

# **Supporting Information: Excited-State Relaxation Mechanisms of 2,2'-(1-Phenyl-1H-1,2,4-triazole-3,5-diyl) diphenol: Single or Double Proton Transfer?**

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### 1. CASSCF Active Space

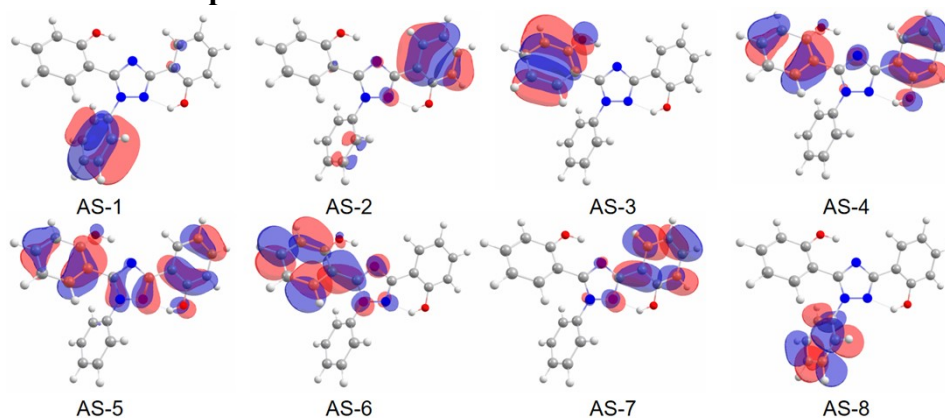


Figure S1. The active space (10e,8o) of ExPh used in the CAS(10,8)/6-31G\* calculations. See text for simulation details.

### 2. OM2/MRCI Active Space

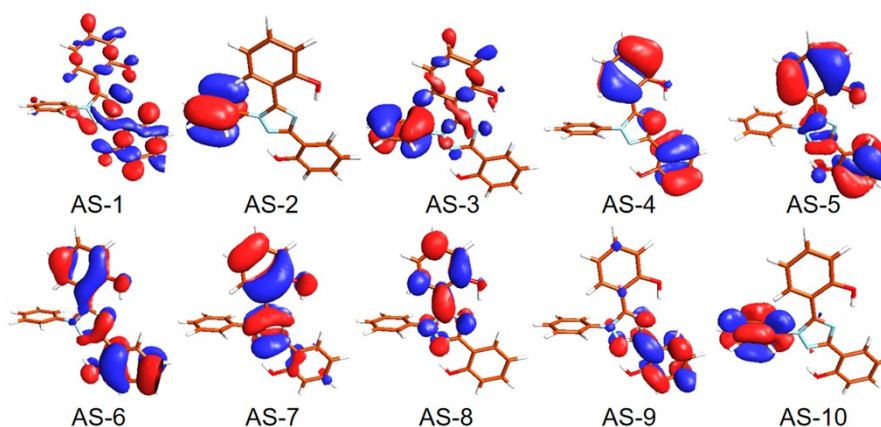


Figure S2. The active space (12e,10o) of ExPh used in the OM2/MRCI calculations. See text for simulation details.

### 3. Molecular orbitals involved in the electronic transitions to the first singlet state

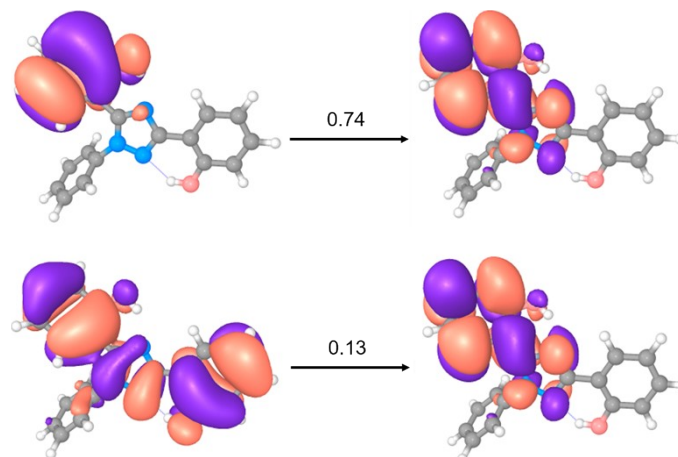


Figure S3. Molecular orbitals involved in the electronic transitions to the first singlet state calculated at the MS-CASPT2//CAS(10,8)/def-TZVP level.

