

SI: Excited-State Proton Transfer in 4-2'-Hydroxyphenylpyridine: Full-Dimensional Surface-Hopping Dynamics Simulations

Wei-Wei Guo, Xiang-Yang Liu, Wen-Kai Chen, and Ganglong Cui*

Email: ganglong.cui@bnu.edu.cn

Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, China

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1. Active Orbitals in CASSCF Computations

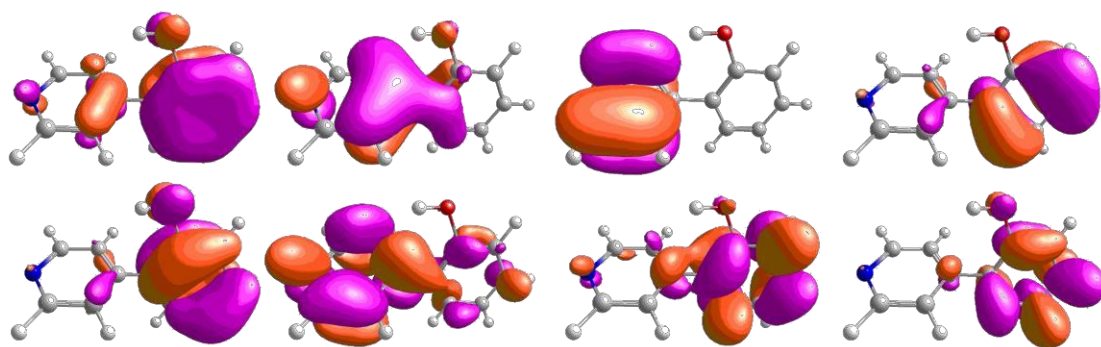


Fig. S1: Natural molecular orbitals used for the active space of CASSCF and CASPT2 methods. See main text for discussion.

2. Active Orbitals in OM2/MRCI Computations

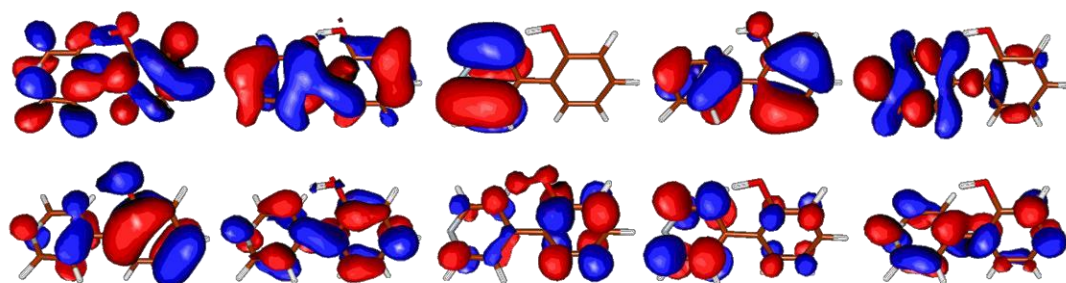


Fig. S2: Canonical molecular orbitals used for the active space of OM2/MRCI method. See main text for details.

3. CASSCF and OM2/MRCI Optimized Geometry Parameters

Table S1: Key Geometry Parameters of Critical Structures Optimized at the CASSCF and OM2/MRCI Levels, Respectively (^a CASSCF/6-31G^{*}; ^b OM2/MRCI)

structure	C9N8C7H14	N8C6C7H14	C6C5C10H13	C5C9C10H13
S0-ENOL ^a	179.9	-179.6	-179.0	178.9
S0-ENOL ^b	179.4	-179.8	-178.4	177.8
S0-KETO ^a	179.9	180.0	-123.0	124.1
S0-KETO ^b	180.0	180.0	-121.7	121.9
S1-ENOL ^a	179.9	-179.7	-175.6	176.3
S1-KETO ^a	-179.9	-179.2	-122.8	123.0
S1S0-ENOL-1 ^a	-68.3	135.8	-168.0	-175.8
S1S0-ENOL-1 ^b	-65.7	144.7	-172.8	-173.9
S1S0-ENOL-2 ^a	-166.0	-176.2	-59.8	116.5
S1S0-ENOL-2 ^b	-176.0	-171.4	-62.1	120.4
S1S0-ENOL-3 ^a	-179.7	179.4	176.8	-177.4
S1S0-ENOL-3 ^b	-179.0	179.0	179.5	-179.7
S1S0-KETO ^a	180.0	179.0	-153.2	140.9

S1S0-KETO ^b	-176.1	177.7	-141.2	128.9
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structure	C4C3C2O11	C3C1C2O11	C2C3C5C10	C2C3C5C6
S0-ENOL ^a	-179.3	179.8	60.2	-120.4
S0-ENOL ^b	178.6	-176.9	47.5	-132.7
S0-KETO ^a	-179.8	180.0	0.1	-180.0
S0-KETO ^b	-180.0	-180.0	0.0	180.0
S1-ENOL ^a	-161.5	172.9	26.3	-154.6
S1-KETO ^a	-177.8	178.2	37.7	-143.4
S1S0-ENOL-1 ^a	-179.1	179.6	58.8	-120.6
S1S0-ENOL-1 ^b	-180.0	-180.0	49.9	-125.9
S1S0-ENOL-2 ^a	-178.4	-179.7	-7.8	-178.1
S1S0-ENOL-2 ^b	-173.8	-180.0	-0.4	-176.4
S1S0-ENOL-3 ^a	-89.5	149.0	-28.5	154.7
S1S0-ENOL-3 ^b	-82.3	139.8	-7.9	174.3
S1S0-KETO ^a	171.6	-177.2	64.0	-99.5
S1S0-KETO ^b	170.3	-172.7	50.8	-113.4

4. S₀ Relaxed Hydrogen Transfer Minimum Energy Path

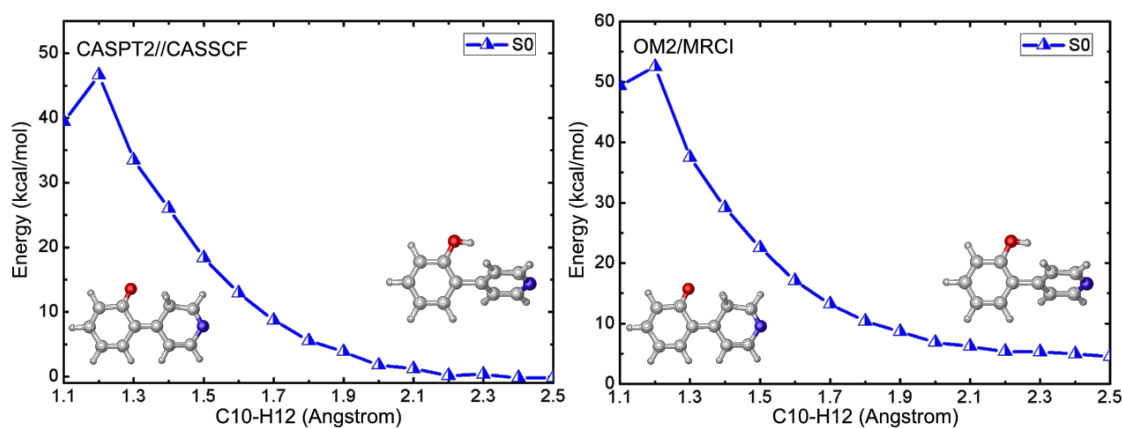
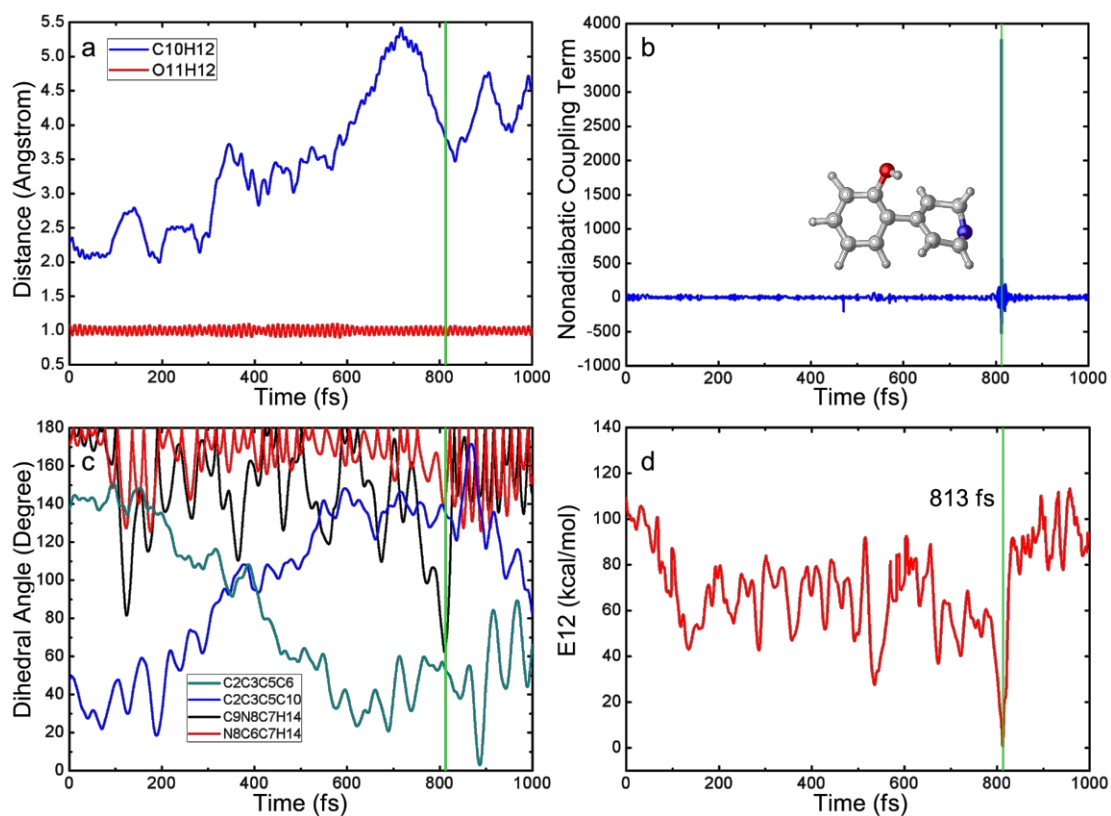


Fig. S3: CASPT2//CASSCF and OM2/MRCI computed S₀ relaxed minimum-energy intramolecular proton transfer path

5. Typical trajectories

(I)



(II)

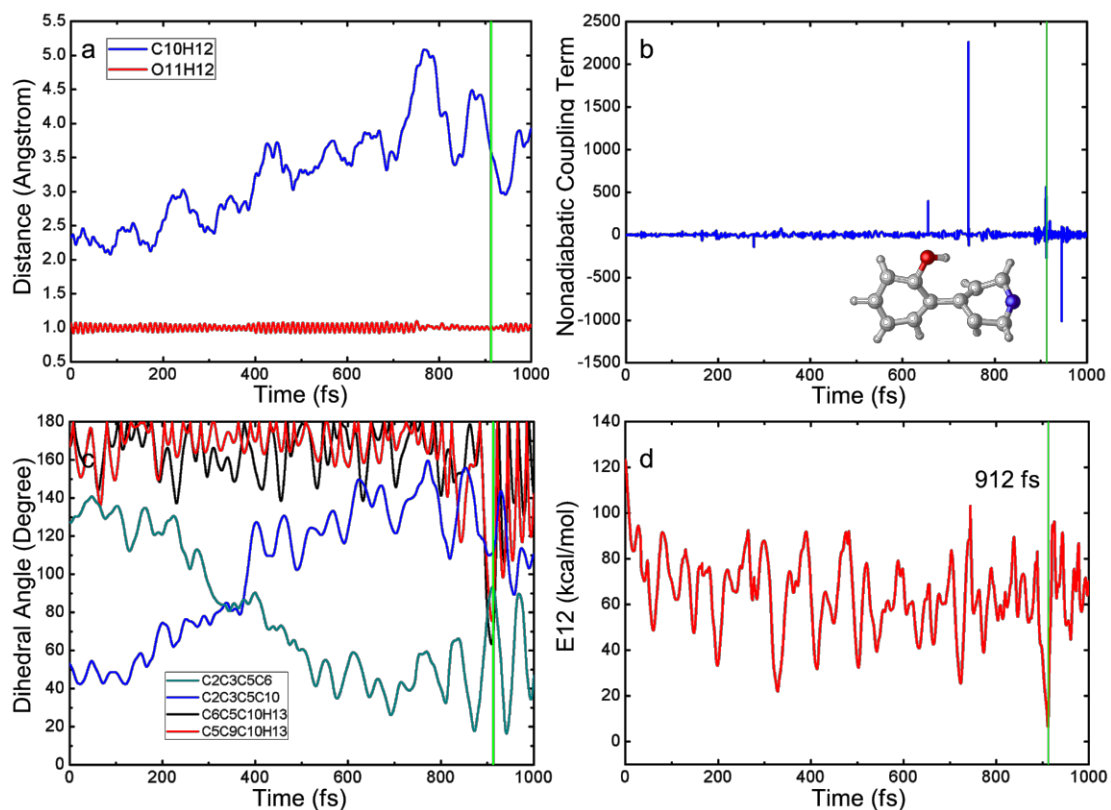


Fig. S4: Time-dependent physical variables of two other typical OM2/MRCI trajectories involved (I) S1-ENOL and S1S0-ENOL-1 and (II) S1-ENOL and S1S0-ENOL-2: (a) two key bond lengths; (b) nonadiabatic coupling term; (c) four key dihedral angles; and (d) S₁-S₀ energy gap.

