652046
N	4.168910582	-0.005176438	0.002812228
O	5.064745348	-0.887688945	-0.299666514
O	5.075533039	0.864699734	0.303480612

S1T1

C	2.139304267	1.129067761	0.438998381
C	0.749865382	1.112547212	0.431486901
C	0.759454423	-1.127044859	-0.440660400
C	2.128300333	-1.147395735	-0.442531084
C	2.834467712	-0.013331012	-0.000799269

H	2.672491361	1.995459322	0.783653254
H	0.220962098	1.978334580	0.785809487
H	0.228631359	-1.990101006	-0.799037458
H	2.670282285	-2.008249944	-0.784218807
C	-1.461208374	-0.014837093	-0.000441630
C	-2.174106529	-1.051779005	0.536553557
C	-2.190032626	1.067897469	-0.559149028
C	-3.582542570	-1.058484639	0.538978749
H	-1.658370647	-1.882058267	0.985695472
C	-3.559557248	1.077304849	-0.561581640
H	-1.657582247	1.888447707	-1.005896914
C	-4.268071365	-0.009615579	-0.000462220
H	-4.109742824	-1.890413526	0.974553809
H	-4.116051336	1.888871917	-0.991880882
C	0.028990970	-0.007837422	-0.003655842
O	-5.614648142	0.068620896	-0.040096215
H	-6.007155550	-0.699214758	0.352071165
N	4.182844131	-0.029942071	-0.005147122
O	5.008152080	-0.882313351	-0.328939541
O	4.976301176	0.958120077	0.371792484

S1T2

C	2.146783547	1.126356473	0.458607732
C	0.750492076	1.125995543	0.431829390
C	0.768318396	-1.145284842	-0.345951505
C	2.138543326	-1.159148323	-0.334639632
C	2.829509015	-0.018574502	0.066774273
H	2.682266964	1.995699272	0.790850049
H	0.225542419	2.007254635	0.751662193
H	0.242786977	-2.020897465	-0.680414038
H	2.681893682	-2.031541977	-0.640917068
C	-1.451225816	-0.009421620	0.012796379
C	-2.183724119	-1.097489622	0.479806684
C	-2.174660736	1.096651759	-0.482430906
C	-3.585737160	-1.091392330	0.458829643
H	-1.675614739	-1.953834652	0.884419662
C	-3.537475364	1.105728477	-0.503937569
H	-1.640915778	1.945498391	-0.870698752
C	-4.256096444	0.000101613	-0.027142602
H	-4.129098757	-1.943221918	0.831861920
H	-4.083602764	1.946293141	-0.890146984
C	0.035367831	-0.005021860	0.033453363
O	-5.604069084	0.082902374	-0.080093326

H	-6.002147554	-0.707667402	0.256744498
N	4.247927566	-0.035187223	0.126817619
O	4.920962444	-1.002607114	-0.282499512
O	4.854952171	1.140862682	-0.210486305

S1T3

C	2.127462153	1.220224087	0.137674008
C	0.781386058	1.208334089	0.132882011
C	0.770613056	-1.222562088	-0.136653008
C	2.145952156	-1.229210089	-0.144533013
C	2.848128206	-0.005622000	-0.005705002
H	2.668709194	2.137533153	0.258005019
H	0.269781018	2.141018155	0.268721017
H	0.261287019	-2.155533154	-0.275198020
H	2.688863195	-2.145106155	-0.265367018
C	-1.435153105	-0.000084002	0.005882001
C	-2.193985157	-1.173011084	0.249963017
C	-2.189914160	1.184586085	-0.234526017
C	-3.567159255	-1.165073086	0.256967017
H	-1.696248122	-2.097795153	0.468149036
C	-3.553543255	1.190213086	-0.231716017
H	-1.684193121	2.104282152	-0.456639034

C	-4.265437306	0.011481003	0.016301004
H	-4.103971294	-2.076894150	0.459403033
H	-4.103041296	2.092097153	-0.428487032
C	0.011903001	-0.007389002	-0.001710999
O	-5.612163406	0.081747005	0.008104000
H	-5.996353434	-0.766495057	0.181203011
N	4.242994306	0.006818999	-0.008027000
O	4.899258351	-1.048940075	-0.130780008
O	4.885800352	1.067437079	0.111183008

Methanol

S0

C	4.570292096	1.385757933	0.506084446
C	3.209220621	1.295604434	0.334197674
C	3.422333544	-0.952758919	-0.476270166
C	4.804046452	-0.883145662	-0.305134175
C	5.363098434	0.289181534	0.184713764
C	1.123758361	0.077593001	-0.360801462
C	0.376558244	-1.046042179	0.022892636
C	0.442396287	1.143732061	-0.920821617
C	-1.000839794	-1.086064060	-0.158284837
C	-0.935265743	1.117797164	-1.103276910