### 4. Structures of Three $S_1/S_0$ Conical Intersections and $S_0$ -ENOL

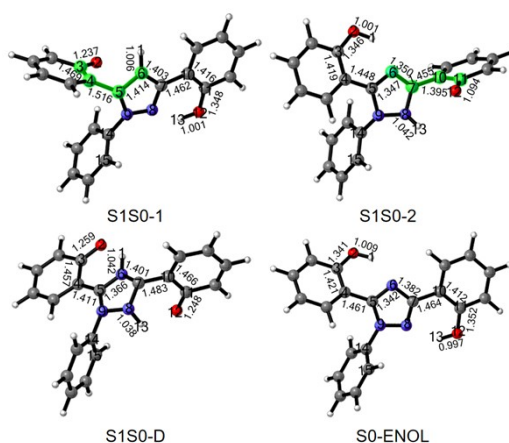


Figure S4. Structures of three  $S_1/S_0$  conical intersections and  $S_0$ -ENOL with selected bond lengths (Å) obtained at the OM2/MRCI level.

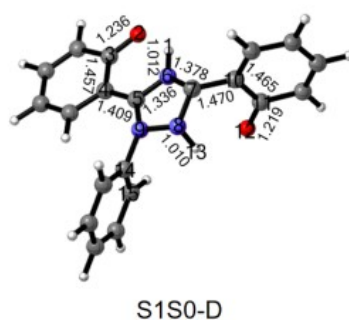


Figure S5. Structure of  $S_1S_0$ -D conical intersection with selected bond lengths (Å) obtained at the CAS(10,8)/6-31G\* level.

## 5. Key Dihedral Angles and Energies (kcal/mol) of All Optimized Structures in the $S_0$ and $S_1$ state

Table S1. Key Dihedral Angles (Degree) of ExPh in Different Structures from OM2/MRCI and CASSCF Optimizations and Relative Energies  $\Delta E$  (kcal/mol) from OM2/MRCI and MS-CASPT2 Single-point Calculations.

structure	N6C5C4C3	N6C7C10C11	C5N9C14C15	$\Delta E$
<b>OM2/MRCI</b>				
S0-ENOL	0	-180.0	-91.1	0
S1S0-1	60.0	-178.6	-95.9	66.0
S1S0-2	1.1	-90.6	-123.1	74.8
S1S0-D	2.9	-66.6	-118.7	81.5
<b>CASSCF</b>				
S0-ENOL	36.1	-175.3	-111.9	0
S0-KETO-1	0.9	177.0	-95.8	16.9

S0-KETO-2	34.1	-178.1	-131.0	27.6
S1-ENOL	21.5	169.7	165.2	77.6
S1S0-1	59.3	178.9	-96.7	66.6
S1S0-2	15.2	91.9	-140.6	69.8
S1S0-D	3.8	66.2	-130.5	92.2

## 6. The $S_1$ Minimum-energy Potential Energy Surface with Respect to the N6-H1 and N8-H13 Reaction Coordinates

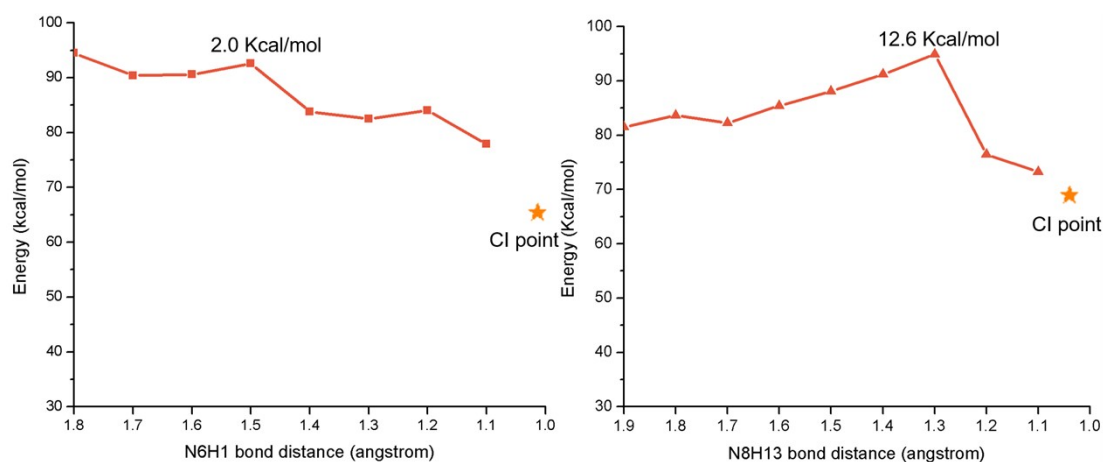


Figure S6. The  $S_1$  minimum-energy potential energy surfaces with respect to the N6-H1 and N8-H13 reaction coordinates computed at the MS-CASPT2//CAS(10,8)/6-31G\* level.

