

Supporting Information: Electronic Structure Calculations and Nonadiabatic Dynamics Simulations on Excited-State Relaxation of Pigment Yellow 101

Meng Che,¹ Yuan-Jun Gao², Yan Zhang¹, Shu-Hua Xia^{1*}, and Ganglong Cui^{2*}

1. College of Life and Environmental Science, Minzu University of China, Beijing 100081, China.

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

Table of Contents

1. Fig. S1 Active spaces of 10 electrons in 8 orbitals and 12 electrons in 10 orbitals used in CASSCF calculations.
2. Table S1 Selected geometric parameters of optimized structures and their relative energies at different computational levels.
3. Table S2 Single-point energies of selected optimized structures relative to S₀-TRANS-ENOL.
4. Fig. S2 Two singly occupied molecular orbitals computed by CASSCF method at the S₁ minimum.
5. Fig. S3 Time-dependent evolution of selected key geometric parameters in a typical trajectory.
6. Fig. S4 Time-dependent evolution of selected key geometric parameters in two typical trajectories.
7. Fig. S5 Schematic enol and keto products in the S₀ state optimized at the CASSCF level.
8. Fig. S6 Spatially superpositions of S₀-TRANS-ENOL and S₀-TRANS-KETO.
9. Fig. S7 Minimum-energy relaxation paths from the enol minimum to the enol conical intersection and the keto minimum to the keto conical intersection.
10. References
11. Cartesian coordinates of CASSCF optimized structures.
12. Cartesian coordinates of OM2/MRCI optimized structures.

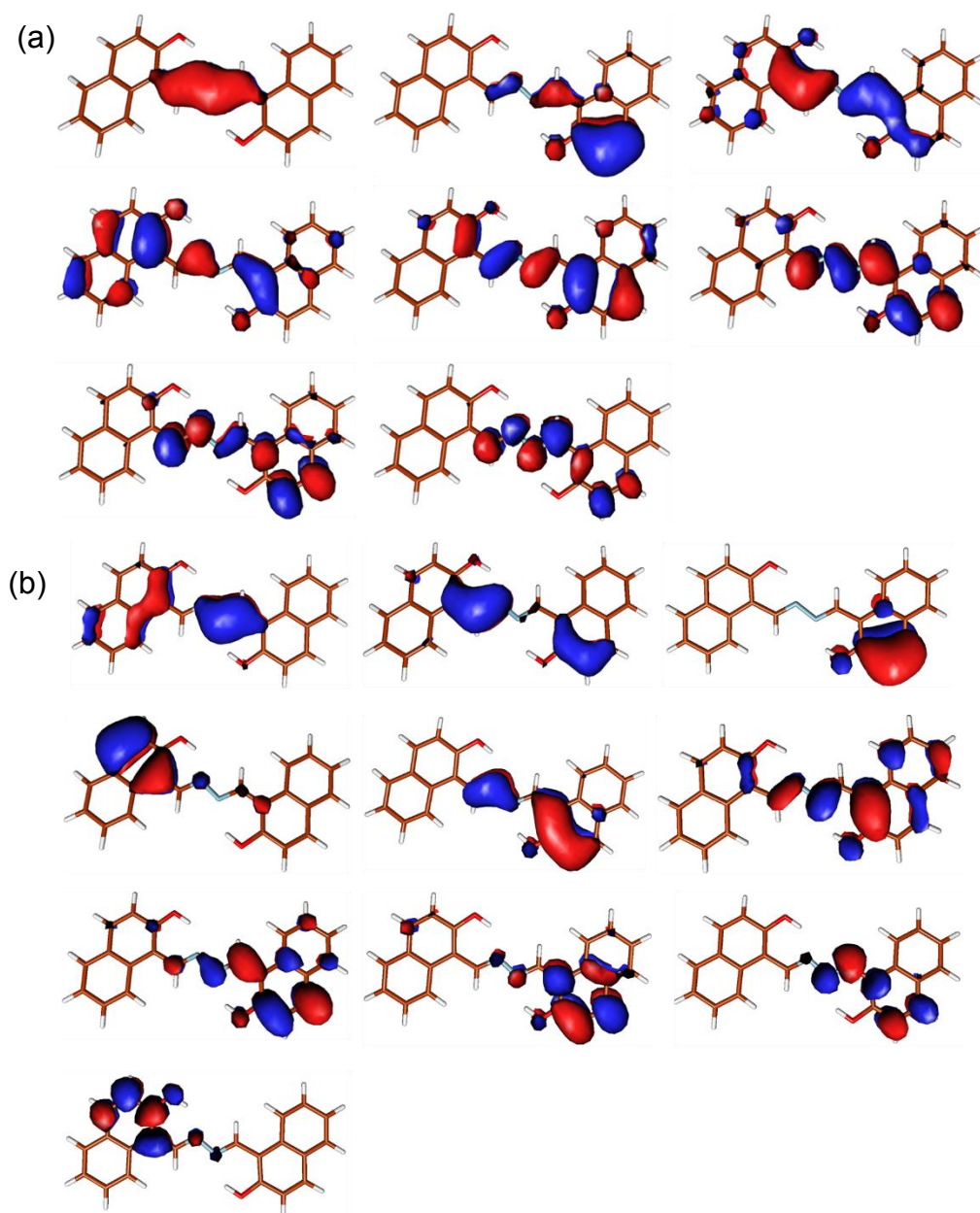


Fig. S1. Active spaces of (a) 10 electrons in 8 orbitals and (b) 12 electrons in 10 orbitals used in CASSCF calculations. These two sets of active spaces give very similar relative energies for S0-TRANS-KETO (difference within 1.0 kcal/mol, CASSCF level).

Table S1. Selected Geometric Parameters of Optimized Structures and Their Relative Energies at Different Computational Levels

	C4C5N6N7	C5N6N7C8	N7C8C9C10	N6N7C8C9	OM2/MRCI	MS-CASPT2 6-31G*	MS-CASPT2 cc-pVDZ
S0-TRANS-ENOL	-180.0	-180.0	0.0	-180.0	0.0	0.0	0.0
S0-TRANS-KETO	180.0	-180.0	0.0	-180.0	4.0	6.1	8.8

S1-TRANS-ENOL	180.0	-180.0	0.0	180.0	65.8	69.7	72.3
S1-TRANS-KETO	-180.0	-180.0	0.0	-180.0	66.2	61.2	56.4
S1-CIS-ENOL	180.0	0.0	0.0	180.0	66.2	66.7	57.5
S1-CIS-KETO	180.0	0.0	0.0	180.0	66.0	63.2	59.8
S1S0-TRANS-ENOL	-177.3	-176.7	5.5	95.4	49.2/49.2	57.5/62.7	58.5/67.5
S1S0-TRANS-KETO	-169.7	172.5	81.8	175.8	52.1/52.1	53.1/62.3	55.0/56.7
S1S0-CIS-ENOL	179.0	0.9	4.3	97.1	45.4/45.4	48.4/57.7	47.2/52.6
S1S0-CIS-KETO	177.7	-42.3	-85.5	130.5	52.2/52.2	43.3/52.4	49.5/58.2