C	-1.656766372	0.003033927	-0.723034852
C	2.601593390	0.136158682	-0.166453683
H	5.015242446	2.282197930	0.889488963
H	2.595761952	2.132487262	0.610908511
H	2.988834436	-1.856023498	-0.864490868
H	5.429223740	-1.719686542	-0.540275911
H	0.864595798	-1.888768621	0.477311629
H	0.984480364	2.017199813	-1.236966928
H	-1.561291853	-1.949517000	0.155759862
H	-1.450026674	1.962781817	-1.523238002
O	-2.987524908	-0.002315029	-0.953850289
H	-3.470252820	-0.610339413	-0.385727706
N	6.799740967	0.365131550	0.390148966
O	7.474651275	-0.567400992	0.030439074
O	7.239270991	1.345898509	0.937242188
C	-4.666423705	0.881430726	-4.029079013
O	-4.875040183	1.309481181	-2.711666401
H	-4.134398911	1.056319314	-2.166780060
H	-5.553716424	1.123843802	-4.597546926
H	-3.817875752	1.387793816	-4.480216672
H	-4.502571326	-0.190830444	-4.086881583

C	-7.615211198	1.179482784	-0.342464703
O	-6.721321571	0.217994049	-0.841853411
H	-6.236101737	0.587247059	-1.576761037
H	-8.351239849	1.454547747	-1.089457161
H	-8.132493765	0.745779520	0.501397602
H	-7.097759787	2.074470423	-0.011812623
C	-5.318102286	-2.678034218	0.711466180
O	-4.863851884	-1.357659425	0.542205000
H	-5.571057076	-0.827404750	0.172103549
H	-5.575572984	-3.134921087	-0.239507888
H	-4.518337522	-3.245562604	1.165623769
H	-6.182806873	-2.711599857	1.364989144
S1			
C	4.493108324	1.408648104	0.500414037
C	3.127846225	1.305351096	0.359082028
C	3.346697240	-0.916008067	-0.506181037
C	4.729136343	-0.844363061	-0.356680023
C	5.298314380	0.324953022	0.148475013
C	1.041879072	0.100940010	-0.360795027
C	0.288044020	-1.025648074	0.038220001
C	0.366306028	1.146203081	-0.944584067

C	-1.074725078	-1.079461077	-0.163088010
C	-1.019441073	1.110776082	-1.146215083
C	-1.735562124	0.007927001	-0.767232053
C	2.519847184	0.158142012	-0.162346013
H	4.923882354	2.313413165	0.887339064
H	2.514271179	2.131472152	0.667252050
H	2.914631208	-1.815286132	-0.906639063
H	5.356282388	-1.673930120	-0.614939042
H	0.778986053	-1.854872136	0.514462036
H	0.907320067	2.016287146	-1.272266093
H	-1.639016116	-1.939793140	0.152922012
H	-1.527025112	1.947273140	-1.591266114
O	-3.061424220	-0.031661003	-1.027480075
H	-3.547420256	-0.610417043	-0.432396033
N	6.691368482	0.420686028	0.243412020
O	7.491914540	-0.516452039	0.162501009
O	7.193161518	1.413050102	1.054663074
C	-4.897550352	0.801252059	-4.047496291
O	-4.964631358	1.314998092	-2.745619196
H	-4.204895301	1.032260075	-2.243032162
H	-5.814480420	1.070003076	-4.553651329

H	-4.061392290	1.224124087	-4.597628329
H	-4.806678346	-0.281125022	-4.052879294
C	-7.613064548	1.340500096	-0.257683020
O	-6.748484488	0.350701024	-0.751622055
H	-6.270240454	0.693335049	-1.503969108
H	-8.322843600	1.654456122	-1.014871072
H	-8.163316588	0.917577067	0.570581040
H	-7.067116508	2.210273159	0.094559005
C	-5.409913391	-2.614249187	0.747654056
O	-4.913675356	-1.311944094	0.558531039
H	-5.618779402	-0.750553053	0.233654018
H	-5.842091423	-3.012347216	-0.165656011
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H	-6.160558441	-2.636303189	1.530129113

S2

C	4.537192324	1.494473107	0.364684025
C	3.211738229	1.394994103	0.172227012
C	3.423444245	-1.022066073	-0.238508018
C	4.807957347	-0.940481070	-0.070476006
C	5.391224390	0.341752023	0.240658017
C	1.145584081	0.051873002	-0.392432027