In order to ensure the accuracy of the computational method used for the system, we have performed the calculations of minimum energy paths in the  $S_1$  excited state at MS-CASPT2//CAS(10,8)/6-31G\* level. The calculations show that the energy barrier of proton-transfer process along N6-H1 reaction coordinate is very small (2.0 Kcal/mol), while there is a larger energy barrier (ca. 12.6 Kcal/mol) in the  $S_1$  state along the N8-H13 bond length. Therefore, the MS-CASPT2//CASSCF calculations indicate that the ESIPT-I reaction is more favorable to take place than the ESIPT-II process, which is in good accordance with the results from OM2/MRCI method. Energetically, the two conical intersections involving the proton transfer reaction coordinates are all accessible.

## 7. Cartesian Coordinates of All Optimized CASSCF Structures

### S0-ENOL

C	-3.10645859	2.81451305	1.38024030
C	-2.13576491	1.80630765	1.25255178
C	-1.40900834	1.71748961	0.10264867
C	-1.59687227	2.63205650	-0.94758112

C	-2.54218548	3.62475430	-0.81165641
C	-3.30700353	3.70965724	0.36669174
H	-3.68342600	2.87713153	2.28462026
H	-1.97003939	1.10718948	2.05101456
H	-0.99755183	2.54951185	-1.83514690
H	-2.69601670	4.33302978	-1.60497195
H	-4.04632082	4.48357519	0.46683378
C	-4.05704273	-2.93910876	-0.31074532
C	-2.94026530	-3.41543261	0.39218929
C	-1.76877078	-2.66878988	0.40761935
C	-1.73633120	-1.42405161	-0.23232107
C	-2.86283001	-0.98142096	-0.95411435
C	-4.00732114	-1.73144778	-0.99642174
H	-4.95344202	-3.53207790	-0.32810910
H	-2.95123347	-4.36475513	0.89150833
H	-2.81939075	-0.04254637	-1.47172984
H	-4.86207340	-1.38704824	-1.54892235
C	3.59387927	-1.42842539	-0.26982360
C	4.97636771	-1.57939360	-0.25371330
C	5.77099399	-0.46759594	-0.03959799
C	5.21261255	0.78155799	0.15383553
C	3.83128089	0.94130454	0.13637622
C	3.00853345	-0.16855988	-0.07298780
H	2.95607618	-2.27440359	-0.43741282
H	5.41720727	-2.54722383	-0.40606025
H	6.84193263	-0.57028440	-0.02375558
H	5.82198517	1.64989362	0.31919620
C	-0.48874486	-0.61144811	-0.16956542
C	1.53662505	-0.05484513	-0.08816734
N	-0.40778398	0.70526287	-0.03897430
N	0.89788908	1.06231591	-0.00060328
N	0.70425909	-1.12644825	-0.19572132
O	3.37089558	2.18522854	0.32882119
O	-0.72565029	-3.19468461	1.05213279
H	2.42018831	2.21744509	0.28689480
H	0.08052353	-2.74636373	0.81072136
S1-ENOL			
C	-3.23464217	2.15783479	2.33596337