Table S2. Single-Point Energies of Selected Optimized Structures Relative to S0-TRANS-ENOL
Computed by MS-CASPT2 Method with Different Basis Sets

Basis Set	S0-TRANS-KETO	S1-TRANS-ENOL	S1-TRANS-KETO
6-31G*	6.1	69.7	61.2
cc-pVDZ ¹	8.8	72.3	56.4
TZVP ²	8.4	73.6	56.5

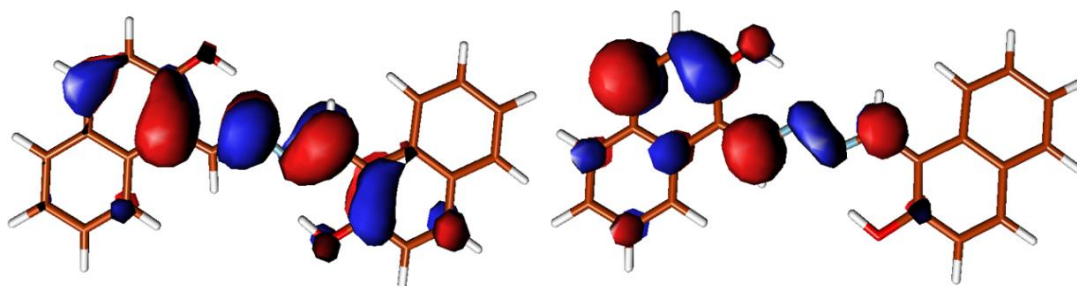


Fig. S2. Two singly occupied molecular orbitals computed by CASSCF method at the S₁ minimum i.e. S1-TRANS-ENOL.

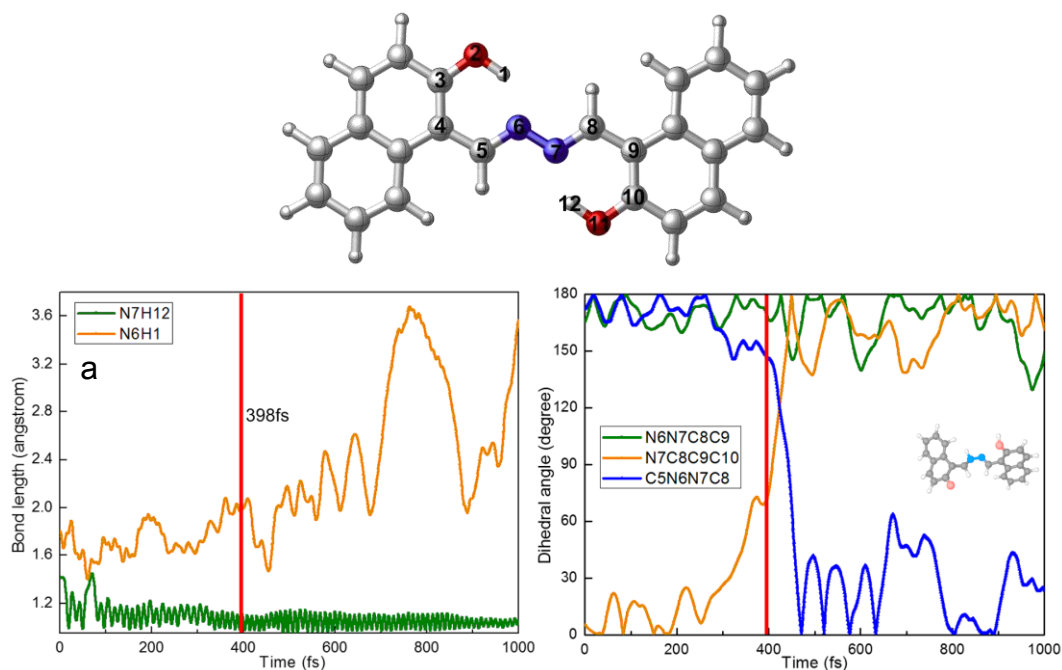


Fig. S3. Time-dependent evolution of selected key geometric parameters (a) N6-H1 and N7-H12 distances and (b) C5N6N7C8, N6N7C8C9, and N7C8C9C10 dihedral angles in a typical trajectory. Therein the system hops to the S_0 state via the trans-keto S_1/S_0 conical intersection and finally stays in the cis-keto region at the end of 1 ps simulation time.