C	0.404420029	-1.139528081	-0.246384017
C	0.414998029	1.208385085	-0.797255057
C	-0.971882072	-1.177267087	-0.472365034
C	-0.923285064	1.170466085	-1.028097074
C	-1.637353118	-0.029166001	-0.854745063
C	2.569333183	0.130632008	-0.152289010
H	4.977254357	2.437345175	0.623526044
H	2.609408189	2.270100166	0.310330023
H	2.997594214	-1.976557142	-0.481690036
H	5.435118394	-1.799745127	-0.156553009
H	0.888406065	-2.040218144	0.079069003
H	0.931673068	2.134021151	-0.959185068
H	-1.515480111	-2.095510150	-0.334758025
H	-1.456422104	2.051842147	-1.333113094
O	-2.952074213	0.012855001	-1.097442080
H	-3.438848245	-0.760148053	-0.783437059
N	6.729985483	0.441715034	0.423099029
O	7.469152536	-0.582461043	0.296166023
O	7.252302520	1.531268108	0.723226054
C	-4.918957355	1.916324140	-3.577378255
O	-4.957976356	1.866732135	-2.174998156

H	-4.187766299	1.412153104	-1.846951135
H	-5.820713419	2.411129173	-3.910904282
H	-4.062879294	2.484464181	-3.929049283
H	-4.888459351	0.923394069	-4.015810290
C	-7.400910531	0.667387049	0.206761013
O	-6.828591493	0.091540007	-0.941005067
H	-6.319785457	0.751292054	-1.406374102
H	-8.079953582	1.471121108	-0.054320002
H	-7.963542572	-0.102808006	0.715160054
H	-6.643587481	1.054209077	0.881998062
C	-5.160463373	-2.571649186	0.821269057
O	-4.820237349	-1.759696125	-0.272106021
H	-5.579859400	-1.239407091	-0.536231039
H	-6.058239437	-3.141568225	0.614661045
H	-4.348337314	-3.263417235	0.986521073
H	-5.312312383	-1.985305141	1.723254122
T1			
C	4.469571319	1.455410105	0.480211033
C	3.109807224	1.349906095	0.339143026
C	3.330935240	-0.886910065	-0.488963038
C	4.719131342	-0.802438057	-0.339961023

C	5.280173380	0.370999025	0.146340010
C	1.025114076	0.119309006	-0.349594023
C	0.277310019	-0.985950070	0.038546001
C	0.333431023	1.197162088	-0.942492065
C	-1.111301079	-1.032654074	-0.160173010
C	-1.019293073	1.160967084	-1.131368083
C	-1.752854128	0.031208001	-0.740184052
C	2.501684180	0.185125014	-0.162304012
H	4.905038353	2.360743170	0.856854062
H	2.493494178	2.180223157	0.631452045
H	2.905315211	-1.794123127	-0.878094062
H	5.341439384	-1.636713115	-0.593362041
H	0.759809056	-1.822095130	0.510697035
H	0.881493063	2.064966150	-1.263745090
H	-1.670096119	-1.896357134	0.156823011
H	-1.539108113	1.992099142	-1.572717112
O	-3.081478222	0.040599002	-0.995375071
H	-3.577332259	-0.554284042	-0.425118030
N	6.700806480	0.508047037	0.242363016
O	7.434970533	-0.561568040	0.138659007
O	7.177396518	1.342957098	1.121850079

C	-4.812410347	0.803853056	-4.052456291
O	-4.925898356	1.360392097	-2.771998201
H	-4.189960300	1.083826080	-2.231623159
H	-5.691637409	1.088985076	-4.613705332
H	-3.934759285	1.179407085	-4.571429330
H	-4.761389341	-0.280883019	-4.020794288
C	-7.647853550	1.359727096	-0.344047023
O	-6.778202489	0.375371030	-0.840521059
H	-6.279809449	0.732251050	-1.572916115
H	-8.352413601	1.679242122	-1.103739078
H	-8.203370591	0.928479066	0.476491034
H	-7.105025512	2.226784161	0.019036003
C	-5.432929389	-2.590325184	0.709361049
O	-4.965090355	-1.277067090	0.524816040
H	-5.672134407	-0.733674050	0.175094015
H	-5.806829417	-3.013587216	-0.217901014
H	-4.604468332	-3.190199228	1.057459077
H	-6.219468447	-2.624386191	1.454770102