C	-2.50290040	1.25296970	1.59160627
C	-1.50719112	1.71775889	0.69804428
C	-1.28535941	3.11721106	0.58813310
C	-2.03583334	3.98543402	1.32709375
C	-3.02032146	3.51790933	2.20995519
H	-3.97767321	1.79091860	3.02022110
H	-2.67095938	0.20400765	1.71014194
H	-0.52283156	3.46900863	-0.07522797
H	-1.86337980	5.04232576	1.23526482
H	-3.59920413	4.21453420	2.78746977
C	-3.81600488	-3.29710105	-0.61689172
C	-2.57404398	-3.76472944	-0.18538838
C	-1.54185741	-2.89405513	0.05347989
C	-1.73987131	-1.47589870	-0.12414564
C	-3.02382520	-1.03990346	-0.58178391
C	-4.03093540	-1.93857768	-0.82544577
H	-4.60784568	-4.00066077	-0.79908778
H	-2.39628035	-4.81431391	-0.04312135
H	-3.17868130	0.00316025	-0.77306395
H	-4.98346703	-1.59166756	-1.18258702
C	3.47490170	-0.77543767	-0.12744861
C	4.81280799	-0.76780086	-0.40019920
C	5.34642385	0.28086371	-1.19539724
C	4.55069366	1.26950356	-1.67826295
C	3.16604921	1.27602806	-1.39312396
C	2.61487036	0.25174520	-0.61812934
H	3.03659482	-1.55303522	0.46587038
H	5.45701669	-1.54119313	-0.02612321
H	6.39831692	0.29236268	-1.41938921
H	4.93946328	2.06770338	-2.28170665
C	-0.70467536	-0.58036307	0.18087173
C	1.20456168	0.20321666	-0.30747979
N	-0.79218837	0.85758620	-0.05227786
N	0.41945954	1.23564535	-0.59007942
N	0.62939705	-0.86266286	0.25569271
O	2.47653680	2.28110928	-1.90578903
O	-0.37368513	-3.38279344	0.46221218
H	1.55238100	2.21993829	-1.65142637
H	0.29956189	-2.69843112	0.46157213
S0-KETO-1			
C	-2.96352607	2.84519188	1.42922488
C	-2.05227349	1.81014946	1.38860563
C	-1.50013872	1.43335397	0.16678689

C	-1.84987306	2.09958841	-1.00539362
C	-2.76088314	3.13392273	-0.94998165
C	-3.32265457	3.50935237	0.26366800
H	-3.39489980	3.13728532	2.36930604
H	-1.76657423	1.29000162	2.28403921
H	-1.40978696	1.79963791	-1.93830020
H	-3.03627339	3.64924518	-1.85205546
H	-4.03307110	4.31478670	0.30097386
C	-4.02684673	-3.52410316	-0.30390308
C	-2.79653559	-4.05563096	-0.24937237
C	-1.60832581	-3.22672111	-0.13798452
C	-1.84080285	-1.78964761	-0.08013961
C	-3.19285480	-1.28166724	-0.14810092
C	-4.24442372	-2.10182643	-0.25529137
H	-4.88139820	-4.17398056	-0.38817031
H	-2.62989692	-5.11599556	-0.28765063
H	-3.35971843	-0.22465381	-0.11566467
H	-5.24448474	-1.71348838	-0.30722674
C	3.48260155	-1.80613680	0.25476119
C	4.84768090	-1.96531754	0.30938430
C	5.65671983	-0.83390015	0.34646222
C	5.10356105	0.42467542	0.33108380
C	3.72029784	0.58812768	0.27740238
C	2.89667230	-0.53909627	0.23614251
H	2.85859414	-2.68056798	0.22807723
H	5.27791676	-2.94905418	0.32334351
H	6.72593284	-0.93990491	0.38885471
H	5.71349254	1.30773024	0.36061069
C	-0.70790043	-0.97004977	0.03219606
C	1.42848895	-0.41144068	0.17158551
N	-0.54314402	0.37925837	0.11904462
N	0.77159221	0.71179456	0.20373381
N	0.55786030	-1.44917925	0.06944871
O	3.27213153	1.84841079	0.26781130
O	-0.48599976	-3.74525316	-0.09737187
H	2.32118330	1.89113172	0.25146884
H	0.67933104	-2.45144181	0.01448179

S0-KETO-2

C	-3.17239265	2.70564162	1.28076065
C	-2.27100665	1.67430506	1.12842428
C	-1.35660237	1.72215461	0.07659588
C	-1.33657448	2.80463563	-0.80136284
C	-2.23490870	3.83564992	-0.62266477