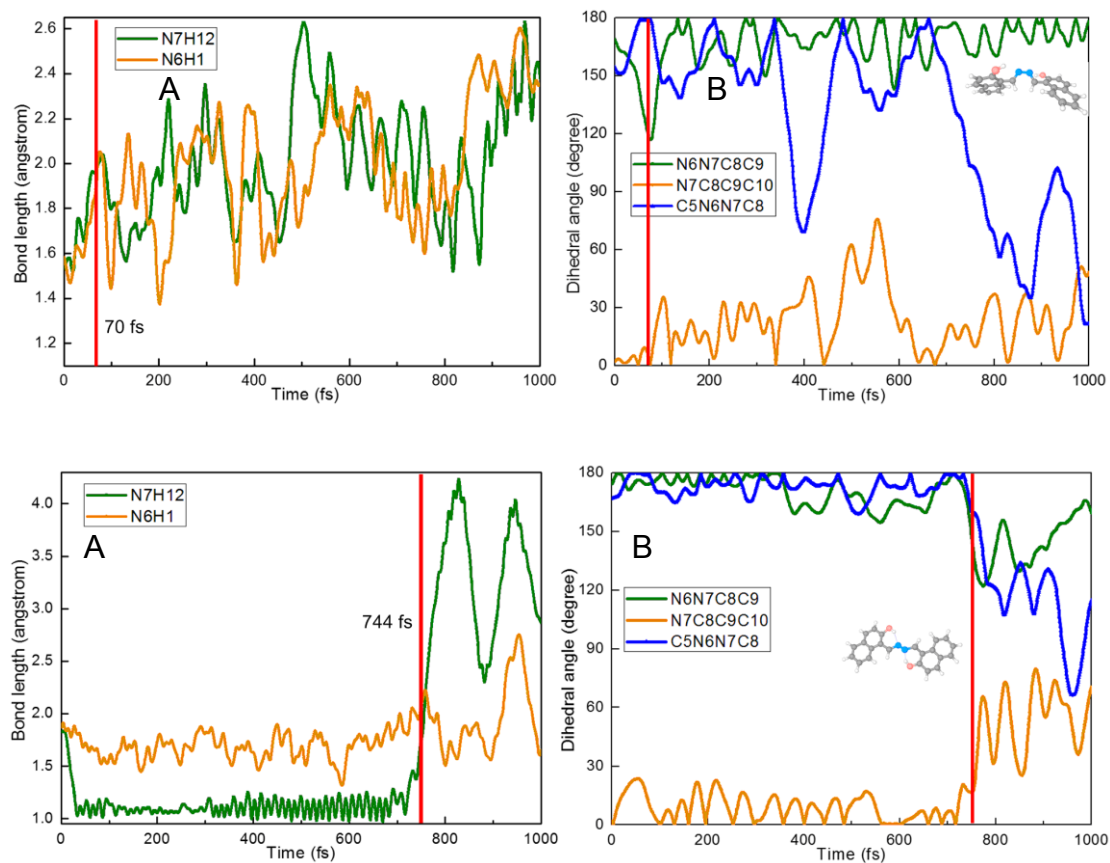


Fig. S4. Time-dependent evolution of selected key geometric parameters (A) N6-H1 and N7-H12 distances and (B) C5N6N7C8, N6N7C8C9, and N7C8C9C10 dihedral angles in two typical trajectories, in which the system hops to the S_0 state through the trans-enol S_1/S_0 conical intersection region and finally stays in the (top) cis-enol and (bottom) trans-enol regions, respectively.

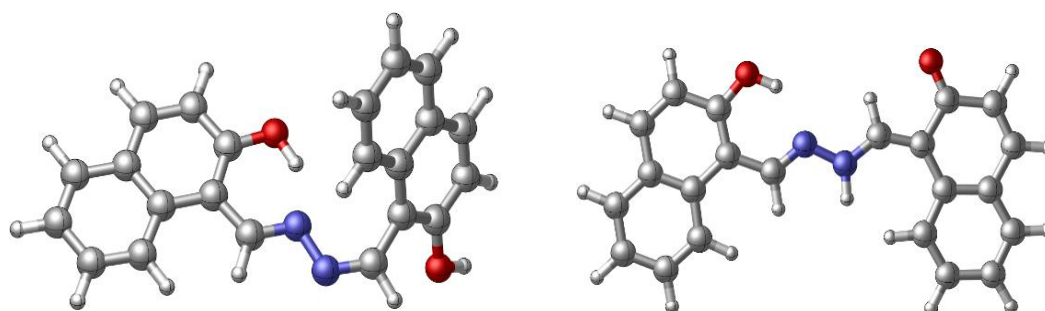


Fig. S5. Schematic (left) enol and (right) keto products in the S_0 state optimized at the CASSCF level.

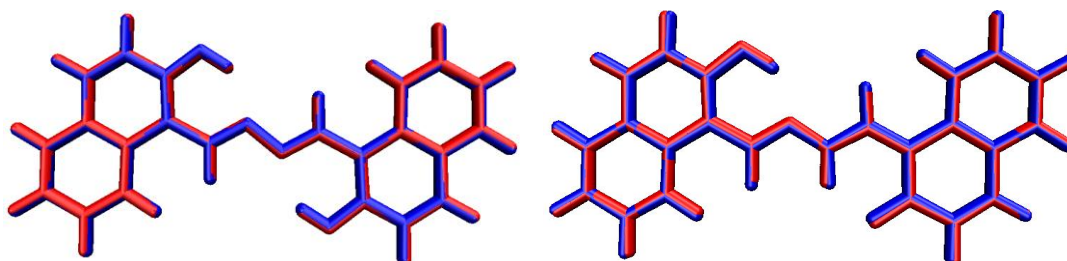


Fig. S6. Spatially superpositions of (left) S_0 -TRANS-ENOL and (right) S_0 -TRANS-KETO optimized by OM2/MRCI (in blue) and CASSCF (in red) methods.

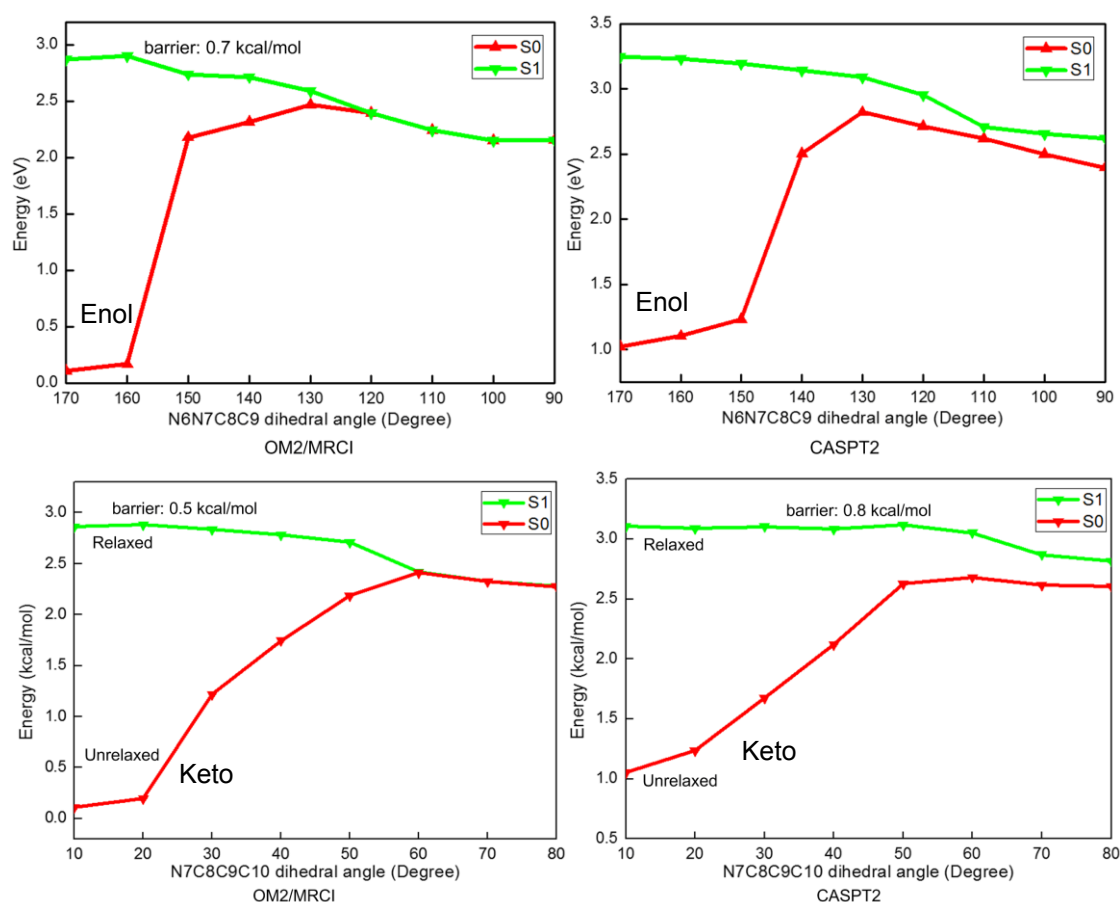


Fig. S7. Minimum-energy relaxation paths from (top) the enol minimum to the enol conical intersection and (bottom) the keto minimum to the keto conical intersection which are computed by (left) OM2/MRCI and (right) CASPT2 methods.