T2

| C | 4.484712324 | 1.441507106 | 0.453227031 |
| C | 3.125297226 | 1.341439095 | 0.308573023 |

C	3.334623241	-0.911517067	-0.486917037
C	4.720588341	-0.838681063	-0.327641025
C	5.285980380	0.342384025	0.141737009
C	1.035119076	0.111631010	-0.361738027
C	0.286565022	-0.992474074	0.027680002
C	0.343001024	1.192056088	-0.950125066
C	-1.102403080	-1.036261073	-0.164929012
C	-1.010546075	1.158346085	-1.133682080
C	-1.745046123	0.030473000	-0.739595052
C	2.511787179	0.172766011	-0.177622011
H	4.922854354	2.353728168	0.813855061
H	2.513669182	2.179764159	0.586367043
H	2.901950210	-1.820836132	-0.862630064
H	5.345748384	-1.678599119	-0.554920039
H	0.768413055	-1.830008134	0.498064035
H	0.890609062	2.059227149	-1.273791092
H	-1.661163120	-1.899380139	0.153403013
H	-1.531479113	1.992196145	-1.568622111
O	-3.073710223	0.043131004	-0.988779072
H	-3.568428259	-0.557557041	-0.423221030
N	6.688081482	0.447790032	0.245797017

O	7.471071539	-0.506818039	0.121525010
O	7.164683516	1.328547094	1.174933082
C	-4.824881345	0.806760059	-4.046267293
O	-4.932804357	1.359515097	-2.763602200
H	-4.193404302	1.083944076	-2.227702162
H	-5.706298413	1.094149079	-4.602732334
H	-3.949265282	1.183278086	-4.567843329
H	-4.774325344	-0.277965019	-4.018051287
C	-7.644828550	1.350440098	-0.319277024
O	-6.767856487	0.373136028	-0.816403060
H	-6.277888451	0.730491054	-1.554044114
H	-8.354182604	1.662749118	-1.077472079
H	-8.194354591	0.915621064	0.503425034
H	-7.108898513	2.222884162	0.041388000
C	-5.422647390	-2.594878188	0.719336051
O	-4.949420359	-1.284860093	0.526692037
H	-5.657570407	-0.737519052	0.185204015
H	-5.813929420	-3.016378218	-0.201724013
H	-4.593104330	-3.200440231	1.054924075
H	-6.198288445	-2.622965186	1.476297107

T3

C	4.514372323	1.454030106	0.540668037
C	3.177300231	1.366758099	0.371375027
C	3.384694246	-0.910050066	-0.496102036
C	4.759453341	-0.843596061	-0.330720022
C	5.332120382	0.348670026	0.184928012
C	1.076974076	0.159209013	-0.389655026
C	0.321173024	-0.986048073	0.051679006
C	0.437226029	1.181385086	-0.995535073
C	-1.099042079	-1.034070072	-0.136284012
C	-0.998564073	1.152800085	-1.180138085
C	-1.735526124	-0.006211001	-0.723202051
C	2.550365185	0.197120012	-0.161825012
H	4.964835355	2.342324171	0.935708066
H	2.557043185	2.196005159	0.655487048
H	2.942903211	-1.806682128	-0.889181067
H	5.389879385	-1.673318121	-0.573110042
H	0.815250057	-1.793216128	0.555359040
H	0.979941071	2.037872148	-1.351562097
H	-1.647508120	-1.889967134	0.216719018
H	-1.529925109	1.996059144	-1.575133113
O	-3.060973218	0.040688005	-0.960271072

H	-3.562631255	-0.575233043	-0.416128028
N	6.749935486	0.424509032	0.392138027
O	7.428972536	-0.515934038	0.050111006
O	7.194369518	1.416601103	0.923429069
C	-4.805928344	0.789402056	-4.040480290
O	-4.915891355	1.347173096	-2.759895197
H	-4.178364301	1.073288076	-2.221122160
H	-5.686611411	1.074696079	-4.599082329
H	-3.929770281	1.164467083	-4.562141327
H	-4.755422344	-0.295078024	-4.007966290
C	-7.655026553	1.334388094	-0.336963022
O	-6.769240486	0.362184028	-0.828693059
H	-6.274059452	0.723182053	-1.560965112
H	-8.361599600	1.642451117	-1.099470078
H	-8.207016591	0.896365066	0.482377035
H	-7.126383513	2.209908159	0.026758001
C	-5.421869388	-2.613156188	0.702663052
O	-4.953286358	-1.300829091	0.513781038
H	-5.662362408	-0.754714053	0.172642014
H	-5.814915420	-3.031509216	-0.219066014
H	-4.588949330	-3.217277233	1.032068073