6. Cartesian Coordinates of All Optimized Structures and Paths

In xyz format (unit: Ångstrom)

CASSCF method

S0-ENOL

C	-5.049394010	0.812987680	0.232104320
C	-4.377811880	1.249015260	-0.890528860
C	-4.150708060	2.600423380	-1.129162400
C	-4.632048140	3.536224220	-0.210602920
C	-5.318914780	3.112444000	0.928130450
C	-5.524088260	1.753661270	1.152969400
H	-5.203417920	-0.237581420	0.396686620
H	-4.003589600	0.531683490	-1.599625280
H	-5.681201250	3.854492580	1.614665210
H	-6.051031670	1.432771150	2.033072100
C	-3.406898030	3.024800010	-2.355126940
C	-2.224876490	3.737502070	-2.282131420
C	-3.877606930	2.702819950	-3.633557900
C	-1.571499400	4.090921860	-3.460161360
H	-1.798353000	4.004006080	-1.332138660
C	-3.157047090	3.094063240	-4.734012150
H	-4.796489730	2.159366450	-3.754085350
N	-2.012581500	3.784749210	-4.666928150
H	-0.646537510	4.638842680	-3.416844040
H	-3.502836820	2.855283150	-5.723837290
O	-4.473405530	4.876638910	-0.359904370
H	-4.122160720	5.085067730	-1.214354370

S0-KETO

C	-5.536493090	0.942604450	0.038788700
C	-4.885079490	1.339006070	-1.082292010
C	-4.078065040	2.555341130	-1.122837620
C	-4.004625950	3.356547650	0.146535030
C	-4.744770950	2.850823640	1.322063980
C	-5.453126700	1.734104120	1.270986800
H	-6.122390110	0.042516920	0.039195960
H	-4.970598550	0.733395370	-1.960615680
H	-4.665432780	3.450704790	2.209268250
H	-5.984144190	1.384915490	2.139192170
C	-3.407947400	2.962670850	-2.263332060
C	-2.563263530	4.221586420	-2.323019800
C	-3.455913100	2.214593530	-3.510086510

C	-1.914308020	4.483883710	-3.652681140
H	-1.786269730	4.196468910	-1.566272090
C	-2.789659030	2.628624370	-4.617477520
H	-4.024372240	1.310711110	-3.583770500
N	-1.998853460	3.788320150	-4.694826170
H	-1.308846930	5.377432760	-3.702382510
H	-2.838127260	2.062613920	-5.527689690
O	-3.375731390	4.376947090	0.237507140
H	-3.155196930	5.091403950	-2.058062120
S1-ENOL			
C	-5.339092790	0.888164760	0.146177830
C	-4.807558180	1.323961440	-1.105329080
C	-4.207971830	2.639746700	-1.242080640
C	-4.449714080	3.523795250	-0.098962050
C	-5.008896660	3.048126500	1.137933460
C	-5.421943910	1.704440240	1.241192050
H	-5.677502670	-0.129944550	0.217221370
H	-4.751334540	0.624838150	-1.914182650
H	-5.155504390	3.757923100	1.927745170
H	-5.824937840	1.337969820	2.166440430
C	-3.430102270	3.032456680	-2.389878260
C	-2.422692550	4.004706020	-2.339732370
C	-3.627754760	2.433911630	-3.659678850
C	-1.714155640	4.322652620	-3.485818860
H	-2.142662340	4.471365040	-1.414155570
C	-2.876299800	2.829983600	-4.725605510
H	-4.387749580	1.690239760	-3.803965080
N	-1.915504070	3.770311910	-4.673257630
H	-0.931346820	5.059719250	-3.434477590
H	-3.038312690	2.385274710	-5.691618470
O	-4.303927070	4.854361860	-0.184115820
H	-4.147533840	5.126178470	-1.079225250
S1-KETO			
C	-5.148982150	0.769561470	0.254443530
C	-4.554208570	1.271017220	-0.946025790
C	-4.177741770	2.606493160	-1.109910990
C	-4.406276180	3.576727150	-0.049341470
C	-5.022204610	3.024410580	1.125807810
C	-5.372135370	1.643227530	1.257828320
H	-5.415609980	-0.267478560	0.327414120
H	-4.358297110	0.578674860	-1.744390810
H	-5.267177450	3.716049390	1.909730580

H	-5.822164000	1.316692580	2.178632020
C	-3.477247360	2.996724850	-2.327193460
C	-2.325084480	3.951003840	-2.233613530
C	-3.804762630	2.511974050	-3.589979310
C	-1.674490330	4.247081340	-3.545169580
H	-1.573439380	3.557952650	-1.546181880
C	-3.068365200	2.893496390	-4.711242580
H	-4.640894060	1.850219110	-3.721996760
N	-2.003774560	3.775609330	-4.673189560
H	-0.842472040	4.934117490	-3.525503380
H	-3.314622950	2.514940260	-5.683983200
O	-4.132308000	4.767764780	-0.155128390
H	-2.660957690	4.868956930	-1.752813080

S1S0-KETO

C	-5.443420320	0.854229680	0.197306950
C	-4.824284360	1.134667860	-0.992747210
C	-4.294579310	2.404311440	-1.236395290
C	-4.274570150	3.429531650	-0.239136220
C	-4.949854150	3.104399830	0.985708850
C	-5.513715960	1.864785610	1.181460170
H	-5.882415170	-0.110209750	0.373234290
H	-4.762565730	0.378903410	-1.757989240
H	-5.005896920	3.871688530	1.735810460
H	-6.012699500	1.656632440	2.112148380
C	-3.567320750	2.811157820	-2.440154900
C	-2.131909990	3.043346790	-2.281548460
C	-4.148404110	3.300186030	-3.606007020
C	-1.409912320	3.504950130	-3.462415400
H	-1.604737990	2.324937770	-1.664755130
C	-3.327346580	3.766920470	-4.624037950
H	-5.212224160	3.270982890	-3.739003500
N	-1.971358720	3.860625630	-4.559114950
H	-0.335892390	3.570502090	-3.419801450
H	-3.755052300	4.075258010	-5.559535660
O	-3.655294600	4.503256600	-0.434092630
H	-2.291395350	3.925713860	-1.559340640

S1S0-ENOL-1

C	-5.592482190	0.963792260	0.000936720
C	-4.891004870	1.322183310	-1.117636880
C	-4.226580280	2.560881280	-1.210854620
C	-4.301865980	3.427061410	-0.138452540
C	-5.015539090	3.072422130	1.016713740

C	-5.653672870	1.851862940	1.085041230
H	-6.087272380	0.011109020	0.050416560
H	-4.826430320	0.646368230	-1.951534530
H	-5.053561590	3.775494620	1.827558090
H	-6.200075780	1.585042930	1.971598130
C	-3.463054170	2.918325200	-2.442681790
C	-2.002861140	3.226777090	-2.324226020
C	-4.046479780	2.987242130	-3.670620330
C	-1.387509340	3.864080910	-3.325088330
H	-1.486617780	2.991607650	-1.412481720
C	-3.064385140	3.206711760	-4.769793380
H	-5.084869630	2.765558170	-3.831361310
N	-2.216302940	4.200229600	-4.389348310
H	-0.377558920	4.226593650	-3.297588590
H	-2.631005280	2.323254360	-5.230918380
O	-3.721456710	4.645460350	-0.123851300
H	-3.322137590	4.849904810	-0.959517790
S1S0-ENOL-2			
C	-5.687654800	1.053997300	-0.102796600
C	-4.840031700	1.388027400	-1.129092100
C	-4.062334600	2.589192300	-1.108372900
C	-4.205523200	3.439241800	0.007137500
C	-5.056122800	3.076634000	1.066021000
C	-5.791992700	1.911613100	1.014524800
H	-6.266460600	0.150174300	-0.147763100
H	-4.763738900	0.741614900	-1.981417900
H	-5.120158600	3.746165800	1.902753800
H	-6.449468900	1.661155600	1.826885400
C	-3.129560900	2.867398700	-2.147126200
C	-2.346713000	4.092777300	-2.285691600
C	-2.958246500	2.049233300	-3.348860200
C	-2.693187900	4.804186500	-3.554267600
H	-1.294168100	3.820374600	-2.412731100
C	-2.903146500	2.746178500	-4.495383600
H	-3.004820300	0.975611500	-3.366789600
N	-2.942784500	4.147621200	-4.610332400
H	-2.645493200	5.878479500	-3.630047700
H	-2.882781600	2.235672900	-5.440676200
O	-3.572021100	4.594783700	0.142337600
H	-2.966112000	4.730066600	-0.603694300
S1S0-ENOL-3			
C	-5.293279000	1.111787000	-0.019273000

C	-5.230215000	1.586475000	-1.277036000
C	-4.675722000	2.914570000	-1.513984000
C	-4.880655000	3.687119000	-0.312808000
C	-4.261047000	3.145090000	0.911705000
C	-4.644033000	1.843694000	1.077189000
H	-5.682168000	0.128855000	0.172979000
H	-5.495029000	0.966971000	-2.117379000
H	-3.744316000	3.727595000	1.650473000
H	-4.411552000	1.315939000	1.988816000
C	-3.552388000	3.111232000	-2.401772000
C	-2.914139000	4.367504000	-2.533632000
C	-3.070694000	2.104636000	-3.224142000
C	-1.879749000	4.509246000	-3.430527000
H	-3.254432000	5.217429000	-1.974855000
C	-2.015023000	2.367436000	-4.095557000
H	-3.472254000	1.113435000	-3.179276000
N	-1.418966000	3.522540000	-4.212771000
H	-1.392832000	5.460931000	-3.543363000
H	-1.644117000	1.572266000	-4.718960000
O	-5.992960000	4.369632000	-0.186580000
H	-6.382290000	4.471503000	-1.060825000

OM2/MRCI method

S0-ENOL

C	-5.140295943	0.814827011	0.177423952
C	-4.492090738	1.214556967	-0.986027211
C	-4.153006675	2.562822902	-1.168679263
C	-4.534316002	3.491756993	-0.179637136
C	-5.201502455	3.098632683	0.987832611
C	-5.505255297	1.748574605	1.153216016
H	-5.368591278	-0.243566004	0.335386879
H	-4.214733924	0.480755161	-1.749918806
H	-5.468625091	3.843076054	1.734823065
H	-6.056972198	1.424830711	2.041730682
C	-3.420781116	3.001493695	-2.371353265
C	-2.309101909	3.849867952	-2.269461488
C	-3.819580209	2.574184994	-3.644485563
C	-1.644094402	4.217494176	-3.446296803
H	-1.953198665	4.182218153	-1.294265909
C	-3.084563597	3.007375129	-4.754534904
H	-4.688670109	1.924525982	-3.760836415
N	-2.019258799	3.806310588	-4.659125702

H	-0.756711037	4.872529630	-3.378088273
H	-3.392692092	2.681762104	-5.764375786
O	-4.224852534	4.818051032	-0.256798722
H	-4.107445159	5.067780694	-1.210364087
S0-KETO			
C	-5.523842495	0.960025119	0.050490242
C	-4.878789354	1.334130290	-1.092844564
C	-4.087330412	2.529625649	-1.145499670
C	-3.990732335	3.347506421	0.079449376
C	-4.703805899	2.893599516	1.269577412
C	-5.436544528	1.745596712	1.243107407
H	-6.124635580	0.044708667	0.076143014
H	-4.967986873	0.706476913	-1.990616131
H	-4.618353513	3.513121527	2.162804822
H	-5.975451335	1.397614571	2.133520206
C	-3.415645508	2.941143710	-2.294988478
C	-2.607864817	4.197436277	-2.282839798
C	-3.466377788	2.192132514	-3.523017946
C	-1.950289949	4.500631403	-3.589393653
H	-1.826329542	4.120828314	-1.496694745
C	-2.791502289	2.633120811	-4.626733074
H	-4.047264693	1.267881824	-3.570405091
N	-2.036804864	3.784316810	-4.655818099
H	-1.343567605	5.430607990	-3.604525575
H	-2.828686214	2.060394262	-5.570148434
O	-3.322780843	4.394393146	0.104074865
H	-3.263896662	5.050034736	-2.004629596
S1S0-KETO			
C	-3.861292613	-2.001756791	7.168916652
C	-3.199091913	-1.728965391	5.966712552
C	-3.081250813	-0.422221491	5.524658752
C	-3.544195813	0.679571809	6.372272752
C	-4.168441313	0.351790709	7.628852152
C	-4.336881513	-0.970085591	7.990848752
H	-4.024250213	-3.042259091	7.472125252
H	-2.808511713	-2.547921491	5.357185252
H	-4.587078113	1.167958809	8.220178952
H	-4.826484013	-1.222202891	8.935858452
C	-2.301326313	0.032011209	4.365299052
C	-1.205661013	0.960653809	4.710108652
C	-2.753334613	-0.112336891	3.073551452
C	-0.486453813	1.435538309	3.506106352