References

- [1] T. H. Dunning, Jr. *J. Chem. Phys.* 1989, **90**, 1007–1023.
- [2] A. Schäfer, C. Huber, and R. Ahlrichs, *J. Chem. Phys.* 1994, **100**, 5829–5835.

Cartesian coordinates of CASSCF optimized structures

S0-TRANS-ENOL

C	-8.25403454	0.91667533	-0.20720144
C	-6.96923290	0.52921381	0.04277019
C	-5.89312233	1.44994035	-0.01508421
C	-6.20581193	2.78075682	-0.34128911
C	-7.54126946	3.15781265	-0.59557837
C	-8.55432000	2.24945745	-0.53218739
H	-9.04480280	0.18958395	-0.15386983

H	-6.79781260	-0.50038689	0.28595327
C	-4.50737317	1.08278565	0.24357430
C	-5.15212864	3.75063319	-0.41266222
H	-7.74683461	4.18485902	-0.84267289
H	-9.56966396	2.54367433	-0.72716966
C	-3.86055528	3.39460926	-0.16867081
C	-3.53267972	2.06239979	0.15975502
H	-5.39556451	4.76740515	-0.66244226
H	-3.05698030	4.10501406	-0.21685232
O	-2.23538369	1.84608583	0.37445025
N	-2.96495151	-0.69336101	0.82423903
N	-2.88837187	-2.03484748	1.12217567
C	-4.16717073	-0.29212123	0.58282435
H	-4.95225295	-1.02207489	0.63813400
C	-1.69206792	-2.44122441	1.36172160
C	-2.03540197	-6.13919515	2.11549189
C	-0.75841745	-6.49669376	2.35331212
C	0.30315763	-5.55024590	2.28264582
C	0.00720887	-4.21180320	1.95671340
C	-1.36569301	-3.83191763	1.70220852
C	-2.34979856	-4.79309371	1.78556469
H	1.82633081	-6.97921768	2.78239633
H	-2.84600373	-6.84106361	2.16488156
H	-0.52412430	-7.51662272	2.60281692
C	1.63696742	-5.94889152	2.53629684
C	1.10023521	-3.30639364	1.89860712
C	2.37581005	-3.71653757	2.14738518
C	2.66013454	-5.05695544	2.47240532
H	0.94491149	-2.27430602	1.65621852
H	3.17817733	-3.00229107	2.09399016
H	3.67200867	-5.36319425	2.66562305
H	-0.89929607	-1.71939599	1.30750591
H	-2.07690638	0.92975579	0.59147265
O	-3.64347061	-4.56695677	1.57393696
H	-3.79469951	-3.64867287	1.35642587

S0-TRANS-KETO

C	-6.67839644	1.67809188	0.00057502
C	-6.66526822	0.31945418	0.00068126
C	-5.44700183	-0.40099316	0.00064189
C	-4.21317298	0.28302849	0.00050450
C	-4.26554105	1.70472987	0.00039175

C	-5.45248787	2.37250577	0.00042382
H	-6.39463741	-2.33851603	0.00085028
H	-7.60618757	2.22054827	0.00060245
H	-7.58778827	-0.23448141	0.00079661
C	-5.45047335	-1.82308171	0.00073714
C	-2.98432864	-0.47401350	0.00047936
H	-3.36661998	2.28777526	0.00026905
H	-5.45196014	3.44797905	0.00032821
C	-3.05043984	-1.84724087	0.00054315
C	-4.29900289	-2.52351865	0.00067956
H	-4.28137906	-3.59682569	0.00073540
C	-1.68637655	0.23834985	0.00044265
H	-1.69220660	1.31289657	0.00060966
O	-1.98961422	-2.65826818	0.00049755
N	-0.55160641	-0.37125123	0.00026289
C	5.54570508	-2.31901842	-0.00039651
C	4.33194947	-1.67671850	-0.00023293
C	4.25063214	-0.25899489	0.00018461
C	5.44375780	0.45091945	0.00042002
C	6.68699553	-0.22494699	0.00025751
C	6.75022142	-1.58101974	-0.00014298
H	5.57669376	-3.39389360	-0.00072099
H	3.44304851	-2.27717308	-0.00043125
C	2.97798928	0.47876687	0.00037672
C	5.41233234	1.90264748	0.00083711
H	7.59017419	0.36047985	0.00045885
H	7.69679477	-2.09005070	-0.00026768
C	4.28105084	2.60622278	0.00099752
C	2.98052336	1.94446439	0.00077174
H	6.35844136	2.41688886	0.00101909
H	4.27019273	3.67992755	0.00129792
C	1.76972158	-0.18286598	0.00020965
H	1.72056265	-1.25206483	-0.00007165
N	0.56014710	0.39608105	0.00038713
O	1.95223232	2.60445638	0.00091909
H	0.51316115	1.39807533	0.00059374
H	-1.17892294	-2.15873243	0.00036046

S0-CIS-ENOL

C	5.18613741	2.98180645	-0.13955749
C	5.78974968	1.76464462	-0.19195824
C	5.03113558	0.57138393	-0.19417503

C	3.62353025	0.61785806	-0.14177780
C	3.02693792	1.90548583	-0.08786932
C	3.78129226	3.04130145	-0.08693136
H	6.75636195	-0.72098860	-0.28927252
H	5.76649302	3.88627309	-0.13806992
H	6.86243557	1.69001623	-0.23286973
C	5.68164439	-0.69501331	-0.24950569
C	2.87238883	-0.62034377	-0.14539335
H	1.96182003	2.01698133	-0.04630634
H	3.29209463	3.99828568	-0.04519651
C	3.56003491	-1.81778433	-0.20034661
C	4.98062981	-1.84480319	-0.25272615
H	5.45581337	-2.80632498	-0.29405332
C	1.40606949	-0.59336557	-0.09137355
H	0.94273858	0.37159640	-0.05042482
O	2.98788057	-3.01357601	-0.20941076
N	0.70652594	-1.67317985	-0.09288996
C	-3.81754559	2.97922226	0.18802326
C	-3.05142300	1.84725772	0.13185691
C	-3.63273777	0.55789090	0.12073604
C	-5.03447093	0.49039391	0.17001262
C	-5.80404391	1.66677774	0.22741214
C	-5.21468727	2.89817383	0.23678574
H	-3.33742259	3.94175124	0.19464621
H	-1.98719887	1.97277804	0.09630964
C	-2.85843437	-0.68042138	0.06160059
C	-5.67639013	-0.79829726	0.16112728
H	-6.87599160	1.57868211	0.26417951
H	-5.80966990	3.79227774	0.28077797
C	-4.94573490	-1.94185612	0.10595977
C	-3.53245101	-1.89043928	0.05585154
H	-6.74983785	-0.84257044	0.19905410
H	-5.40463660	-2.91226718	0.09838010
C	-1.40572694	-0.63264692	0.00995456
H	-0.95721546	0.34031963	0.01796367
N	-0.67876470	-1.69661248	-0.04308788
O	-2.93925348	-3.07575412	0.00463509
H	-1.98692580	-2.97590421	-0.02749811
H	2.03335259	-2.92964779	-0.17257086