| H | -6.194463446 | -2.646988193 | 1.462679106 |

S1S0

C	4.465167427	1.704520692	0.544158728
C	3.105904346	1.578039069	0.358086349
C	3.365892954	-0.725957487	-0.248413973
C	4.740858957	-0.625111819	-0.049898515
C	5.278781236	0.599624272	0.343689294
C	1.054359802	0.280695531	-0.296484513
C	0.305225516	-0.819359611	0.087777456
C	0.370043014	1.339241681	-0.948301172
C	-1.078777739	-0.890227747	-0.167369731
C	-0.969523715	1.279558817	-1.186411281
C	-1.707755563	0.148413020	-0.794821503
C	2.523103037	0.372059063	-0.055180492
H	4.883783324	2.642928647	0.860759427
H	2.477830769	2.424869948	0.562542007
H	2.955050941	-1.667283754	-0.564633178
H	5.380325053	-1.473629233	-0.196311980
H	0.773551752	-1.638738626	0.601342801
H	0.918004621	2.206725263	-1.269341092
H	-1.636543249	-1.756239084	0.144465929

H	-1.483736514	2.095168825	-1.662073882
O	-3.025754265	0.140322201	-1.101599868
H	-3.539384546	-0.441600748	-0.533267620
N	6.675775565	0.735502977	0.437441473
O	7.459518446	-0.230719312	0.767884719
O	7.234381986	1.547018006	1.334085696
C	-4.895628602	0.839720684	-4.124987182
O	-4.885484036	1.465274038	-2.870840107
H	-4.142586686	1.155339136	-2.359436134
H	-5.782565343	1.167002281	-4.649236960
H	-4.024285990	1.115223161	-4.712604745
H	-4.929496872	-0.242432227	-4.039524442
C	-7.399918885	1.748650423	-0.226021409
O	-6.713622391	0.677056138	-0.818843795
H	-6.224985131	0.989632281	-1.577456503
H	-8.066250299	2.229828899	-0.932937982
H	-7.991986913	1.352871245	0.586330990
H	-6.716043631	2.491832593	0.173427837
C	-5.446243838	-2.402392769	0.660041010
O	-4.933917545	-1.111322966	0.434429761
H	-5.631803968	-0.534961040	0.121461419

H	-5.889277000	-2.819654898	-0.239580136
H	-4.624671425	-3.033905902	0.967288798
H	-6.191123121	-2.394763499	1.447472955

S2S1

C	4.531130329	1.503674108	0.363537028
C	3.206669230	1.402945102	0.171324013
C	3.425124245	-1.013166074	-0.237168019
C	4.808564345	-0.929070067	-0.070157007
C	5.388064387	0.355250028	0.240047019
C	1.148167085	0.051513003	-0.388927027
C	0.407636030	-1.141179083	-0.241924016
C	0.416538030	1.207756089	-0.793890056
C	-0.967908068	-1.179976083	-0.468043031
C	-0.921216065	1.169246083	-1.026954073
C	-1.633634119	-0.030790004	-0.853129062
C	2.571348185	0.132374012	-0.150291011
H	4.968382356	2.448713177	0.620578045
H	2.601409188	2.275865166	0.310208021
H	3.001784219	-1.968987140	-0.481032036
H	5.440002393	-1.784970128	-0.155432011
H	0.892715066	-2.041131145	0.083235004

H	0.932981067	2.133526154	-0.954643070
H	-1.511491109	-2.097933152	-0.329345023
H	-1.455090107	2.050301146	-1.331319093
O	-2.946718214	0.010512000	-1.093952077
H	-3.434489248	-0.762841057	-0.780852054
N	6.730313483	0.436064030	0.415184029
O	7.464270537	-0.599653043	0.287097020
O	7.251603520	1.519308110	0.715882053
C	-4.916708351	1.916009137	-3.576299258
O	-4.954142355	1.864075136	-2.173855154
H	-4.183765301	1.409490104	-1.847133135
H	-5.818887419	2.410971171	-3.908197281
H	-4.061348294	2.484926179	-3.928231281
H	-4.886162351	0.923949065	-4.016577290
C	-7.399560531	0.665872046	0.207974014
O	-6.825794490	0.090288005	-0.939319066
H	-6.318178457	0.750489054	-1.405065103
H	-8.078590580	1.469393106	-0.053491004
H	-7.962493574	-0.104221009	0.716042050
H	-6.643211479	1.053411078	0.883869064
C	-5.157392373	-2.572159186	0.822233059

O	-4.816308346	-1.759745127	-0.270795022
H	-5.576054403	-1.239939089	-0.535622041
H	-6.055221434	-3.141649226	0.614939042
H	-4.345831311	-3.264483236	0.987661069
H	-5.309419382	-1.986166144	1.724381122