H	-0.505977413	0.561361709	5.484059752
C	-1.944431113	0.423797809	2.038258952
H	-3.646026713	-0.687235991	2.831765652
N	-0.859626413	1.183858409	2.276938152
H	0.410763987	2.055991309	3.681875952
H	-2.188634613	0.180028009	0.991377352
O	-3.260300513	1.858230009	6.033940052
H	-1.746814213	1.844193709	5.227410252
S1S0-ENOL-1			
C	-5.647683996	0.999330202	-0.037600155
C	-4.952577107	1.332203439	-1.199530055
C	-4.220244780	2.521342693	-1.259393689
C	-4.214396772	3.379907057	-0.139705418
C	-4.920009335	3.054980805	1.031119320
C	-5.625012362	1.856681206	1.067510935
H	-6.212532615	0.065063060	0.009067234
H	-4.965995386	0.657362085	-2.062138742
H	-4.893038673	3.740398622	1.875558081
H	-6.179216729	1.584818318	1.972848707
C	-3.469693806	2.886937367	-2.470896205
C	-2.078796678	3.293825454	-2.323195921
C	-4.103957304	2.923379806	-3.696828534
C	-1.441974339	3.984600172	-3.351320798
H	-1.583793810	3.138267815	-1.368627376
C	-2.983435551	3.089287201	-4.633906786
H	-5.145133925	2.759549025	-3.913280589
N	-2.260773456	4.180897543	-4.434562633
H	-0.481696813	4.494391397	-3.234158978
H	-2.486950053	2.117141184	-4.942225259
O	-3.533092068	4.555072903	-0.105239237
H	-3.252718948	4.806527007	-1.027186343
S1S0-ENOL-2			
C	-5.662272177	1.019380978	0.039562024
C	-4.932181560	1.286549981	-1.108689733
C	-4.202346643	2.486716103	-1.207710496
C	-4.295453328	3.443514681	-0.145705789
C	-4.997867852	3.139114924	1.038285808
C	-5.711778121	1.949812561	1.092604300
H	-6.189461309	0.065974661	0.141289385
H	-4.901726654	0.560928759	-1.929025171
H	-5.035231623	3.876658521	1.837680592
H	-6.344441550	1.738949300	1.962394213

C	-3.261233581	2.790097129	-2.232829493
C	-2.456962277	4.003020062	-2.196284689
C	-3.002662839	2.067630267	-3.439611677
C	-2.690376017	4.862958820	-3.393224554
H	-1.357945228	3.740348285	-2.199823133
C	-2.660301053	2.850714869	-4.536174964
H	-3.295891033	1.025645039	-3.563270500
N	-2.627738445	4.232706087	-4.519673218
H	-2.811898678	5.950270268	-3.308613932
H	-2.533610081	2.379408825	-5.523328774
O	-3.721472993	4.640702169	-0.251821386
H	-2.889669413	4.589098375	-0.961411352
S1S0-ENOL-3			
C	-5.394292368	1.202170520	0.157730808
C	-4.991223916	1.522263861	-1.132930300
C	-4.334330539	2.749197952	-1.403331544
C	-4.661208279	3.565229321	-0.261344196
C	-4.402134955	3.220411267	1.106290054
C	-5.007760147	1.981466964	1.275100809
H	-5.891570518	0.250698714	0.339227081
H	-5.092253105	0.793975576	-1.946743375
H	-3.861546839	3.790356840	1.832111135
H	-5.081323837	1.554422799	2.281254279
C	-3.365428223	3.044750712	-2.434256260
C	-2.753556124	4.309233098	-2.466201186
C	-3.051399031	2.113454808	-3.437552892
C	-1.851258011	4.580194529	-3.502641327
H	-2.975585760	5.064642667	-1.710953785
C	-2.142378802	2.496670874	-4.429922756
H	-3.489124342	1.114502036	-3.438081564
N	-1.558310563	3.698057655	-4.460555060
H	-1.360322921	5.568574380	-3.539652515
H	-1.877060676	1.772449949	-5.220659241
O	-5.869075193	4.149351279	-0.353724090
H	-6.296714868	4.073808824	-1.254741959

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2.40

C	-5.352811070	0.895798810	0.139819200
C	-4.831389810	1.340412480	-1.109233970
C	-4.210158570	2.642037180	-1.243831640
C	-4.441537930	3.520791630	-0.097877720

C	-4.987732420	3.040804980	1.145405950
C	-5.410892780	1.696392600	1.247015990
H	-5.704523130	-0.118600070	0.199347420
H	-4.817663130	0.655038520	-1.931507660
H	-5.125565080	3.749646080	1.937663440
H	-5.801314880	1.324595640	2.175192010
C	-3.430298380	3.027869630	-2.385327550
C	-2.436108810	4.014217760	-2.341141290
C	-3.613415140	2.412896050	-3.651609080
C	-1.725985590	4.331896750	-3.497593720
H	-2.157784280	4.489116130	-1.419566550
C	-2.852143670	2.817875130	-4.724299300
H	-4.361291730	1.657872950	-3.796890370
N	-1.911300970	3.773821240	-4.664961070
H	-0.956854530	5.084462450	-3.444708870
H	-2.999315980	2.363948320	-5.688170530
O	-4.312067370	4.851930320	-0.180689450
H	-4.142343080	5.127358370	-1.072408600
2.20			
C	-5.367155030	0.894124430	0.146706810
C	-4.789337840	1.305510220	-1.089880230
C	-4.164726990	2.599667950	-1.232070710
C	-4.410156730	3.497066780	-0.106438070
C	-5.009224020	3.053021880	1.123143700
C	-5.460626230	1.718373110	1.234062100
H	-5.734788540	-0.114177080	0.212530210
H	-4.747807720	0.601742330	-1.895833580
H	-5.153818700	3.777532030	1.899859710
H	-5.893759670	1.371357170	2.152712630
C	-3.408871550	3.000153350	-2.377394060
C	-2.434118080	4.011787640	-2.340374460
C	-3.602761600	2.397402800	-3.649157360
C	-1.761404560	4.363344420	-3.509217090
H	-2.110050570	4.452974280	-1.416924350
C	-2.879463030	2.840019970	-4.732320830
H	-4.335144070	1.625903430	-3.787973650
N	-1.963574600	3.822272600	-4.681749320
H	-1.007423050	5.131638810	-3.462142900
H	-3.038242600	2.397404390	-5.699600730
O	-4.234658900	4.816132530	-0.216844820
H	-3.923252580	5.038015620	-1.087643570
2.00			

C	-5.387458830	0.898273980	0.157339830
C	-4.768438330	1.273599310	-1.074026590
C	-4.125925370	2.550614490	-1.226727050
C	-4.376141880	3.470266580	-0.124353590
C	-5.009660740	3.066929470	1.098615050
C	-5.493086450	1.745486970	1.225196690
H	-5.777407660	-0.100881300	0.232260120
H	-4.730235030	0.556610760	-1.868803910
H	-5.150833860	3.809083980	1.859288760
H	-5.955751550	1.425948310	2.139225450
C	-3.387571740	2.963700770	-2.368707120
C	-2.436570550	4.006568510	-2.327789710
C	-3.582411590	2.376651140	-3.650261790
C	-1.803587640	4.402010070	-3.505134310
H	-2.057209860	4.399507040	-1.403624830
C	-2.900757360	2.868995350	-4.736875000
H	-4.289920800	1.582150050	-3.789693660
N	-2.019341530	3.886009040	-4.686251070
H	-1.068259140	5.188413380	-3.456830220
H	-3.064667640	2.441654210	-5.710156970
O	-4.155169000	4.771857870	-0.275749220
H	-3.746986500	4.924858850	-1.127975960
1.80			
C	-5.410778870	0.908035370	0.173423780
C	-4.765470930	1.247027990	-1.061564130
C	-4.098964790	2.497476120	-1.230250660
C	-4.346992750	3.443155210	-0.154472180
C	-4.995355080	3.082446360	1.069435620
C	-5.511143100	1.778047050	1.221209320
H	-5.822923200	-0.080906920	0.261831720
H	-4.744339840	0.516959000	-1.845550090
H	-5.123237560	3.844798220	1.812542440
H	-5.990043050	1.488832750	2.136818310
C	-3.365532050	2.914496220	-2.360417970
C	-2.442037420	3.996348880	-2.303268400
C	-3.552966710	2.349162270	-3.658484780
C	-1.850897820	4.444450480	-3.485602970
H	-1.987794480	4.313995080	-1.383037700
C	-2.918893500	2.904907030	-4.739626570
H	-4.227701060	1.527696770	-3.807801700
N	-2.079745430	3.964439460	-4.677828330
H	-1.136950000	5.250368150	-3.428273240

H	-3.082657170	2.499928420	-5.722417730
O	-4.086023970	4.719633180	-0.351357990
H	-3.603970690	4.804051920	-1.190826410
1.60			
C	-5.273419840	0.850857790	0.242249710
C	-4.538651660	1.133720630	-0.916690570
C	-4.123712920	2.431634210	-1.205052550
C	-4.497535400	3.483148030	-0.261855360
C	-5.184846770	3.150602750	0.954215880
C	-5.582232110	1.876887810	1.174274070
H	-5.593433390	-0.154740160	0.439727440
H	-4.281845670	0.341056050	-1.593464750
H	-5.411644860	3.953777350	1.628506290
H	-6.136277980	1.629030690	2.060989060
C	-3.341015540	2.824903190	-2.374258000
C	-2.363406550	3.920280450	-2.191662930
C	-3.698009410	2.463213230	-3.675777610
C	-1.797134090	4.418380150	-3.428648140
H	-1.633342090	3.784185900	-1.398456890
C	-3.084155460	3.085128970	-4.758833690
H	-4.474972820	1.739114650	-3.852978370
N	-2.125386140	4.076317810	-4.615468580
H	-1.019894660	5.164659670	-3.347844540
H	-3.321269810	2.806004130	-5.767146650
O	-4.245670460	4.686486530	-0.518187790
H	-3.416561830	4.750699170	-1.319155700
1.40			
C	-5.268510200	0.832266600	0.238724200
C	-4.564410000	1.182897000	-0.932855100
C	-4.176348800	2.497943500	-1.188113300
C	-4.530947200	3.534199300	-0.216067600
C	-5.209363700	3.128413300	0.983974600
C	-5.576627700	1.813906900	1.183431900
H	-5.558590800	-0.188154900	0.402836200
H	-4.306154200	0.416767300	-1.639511300
H	-5.463466000	3.899004300	1.686343300
H	-6.107341500	1.543128300	2.078102800
C	-3.410280300	2.893700300	-2.365290100
C	-2.398117000	3.965671400	-2.193160300
C	-3.720288000	2.474022100	-3.658678300
C	-1.788217600	4.415413100	-3.453686300
H	-1.653107900	3.762512300	-1.426660000

C	-3.051289700	3.029408400	-4.747624600
H	-4.498577800	1.751287900	-3.830970400
N	-2.083137200	4.014532500	-4.625711700
H	-1.015523800	5.166560400	-3.380392100
H	-3.260796600	2.706789000	-5.748896600
O	-4.287732200	4.745477500	-0.416989700
H	-3.221641280	4.835988590	-1.469036170
1.20			
C	-5.261064800	0.816654400	0.225795900
C	-4.589288300	1.243044400	-0.951618400
C	-4.228915600	2.575399500	-1.166926000
C	-4.565091800	3.585399800	-0.164454100
C	-5.234727600	3.103174000	1.013466000
C	-5.570350500	1.748688900	1.185198200
H	-5.520015800	-0.217656700	0.349047100
H	-4.328446900	0.509076800	-1.691207300
H	-5.516376700	3.836674500	1.744807800
H	-6.078544300	1.450239100	2.084548600
C	-3.477657400	2.973350900	-2.351656800
C	-2.430623000	4.025216500	-2.199501800
C	-3.743081800	2.488860300	-3.629782000
C	-1.778581300	4.407893500	-3.480219700
H	-1.677494600	3.751282000	-1.460235000
C	-3.022176600	2.966950600	-4.724195700
H	-4.522920000	1.766682500	-3.792416000
N	-2.041452500	3.941761100	-4.631007000
H	-1.006533700	5.160588100	-3.422972300
H	-3.207903600	2.593459100	-5.712236200
O	-4.326001400	4.794249200	-0.313795700
H	-3.021967240	4.901449090	-1.631585930
1.00			
C	-5.225661250	0.804531660	0.203353790
C	-4.594902700	1.305810380	-0.979139000
C	-4.252766170	2.651437890	-1.154453540
C	-4.553048550	3.629595430	-0.119518210
C	-5.207561510	3.076642970	1.037116250
C	-5.520828000	1.686446140	1.179708450
H	-5.460806720	-0.239558350	0.282951850
H	-4.344141260	0.605990480	-1.754918990
H	-5.503554670	3.772756380	1.799046510
H	-6.001617930	1.361871670	2.085471490
C	-3.522609340	3.042094280	-2.354971630