S0-CIS-KETO

C	5.20164756	2.96216058	-0.13222218
---	------------	------------	-------------

C	5.80424753	1.74554283	-0.18792736
C	5.04584043	0.55082417	-0.19378193
C	3.63643497	0.59801892	-0.14147833
C	3.04127562	1.88930538	-0.08394612
C	3.79542852	3.02344504	-0.07963011
H	6.76940807	-0.74249683	-0.29215636
H	5.78270057	3.86624385	-0.12805824
H	6.87690159	1.67055381	-0.22882251
C	5.69485138	-0.71325708	-0.25248271
C	2.88491182	-0.63453516	-0.14865574
H	1.97646090	2.00249275	-0.04224817
H	3.30758409	3.98102482	-0.03529785
C	3.56790778	-1.82744572	-0.20661587
C	4.98709492	-1.85976077	-0.25883862
H	5.45797731	-2.82342465	-0.30272175
C	1.40323393	-0.59015842	-0.09384576
H	0.94753558	0.37754843	-0.05039373
O	2.99525673	-3.03126297	-0.21947441
N	0.69016578	-1.65660935	-0.09780916
C	-3.90416240	3.02022717	0.19879911
C	-3.10769925	1.90075866	0.13873301
C	-3.66856151	0.59671748	0.12256255
C	-5.05469926	0.49828856	0.16988606
C	-5.86028026	1.65772684	0.23138940
C	-5.30889537	2.89970273	0.24618110
H	-3.44924657	3.99444643	0.20959656
H	-2.04507977	2.04352531	0.10432551
C	-2.86433514	-0.63326832	0.05915232
C	-5.68258702	-0.81266215	0.15592991
H	-6.92931262	1.53911077	0.26669101
H	-5.92666882	3.77782250	0.29304639
C	-4.99148499	-1.94836017	0.09925120
C	-3.53116217	-1.94312115	0.04666783
H	-6.75815390	-0.84439391	0.19387481
H	-5.46427146	-2.91229138	0.08939547
C	-1.48817801	-0.58116814	0.01088062
H	-1.00594766	0.37065534	0.01999326
N	-0.66608931	-1.64114216	-0.04837833
O	-2.91414928	-2.99190091	-0.00488604
H	-1.08701434	-2.54582263	-0.05841418
H	2.04533934	-2.95620627	-0.18301893

S1-TRANS-ENOL

C	-8.28294209	1.41627098	-0.34541940
C	-7.03934449	0.92211797	-0.07075017
C	-5.89414635	1.75532807	-0.08002956
C	-6.09217920	3.11737182	-0.38503166
C	-7.38707671	3.60402543	-0.66535015
C	-8.46853200	2.77534264	-0.64803951
H	-9.12986927	0.75385185	-0.32915293
H	-6.95192881	-0.12119670	0.15381852
C	-4.55728250	1.26386283	0.20715971
C	-4.97244732	3.99845646	-0.40770541
H	-7.50569549	4.64857092	-0.89459426
H	-9.45208559	3.15210176	-0.86241542
C	-3.72709123	3.54855463	-0.14185497
C	-3.50458604	2.18741001	0.16640271
H	-5.13321133	5.03574044	-0.64137923
H	-2.87189030	4.19732490	-0.15426873
O	-2.23754532	1.87190456	0.40793746
N	-3.13578981	-0.61341071	0.78820290
N	-3.04979215	-1.87401413	1.05700819
C	-4.34622951	-0.12483644	0.51957078
H	-5.16806361	-0.81165631	0.54468969
C	-1.73678806	-2.25876000	1.31877260
C	-1.96863501	-5.90232439	2.02840365
C	-0.61320473	-6.20641265	2.27943766
C	0.42219617	-5.19911541	2.21898703
C	0.08357027	-3.86841053	1.90090559
C	-1.35412146	-3.52803165	1.63083277
C	-2.35070281	-4.63675519	1.71749418
H	1.98519225	-6.56077394	2.71430598
H	-2.72114438	-6.66559853	2.07877159
H	-0.33434244	-7.21383514	2.52337422
C	1.74733448	-5.53955599	2.47328931
C	1.10470206	-2.93449271	1.85347616
C	2.42578067	-3.28613032	2.10949313
C	2.75248909	-4.59017773	2.42045161
H	0.90072709	-1.90861828	1.61627067
H	3.18947582	-2.53083198	2.06244927
H	3.77184836	-4.86743056	2.61919238
H	-1.00888773	-1.47243342	1.26018828
H	-2.16167520	0.93881459	0.60845669
O	-3.62818529	-4.41409121	1.49396355
H	-3.79318427	-3.48878465	1.28242304

S1-TRANS-KETO

C	-6.56897614	1.80536292	0.00011046
C	-6.62290655	0.44393762	0.00053810
C	-5.44302135	-0.33033936	0.00068873
C	-4.18091773	0.29622131	0.00041218
C	-4.15993479	1.71074354	-0.00004650
C	-5.31572918	2.43951101	-0.00019252
H	-6.48693235	-2.22003474	0.00129793
H	-7.47051435	2.39032100	-0.00000955
H	-7.57168265	-0.06326067	0.00075933
C	-5.51797931	-1.75388880	0.00109494
C	-2.97291334	-0.51679807	0.00057646
H	-3.23137967	2.24506410	-0.00031399
H	-5.26220884	3.51333589	-0.00055402
C	-3.12414070	-1.91753077	0.00095309
C	-4.40189734	-2.51672213	0.00121274
H	-4.44448633	-3.58919002	0.00151031
C	-1.68597522	0.08916541	0.00037163
H	-1.60710890	1.16024884	0.00019972
O	-2.10802022	-2.76247402	0.00111449
N	-0.56491265	-0.62484702	0.00038991
C	5.68517874	-2.22707298	-0.00057668
C	4.44648723	-1.67464859	-0.00033507
C	4.25505303	-0.24995566	-0.00041436
C	5.42753108	0.55455250	-0.00077040
C	6.69138759	-0.04833297	-0.00100320
C	6.83150157	-1.40899805	-0.00091086
H	5.79384337	-3.29695059	-0.00051701
H	3.59999156	-2.33127151	-0.00009706
C	2.98008956	0.35025440	-0.00015656
C	5.30078656	1.98623608	-0.00089485
H	7.56326218	0.58240776	-0.00126528
H	7.81004386	-1.85428789	-0.00109937
C	4.05881393	2.57862639	-0.00068002
C	2.84330822	1.79331795	-0.00030592
H	6.19187270	2.58691922	-0.00116397
H	3.93652302	3.64497430	-0.00077024
C	1.76436049	-0.49124787	0.00023240
H	1.78732092	-1.55739757	0.00062835
N	0.55241595	0.05553441	0.00015798
O	1.74099024	2.35965185	-0.00013714
H	0.55437343	1.07308824	-0.00007753
H	-1.27252760	-2.29008546	0.00089332