T2T1

C	4.143744298	1.196507088	0.666381046
C	2.827243205	1.079016076	0.344469026
C	3.184822232	-1.127359079	-0.549095041
C	4.538854327	-1.041437077	-0.227199019
C	5.018210363	0.123205010	0.385668030
C	0.850630059	-0.175094015	-0.592412041
C	0.113492010	-1.318506093	-0.312631024
C	0.169307012	0.915289063	-1.175493084
C	-1.256095092	-1.389505101	-0.601569046
C	-1.169131082	0.852715060	-1.454011104
C	-1.893129137	-0.311747022	-1.162576084
C	2.300267164	-0.080937004	-0.273978018
H	4.518235327	2.084786151	1.140032080
H	2.161499156	1.885749136	0.590424044
H	2.821332205	-2.020275147	-1.024195075

H	5.205571374	-1.855221133	-0.436013033
H	0.584377040	-2.165125158	0.153383010
H	0.708740049	1.815160129	-1.411753104
H	-1.808675131	-2.280562164	-0.360116024
H	-1.685270123	1.695918122	-1.875981138
O	-3.209721233	-0.330336024	-1.484292107
H	-3.721559270	-0.860965060	-0.865052060
N	6.327802455	0.223013015	0.726364054
O	7.273516522	-0.606488045	0.562185040
O	6.949078501	1.159638082	1.304621096
C	-5.542572401	0.469111033	-4.124519299
O	-5.159558369	1.195484088	-2.986126213
H	-4.384814317	0.799938059	-2.594479189
H	-6.448780465	0.915682067	-4.508983324
H	-4.779727344	0.511811038	-4.897418354
H	-5.743551412	-0.572716043	-3.891398279
C	-7.759955559	1.369420099	-0.349358025
O	-6.745453487	0.477681032	-0.729011052
H	-6.296671455	0.808979058	-1.504066107
H	-8.491887611	1.492891105	-1.140406082
H	-8.260599597	0.957799068	0.515178040

H	-7.359916530	2.343489171	-0.086243006
C	-5.537760397	-2.671889195	0.469018035
O	-4.967917358	-1.392616102	0.353256024
H	-5.650663405	-0.759829054	0.130636008
H	-5.971082431	-3.003881216	-0.469851034
H	-4.752369340	-3.357937240	0.752906055
H	-6.304871453	-2.691651192	1.235047088

T3T2

C	4.549917328	1.582163112	0.407836027
C	3.222975234	1.461479107	0.240603015
C	3.445142248	-0.949833066	-0.154687014
C	4.808242346	-0.841344062	-0.015799000
C	5.384513385	0.424103031	0.274113021
C	1.145697082	0.106558010	-0.234238018
C	0.430052031	-1.114445080	-0.076261003
C	0.361698026	1.244093088	-0.583696042
C	-0.927557064	-1.186366084	-0.248382016
C	-0.988731071	1.168323087	-0.764029054
C	-1.656521119	-0.048198004	-0.599231046
C	2.574960184	0.197295016	-0.053741003
H	4.990837358	2.529009184	0.650949046

H	2.615842191	2.333655168	0.380375025
H	3.030332220	-1.912428136	-0.382851029
H	5.440338394	-1.699207123	-0.118090010
H	0.949978066	-2.005865143	0.219489017
H	0.839319060	2.191059156	-0.744538054
H	-1.439288101	-2.120609154	-0.092193006
H	-1.557940113	2.040942149	-1.028642074
O	-2.985905213	-0.079524006	-0.840689063
H	-3.464924248	-0.709467049	-0.292812023
N	6.766660488	0.534371039	0.479095036
O	7.502788540	-0.456621031	0.389814028
O	7.275286525	1.626115119	0.779778057
C	-4.597399333	0.939955068	-3.922787285
O	-4.844032349	1.288009095	-2.588388184
H	-4.117157295	1.005413071	-2.039680146
H	-5.469379393	1.213851089	-4.500598326
H	-3.738504271	1.473497108	-4.319714313
H	-4.428764319	-0.126631010	-4.040816291
C	-7.640470548	1.094886080	-0.281517021
O	-6.725477486	0.152634012	-0.779448057
H	-6.233002446	0.538452038	-1.500572108

H	-8.365854603	1.373883100	-1.037743076
H	-8.168188586	0.640494044	0.545124037
H	-7.140120516	1.991063145	0.072940003
C	-5.356681387	-2.714785197	0.861529063
O	-4.874890352	-1.415625104	0.624883045
H	-5.578049402	-0.884327061	0.249067020
H	-5.734908413	-3.172339226	-0.047710002
H	-4.535844324	-3.310588238	1.234970088
H	-6.145170443	-2.709147194	1.606547118