C	-3.15940555	3.79061944	0.41313185
H	-3.88006165	2.67263480	2.08881136
H	-2.26559504	0.84396089	1.80845313
H	-0.62728660	2.82800362	-1.60817591
H	-2.21930042	4.67341973	-1.29529021
H	-3.85973546	4.59440758	0.54563135
C	-4.08121292	-2.93826596	-0.26002888
C	-2.98166248	-3.42713498	0.40647867
C	-1.79243691	-2.70103280	0.42947560
C	-1.73825286	-1.45124877	-0.19285690
C	-2.85853498	-0.98888966	-0.88611518
C	-4.02498082	-1.71743762	-0.92581077
H	-4.98761829	-3.51656543	-0.27693481
H	-3.00257686	-4.37748570	0.90536097
H	-2.80723508	-0.04934556	-1.40324840
H	-4.87627542	-1.34817119	-1.46644273
C	3.70310723	-1.50149568	-0.16224890
C	5.04231627	-1.54807034	-0.13566033
C	5.77997571	-0.31404649	-0.06155090
C	5.17714244	0.88753167	-0.01828263
C	3.73142919	1.00658449	-0.04590640
C	3.00797050	-0.24342531	-0.11936103
H	3.12145565	-2.40361063	-0.22139809
H	5.57022735	-2.48288843	-0.17043817
H	6.85585935	-0.36242758	-0.04061931
H	5.73711282	1.80280234	0.03635798
C	-0.48378347	-0.66823267	-0.14541304
C	1.61440447	-0.18215515	-0.13380686
N	-0.40172707	0.68204852	-0.08997707
N	0.91798479	0.96822617	-0.12005807
N	0.71114257	-1.21153777	-0.16247184
O	3.16403241	2.10862409	-0.00639676
O	-0.75966934	-3.25424480	1.07405656
H	1.35287987	1.87030825	0.00426721
H	0.06151945	-2.84197792	0.82050732
S1S0-1			
C	-2.720615407	2.526458010	1.811142610
C	-1.721768452	1.674982531	1.362238200
C	-1.361006387	1.720154133	0.002974601
C	-1.973089740	2.619176558	-0.881990495
C	-2.982672284	3.448745246	-0.410028700
C	-3.362567472	3.403399217	0.932470168
H	-3.002127596	2.521548531	2.872575004



H	-1.194510407	1.013492555	2.052455940
H	-1.650799639	2.646734723	-1.926227200
H	-3.474485248	4.151870619	-1.093174827
H	-4.151024311	4.066363762	1.297880224
C	-3.888675678	-2.681292780	0.894950697
C	-2.851277753	-2.320314266	1.718056364
C	-1.678708580	-1.610309277	1.170668226
C	-1.671875160	-1.268472929	-0.269230557
C	-2.717271944	-1.658537660	-1.024968203
C	-3.833346916	-2.372734458	-0.461235621
H	-4.766113534	-3.206977650	1.287874604
H	-2.855023994	-2.535787045	2.787946322
H	-2.733108515	-1.419904984	-2.091494298
H	-4.661082217	-2.663283550	-1.116778968
C	3.718810358	-1.400272662	-0.622151734
C	5.102669016	-1.512405527	-0.493890207
C	5.860366131	-0.426383092	-0.048117034
C	5.251158057	0.783059925	0.266601387
C	3.854486727	0.900743505	0.139198498
C	3.078984803	-0.197037752	-0.304890864
H	3.134256223	-2.256534892	-0.981514532
H	5.596202203	-2.455511025	-0.743215582
H	6.947235393	-0.527236449	0.052643913
H	5.824744099	1.643815029	0.604435414
C	-0.546591091	-0.494584668	-0.941519147
C	1.627329845	-0.054165636	-0.432612043
N	-0.330749756	0.865916514	-0.508995069
N	0.961497577	1.072936035	-0.210515018
N	0.751747163	-1.060748189	-0.883180593
O	3.355442603	2.110517670	0.459771134
O	-0.735067363	-1.374346130	1.921743709
H	2.362801643	2.130882453	0.348183834
H	0.965349882	-2.040532486	-0.816663251
S1S0-2			
C	-3.53169634	-0.20424871	0.48429185
C	-2.60038510	0.80928716	0.47235525
C	-1.25165460	0.52975575	0.27229091
C	-0.84135596	-0.79741567	0.05359459
C	-1.81106082	-1.80911788	0.09104514
C	-3.13952493	-1.52725697	0.30242672
H	-4.56804700	0.03219126	0.64712644
H	-2.88304201	1.83369897	0.62617438
H	-1.50443791	-2.82833879	-0.03892078