S1-CIS-ENOL

C	5.25798286	2.94326270	-0.14309290
C	5.82991278	1.70679373	-0.19484790
C	5.04110016	0.53752063	-0.19538268
C	3.63406659	0.62583317	-0.14195184
C	3.07444886	1.92622531	-0.08903863
C	3.85890924	3.04511670	-0.08960672
H	6.73307951	-0.80268178	-0.29049518
H	5.86582300	3.82973232	-0.14304565
H	6.90020778	1.60468105	-0.23636668
C	5.66005856	-0.74511890	-0.24999575
C	2.82786710	-0.58259549	-0.14284369
H	2.01311416	2.06178594	-0.04700060
H	3.39647987	4.01519422	-0.04849885
C	3.50697209	-1.81211528	-0.19830967
C	4.91854172	-1.87329500	-0.25122041
H	5.36513028	-2.84867942	-0.29187130
C	1.38873886	-0.50118892	-0.08844508
H	0.93770936	0.46511752	-0.04788967
O	2.90047770	-2.98826563	-0.20565079
N	0.65558665	-1.61346756	-0.08956352
C	-3.91639599	3.01293831	0.19240732
C	-3.10415120	1.89060745	0.13481674
C	-3.63583342	0.60818968	0.12209358
C	-5.03610076	0.47755814	0.16975275
C	-5.84353952	1.61378666	0.22751498
C	-5.29283672	2.87856745	0.23910181
H	-3.46664489	3.98936722	0.20046047
H	-2.04368350	2.04650771	0.10015243
C	-2.78800900	-0.62817966	0.06035157
C	-5.63332201	-0.83642398	0.15863338
H	-6.91169514	1.49127387	0.26329704
H	-5.92551083	3.74632801	0.28379852
C	-4.86067153	-2.00059913	0.10144142
C	-3.49516961	-1.93975974	0.05329818
H	-6.70355625	-0.91289904	0.19564472
H	-5.32220062	-2.96933847	0.09401907
C	-1.42645348	-0.56259384	0.01245336
H	-0.96333194	0.39948348	0.01964696
N	-0.62952533	-1.71386114	-0.04531201
O	-2.83454302	-3.06700022	0.00110428

H	-1.87572953	-2.90422006	-0.02971027
H	1.94720131	-2.86422656	-0.16784736

S1-CIS-KETO

C	5.33753899	2.90970359	-0.14622614
C	5.88973334	1.66561418	-0.19658456
C	5.08087899	0.50877923	-0.19593177
C	3.67685786	0.61951232	-0.14280318
C	3.13640069	1.92732134	-0.09130231
C	3.93910487	3.03232548	-0.09300521
H	6.75043725	-0.85646495	-0.28938138
H	5.95791499	3.78718483	-0.14696720
H	6.95810902	1.54588076	-0.23788408
C	5.67827713	-0.78432626	-0.24911574
C	2.85927517	-0.58380297	-0.14297978
H	2.07692638	2.08134302	-0.04948437
H	3.49194517	4.00944443	-0.05296984
C	3.51569968	-1.82461226	-0.19700270
C	4.92623019	-1.90598063	-0.24964134
H	5.36238829	-2.88583484	-0.28934720
C	1.43158901	-0.49701891	-0.08958364
H	0.98997973	0.47540611	-0.04984909
O	2.89110482	-2.98753794	-0.20312040
N	0.67542802	-1.57894438	-0.08899017
C	-4.05360417	2.97777526	0.19293167
C	-3.22726643	1.90145204	0.13675907
C	-3.73553961	0.55707223	0.12192467
C	-5.15629736	0.41418266	0.16944545
C	-5.97632580	1.54698671	0.22677994
C	-5.45082078	2.81044054	0.23899932
H	-3.63663048	3.96912340	0.20235606
H	-2.17175158	2.08144846	0.10328288
C	-2.91063235	-0.57817598	0.06434381
C	-5.72805518	-0.90180009	0.15759934
H	-7.04273728	1.40761903	0.26165647
H	-6.09559324	3.66919739	0.28329385
C	-4.92639052	-2.01133750	0.10149902
C	-3.47909323	-1.90729599	0.05206747
H	-6.79769371	-1.00237504	0.19354754
H	-5.32958573	-3.00611550	0.09150408
C	-1.43168552	-0.41492800	0.01521660
H	-0.98183204	0.54768849	0.02264167

N	-0.63653267	-1.47753321	-0.03939305
O	-2.79180211	-2.93409929	0.00212157
H	-1.12921299	-2.36246222	-0.04342587
H	1.93955318	-2.86309551	-0.16590146

12. Cartesian coordinates of OM2/MRCI optimized structures

S0-TRANS-ENOL

C	-8.33281903	0.96860357	-0.23855417
C	-7.05939033	0.51078304	0.02718388
C	-5.95441879	1.39414656	-0.00412400
C	-6.19201987	2.76494753	-0.31649103
C	-7.50779866	3.20907861	-0.58514289
C	-8.56231475	2.32404697	-0.54674047
H	-9.18231839	0.27626407	-0.21180317
H	-6.91051432	-0.54963632	0.26416412
C	-4.61198100	0.96931266	0.26413041
C	-5.10918074	3.69299801	-0.35985691
H	-7.67570571	4.26705088	-0.82415374
H	-9.58280020	2.66264358	-0.75393603
C	-3.82735014	3.29359299	-0.10493676
C	-3.57720446	1.92155798	0.20935752
H	-5.32673988	4.74206115	-0.60372158
H	-2.98033922	3.97647100	-0.13003962
O	-2.28786242	1.65028536	0.43908937
N	-3.05298353	-0.73920442	0.82437044
N	-2.82571727	-2.02070964	1.11690422
C	-4.29849486	-0.40858447	0.58816537
H	-5.12828828	-1.14874888	0.62709318
C	-1.58013274	-2.35135669	1.35440682
C	-2.06108963	-6.04879264	2.04255331
C	-0.78080332	-6.45196912	2.29980662
C	0.30356436	-5.52460484	2.25901036
C	0.07278306	-4.16088357	1.94943076
C	-1.26955218	-3.72980659	1.67796522
C	-2.30591219	-4.67695441	1.72938447
H	1.78137082	-7.03439494	2.76886124
H	-2.90959312	-6.73024410	2.06547128
H	-0.56550333	-7.50099017	2.54312206
C	1.62046978	-5.97541387	2.53098163
C	1.17885253	-3.27991349	1.92112567
C	2.45012080	-3.74098211	2.18894928