S0T1

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C	2.942155214	1.356113095	0.331670022
C	3.218494230	-0.866579065	-0.524935036
C	4.612975332	-0.734473055	-0.401769031
C	5.137943368	0.443779032	0.082432004
C	0.886071065	0.063286006	-0.333483025
C	0.179776011	-1.075328075	0.028662002
C	0.155601009	1.137882081	-0.881884062
C	-1.208362087	-1.157448081	-0.147120012
C	-1.198766088	1.069325078	-1.050716073
C	-1.892320136	-0.093182007	-0.678533051

C	2.363074169	0.170837011	-0.169429013
H	4.707318338	2.419730177	0.825772059
H	2.301486166	2.160722155	0.643038047
H	2.815908202	-1.783264129	-0.915820066
H	5.256631379	-1.544052110	-0.680858049
H	0.692491048	-1.913554135	0.464320031
H	0.672537049	2.030813146	-1.185117088
H	-1.734622125	-2.046274149	0.154939013
H	-1.749821127	1.899414138	-1.454136106
O	-3.225654231	-0.110216006	-0.900269066
H	-3.691771263	-0.745256052	-0.347784025
N	6.564727471	0.671036048	0.143345010
O	7.296181528	-0.440009030	0.145870011
O	6.972307504	1.165999083	1.309871095
C	-4.837975349	0.859284060	-3.974577285
O	-5.101098365	1.216735090	-2.645461189
H	-4.376773315	0.944207065	-2.087967152
H	-5.691268409	1.154440085	-4.569507327
H	-3.957586282	1.369578101	-4.355492315
H	-4.696574336	-0.211905013	-4.087193295
C	-8.016523576	0.550327040	-0.520886036

O	-6.948889500	-0.227562018	-0.999523074
H	-6.460113463	0.269090018	-1.651676121
H	-8.701974625	0.805522059	-1.321884096
H	-8.549494613	-0.037288004	0.213520014
H	-7.665560551	1.464001107	-0.051605005
C	-5.379591386	-2.905347211	0.766855057
O	-5.053666366	-1.552896112	0.567485041
H	-5.781948418	-1.117258080	0.121841008
H	-5.527652397	-3.423932247	-0.175735012
H	-4.557239326	-3.369142240	1.292973095
H	-6.276969450	-3.007507218	1.367389101

S1T1

C	4.470358322	1.458136104	0.479807033
C	3.098955222	1.357219097	0.326324025
C	3.320065241	-0.892387066	-0.479393037
C	4.704481339	-0.818574057	-0.318218024
C	5.272727380	0.360564026	0.162778012
C	1.015283074	0.129716007	-0.374398026
C	0.260556019	-0.964243071	0.032315002
C	0.340069023	1.188001088	-0.996487073
C	-1.115299082	-1.015919071	-0.181385011

C	-1.018183071	1.151647082	-1.205481088
C	-1.753498126	0.039801003	-0.799785058
C	2.491692181	0.191833013	-0.168943012
H	4.907729351	2.366447171	0.848661060
H	2.485275177	2.192628156	0.607995046
H	2.889981211	-1.800668129	-0.860850060
H	5.325590382	-1.660357120	-0.551315041
H	0.737521052	-1.789300126	0.529907037
H	0.893313062	2.047632145	-1.330853095
H	-1.680217121	-1.870615132	0.148873012
H	-1.527513109	1.976666142	-1.669743121
O	-3.077574222	0.030204003	-1.075567078
H	-3.577506258	-0.557873039	-0.502455036
N	6.676230483	0.470123031	0.263327018
O	7.441570537	-0.553115042	0.228619018
O	7.204280521	1.361904099	1.071750075
C	-4.908218353	0.686307051	-4.110939299
O	-4.951305357	1.314869095	-2.859326205
H	-4.202458302	1.044660073	-2.334206169
H	-5.807448417	0.957988069	-4.646355336
H	-4.048391294	1.013111071	-4.689071338

H	-4.875759351	-0.395614028	-4.021369292
C	-7.608045546	1.509885109	-0.351315023
O	-6.764513489	0.490640038	-0.819963058
H	-6.276041453	0.802664058	-1.578930114
H	-8.305795599	1.827264133	-1.118368082
H	-8.173055588	1.116198080	0.481365037
H	-7.044983506	2.373337170	-0.010961002
C	-5.505520394	-2.551605185	0.645629047
O	-4.976564357	-1.263813090	0.449173031
H	-5.670140409	-0.674752047	0.151380011
H	-5.989134429	-2.926082212	-0.251433019
H	-4.689203336	-3.211817230	0.900898067
H	-6.220658445	-2.561757186	1.460504103