H	-3.86270140	-2.32106954	0.32987587
C	4.73618875	0.33899877	-0.91023933
C	6.01310281	0.79054170	-0.62233327
C	6.63017110	0.46342978	0.60116351
C	5.99312560	-0.31499519	1.51186248
C	4.66609830	-0.83724089	1.25012073
C	4.04006762	-0.42854067	0.00205194
H	4.27245688	0.60505715	-1.84266042
H	6.53363345	1.40653975	-1.33223530
H	7.61772029	0.83615546	0.80645602
H	6.44300051	-0.58269654	2.44963071
C	0.56290831	-1.11264870	-0.17832481
C	2.67728640	-0.91270410	-0.24174970
N	1.02343592	-2.34059660	-0.65942802
N	2.43266591	-2.19669418	-0.72846743
N	1.54498548	-0.29632202	0.07452570
O	4.10373981	-1.61633116	2.00862889
O	-0.41667342	1.57156287	0.29156985
H	2.88466342	-2.90585088	-0.17560854
H	0.49195450	1.27805263	0.29795758
C	0.46237677	-2.94730618	-1.83705602
C	0.27618748	-4.32438945	-1.84083394
C	0.14784850	-2.19478193	-2.96979854
C	-0.22779061	-4.95189051	-2.97713522
H	0.52147603	-4.89154630	-0.96149959
C	-0.36532188	-2.82995472	-4.09443046
H	0.29737385	-1.13047861	-2.96759631
C	-0.54977082	-4.21145659	-4.09453087
H	-0.37019361	-6.01752902	-2.97588629
H	-0.61528283	-2.25245738	-4.96578176
H	-0.94534636	-4.69830447	-4.96775558

S1S0-D

C	-1.68424937	1.63023097	3.34870416
C	-1.07698772	0.74525872	2.43983951
C	-1.15323397	1.00193514	1.09836029
C	-1.80244575	2.15328596	0.62032483
C	-2.38065786	3.02023548	1.50387995
C	-2.32816182	2.75791045	2.88618385
H	-1.63585451	1.42259544	4.40191746
H	-0.56854165	-0.13313708	2.79402931
H	-1.83362646	2.32914679	-0.43880073
H	-2.88089498	3.90124315	1.14468097
H	-2.78983977	3.43924937	3.57770493

C	-3.84325696	-3.82903065	0.73875855
C	-2.68272514	-4.33270394	0.28033945
C	-1.54128842	-3.48442284	-0.01118881
C	-1.71829333	-2.06708829	0.27515446
C	-2.98551845	-1.58975447	0.74155635
C	-4.01796132	-2.42642566	0.96819424
H	-4.66896132	-4.49256490	0.93266241
H	-2.55036602	-5.38250263	0.09529149
H	-3.12631319	-0.53915453	0.89909410
H	-4.96533844	-2.05186414	1.30881378
C	3.43606199	-0.72346028	-2.19977527
C	4.80991188	-0.89456354	-2.27802265
C	5.58101720	-1.07082062	-1.10252227
C	5.00079074	-1.06169040	0.11812021
C	3.56362822	-0.86392974	0.26093505
C	2.79816886	-0.73052100	-0.98066456
H	2.86057309	-0.59547433	-3.09842271
H	5.29447670	-0.90120769	-3.23630066
H	6.64316971	-1.21091514	-1.19416991
H	5.56450319	-1.19341390	1.02258186
C	-0.63066022	-1.21003349	0.01613179
C	1.34153555	-0.57748178	-0.85001104
N	-0.52249462	0.14373291	0.15277897
N	0.77593472	0.56618163	-0.25905567
N	0.50776214	-1.63020219	-0.54188938
O	3.01636268	-0.77715380	1.34619324
O	-0.50265410	-3.96872818	-0.47426678
H	1.30348797	0.81395509	0.56539311
H	0.57518889	-2.60712312	-0.79845460

## 8. Cartesian Coordinates of All Optimized OM2/MRCI Structures

S0-ENOL

C	-2.9008600921	3.1522809236	1.3595839215
C	-1.9264268138	2.1585919319	1.3241034815
C	-1.4187804943	1.7840787225	0.0744951539
C	-1.8335215301	2.3792544673	-1.1226845906
C	-2.8092434323	3.3698828975	-1.0532559290
C	-3.3384363117	3.7497161973	0.1788770459
H	-3.3162704141	3.4669955382	2.3212653672
H	-1.5616712598	1.6860108251	2.2365782446
H	-1.3979624605	2.0748382951	-2.0748447542
H	-3.1532610876	3.8541633999	-1.9717159753