C	2.67466168	-5.09602222	2.49585458
H	1.03236845	-2.21943418	1.68494615
H	3.30137368	-3.05051454	2.16461149
H	3.69408654	-5.43721877	2.70478608
H	-0.74946171	-1.61116391	1.31686802
H	-2.16657789	0.66261340	0.65743219
O	-3.59224033	-4.39826039	1.49667545
H	-3.70625296	-3.40565856	1.27874969

S0-TRANS-KETO

C	-6.71588263	1.64464446	0.00036501
C	-6.66907629	0.27092388	0.00041980
C	-5.42290377	-0.40356184	0.00051161
C	-4.21041890	0.34447545	0.00055330
C	-4.29513671	1.75750260	0.00050241
C	-5.51923651	2.38989842	0.00040860
H	-6.34442716	-2.37565957	0.00054234
H	-7.67593399	2.17164630	0.00029277
H	-7.59352328	-0.32051382	0.00039657
C	-5.39273118	-1.82805418	0.00055819
C	-2.96170734	-0.36130903	0.00062543
H	-3.38208318	2.36564603	0.00053931
H	-5.57278985	3.48461523	0.00036792
C	-2.98435714	-1.76318204	0.00062967
C	-4.20375850	-2.50433275	0.00061628
H	-4.14386661	-3.59129087	0.00064395
C	-1.69511435	0.35703554	0.00070526
H	-1.72557982	1.46833854	0.00087460
O	-1.89622570	-2.55557025	0.00065538
N	-0.57260367	-0.30744309	0.00060151
C	5.55606315	-2.34271162	-0.00043433
C	4.32135644	-1.71333405	-0.00016658
C	4.23113157	-0.30931698	0.00020841
C	5.42889341	0.44313504	0.00030331
C	6.67557035	-0.21237802	0.00002809
C	6.73819660	-1.59314462	-0.00033434
H	5.61104496	-3.43763856	-0.00072816
H	3.41367532	-2.33009484	-0.00025154
C	2.96262600	0.39421256	0.00049611
C	5.39482078	1.88725032	0.00067688
H	7.59718030	0.38408670	0.00010441
H	7.70570054	-2.10489524	-0.00054331

C	4.22626204	2.56728287	0.00093572
C	2.95193429	1.85231126	0.00085407
H	6.35915455	2.41793656	0.00074264
H	4.17632960	3.65596521	0.00121246
C	1.74763498	-0.28805881	0.00042984
H	1.70886453	-1.39501757	0.00016655
N	0.56317224	0.38133827	0.00068844
O	1.87529300	2.49074267	0.00109220
H	0.60775103	1.43739976	0.00091710
H	-1.05638398	-2.00826031	0.00067150

S0-CIS-ENOL

C	5.52483000	2.82055000	-0.15511000
C	6.01025000	1.53028000	-0.20421000
C	5.12325000	0.43082000	-0.19938000
C	3.71701000	0.65512000	-0.14340000
C	3.25241000	1.98786000	-0.09398000
C	4.13777000	3.04623000	-0.09978000
H	6.73212000	-1.03416000	-0.29310000
H	6.21005000	3.67392000	-0.15875000
H	7.09112000	1.34477000	-0.24753000
C	5.64440000	-0.89505000	-0.25065000
C	2.82435000	-0.47466000	-0.13909000
H	2.17479000	2.19363000	-0.05024000
H	3.76449000	4.07593000	-0.06109000
C	3.40266000	-1.78030000	-0.19191000
C	4.80658000	-1.98119000	-0.24725000
H	5.17850000	-3.00328000	-0.28570000
C	1.40780000	-0.32356000	-0.08450000
H	0.98244000	0.69654000	-0.04419000
O	2.69451000	-2.90624000	-0.19412000
N	0.65187000	-1.42667000	-0.08439000
C	-4.26270000	2.99238000	0.20077000
C	-3.33848000	1.96457000	0.14225000
C	-3.75506000	0.61492000	0.12402000
C	-5.15259000	0.33798000	0.16740000
C	-6.07370000	1.40064000	0.22665000
C	-5.63476000	2.71136000	0.24316000
H	-3.92531000	4.03485000	0.21431000
H	-2.26783000	2.21082000	0.10983000
C	-2.83304000	-0.47307000	0.06417000
C	-5.63099000	-1.01429000	0.15133000

H	-7.14815000	1.17789000	0.25977000
H	-6.35423000	3.53611000	0.28935000
C	-4.76680000	-2.06874000	0.09440000
C	-3.34748000	-1.84261000	0.04900000
H	-6.71653000	-1.18000000	0.18622000
H	-5.10838000	-3.10287000	0.08125000
C	-1.42508000	-0.28253000	0.01829000
H	-0.99189000	0.72820000	0.02753000
N	-0.62948000	-1.39358000	-0.03754000
O	-2.54564000	-2.82984000	-0.00403000
H	-1.63304404	-2.50203103	-0.02872612
H	1.69330000	-2.71009000	-0.15332000

S0-CIS-KETO

C	5.40543099	2.87253193	-0.14191122
C	5.94315882	1.60826513	-0.19669554
C	5.10038580	0.46981588	-0.19799903
C	3.68574709	0.63093695	-0.14231949
C	3.16713358	1.94720405	-0.08678342
C	4.00706667	3.03926360	-0.08665729
H	6.76983548	-0.92363934	-0.29732833
H	6.05187366	3.75630817	-0.14061313
H	7.03028989	1.46478997	-0.24005057
C	5.67659957	-0.83227126	-0.25522063
C	2.85425309	-0.53771878	-0.14488412
H	2.08216295	2.11163955	-0.04294163
H	3.59233609	4.05330161	-0.04331480
C	3.46784457	-1.79754433	-0.20226649
C	4.88639987	-1.94823655	-0.25779990
H	5.29223739	-2.95749418	-0.30067945
C	1.40209961	-0.42704357	-0.08929072
H	0.97566552	0.59924535	-0.04524231
O	2.82475634	-2.97734844	-0.21194120
N	0.67764965	-1.50977335	-0.09331678
C	-4.12506614	3.01609347	0.20647213
C	-3.24295191	1.94905298	0.14483508
C	-3.71709531	0.62448953	0.12505415
C	-5.11465085	0.40802269	0.16955601
C	-5.99746713	1.50373294	0.23201624
C	-5.50669640	2.79600704	0.25029559
H	-3.74118996	4.04296144	0.22121953
H	-2.16475445	2.15481865	0.11159771