S1T2

C	4.497407323	1.442674105	0.458267032
C	3.139757227	1.356130098	0.304397020
C	3.333851240	-0.901741067	-0.484958034
C	4.716495341	-0.841765060	-0.317226023
C	5.290096379	0.333030023	0.154591010
C	1.043734077	0.142338012	-0.376703027
C	0.286220020	-0.963303072	-0.001430001

C	0.359998028	1.231401089	-0.955692069
C	-1.100478081	-0.996829070	-0.200859015
C	-0.993640073	1.206914089	-1.146462081
C	-1.735090124	0.078837006	-0.770273055
C	2.518210179	0.191775015	-0.183442013
H	4.941578354	2.352702168	0.816540059
H	2.533742182	2.200181156	0.576831041
H	2.894954207	-1.807739128	-0.861435060
H	5.334831383	-1.688573121	-0.538416038
H	0.761377056	-1.807495129	0.463674033
H	0.912892065	2.099245152	-1.268119089
H	-1.666220118	-1.859288136	0.106868007
H	-1.507518110	2.047844150	-1.576183112
O	-3.062352222	0.098567004	-1.026192073
H	-3.563135259	-0.499687037	-0.463670032
N	6.690987480	0.425250028	0.277695022
O	7.469034540	-0.532380036	0.131311011
O	7.167586514	1.293893091	1.206499087
C	-4.819016347	0.791795059	-4.091633293
O	-4.908087356	1.399039102	-2.832286206
H	-4.175416303	1.124304081	-2.287045162

H	-5.683630407	1.096476078	-4.664954334
H	-3.924763280	1.106076078	-4.622523330
H	-4.817845346	-0.292128019	-4.021337287
C	-7.642579552	1.413485101	-0.385118030
O	-6.764974487	0.438370031	-0.885234066
H	-6.270396450	0.798799058	-1.618127114
H	-8.348878602	1.732341122	-1.143471082
H	-8.196047588	0.973815072	0.432343030
H	-7.107078514	2.282608164	-0.016013999
C	-5.429385393	-2.540268181	0.671532046
O	-4.956038355	-1.231712086	0.468000036
H	-5.661778408	-0.685950052	0.119787007
H	-5.810790420	-2.973929212	-0.248097017
H	-4.602207332	-3.140261226	1.022593075
H	-6.212448445	-2.561001182	1.421195102

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C	4.403425317	1.961515142	0.433350033
C	3.091182222	1.772621126	0.220539016
C	3.408071244	-0.657033045	0.152576009
C	4.759415341	-0.482479034	0.347496025
C	5.282979379	0.830891060	0.488549036

C	1.081099076	0.296009021	-0.176530011
C	0.390108029	-0.898697065	0.130751009
C	0.298173023	1.349557097	-0.732057054
C	-0.970362069	-1.030296076	-0.081043004
C	-1.039603076	1.215142086	-0.948951071
C	-1.695971125	0.020385003	-0.615222046
C	2.502923180	0.458693036	0.056037003
H	4.797291345	2.947555214	0.575657041
H	2.451746178	2.632838189	0.217876016
H	3.035434219	-1.656130121	0.032461002
H	5.419062389	-1.324183096	0.395844030
H	0.913096068	-1.726034123	0.571663043
H	0.765862056	2.272252166	-1.018517072
H	-1.467271105	-1.945621139	0.191701015
H	-1.610182115	2.022815145	-1.369733097
O	-3.018796219	-0.056359002	-0.876996062
H	-3.483879250	-0.691365049	-0.324351024
N	6.649110477	1.021815074	0.702870050
O	7.439972533	0.068538005	0.748307055
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C	-4.581110332	0.895176063	-3.973043285

O	-4.935361357	1.218897086	-2.655345193
H	-4.220944305	0.989906072	-2.067109149
H	-5.424070390	1.132563082	-4.607278332
H	-3.723929269	1.473126108	-4.305338308
H	-4.354354314	-0.161293014	-4.083285295
C	-7.958860571	0.394866031	-0.713211052
O	-6.827266492	-0.312166025	-1.153915082
H	-6.330271453	0.224329015	-1.767332127
H	-8.612456620	0.642552046	-1.542720113
H	-8.499484612	-0.242998018	-0.027984004
H	-7.682548553	1.309216095	-0.196618014
C	-5.298654382	-2.767161198	0.928473065
O	-4.921058352	-1.472987109	0.531153038
H	-5.632361408	-1.086485079	0.017916000
H	-5.440454390	-3.422520248	0.074809005
H	-4.508369325	-3.166981227	1.547640112
H	-6.214805449	-2.746491196	1.508714108