H	-4.1030892460	4.5328433190	0.2204685642
C	-4.0526491620	-2.9915815786	-0.4562458562
C	-2.8109143381	-3.6038085082	-0.4643236685
C	-1.6518928615	-2.8068287593	-0.3484076771
C	-1.7654704610	-1.3955527328	-0.2254183105
C	-3.0335142211	-0.8022232663	-0.2200542718
C	-4.1668365571	-1.5998786854	-0.3350329693
H	-4.9595275473	-3.6006198828	-0.5456191656
H	-2.6972302220	-4.6821687243	-0.5572913663
H	-3.1348609459	0.2815170908	-0.1261406969
H	-5.1572775154	-1.1360166280	-0.3307916749
C	3.6139705842	-1.4842395217	-0.0290308927
C	5.0009105203	-1.6047113813	0.0127407923
C	5.8067773243	-0.4709890505	0.1454986166
C	5.2447378784	0.7956424855	0.2383367362
C	3.8431956272	0.9256120912	0.1968803873
C	3.0254123511	-0.2175381503	0.0628078994
H	2.9809569384	-2.3694646641	-0.1328411011
H	5.4611841793	-2.5943699591	-0.0589892320
H	6.8972281070	-0.5818646195	0.1768782513
H	5.8545796822	1.6914098828	0.3422099235
C	-0.5327114601	-0.6198829699	-0.1086270440
C	1.5667277597	-0.0965358138	0.0183351477
N	-0.3916259257	0.7742597600	0.0224343949
N	0.8918206085	1.0785840038	0.0986412172
N	0.6951890558	-1.1607983409	-0.1107379124
O	3.3899574701	2.1951827901	0.2941225221
O	-0.4913372465	-3.4789008579	-0.3649467364
H	2.3942365173	2.2221856617	0.2587834063
H	0.2946140462	-2.8527871641	-0.2785982730
S1S0-1			
C	-2.7427744336	2.5215342209	1.8099927690
C	-1.7450977594	1.6589173212	1.3779138848
C	-1.3650210082	1.7047087567	0.0256350211
C	-1.9454299395	2.6117179629	-0.8737971966
C	-2.9524344105	3.4504870417	-0.4165047495
C	-3.3575026471	3.4050711191	0.9200300604
H	-3.0431973110	2.5183533566	2.8658213751
H	-1.2343622134	0.9873812289	2.0698725561
H	-1.6066362652	2.6401334461	-1.9130760719
H	-3.4282868636	4.1593021490	-1.1050229747
H	-4.1476445954	4.0747036688	1.2733703995
C	-3.8971525368	-2.6717575788	0.8904537368

C	-2.8683392487	-2.3301034476	1.7235038299
C	-1.6923123667	-1.6293930848	1.1868962801
C	-1.6774612385	-1.2842073203	-0.2408215143
C	-2.7366147280	-1.6564868436	-1.0209472848
C	-3.8395798883	-2.3502776496	-0.4768895569
H	-4.7799891904	-3.1938486511	1.2753509270
H	-2.8843268311	-2.5528511060	2.7927089187
H	-2.7375025795	-1.4039654536	-2.0850819874
H	-4.6744073152	-2.6320943207	-1.1290366532
C	3.7312406195	-1.3940801845	-0.6405553936
C	5.1136187069	-1.5003237069	-0.5077920163
C	5.8673801541	-0.4118471812	-0.0587188682
C	5.2546091788	0.7954400987	0.2545193735
C	3.8571562617	0.9097857010	0.1197834627
C	3.0869953361	-0.1904167386	-0.3277173547
H	3.1506932551	-2.2544112906	-0.9975222557
H	5.6120265986	-2.4427511892	-0.7546491322
H	6.9537532510	-0.5120902482	0.0471020085
H	5.8241627624	1.6572761263	0.5978045314
C	-0.5429397418	-0.5157330239	-0.8900623209
C	1.6364449445	-0.0563229595	-0.4464101934
N	-0.3307071670	0.8295839515	-0.4470744782
N	0.9605684425	1.0732017070	-0.2284150775
N	0.7567538014	-1.0723338098	-0.8491048087
O	3.3551048032	2.1194491564	0.4368984148
O	-0.7416259826	-1.3862849106	1.9395503425
H	2.3606986089	2.1397886508	0.3247338833
H	0.9796620348	-2.0518312945	-0.8013253375