C	-2.428872560	4.069196440	-2.249838250
C	-3.759628830	2.485711970	-3.607485410
C	-1.748357930	4.356154550	-3.553207550
H	-1.672907770	3.715502740	-1.544045900
C	-2.999018840	2.865801260	-4.714835390
H	-4.547467530	1.768807310	-3.748448310
N	-1.995347930	3.817639340	-4.670947770
H	-0.966676690	5.100251380	-3.530905680
H	-3.178543410	2.432437300	-5.679134640
O	-4.304426720	4.824077610	-0.227545290
H	-2.783778710	4.910310850	-1.841710570

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2.50

C	-5.061258810	0.815600160	0.249140270
C	-4.385539860	1.236146130	-0.879282150
C	-4.154352860	2.586732550	-1.128691390
C	-4.632492260	3.521226300	-0.212465430
C	-5.315173980	3.107154420	0.923688260
C	-5.524404140	1.762546130	1.152044330
H	-5.222021210	-0.232241950	0.424971370
H	-4.014356100	0.510809380	-1.581675350
H	-5.674050380	3.854630580	1.606407240
H	-6.052783120	1.452198290	2.035774570
C	-3.416526680	3.014868050	-2.356020210
C	-2.224235780	3.747411240	-2.280630110
C	-3.881540180	2.696571290	-3.637634030
C	-1.571638990	4.114333820	-3.458112840
H	-1.797401310	4.006406080	-1.328511920
C	-3.151127100	3.107987280	-4.751989100
H	-4.795907170	2.147381370	-3.766031780
N	-2.018380250	3.805872120	-4.674443450
H	-0.652933980	4.671562250	-3.416551780
H	-3.494822420	2.871102250	-5.742894340
O	-4.470826650	4.853312230	-0.373029100
H	-4.070725110	5.048572980	-1.209436400

2.40

C	-5.091418380	0.806772250	0.229030550
C	-4.407472280	1.229233850	-0.904116720
C	-4.149192310	2.589039380	-1.130615410
C	-4.601461260	3.522802730	-0.206850010
C	-5.293670970	3.112693940	0.925371650

C	-5.536132230	1.762610680	1.147899640
H	-5.272391170	-0.239095260	0.395681410
H	-4.050863760	0.508651600	-1.618092400
H	-5.632238300	3.862069200	1.616299220
H	-6.068740880	1.458981840	2.030931610
C	-3.407891700	3.016916880	-2.355150160
C	-2.259815290	3.781032930	-2.282296290
C	-3.855748870	2.662455600	-3.634291130
C	-1.612530140	4.150093940	-3.461092420
H	-1.843200540	4.067594730	-1.333506720
C	-3.145183300	3.072341220	-4.733010060
H	-4.751118210	2.081412200	-3.755433680
N	-2.031268120	3.813462990	-4.666181760
H	-0.712102510	4.737458880	-3.416678560
H	-3.473499450	2.809427580	-5.722623700
O	-4.407769750	4.854154770	-0.352866910
H	-3.978788900	5.040071030	-1.177781530
2.30			
C	-5.128332900	0.809906240	0.214368070
C	-4.439878310	1.227100920	-0.918115930
C	-4.146391730	2.582351990	-1.129031400
C	-4.569256340	3.517541430	-0.190898700
C	-5.267952660	3.112913810	0.937858870
C	-5.544271610	1.766619470	1.145633310
H	-5.335296170	-0.232707200	0.370546600
H	-4.105683640	0.505016950	-1.641263300
H	-5.584501970	3.862393990	1.639038160
H	-6.080638400	1.466689830	2.027635940
C	-3.406928450	3.011033710	-2.351930360
C	-2.295256910	3.817509910	-2.284777580
C	-3.832975380	2.616623430	-3.633770720
C	-1.649503690	4.194270940	-3.473598520
H	-1.887038180	4.129251770	-1.340336890
C	-3.123150860	3.043571370	-4.736171890
H	-4.705829370	2.002692490	-3.753488670
N	-2.040675490	3.829727870	-4.660866790
H	-0.774246790	4.819445860	-3.424696430
H	-3.429969550	2.758847410	-5.726299520
O	-4.338834800	4.843414760	-0.326956500
H	-3.895885120	5.015966010	-1.148251140
2.20			
C	-5.142591290	0.809026140	0.218394810

C	-4.447963850	1.212294320	-0.915928250
C	-4.142892890	2.563467330	-1.132242820
C	-4.553456570	3.507405670	-0.198670400
C	-5.258421480	3.118243610	0.931512590
C	-5.550234270	1.775338260	1.144008070
H	-5.360883660	-0.230387510	0.380448440
H	-4.120786820	0.483225640	-1.635318800
H	-5.566305790	3.874065730	1.629735110
H	-6.090903700	1.484976470	2.026613790
C	-3.407224300	2.997289420	-2.355526970
C	-2.307737960	3.830232620	-2.280291020
C	-3.823243390	2.607644570	-3.634753100
C	-1.673688460	4.226839090	-3.457763880
H	-1.900138890	4.134647980	-1.333223850
C	-3.129219900	3.050307580	-4.731153830
H	-4.683722130	1.976879250	-3.758789150
N	-2.062454950	3.857880200	-4.663020960
H	-0.808771600	4.865221140	-3.411136280
H	-3.433715640	2.760554130	-5.720876120
O	-4.298437170	4.827023980	-0.349342430
H	-3.819703580	4.968007330	-1.158048310

2.10

C	-5.172470020	0.812336810	0.211549690
C	-4.471599010	1.205805810	-0.922631740
C	-4.136792050	2.551267640	-1.129900100
C	-4.525280160	3.499907400	-0.189515250
C	-5.238750280	3.120869590	0.937239490
C	-5.558478930	1.782694910	1.142149560
H	-5.412710350	-0.222850080	0.369253320
H	-4.161958380	0.473141620	-1.646063170
H	-5.530342750	3.878815610	1.640127290
H	-6.104247080	1.499036990	2.023776500
C	-3.403552160	2.987710270	-2.350916630
C	-2.338209050	3.855717740	-2.279182040
C	-3.803222750	2.572103540	-3.633609230
C	-1.709094170	4.265471700	-3.466161730
H	-1.929070070	4.170997100	-1.336644050
C	-3.113556400	3.037471060	-4.733364500
H	-4.643172480	1.914853920	-3.757280900
N	-2.076802820	3.882366780	-4.655069070
H	-0.868217720	4.935989690	-3.414224130
H	-3.401751370	2.737144770	-5.724461460

O	-4.236730220	4.811413940	-0.341367490
H	-3.746490040	4.927916160	-1.149077740
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C	-5.182295190	0.811186620	0.220986680
C	-4.474844200	1.186703300	-0.915866140
C	-4.131411250	2.527440520	-1.133368970
C	-4.510765450	3.488196100	-0.203099630
C	-5.230794540	3.128615990	0.925821830
C	-5.562994240	1.794340570	1.140997000
H	-5.431616760	-0.220218680	0.389136500
H	-4.169920360	0.444946590	-1.632084510
H	-5.516307930	3.895022150	1.621980870
H	-6.113283700	1.522978680	2.023722960
C	-3.402109230	2.969131950	-2.354908240
C	-2.346280180	3.859514350	-2.271082070
C	-3.797015760	2.569614330	-3.635216460
C	-1.733383060	4.295118030	-3.444630690
H	-1.929655120	4.155758390	-1.325780660
C	-3.125555350	3.057007770	-4.728380210
H	-4.626218260	1.899769430	-3.765812940
N	-2.104564940	3.918962020	-4.654223490
H	-0.901174710	4.975126810	-3.393171290
H	-3.415434140	2.759773120	-5.720304690
O	-4.198700970	4.791425180	-0.376935020
H	-3.678172980	4.869769740	-1.173154170
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C	-5.205686600	0.814354320	0.219502560
C	-4.490696170	1.176775690	-0.917181730
C	-4.121817080	2.511434940	-1.130023670
C	-4.485711740	3.479941700	-0.199290390
C	-5.216259600	3.133656380	0.925640130
C	-5.571032040	1.804329920	1.138579900
H	-5.474006300	-0.212226580	0.387701080
H	-4.199283830	0.429820430	-1.633618970
H	-5.490777890	3.903912220	1.621941630
H	-6.127653920	1.541830410	2.020003600
C	-3.395224400	2.957067320	-2.348630510
C	-2.372635650	3.876807840	-2.265677870
C	-3.779968240	2.542134360	-3.634349930
C	-1.766995720	4.329260370	-3.449465070
H	-1.944225210	4.172300390	-1.325856710
C	-3.116812880	3.055646100	-4.729666770

H	-4.590640250	1.850463800	-3.764939730
N	-2.122830170	3.948632400	-4.643038900
H	-0.956822770	5.036012400	-3.390807960
H	-3.395027020	2.756346770	-5.723936750
O	-4.143265050	4.772726820	-0.382202300
H	-3.615125820	4.818954950	-1.180054980
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C	-5.213572300	0.813232110	0.232787550
C	-4.491875850	1.153749100	-0.907176750
C	-4.115003550	2.482851550	-1.134373180
C	-4.471047850	3.466951410	-0.218511270
C	-5.207237500	3.143404160	0.909768980
C	-5.573853800	1.818971540	1.137483880
H	-5.491260280	-0.208578730	0.414566350
H	-4.204737540	0.395729970	-1.613794750
H	-5.476533370	3.924171530	1.596330370
H	-6.135149740	1.571925690	2.020466050
C	-3.392897970	2.931792110	-2.354707700
C	-2.377407500	3.875450440	-2.255217230
C	-3.774797990	2.541176870	-3.635353060
C	-1.793831890	4.358919000	-3.419938030
H	-1.935025670	4.141352220	-1.313195310
C	-3.130861910	3.084809250	-4.724306810
H	-4.574465230	1.838512700	-3.776950430
N	-2.157307260	3.992695770	-4.638851480
H	-0.992128880	5.074095750	-3.360571510
H	-3.412725780	2.792796540	-5.720246770
O	-4.107698330	4.749787320	-0.428437550
H	-3.553078110	4.756386650	-1.215144710
1.70			
C	-5.224637690	0.814189700	0.245815420
C	-4.494860090	1.131806630	-0.896327170
C	-4.105619500	2.454396650	-1.136330210
C	-4.454864290	3.455205730	-0.235303320
C	-5.199755240	3.154658030	0.892920670
C	-5.579624510	1.835792940	1.135053270
H	-5.513155570	-0.202183040	0.440612110
H	-4.212595280	0.362372990	-1.592517840
H	-5.465404580	3.946105900	1.568568950
H	-6.147308120	1.605247580	2.018425470
C	-3.387986430	2.903939210	-2.357734910
C	-2.387338850	3.875409210	-2.244514550

C	-3.763684050	2.527438210	-3.634366170
C	-1.824026100	4.389514310	-3.396125300
H	-1.928534170	4.115141200	-1.303536210
C	-3.133684370	3.110526440	-4.722367820
H	-4.549591050	1.811768430	-3.787435600
N	-2.190203770	4.037475700	-4.626666080
H	-1.037449320	5.120332340	-3.331361530
H	-3.416107320	2.828254970	-5.721242100
O	-4.070624520	4.726888050	-0.470858510
H	-3.495443470	4.695901760	-1.250081920
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C	-5.235997910	0.815086740	0.253494660
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C	-4.094510430	2.430150750	-1.136275470
C	-4.433871320	3.444653000	-0.245703930
C	-5.188121030	3.162897690	0.880995410
C	-5.582985400	1.849322430	1.132006930
H	-5.537080940	-0.195936490	0.456855550
H	-4.224405480	0.335569230	-1.579391790
H	-5.447334350	3.962047500	1.550009480
H	-6.156045620	1.632264230	2.015352460
C	-3.381027440	2.883387010	-2.357381330
C	-2.401145030	3.876027270	-2.232774370
C	-3.757293240	2.519501500	-3.636470540
C	-1.854573250	4.417374450	-3.380966580
H	-1.918583450	4.089105570	-1.297373250
C	-3.146227080	3.133389280	-4.718762960
H	-4.530394690	1.791481110	-3.795997420
N	-2.223078420	4.079472890	-4.614660840
H	-1.080367620	5.160782020	-3.309831280
H	-3.428643400	2.860538860	-5.720242840
O	-4.024703830	4.703481750	-0.499471920
H	-3.436953380	4.635875880	-1.278975930
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C	-5.249250290	0.830792980	0.281713790
C	-4.498465530	1.100472000	-0.868653730
C	-4.080403700	2.390422970	-1.137098840
C	-4.424040150	3.435745300	-0.250792010
C	-5.175816420	3.174867740	0.864924210
C	-5.582007210	1.860048280	1.126097910
H	-5.563862170	-0.174565420	0.494341840
H	-4.238919050	0.302549760	-1.542237870