S1S0-2

C	-3.539254779	-0.227618697	0.454594623
C	-2.575798414	0.733448715	0.722992754
C	-1.221422039	0.428615039	0.499667184
C	-0.840525795	-0.846016512	0.006192590
C	-1.840420780	-1.802390539	-0.245885304
C	-3.170581885	-1.492002272	-0.019192587
H	-4.598937409	0.005890495	0.610549621
H	-2.838373456	1.718689103	1.103266209
H	-1.560698940	-2.792980608	-0.616241794
H	-3.944859044	-2.240122425	-0.213877100
C	4.742328600	0.362742960	-0.969318700
C	6.007812071	0.866333771	-0.675402471
C	6.629583643	0.601953202	0.558578174
C	6.013236445	-0.183533135	1.511243267

C	4.703454571	-0.750392552	1.263116698
C	4.074414971	-0.400034650	-0.011815053
H	4.267099502	0.585905066	-1.928580111
H	6.526952996	1.486549140	-1.414462581
H	7.621960502	1.025284976	0.752749944
H	6.475548619	-0.388150522	2.477755582
C	0.564634265	-1.135808225	-0.188772955
C	2.723040784	-0.890572456	-0.234202629
N	1.111432483	-2.376102542	-0.672467289
N	2.459333550	-2.193055030	-0.750711314
N	1.564033830	-0.276382304	0.086915428
O	4.144923785	-1.545042117	2.043755026
O	-0.367181368	1.430820146	0.778743510
H	3.043206752	-2.952544691	-0.340416582
H	0.585577124	1.134982671	0.697265262
C	0.510075172	-2.999316092	-1.836266060
C	0.038578262	-4.309577055	-1.706256740
C	0.404549946	-2.297282038	-3.041516117
C	-0.549405846	-4.921610639	-2.808822575
H	0.145220080	-4.835135841	-0.754719494
C	-0.194162647	-2.929627898	-4.126618210
H	0.778965857	-1.274422289	-3.116740000
C	-0.665964004	-4.234771061	-4.015446338
H	-0.918027201	-5.949802577	-2.732514972
H	-0.294795978	-2.397061006	-5.078629644
H	-1.127372101	-4.726751943	-4.877632875

S1S0-D

C	-0.7326453626	1.5526675790	3.0903977241
C	-0.3530197663	0.8226536417	1.9674797111
C	-1.0904649450	1.0028481571	0.7896621125
C	-2.1682426248	1.8898590818	0.7073002578
C	-2.5230981749	2.6052081690	1.8474005327
C	-1.8106798762	2.4329956376	3.0316013935
H	-0.1787786822	1.4284567317	4.0261037425
H	0.4921825296	0.1350216089	1.9974514217
H	-2.7055844613	2.0101300116	-0.2351469460
H	-3.3650678805	3.3036371497	1.8110457677
H	-2.1010698184	2.9961497760	3.9261280204
C	-3.8301099170	-3.7572456925	0.9070894448
C	-2.6980881076	-4.2829545818	0.3577797222
C	-1.6313127387	-3.4168276405	-0.0975376978
C	-1.8387755375	-1.9848082325	0.0736117650
C	-3.0272827452	-1.4809017893	0.6642648730

C	-4.0015870589	-2.3523216652	1.0765806678
H	-4.6506670416	-4.4180919216	1.2252575824
H	-2.5522576445	-5.3549209558	0.2282059929
H	-3.1544468927	-0.3999825281	0.7951456821
H	-4.9178325039	-1.9836485348	1.5441058152
C	3.5742924047	-0.7713867388	-2.0931473795
C	4.9328230586	-0.9164341048	-1.7823318084
C	5.3797325840	-1.0138057227	-0.4549043388
C	4.4887809739	-0.9232816702	0.6002626327
C	3.0737338989	-0.7479030194	0.3354452200
C	2.6456581175	-0.7037913546	-1.0662764611
H	3.2486681708	-0.7170303288	-3.1338761788
H	5.6651314325	-0.9703021773	-2.5969404303
H	6.4456145470	-1.1695661431	-0.2615888095
H	4.8074175558	-1.0465981084	1.6362284071
C	-0.7824975020	-1.1551030092	-0.3595462025
C	1.1908532249	-0.5710150420	-1.3219935103
N	-0.7118735627	0.2708270717	-0.3975058028
N	0.5051917292	0.6143345691	-0.9456902429
N	0.3488221575	-1.6302637772	-0.9603181979
O	2.2440804305	-0.5290972473	1.2410963749
O	-0.5732223005	-3.8608424698	-0.6145409221
H	1.0529281393	1.3326168363	-0.4345806003
H	0.4849423999	-2.6596868888	-1.0496411880