H	-5.439689100	3.980302530	1.524684050
H	-6.162493520	1.661926560	2.009724680
C	-3.368842410	2.845473830	-2.355259910
C	-2.412494590	3.865783060	-2.219901870
C	-3.746848430	2.502258310	-3.653608600
C	-1.883779170	4.447634470	-3.362987740
H	-1.909407530	4.058758360	-1.290971590
C	-3.149536700	3.163353460	-4.727051910
H	-4.503145750	1.760453590	-3.828238030
N	-2.248505460	4.131802430	-4.590324660
H	-1.129957560	5.210344410	-3.273850540
H	-3.425612560	2.914644420	-5.735897060
O	-3.996715030	4.675111910	-0.547003460
H	-3.392705990	4.562002010	-1.322982000
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C	-5.251411700	0.817301610	0.278777770
C	-4.501305980	1.071484000	-0.868170510
C	-4.073310500	2.374968280	-1.140225950
C	-4.399598920	3.423820080	-0.280934500
C	-5.170354290	3.183828480	0.844099340
C	-5.587748520	1.881960130	1.125314630
H	-5.571038930	-0.182323890	0.508566560
H	-4.236289410	0.271717450	-1.536614300
H	-5.422614800	4.003015000	1.491181110
H	-6.170507150	1.697261990	2.009780730
C	-3.370817500	2.826756640	-2.364643950
C	-2.421270980	3.868869290	-2.206053010
C	-3.741831410	2.498097810	-3.638204310
C	-1.916037950	4.472141980	-3.328161640
H	-1.889723490	4.011656310	-1.283553020
C	-3.166848610	3.193738760	-4.712775610
H	-4.491403510	1.751286650	-3.821887440
N	-2.300539920	4.172863920	-4.580299290
H	-1.166160990	5.237921350	-3.242161200
H	-3.452881980	2.946112450	-5.720107190
O	-3.954198500	4.657179830	-0.579250050
H	-3.326603280	4.520524840	-1.360051510
1.30			
C	-5.319720530	0.844177130	0.228562090
C	-4.528483990	1.084560250	-0.886003420
C	-4.003381320	2.361250250	-1.109145990
C	-4.307947130	3.414425090	-0.214446490

C	-5.136216640	3.176736660	0.861727370
C	-5.617686850	1.885871080	1.082811690
H	-5.702506450	-0.141650640	0.419037880
H	-4.302488090	0.287090950	-1.571661510
H	-5.381912830	3.984866500	1.524484930
H	-6.237750620	1.705380860	1.943293100
C	-3.321733890	2.818631550	-2.313444280
C	-2.448479160	3.924445860	-2.200921740
C	-3.679192930	2.427640950	-3.612011450
C	-2.006085450	4.542618800	-3.373043640
H	-1.841247420	4.081689900	-1.329907550
C	-3.180718460	3.143012660	-4.695249320
H	-4.372449580	1.623722300	-3.769393520
N	-2.380366370	4.199980980	-4.582715080
H	-1.313115390	5.363336150	-3.306004860
H	-3.455757610	2.864669910	-5.696487970
O	-3.810277150	4.622137070	-0.473721770
H	-3.234980470	4.485588680	-1.331131800
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C	-5.569794590	0.937399570	-0.010876070
C	-4.933100980	1.367812310	-1.096481370
C	-4.188121070	2.636004170	-1.128742090
C	-4.193776730	3.427444050	0.134368870
C	-4.924930580	2.873318580	1.296085040
C	-5.566364140	1.714872360	1.225095950
H	-6.097135060	0.001001710	-0.028775160
H	-4.956631200	0.758667040	-1.976490080
H	-4.901830400	3.470500000	2.188611470
H	-6.094485970	1.327839910	2.078560610
C	-3.528219650	3.062490780	-2.260985040
C	-2.727968630	4.345314300	-2.317107270
C	-3.552091810	2.321987590	-3.522158880
C	-1.980716140	4.574142810	-3.598040480
H	-2.041264400	4.427243120	-1.485215030
C	-2.846534670	2.730358930	-4.597512820
H	-4.140953380	1.433846810	-3.622472990
N	-2.018260960	3.867991420	-4.635564810
H	-1.350789360	5.451441820	-3.616996080
H	-2.879704010	2.176885210	-5.516296160
O	-3.634159810	4.506689330	0.248400310
H	-3.455664760	5.286931110	-2.162781300

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C	-5.595691970	0.950840320	-0.016643690
C	-4.944426190	1.373146380	-1.099454950
C	-4.191960180	2.618920260	-1.127342820
C	-4.176550210	3.427726700	0.132148010
C	-4.920811690	2.893787750	1.286672830
C	-5.591538880	1.723138510	1.215962230
H	-6.138087130	0.023128860	-0.041039390
H	-4.978664150	0.765899910	-1.980608170
H	-4.892121600	3.494003360	2.176388040
H	-6.128989310	1.349471370	2.068722270
C	-3.517084690	3.050190160	-2.256072950
C	-2.724006990	4.340478170	-2.303705530
C	-3.511399860	2.299776730	-3.503750970
C	-2.049248890	4.621771080	-3.615109730
H	-1.973062580	4.358234400	-1.521216480
C	-2.836813770	2.735920530	-4.593356100
H	-4.046666920	1.377100060	-3.589004130
N	-2.083602570	3.920333910	-4.656800130
H	-1.473560270	5.535155340	-3.652210130
H	-2.846193840	2.167768080	-5.503641070
O	-3.592477100	4.476059270	0.235311390
H	-3.369539510	5.197331780	-2.060621900

CASSCF: S1 LIIC path S1-KETO_S1S0-KETO

coord_1

C	-5.1489836	0.7695617	0.2544436
C	-4.5542098	1.2710176	-0.9460261
C	-4.1777429	2.6064939	-1.1099113
C	-4.4062774	3.5767282	-0.0493415
C	-5.022206	3.0244114	1.1258081
C	-5.3721369	1.643228	1.2578287
H	-5.4156115	-0.2674786	0.3274142
H	-4.3582983	0.578675	-1.7443913
H	-5.2671789	3.7160504	1.9097311
H	-5.8221656	1.3166929	2.1786326
C	-3.4772483	2.9967257	-2.3271941
C	-2.3250851	3.9510049	-2.2336142
C	-3.8047637	2.5119748	-3.5899803
C	-1.6744908	4.2470825	-3.5451706
H	-1.5734398	3.5579536	-1.5461823
C	-3.0683661	2.8934972	-4.7112439
H	-4.6408954	1.8502196	-3.7219978

N	-2.0037751	3.7756104	-4.6731909
H	-0.8424723	4.9341189	-3.5255044
H	-3.3146239	2.514941	-5.6839848
O	-4.1323092	4.7677661	-0.1551284
H	-2.6609584	4.8689583	-1.7528136
coord_2			
C	-5.1160004	0.7612024	0.2837079
C	-4.520597	1.2341336	-0.9200703
C	-4.1753028	2.5727374	-1.1184274
C	-4.4260902	3.5666315	-0.0890444
C	-5.044307	3.0413658	1.0971479
C	-5.3691772	1.6641214	1.2631858
H	-5.3640509	-0.2778721	0.3880106
H	-4.3031497	0.5237934	-1.6971464
H	-5.3046528	3.7515409	1.8593567
H	-5.8241214	1.3532163	2.1870674
C	-3.4732046	2.9711657	-2.3337311
C	-2.3105844	3.9063322	-2.2240227
C	-3.8292097	2.5451282	-3.6096717
C	-1.6573171	4.2309118	-3.52444
H	-1.5700881	3.5175208	-1.5260028
C	-3.0938974	2.950803	-4.7219026
H	-4.6805286	1.9063291	-3.7552341
N	-2.0096441	3.8033198	-4.6651295
H	-0.8079743	4.8953107	-3.4884932
H	-3.3567184	2.6116518	-5.7049621
O	-4.1563091	4.7584531	-0.2277842
H	-2.6703139	4.8174368	-1.7342307
coord_3			
C	-5.082354	0.7542195	0.3116931
C	-4.4854732	1.1996966	-0.8939392
C	-4.1716849	2.5401442	-1.126255
C	-4.4456617	3.5556598	-0.1282705
C	-5.0671623	3.056679	1.067392
C	-5.3668641	1.6844643	1.2663922
H	-5.3117188	-0.2856988	0.4468296
H	-4.2457526	0.4729417	-1.6493746
H	-5.3437063	3.7839612	1.8075636
H	-5.8272047	1.3883138	2.1925333
C	-3.4690839	2.9462022	-2.3401401
C	-2.2963116	3.8616215	-2.2159243
C	-3.853446	2.5792522	-3.6259938

C	-1.6411517	4.2130153	-3.5049904
H	-1.5665581	3.4766427	-1.5077296
C	-3.119475	3.0080201	-4.729269
H	-4.7197429	1.9641074	-3.7830128
N	-2.0161388	3.8300597	-4.6564058
H	-0.7749275	4.8538804	-3.4550937
H	-3.3989552	2.7083721	-5.7207013
O	-4.18023	4.7475307	-0.2989404
H	-2.6796357	4.7661478	-1.7181802
coord_4			
C	-5.0481225	0.7486253	0.338456
C	-4.4490079	1.1677712	-0.8676793
C	-4.1670409	2.5087802	-1.1334761
C	-4.465047	3.5438973	-0.167043
C	-5.0907315	3.0703514	1.0366157
C	-5.3651742	1.7042106	1.2675648
H	-5.2587249	-0.2909814	0.5039266
H	-4.1863528	0.4261964	-1.60117
H	-5.3842216	3.8133047	1.754483
H	-5.8313135	1.4219082	2.1952166
C	-3.464951	2.9218589	-2.3464922
C	-2.2823027	3.8168809	-2.2092841
C	-3.8774421	2.6142602	-3.6390501
C	-1.625919	4.1934117	-3.4868336
H	-1.5629057	3.4353345	-1.4912605
C	-3.1449597	3.0650506	-4.7334482
H	-4.75851	2.0234271	-3.8054716
N	-2.0230822	3.855777	-4.6470378
H	-0.7432395	4.8099089	-3.4252595
H	-3.441122	2.8049576	-5.7313499
O	-4.2041228	4.7351603	-0.3686343
H	-2.6889459	4.7151418	-1.7045894
coord_5			
C	-5.0133743	0.7444362	0.3640498
C	-4.4113628	1.1384222	-0.8413386
C	-4.1615198	2.4787099	-1.1401641
C	-4.4843033	3.5314235	-0.2053744
C	-5.1149751	3.0823845	1.0049036
C	-5.3640787	1.7233194	1.2668228
H	-5.2051629	-0.2937384	0.5593509
H	-4.1251853	0.3836348	-1.5526308
H	-5.4260866	3.8395657	1.7002561

H	-5.8363398	1.4539295	2.195305
C	-3.460876	2.8981589	-2.3528488
C	-2.268604	3.7721118	-2.2040685
C	-3.9011566	2.6500761	-3.648947
C	-1.6115606	4.1721089	-3.4699786
H	-1.559198	3.3936059	-1.4765
C	-3.1702065	3.1218026	-4.7345521
H	-4.7967794	2.0841765	-3.8227571
N	-2.0303061	3.8804124	-4.6370512
H	-0.7128467	4.7634561	-3.3989404
H	-3.4829934	2.9012745	-5.7370649
O	-4.2280486	4.7214955	-0.4368922
H	-2.6982745	4.6644669	-1.6933965
coord_6			
C	-4.9781689	0.7416715	0.3885253
C	-4.372692	1.1117141	-0.8149664
C	-4.1552694	2.4499964	-1.1463858
C	-4.5034915	3.5183144	-0.2432671
C	-5.1398554	3.09278	0.9723494
C	-5.3635427	1.7417534	1.2642889
H	-5.1511102	-0.2939851	0.6131467
H	-4.0624749	0.3453342	-1.5038597
H	-5.4691954	3.8627396	1.6450348
H	-5.8421693	1.4843137	2.1929895
C	-3.4569342	2.8751251	-2.3592638
C	-2.2552731	3.7273101	-2.2002445
C	-3.9245371	2.6866339	-3.6557947
C	-1.5980347	4.1491054	-3.454432
H	-1.555514	3.3514624	-1.4633577
C	-3.1950633	3.1781898	-4.7326994
H	-4.83448	2.1462592	-3.8350263
N	-2.0376488	3.9039011	-4.6264796
H	-0.6837124	4.7145624	-3.376081
H	-3.5243307	2.9971982	-5.7380139
O	-4.2520803	4.7066831	-0.5037307
H	-2.7076607	4.6141705	-1.6845491
coord_7			
C	-4.9425559	0.7403526	0.4119307
C	-4.3331428	1.087711	-0.7886132
C	-4.148437	2.4227017	-1.1522018
C	-4.5226778	3.5046423	-0.2807141
C	-5.1653364	3.1015402	0.9390572

C	-5.3635259	1.7594786	1.2600908
H	-5.0966266	-0.291734	0.6653537
H	-3.9984358	0.3113718	-1.4549649
H	-5.5134485	3.8828221	1.5889835
H	-5.8486797	1.5130021	2.1884662
C	-3.4532066	2.852779	-2.3657838
C	-2.2423781	3.6824668	-2.1977791
C	-3.9475208	2.7238762	-3.6597084
C	-1.5853148	4.124391	-3.4401971
H	-1.5519437	3.3089071	-1.4517475
C	-3.2193707	3.2341305	-4.7280171
H	-4.8715216	2.2095945	-3.8424486
N	-2.0449533	3.9261727	-4.6153642
H	-0.6558247	4.6632514	-3.3566213
H	-3.5648805	3.0926124	-5.7343769
O	-4.2763053	4.6908637	-0.5691574
H	-2.7171527	4.5642998	-1.6780037
coord_8			
C	-4.906575	0.7405035	0.4343126
C	-4.2928551	1.0664766	-0.7623321
C	-4.141171	2.3968861	-1.1576678
C	-4.5419346	3.4904762	-0.317699
C	-5.1913847	3.108667	0.9051417
C	-5.3639815	1.7764634	1.2543614
H	-5.0417534	-0.2869955	0.716008
H	-3.9332717	0.2818252	-1.4060612
H	-5.5587536	3.8998082	1.5322802
H	-5.8557408	1.53994	2.1819378
C	-3.4497796	2.8311407	-2.3724491
C	-2.2299977	3.6375683	-2.1966391
C	-3.9700343	2.7617542	-3.6608095
C	-1.5733891	4.0979479	-3.4272745
H	-1.5485887	3.265943	-1.4415863
C	-3.2429608	3.2895472	-4.720641
H	-4.9077959	2.2741169	-3.8452075
N	-2.0520662	3.947151	-4.6037542
H	-0.6291957	4.6095307	-3.3404947
H	-3.6043744	3.1874081	-5.7263468
O	-4.3008272	4.6741722	-0.6331716
H	-2.7268081	4.5149028	-1.6737243
coord_9			
C	-4.8702559	0.7421496	0.4557159

C	-4.251962	1.0480741	-0.7361781
C	-4.1336217	2.3726088	-1.162835
C	-4.5613423	3.4758814	-0.3541962
C	-5.2179703	3.1141616	0.8707289
C	-5.3648573	1.7926782	1.2472405
H	-4.986513	-0.2797776	0.7651416
H	-3.8671757	0.2567721	-1.3572705
H	-5.6050267	3.9136916	1.4751174
H	-5.8632139	1.5650761	2.1736146
C	-3.446745	2.8102283	-2.3792944
C	-2.2182211	3.592598	-2.1967901
C	-3.9919932	2.8002267	-3.6592266
C	-1.56226	4.0697515	-3.415661
H	-1.5455614	3.2225752	-1.432793
C	-3.2656563	3.3443651	-4.7107163
H	-4.9431766	2.3397767	-3.8435033
N	-2.0588362	3.9667538	-4.591706
H	-0.6038603	4.5533946	-3.3276274
H	-3.6425275	3.2814818	-5.7141317
O	-4.3257679	4.6567371	-0.6957641
H	-2.7366948	4.4660288	-1.6716822
coord_10			
C	-5.44342032	0.85422968	0.19730695
C	-4.82428436	1.13466786	-0.99274721
C	-4.29457931	2.40431144	-1.23639529
C	-4.27457015	3.42953165	-0.23913622
C	-4.94985415	3.10439983	0.98570885
C	-5.51371596	1.86478561	1.18146017
H	-5.88241517	-0.11020975	0.37323429
H	-4.76256573	0.37890341	-1.75798924
H	-5.00589692	3.87168853	1.73581046
H	-6.0126995	1.65663244	2.11214838
C	-3.56732075	2.81115782	-2.4401549
C	-2.13190999	3.04334679	-2.28154846
C	-4.14840411	3.30018603	-3.60600702
C	-1.40991232	3.50495013	-3.4624154
H	-1.60473799	2.32493777	-1.66475513
C	-3.32734658	3.76692047	-4.62403795
H	-5.21222416	3.27098289	-3.7390035
N	-1.97135872	3.86062563	-4.55911495
H	-0.33589239	3.57050209	-3.41980145
H	-3.7550523	4.07525801	-5.55953566

O	-3.6552946	4.5032566	-0.43409263
H	-2.29139535	3.92571386	-1.55934064

CASSCF: S1 LIIC path S1-ENOL_S1S0-ENOL-1

coord_1

C	-5.339094300	0.888165000	0.146177900
C	-4.807559500	1.323961800	-1.105329400
C	-4.207973000	2.639747400	-1.242081000
C	-4.449715300	3.523796200	-0.098962100
C	-5.008898100	3.048127400	1.137933800
C	-5.421945400	1.704440700	1.241192400
H	-5.677504300	-0.129944600	0.217221400
H	-4.751335900	0.624838300	-1.914183200
H	-5.155505800	3.757924200	1.927745700
H	-5.824939500	1.337970200	2.166441000
C	-3.430103200	3.032457500	-2.389878900
C	-2.422693200	4.004707100	-2.339733000
C	-3.627755800	2.433912300	-3.659679900
C	-1.714156100	4.322653800	-3.485819800
H	-2.142662900	4.471366300	-1.414156000
C	-2.876300600	2.829984400	-4.725606800
H	-4.387750800	1.690240200	-3.803966100
N	-1.915504600	3.770313000	-4.673258900
H	-0.931347100	5.059720700	-3.434478600
H	-3.038313500	2.385275400	-5.691620100
O	-4.303928300	4.854363200	-0.184115900
H	-4.147535000	5.126179900	-1.079225600

coord_2

C	-5.322350900	0.879237400	0.155467400
C	-4.778041300	1.304098800	-1.086706700
C	-4.207213700	2.625220300	-1.236302800
C	-4.457969200	3.520145200	-0.115668600
C	-5.027188300	3.059034300	1.117680600
C	-5.430301800	1.717197500	1.236611900
H	-5.650843500	-0.141088300	0.239194700
H	-4.699421100	0.597175700	-1.887565200
H	-5.183479800	3.777273400	1.898243300
H	-5.843550000	1.362962100	2.162279200
C	-3.436547500	3.023873000	-2.394724500
C	-2.397482700	3.974094300	-2.323338400
C	-3.673214100	2.466080000	-3.668434700
C	-1.719574900	4.336366900	-3.467452000

H	-2.089153000	4.389599500	-1.382506200
C	-2.909518800	2.866660000	-4.743307100
H	-4.450506200	1.741629200	-3.818916200
N	-1.986641100	3.848307700	-4.678940300
H	-0.923571600	5.058570500	-3.414833400
H	-2.984516900	2.335570900	-5.677193200
O	-4.296011700	4.848991900	-0.212482200
H	-4.115424000	5.109200300	-1.106488500
coord_3			
C	-5.304320600	0.870566000	0.164083000
C	-4.747836100	1.286049900	-1.068270000
C	-4.206573600	2.612310700	-1.230572300
C	-4.467064300	3.516861100	-0.132171800
C	-5.046021400	3.069133900	1.097059600
C	-5.438242300	1.729043400	1.230995400
H	-5.622184500	-0.151976100	0.260092600
H	-4.646276500	0.572281100	-1.861134200
H	-5.212658600	3.795174600	1.868507400
H	-5.861599300	1.386064000	2.156510100
C	-3.443957800	3.015716500	-2.400246900
C	-2.372076900	3.941616400	-2.312080600
C	-3.719786000	2.498487300	-3.675515000
C	-1.724254700	4.346386000	-3.452260800
H	-2.035231400	4.306297300	-1.360019100
C	-2.942536100	2.901697900	-4.758799700
H	-4.515275200	1.794876000	-3.830375700
N	-2.059221200	3.922119000	-4.679540600
H	-0.915725000	5.054126900	-3.401023200
H	-2.924801500	2.295865000	-5.650487000
O	-4.290671200	4.844042300	-0.239097400
H	-4.086208100	5.093461100	-1.131036800
coord_4			
C	-5.285100100	0.862214900	0.172009000
C	-4.717008600	1.269880400	-1.050050500
C	-4.206065400	2.600997600	-1.224925600
C	-4.476973400	3.513947100	-0.148485200
C	-5.065401700	3.078408100	1.076084700
C	-5.445843800	1.739984300	1.224366400
H	-5.591669000	-0.162525300	0.279873900
H	-4.591993500	0.550274600	-1.834953200
H	-5.243022900	3.811589700	1.838574400
H	-5.879194400	1.407266300	2.149178000

C	-3.452249000	3.007899000	-2.406439200
C	-2.346562500	3.907347200	-2.305869600
C	-3.767121800	2.531032900	-3.680986600
C	-1.728099900	4.352811200	-3.440277600
H	-1.981245200	4.221640900	-1.346365800
C	-2.974748500	2.934681100	-4.772044900
H	-4.581576400	1.849906400	-3.838407900
N	-2.132769100	3.991401600	-4.675111800
H	-0.907760400	5.046572800	-3.392784900
H	-2.860591600	2.266181400	-5.611785400
O	-4.287788900	4.839592800	-0.264023400
H	-4.059735900	5.079095400	-1.152957700
coord_5			
C	-5.264767600	0.854252200	0.179210600
C	-4.685620000	1.255680600	-1.032090700
C	-4.205706900	2.591298100	-1.219389500
C	-4.487675800	3.511424800	-0.164599800
C	-5.085328700	3.086836000	1.054786200
C	-5.453164000	1.750017000	1.216742700
H	-5.559407300	-0.172656200	0.298462600
H	-4.536658900	0.531311800	-1.809107600
H	-5.274551600	3.826464700	1.808508900
H	-5.896412700	1.426534300	2.140315600
C	-3.461347800	3.000369900	-2.413285700
C	-2.321035500	3.871361500	-2.304607700
C	-3.814880200	2.563659800	-3.684935600
C	-1.731051500	4.355741300	-3.431542100
H	-1.927529800	4.135785000	-1.341211800
C	-3.005551500	2.965219500	-4.782990200
H	-4.648921200	1.906695000	-3.843117000
N	-2.206885600	4.055816100	-4.665695900
H	-0.899647400	5.036054000	-3.389891900
H	-2.793226400	2.246358300	-5.561373800
O	-4.287265900	4.835728300	-0.287279300
H	-4.035886200	5.066248500	-1.172290900
coord_6			
C	-5.243386100	0.846750100	0.185638900
C	-4.653733900	1.243560800	-1.014443100
C	-4.205524700	2.583259700	-1.213985000
C	-4.499156100	3.509332500	-0.180488500
C	-5.105792600	3.094396200	1.033210400
C	-5.460240300	1.759132200	1.208141300

H	-5.525484600	-0.182291200	0.315756300
H	-4.480364300	0.515577100	-1.783702700
H	-5.307213200	3.839734400	1.778402700
H	-5.913298900	1.443814500	2.129953200
C	-3.471195600	2.993108700	-2.420765500
C	-2.295602900	3.833729700	-2.308193200
C	-3.862729600	2.596348400	-3.687473400
C	-1.733091400	4.355272500	-3.426104300
H	-1.874411300	4.048853300	-1.344222700
C	-3.034338700	2.992943300	-4.791560600
H	-4.716815300	1.965256900	-3.844658100
N	-2.281257600	4.115018500	-4.651311900
H	-0.891378200	5.022681600	-3.392161400
H	-2.723925100	2.236108900	-5.499521800
O	-4.289017200	4.832539200	-0.308851800
H	-4.014564500	5.055073200	-1.189041700
coord_7			
C	-5.221006600	0.839784300	0.191234500
C	-4.621421000	1.233646800	-0.997169100
C	-4.205556700	2.576953400	-1.208729600
C	-4.511403500	3.507723600	-0.196110200
C	-5.126771700	3.101069400	1.011419100
C	-5.467089300	1.767317800	1.198582000
H	-5.489964700	-0.191353800	0.331633100
H	-4.423214300	0.503277000	-1.758861900
H	-5.340960100	3.851327400	1.748374200
H	-5.929863500	1.459041100	2.118123700
C	-3.481750700	2.986119000	-2.428854300
C	-2.270383600	3.794513100	-2.316524800
C	-3.910348400	2.629109200	-3.688740500
C	-1.734248000	4.351494600	-3.424029200
H	-1.822208100	3.960932900	-1.355071600
C	-3.060497700	3.017495800	-4.797644900
H	-4.784759900	2.025639600	-3.843246600
N	-2.355667700	4.168643500	-4.631936700
H	-0.882974900	5.006532400	-3.399465600
H	-2.653763900	2.235088700	-5.426463900
O	-4.292967600	4.830120400	-0.328706100
H	-3.995700400	5.045724400	-1.203194600
coord_8			
C	-5.197671200	0.833435300	0.195930000
C	-4.588762400	1.226075300	-0.980338900

C	-4.205854200	2.572468700	-1.203639400
C	-4.524410700	3.506665700	-0.211413300
C	-5.148230600	3.106841400	0.989488100
C	-5.473706900	1.774562500	1.188088800
H	-5.452894800	-0.199767500	0.345956400
H	-4.365332100	0.494633800	-1.734725700
H	-5.375724400	3.861171500	1.718565200
H	-5.946082400	1.472142800	2.104867000
C	-3.492988200	2.979421400	-2.437525600
C	-2.245507800	3.753758100	-2.329506900
C	-3.957422200	2.661974700	-3.688910900
C	-1.734601600	4.344486000	-3.425401500
H	-1.771229800	3.872069400	-1.373447300
C	-3.083402500	3.038526500	-4.801076400
H	-4.852250200	2.087913600	-3.839168600
N	-2.430000900	4.216282100	-4.607481700
H	-0.874498300	4.987646600	-3.411745700
H	-2.583662700	2.242970900	-5.342374400
O	-4.299046100	4.828569400	-0.346796000
H	-3.979242100	5.038352100	-1.214726200
coord_9			
C	-5.173416000	0.827788700	0.199651300
C	-4.555852200	1.220990200	-0.964031600
C	-4.206483000	2.569906800	-1.198730300
C	-4.538173700	3.506239400	-0.226340000
C	-5.170119500	3.111706200	0.967504900
C	-5.480069800	1.780859800	1.176691000
H	-5.414310500	-0.207453100	0.358578100
H	-4.306864200	0.489878600	-1.711450300
H	-5.411415400	3.869198600	1.689138700
H	-5.961898400	1.483050500	2.090231600
C	-3.504899700	2.973048200	-2.446751200
C	-2.221115100	3.711489700	-2.347055600
C	-4.003639600	2.694991400	-3.688196300
C	-1.734292100	4.334308800	-3.430332900
H	-1.721776000	3.782259300	-1.399064900
C	-3.102401900	3.055685900	-4.801606100
H	-4.918772300	2.152163600	-3.832793100
N	-2.504251500	4.257451500	-4.577760900
H	-0.866059200	4.966025300	-3.429030600
H	-2.514383700	2.259534200	-5.247338800
O	-4.307179300	4.827984600	-0.363076100

H	-3.965149300	5.033092300	-1.223619800
coord_10			
C	-5.148275800	0.822936000	0.202318300
C	-4.522800300	1.218537100	-0.948334900
C	-4.207523700	2.569375000	-1.194019600
C	-4.552690300	3.506537400	-0.240830300
C	-5.192374000	3.115669700	0.945565900
C	-5.486138000	1.786213500	1.164421800
H	-5.374241600	-0.214326800	0.369341800
H	-4.247984500	0.489244600	-1.689206400
H	-5.447917600	3.875351100	1.660273900
H	-5.977224900	1.491706600	2.074274600
C	-3.517490300	2.967036200	-2.456500200
C	-2.197351600	3.667703700	-2.369105000
C	-4.048683700	2.728210200	-3.686851700
C	-1.733529600	4.321001100	-3.438970400
H	-1.674133200	3.691439500	-1.431678000
C	-3.116804600	3.068622900	-4.798867900
H	-4.983796400	2.218476100	-3.824586700
N	-2.578525000	4.291555400	-4.542447100
H	-0.857834000	4.941624600	-3.451461700
H	-2.446541500	2.284770200	-5.141321300
O	-4.317280800	4.828461900	-0.377515700
H	-3.953380800	5.030054600	-1.229882700

CASSCF: S1 LIIC path S1-ENOL_S1S0-ENOL-2

coord_1			
C	-5.339094300	0.888165000	0.146177900
C	-4.807559500	1.323961800	-1.105329400
C	-4.207973000	2.639747400	-1.242081000
C	-4.449715300	3.523796200	-0.098962100
C	-5.008898100	3.048127400	1.137933800
C	-5.421945400	1.704440700	1.241192400
H	-5.677504300	-0.129944600	0.217221400
H	-4.751335900	0.624838300	-1.914183200
H	-5.155505800	3.757924200	1.927745700
H	-5.824939500	1.337970200	2.166441000
C	-3.430103200	3.032457500	-2.389878900
C	-2.422693200	4.004707100	-2.339733000
C	-3.627755800	2.433912300	-3.659679900
C	-1.714156100	4.322653800	-3.485819800
H	-2.142662900	4.471366300	-1.414156000

C	-2.876300600	2.829984400	-4.725606800
H	-4.387750800	1.690240200	-3.803966100
N	-1.915504600	3.770313000	-4.673258900
H	-0.931347100	5.059720700	-3.434478600
H	-3.038313500	2.385275400	-5.691620100
O	-4.303928300	4.854363200	-0.184115900
H	-4.147535000	5.126179900	-1.079225600
coord_2			
C	-5.383779100	0.898067900	0.134379100
C	-4.822199400	1.319227700	-1.101869100
C	-4.200768600	2.621830200	-1.233793900
C	-4.421116300	3.511434400	-0.098396100
C	-5.006656300	3.051916500	1.128253300
C	-5.460457700	1.724805500	1.228092500
H	-5.751872500	-0.109705900	0.203472500
H	-4.772451000	0.621126800	-1.912298200
H	-5.135568000	3.764008500	1.919326800
H	-5.887639300	1.373516400	2.148494400
C	-3.411249200	3.002992900	-2.375923400
C	-2.434394000	4.017404700	-2.329098200
C	-3.576804900	2.374460100	-3.641814300
C	-1.797124700	4.409604100	-3.509078500
H	-2.067540200	4.369771600	-1.382020000
C	-2.875525300	2.826049400	-4.716220700
H	-4.273687600	1.569219000	-3.775270800
N	-1.993827000	3.849812400	-4.686564900
H	-1.078999900	5.211316800	-3.484022300
H	-3.012072100	2.366543900	-5.679090400
O	-4.211822100	4.832138100	-0.175620200
H	-4.006967200	5.094659500	-1.066320600
coord_3			
C	-5.427407300	0.909324300	0.119611000
C	-4.834339800	1.316596300	-1.099372500
C	-4.191800000	2.606328900	-1.223782300
C	-4.393555000	3.499280900	-0.095348600
C	-5.007060500	3.055127500	1.119063300
C	-5.500232200	1.745336700	1.212669900
H	-5.824325300	-0.087608200	0.184542800
H	-4.788789300	0.620523100	-1.912058800
H	-5.120465600	3.767972100	1.912072100
H	-5.952663000	1.408762900	2.126612200
C	-3.388975500	2.975938000	-2.358623700

C	-2.443517900	4.030643400	-2.318797700
C	-3.519904600	2.318279700	-3.619810000
C	-1.888562500	4.491147200	-3.530386400
H	-1.976243500	4.275129600	-1.380347800
C	-2.875145100	2.821133500	-4.703381000
H	-4.148349900	1.456581600	-3.741518200
N	-2.081559400	3.922567300	-4.696979400
H	-1.241849400	5.352086900	-3.530023200
H	-2.986019500	2.348523300	-5.663051400
O	-4.122964900	4.807548200	-0.161340800
H	-3.868792300	5.058977300	-1.045132500
coord_4			
C	-5.469997700	0.922192300	0.101403000
C	-4.843973300	1.316343800	-1.098111600
C	-4.180860100	2.593428300	-1.212118800
C	-4.366728800	3.487538200	-0.089716700
C	-5.009860800	3.057943500	1.110293400
C	-5.541204300	1.766220600	1.194571500
H	-5.895020900	-0.063377200	0.159729500
H	-4.800402400	0.623350600	-1.913802200
H	-5.109905700	3.769987100	1.906054100
H	-6.020009100	1.443867100	2.100296800
C	-3.363070400	2.951401600	-2.337983800
C	-2.449112900	4.043809300	-2.308820200
C	-3.456905000	2.265529300	-3.593485300
C	-1.988320700	4.566137100	-3.549199000
H	-1.870617300	4.187854900	-1.410483600
C	-2.875553600	2.815200500	-4.686909600
H	-4.011887500	1.352936100	-3.702380800
N	-2.179304200	3.987815000	-4.704021900
H	-1.418953000	5.480006300	-3.571551400
H	-2.961086600	2.331426400	-5.643455400
O	-4.036985100	4.780947800	-0.140789300
H	-3.732763000	5.019641800	-1.014901500
coord_5			
C	-5.511508900	0.936993200	0.079318100
C	-4.851070500	1.318787300	-1.098319600
C	-4.167729100	2.583318700	-1.198825600
C	-4.340294600	3.476377300	-0.081349400
C	-5.014732900	3.060533000	1.101913800
C	-5.583220300	1.787679600	1.173482600
H	-5.964046000	-0.036638100	0.128359000

H	-4.807334000	0.629997700	-1.917821500
H	-5.103504300	3.770180300	1.901381300
H	-6.089556600	1.479038500	2.069086800
C	-3.333343900	2.929476600	-2.313967600
C	-2.450138800	4.056365700	-2.299325900
C	-3.387708100	2.216585400	-3.562754100
C	-2.095925300	4.633264200	-3.564668900
H	-1.754058100	4.108377400	-1.475057000
C	-2.877075700	2.808165400	-4.666542000
H	-3.864653800	1.259200500	-3.657820600
N	-2.287295100	4.044426500	-4.706809900
H	-1.608958400	5.593093700	-3.607186700
H	-2.938245300	2.315373100	-5.620198000
O	-3.953483200	4.752584400	-0.113437700
H	-3.598639300	4.977020100	-0.974840300
coord_6			
C	-5.551758600	0.954112900	0.052939300
C	-4.855534100	1.324316600	-1.100215500
C	-4.152187700	2.576260800	-1.183899700
C	-4.313912500	3.465985100	-0.070065600
C	-5.021285700	3.063064900	1.093926200
C	-5.625982800	1.809963300	1.149121100
H	-6.031287000	-0.006931600	0.089777100
H	-4.809553900	0.640955800	-1.924393900
H	-5.100818500	3.768637900	1.898193100
H	-6.160982100	1.514505700	2.032558300
C	-3.299685700	2.910298600	-2.286556300
C	-2.445499300	4.067855900	-2.290720900
C	-3.312365500	2.171996500	-3.527653300
C	-2.210398200	4.691091200	-3.575741500
H	-1.632059800	4.037078300	-1.577321300
C	-2.879927200	2.799837800	-4.641960100
H	-3.707343100	1.176488400	-3.608074800
N	-2.405180200	4.090958000	-4.704143000
H	-1.809847400	5.689404100	-3.635141700
H	-2.918443000	2.300243600	-5.593107000
O	-3.872142200	4.722659500	-0.078737600
H	-3.466327700	4.931417200	-0.924165800
coord_7			
C	-5.590346800	0.973982400	0.021878100
C	-4.857154800	1.333407700	-1.104016200
C	-4.134039500	2.572641200	-1.167345200

C	-4.287306600	3.456618100	-0.055690900
C	-5.029086900	3.065727900	1.086345600
C	-5.669007900	1.833332300	1.121241800
H	-6.096299800	0.026239000	0.043377000
H	-4.806887900	0.656829500	-1.933788000
H	-5.101401400	3.765427000	1.896636100
H	-6.233691600	1.550473100	1.990345900
C	-3.262135300	2.894096500	-2.255821900
C	-2.434076800	4.077866600	-2.283719100
C	-3.231141800	2.132402400	-3.488359300
C	-2.330130100	4.738185100	-3.581263700
H	-1.512603800	3.973921400	-1.720466500
C	-2.884172800	2.789912700	-4.612830300
H	-3.541049800	1.105940600	-3.553591300
N	-2.531889500	4.125833100	-4.694612700
H	-2.018697600	5.767158000	-3.653400900
H	-2.902502800	2.285607400	-5.561940900
O	-3.792861900	4.691413100	-0.036180800
H	-3.336036900	4.883185400	-0.862179800
coord_8			
C	-5.626597200	0.997033000	-0.014209300
C	-4.855565500	1.346614800	-1.109936400
C	-4.113122800	2.573012200	-1.149196200
C	-4.260325100	3.448647200	-0.038091900
C	-5.037708700	3.068737700	1.079180000
C	-5.711615300	1.858018500	1.089643000
H	-6.158207200	0.063326900	-0.011362800
H	-4.798940000	0.678323200	-1.946253400
H	-5.104882900	3.760610000	1.896830600
H	-6.306801200	1.587052300	1.942161700
C	-3.220931900	2.881214200	-2.221996900
C	-2.414727900	4.085931700	-2.279400900
C	-3.144529700	2.098436500	-3.445182500
C	-2.452791500	4.773289400	-3.580103800
H	-1.406474400	3.918064100	-1.906985800
C	-2.889687500	2.777994300	-4.578842200
H	-3.367248400	1.048553200	-3.494923400
N	-2.665583000	4.147583700	-4.676727100
H	-2.231481800	5.824963500	-3.659877600
H	-2.891022700	2.270722100	-5.526395200
O	-3.715878100	4.659216500	0.014638600
H	-3.208399600	4.832855600	-0.788351700

coord_9			
C	-5.659508500	1.023629400	-0.055636100
C	-4.850176500	1.364566000	-1.118198600
C	-4.089291200	2.578146300	-1.129518300
C	-4.232987600	3.442600500	-0.017184000
C	-5.046790600	3.072317200	1.072415200
C	-5.752947700	1.884150200	1.054148400
H	-6.215614500	0.104632800	-0.074892300
H	-4.784983800	0.706243300	-1.962028100
H	-5.111079000	3.754222700	1.898851000
H	-6.379171400	1.624136900	1.887774400
C	-3.176526100	2.872113900	-2.185528000
C	-2.386178600	4.091342600	-2.279310500
C	-3.053239400	2.070621100	-3.398535300
C	-2.575225800	4.795472500	-3.571297300
H	-1.327664200	3.867700500	-2.138049500
C	-2.896149800	2.763615400	-4.539746100
H	-3.187754500	1.005027300	-3.432579900
N	-2.803658100	4.155071500	-4.649045500
H	-2.442827500	5.862056100	-3.652608700
H	-2.884349700	2.254550600	-5.486112800
O	-3.641859400	4.626675400	0.074021700
H	-3.084538500	4.781308100	-0.702322700
coord_10			
C	-5.687654800	1.053997300	-0.102796600
C	-4.840031700	1.388027400	-1.129092100
C	-4.062334600	2.589192300	-1.108372900
C	-4.205523200	3.439241800	0.007137500
C	-5.056122800	3.076634000	1.066021000
C	-5.791992700	1.911613100	1.014524800
H	-6.266460600	0.150174300	-0.147763100
H	-4.763738900	0.741614900	-1.981417900
H	-5.120158600	3.746165800	1.902753800
H	-6.449468900	1.661155600	1.826885400
C	-3.129560900	2.867398700	-2.147126200
C	-2.346713000	4.092777300	-2.285691600
C	-2.958246500	2.049233300	-3.348860200
C	-2.693187900	4.804186500	-3.554267600
H	-1.294168100	3.820374600	-2.412731100
C	-2.903146500	2.746178500	-4.495383600
H	-3.004820300	0.975611500	-3.366789600
N	-2.942784500	4.147621200	-4.610332400

H	-2.645493200	5.878479500	-3.630047700
H	-2.882781600	2.235672900	-5.440676200
O	-3.572021100	4.594783700	0.142337600
H	-2.966112000	4.730066600	-0.603694300

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coord_1

C	-4.939802300	0.839359400	0.382464400
C	-4.412646300	1.213476700	-0.890666100
C	-4.161908300	2.607438800	-1.212375800
C	-4.739902700	3.551320500	-0.252317300
C	-5.281830500	3.129626200	1.011544100
C	-5.342721200	1.754770800	1.316223100
H	-5.009641500	-0.210327500	0.604715700
H	-4.095000900	0.444471100	-1.564395300
H	-5.687095600	3.881466700	1.659312800
H	-5.730662800	1.433343800	2.264366500
C	-3.397679000	3.022664100	-2.361412100
C	-2.685813700	4.228012600	-2.416561900
C	-3.302377700	2.212514800	-3.520848600
C	-1.969084000	4.553576500	-3.555393100
H	-2.632503000	4.884298000	-1.568429800
C	-2.572825000	2.635847000	-4.591503100
H	-3.825814500	1.277792900	-3.582232800
N	-1.897734200	3.798517500	-4.641868300
H	-1.412452200	5.474497300	-3.582949900
H	-2.514256400	2.026480300	-5.476058300
O	-4.934240300	4.843893400	-0.552986100
H	-4.761891800	5.012861700	-1.470215700

coord_2

C	-4.968682300	0.859997400	0.322342400
C	-4.505994400	1.252700100	-0.960663600
C	-4.227646200	2.641928700	-1.251804000
C	-4.756864600	3.581857700	-0.237200600
C	-5.167134100	3.146146200	1.076215200
C	-5.255869900	1.769832500	1.327924900
H	-5.074239500	-0.191389800	0.520765500
H	-4.255671100	0.497518600	-1.677825200
H	-5.474947000	3.875704500	1.797264300
H	-5.565126900	1.427704900	2.298131900
C	-3.418439000	3.026047300	-2.372627900
C	-2.711904000	4.236405300	-2.424448000

C	-3.274671700	2.193707700	-3.506685800
C	-1.951176400	4.540480400	-3.539347500
H	-2.708425600	4.915760200	-1.593147200
C	-2.501026300	2.598714100	-4.557678800
H	-3.786554200	1.252840800	-3.566426800
N	-1.831380900	3.759593800	-4.605383400
H	-1.400605400	5.464830200	-3.567457000
H	-2.403105300	1.968635000	-5.424138500
O	-5.081159400	4.827716300	-0.562343100
H	-4.987259600	4.969170600	-1.497054300
coord_3			
C	-5.001004600	0.883814200	0.267747600
C	-4.598678000	1.291531100	-1.021518200
C	-4.290349600	2.675477000	-1.290797700
C	-4.772015000	3.606896800	-0.231299300
C	-5.048863800	3.157870700	1.116703900
C	-5.170057500	1.784381000	1.328647200
H	-5.142741900	-0.166214800	0.449646700
H	-4.415133900	0.550391900	-1.773525500
H	-5.254297700	3.865852100	1.892600100
H	-5.402393700	1.421869000	2.313431900
C	-3.437420700	3.031613100	-2.383118400
C	-2.736596800	4.247016600	-2.434044600
C	-3.248183100	2.176889800	-3.488991900
C	-1.934734300	4.529516900	-3.524423300
H	-2.780801400	4.949089400	-1.623210100
C	-2.432926000	2.563448800	-4.519759700
H	-3.748706800	1.230009100	-3.544496600
N	-1.769019000	3.722629600	-4.567042600
H	-1.390172000	5.457143200	-3.555250200
H	-2.297763400	1.912623100	-5.365716200
O	-5.227772500	4.800757900	-0.551868700
H	-5.208252000	4.923296000	-1.495302100
coord_4			
C	-5.036154900	0.909953700	0.217363200
C	-4.690311300	1.330875300	-1.074406200
C	-4.350413300	2.709167700	-1.327973000
C	-4.786557100	3.628335400	-0.232455200
C	-4.929951800	3.165383800	1.136082600
C	-5.086278000	1.797331500	1.318686200
H	-5.214022000	-0.136356900	0.388068600
H	-4.572499900	0.604635800	-1.854480500

H	-5.030268600	3.852275100	1.950209800
H	-5.243955800	1.414083100	2.310985700
C	-3.455180700	3.039365700	-2.391878600
C	-2.760880700	4.260094700	-2.445153400
C	-3.222533300	2.161689000	-3.466439200
C	-1.920512400	4.520752800	-3.510566400
H	-2.851022200	4.984978500	-1.658738400
C	-2.368025800	2.529469700	-4.476657100
H	-3.711370400	1.208666500	-3.514800400
N	-1.710676800	3.687279900	-4.526388500
H	-1.382331500	5.451716700	-3.546683600
H	-2.197167100	1.857463200	-5.299362700
O	-5.368716700	4.764656600	-0.525765800
H	-5.419053500	4.874084700	-1.471234700
coord_5			
C	-5.073701900	0.938183500	0.170427500
C	-4.780933800	1.371070500	-1.120611100
C	-4.408361700	2.743322000	-1.363185000
C	-4.801379600	3.646690800	-0.238896000
C	-4.812030400	3.169301300	1.136843700
C	-5.004992100	1.808575400	1.298857600
H	-5.287429600	-0.102377900	0.334434700
H	-4.727813600	0.660680100	-1.922974800
H	-4.805946400	3.835793200	1.973689500
H	-5.090371300	1.403857700	2.292094100
C	-3.472152500	3.049041700	-2.398649800
C	-2.785258800	4.275399600	-2.457628700
C	-3.197395700	2.148012900	-3.438683700
C	-1.908583300	4.514117500	-3.497470800
H	-2.919909700	5.023122300	-1.699650800
C	-2.305644500	2.496803400	-4.427905800
H	-3.673973800	1.188682600	-3.477100900
N	-1.655833000	3.653604300	-4.482965600
H	-1.377301300	5.448513100	-3.541391100
H	-2.100171900	1.803243400	-5.224479800
O	-5.501386800	4.719823500	-0.487049800
H	-5.617311900	4.820441400	-1.429291000
coord_6			
C	-5.113409700	0.968492700	0.126550200
C	-4.870828500	1.412180100	-1.161173000
C	-4.464645500	2.777862800	-1.396634600
C	-4.816868900	3.661954500	-0.249277600

C	-4.696017400	3.170143400	1.120813700
C	-4.926433900	1.818320800	1.269993900
H	-5.362662500	-0.064433100	0.288058500
H	-4.881600100	0.718468900	-1.980604500
H	-4.583443300	3.817244800	1.965570800
H	-4.941970800	1.391219900	2.257998600
C	-3.488681200	3.060228300	-2.403412000
C	-2.810013500	4.292450200	-2.471271000
C	-3.172519100	2.135899300	-3.405765200
C	-1.898837500	4.509498800	-3.484688300
H	-2.987951600	5.062733500	-1.745685300
C	-2.245190400	2.465792200	-4.373304200
H	-3.636116400	1.170142800	-3.431725700
N	-1.603930400	3.621896600	-4.436323400
H	-1.375022000	5.447388100	-3.538667000
H	-2.005843500	1.750597100	-5.140851300
O	-5.624130100	4.666303200	-0.438228300
H	-5.801767500	4.761517600	-1.372961700
coord_7			
C	-5.155198100	1.000931200	0.085578800
C	-4.960368900	1.454201900	-1.196803100
C	-4.519538900	2.812555000	-1.428490800
C	-4.832982200	3.673930700	-0.262584200
C	-4.582492900	3.168214700	1.089327800
C	-4.850799700	1.826752400	1.232812600
H	-5.439659600	-0.022506500	0.248691300
H	-5.034558300	0.777880800	-2.028407900
H	-4.364469000	3.797185700	1.927725700
H	-4.799183300	1.376256300	2.209749000
C	-3.504983800	3.072473100	-2.406170900
C	-2.835287800	4.310701400	-2.485864000
C	-3.147681500	2.125427500	-3.367800400
C	-1.891155900	4.506787500	-3.471802400
H	-3.055400000	5.102882300	-1.796517200
C	-2.186214600	2.436888100	-4.312760900
H	-3.597443800	1.153196100	-3.379073100
N	-1.554538400	3.592539100	-4.386102700
H	-1.375417800	5.448188100	-3.537831300
H	-1.913503400	1.700343100	-5.048419900
O	-5.735621000	4.604182300	-0.381594200
H	-5.971384800	4.696891600	-1.305249400
coord_8			

C	-5.199077600	1.035567300	0.047520400
C	-5.049922100	1.497170100	-1.227912700
C	-4.573116800	2.847111600	-1.458778000
C	-4.849371100	3.682342700	-0.278021000
C	-4.471896400	3.163566000	1.043419500
C	-4.778321900	1.833908400	1.187926600
H	-5.518496600	0.023523100	0.216304600
H	-5.187390400	0.838924000	-2.066995900
H	-4.150595000	3.775780500	1.861679700
H	-4.662625200	1.358917400	2.148249500
C	-3.521123800	3.085334200	-2.406889000
C	-2.861114600	4.329622000	-2.501212100
C	-3.122643900	2.116679900	-3.324870800
C	-1.885449100	4.505890700	-3.458526000
H	-3.122332600	5.142639400	-1.851830200
C	-2.128380900	2.410559500	-4.246250400
H	-3.557573800	1.137997900	-3.319413600
N	-1.507364900	3.565931900	-4.332093500
H	-1.378469100	5.450781200	-3.538413800
H	-1.822674400	1.653325400	-4.947213300
O	-5.834753900	4.533715500	-0.319350400
H	-6.125189600	4.626613800	-1.228916900
coord_9			
C	-5.245093000	1.072484400	0.012499300
C	-5.139796300	1.541195400	-1.254666400
C	-4.625268300	2.881226100	-1.487363600
C	-4.865485600	3.686862100	-0.294941200
C	-4.364619200	3.155999500	0.983954100
C	-4.709286800	1.839654700	1.135882600
H	-5.599298000	0.073872100	0.191002100
H	-5.340716100	0.901809400	-2.096647300
H	-3.943362400	3.752789400	1.768812600
H	-4.533097000	1.338957700	2.074333000
C	-3.537006800	3.098390500	-2.405471700
C	-2.887438100	4.348714300	-2.517165000
C	-3.097110700	2.109729100	-3.276996600
C	-1.881658100	4.506732500	-3.444744200
H	-3.188709200	5.181112200	-1.911348600
C	-2.071410900	2.387261500	-4.173812200
H	-3.516042200	1.124695800	-3.252840300
N	-1.462219400	3.542469700	-4.274264600
H	-1.384229600	5.455060300	-3.540223300

H	-1.732993800	1.610365700	-4.837333600
O	-5.920695700	4.455336900	-0.253650300
H	-6.262346600	4.551183300	-1.146602100
coord_10			
C	-5.293280500	1.111787300	-0.019273000
C	-5.230216500	1.586475400	-1.277036400
C	-4.675723300	2.914570800	-1.513984400
C	-4.880656400	3.687120000	-0.312808100
C	-4.261048200	3.145090900	0.911705300
C	-4.644034300	1.843694500	1.077189300
H	-5.682169600	0.128855000	0.172979000
H	-5.495030500	0.966971300	-2.117379600
H	-3.744317000	3.727596000	1.650473500
H	-4.411553200	1.315939400	1.988816600
C	-3.552389000	3.111232900	-2.401772700
C	-2.914139800	4.367505200	-2.533632700
C	-3.070694900	2.104636600	-3.224142900
C	-1.879749500	4.509247300	-3.430528000
H	-3.254432900	5.217430500	-1.974855600
C	-2.015023600	2.367436700	-4.095558100
H	-3.472255000	1.113435300	-3.179276900
N	-1.418966400	3.522541000	-4.212772200
H	-1.392832400	5.460932500	-3.543364000
H	-1.644117500	1.572266400	-4.718961300
O	-5.992961700	4.369633200	-0.186580100
H	-6.382291800	4.471504300	-1.060825300