C	-2.83539040	-0.52381132	0.06117396
C	-5.65662377	-0.93078534	0.15184177
H	-7.07937829	1.32179973	0.26606245
H	-6.19093121	3.64879139	0.29881014
C	-4.85530707	-2.01859616	0.09255544
C	-3.40447624	-1.86463430	0.04439168
H	-6.75147481	-1.03580242	0.18850247
H	-5.24084056	-3.03745996	0.07810445
C	-1.44547157	-0.39402282	0.01452678
H	-0.98566593	0.61570984	0.02602039
N	-0.64372296	-1.48496180	-0.04485160
O	-2.66529217	-2.87602994	-0.01051531
H	-1.15482251	-2.43110688	-0.05274174
H	1.83056834	-2.84964694	-0.17241960

S1-TRANS-ENOL

C	-8.33751256	0.91180174	-0.25077772
C	-7.05690723	0.47466741	0.01685676
C	-5.96699557	1.37310426	-0.01271212
C	-6.22200481	2.73899140	-0.32519766
C	-7.54299690	3.16260286	-0.59567918
C	-8.58635354	2.26190599	-0.55903396
H	-9.17560893	0.20606763	-0.22503466
H	-6.89197195	-0.58366143	0.25427260
C	-4.61579098	0.95708656	0.26067664
C	-5.15586736	3.68399008	-0.36776501
H	-7.72719609	4.21785772	-0.83523656
H	-9.61042078	2.58682908	-0.76798919
C	-3.86388517	3.30092620	-0.10959214
C	-3.58920025	1.94517426	0.20374052
H	-5.38541380	4.72919469	-0.61172682
H	-3.03238726	4.00300572	-0.13577541
O	-2.30018837	1.69165709	0.43530017
N	-3.01171933	-0.70826551	0.82338712
N	-2.74161241	-1.94322544	1.11250888
C	-4.29020593	-0.39155463	0.58020692
H	-5.09228208	-1.15496432	0.62322705
C	-1.46241622	-2.33546622	1.37148858
C	-2.10418717	-6.02563711	2.03456598
C	-0.84193139	-6.46598910	2.30127867
C	0.27645021	-5.56842667	2.27458803
C	0.09235507	-4.18653672	1.96661565

C	-1.21548665	-3.70725823	1.68573836
C	-2.34602958	-4.63907746	1.71759848
H	1.69745404	-7.12038324	2.79052442
H	-2.96835549	-6.68931577	2.04904501
H	-0.65321164	-7.52084596	2.54312572
C	1.56618482	-6.05646991	2.55482856
C	1.23345706	-3.34566279	1.95455330
C	2.48906844	-3.85033477	2.23336372
C	2.65866774	-5.20892912	2.53464059
H	1.12722049	-2.27777338	1.72152025
H	3.36226407	-3.18897670	2.22046144
H	3.66136335	-5.59272499	2.75340802
H	-0.65648798	-1.59024089	1.33244044
H	-2.15917761	0.70721249	0.65491194
O	-3.51711223	-4.23214877	1.47047128
H	-3.48261475	-2.73679469	1.17044010

S1-TRANS-KETO

C	-6.69237000	1.67584000	-0.00007000
C	-6.65660000	0.29747000	0.00102000
C	-5.41965000	-0.38634000	0.00111000
C	-4.20244000	0.35308000	0.00014000
C	-4.27219000	1.76414000	-0.00100000
C	-5.49151000	2.40908000	-0.00111000
H	-6.35713000	-2.35204000	0.00293000
H	-7.64863000	2.20830000	-0.00014000
H	-7.58810000	-0.28321000	0.00182000
C	-5.40188000	-1.81153000	0.00216000
C	-2.95033000	-0.35810000	0.00032000
H	-3.35170000	2.36107000	-0.00183000
H	-5.53381000	3.50422000	-0.00202000
C	-2.99278000	-1.78346000	0.00126000
C	-4.21592000	-2.50154000	0.00219000
H	-4.17547000	-3.58936000	0.00292000
C	-1.69725000	0.31773000	-0.00026000
H	-1.67056000	1.42555000	-0.00069000
O	-1.90756000	-2.55918000	0.00140000
N	-0.57110000	-0.40736000	-0.00019000
C	5.63069000	-2.31964000	-0.00137000
C	4.37700000	-1.73890000	-0.00118000
C	4.22832000	-0.32921000	-0.00060000
C	5.40917000	0.47324000	-0.00023000

C	6.67381000	-0.14386000	-0.00041000
C	6.78378000	-1.52233000	-0.00098000
H	5.73082000	-3.41051000	-0.00183000
H	3.48938000	-2.38551000	-0.00151000
C	2.95785000	0.30715000	-0.00044000
C	5.31940000	1.90470000	0.00032000
H	7.57572000	0.48164000	-0.00011000
H	7.77030000	-1.99912000	-0.00114000
C	4.11012000	2.53396000	0.00034000
C	2.88575000	1.77079000	-0.00013000
H	6.25415000	2.48181000	0.00069000
H	4.01797000	3.61976000	0.00070000
C	1.74132000	-0.44223000	-0.00047000
H	1.73104000	-1.54055000	-0.00049000
N	0.55705000	0.23214000	-0.00039000
O	1.76504000	2.35569000	-0.00026000
H	0.64907000	1.31553000	-0.00041000
H	-1.05980000	-1.99477000	0.00079000

S1-CIS-ENOL

C	5.58775387	2.79264831	-0.15888118
C	6.04644169	1.49051142	-0.20813831
C	5.13821485	0.41086602	-0.20207422
C	3.73493010	0.66838857	-0.14454719
C	3.29869397	2.00817622	-0.09514501
C	4.20791360	3.04993527	-0.10220003
H	6.71420871	-1.08942177	-0.29695959
H	6.29294002	3.63022210	-0.16360983
H	7.12378238	1.28405624	-0.25252229
C	5.62909995	-0.92748296	-0.25341400
C	2.81840951	-0.43858552	-0.13888760
H	2.22517330	2.23520977	-0.05037111
H	3.85633845	4.08694564	-0.06346097
C	3.36810160	-1.76835185	-0.19216170
C	4.76901761	-1.99676886	-0.24885335
H	5.12047767	-3.02579225	-0.28738151
C	1.40594614	-0.27376569	-0.08337130
H	0.98329001	0.74612349	-0.04248905
O	2.61687586	-2.85394171	-0.19198471
N	0.64779524	-1.38652691	-0.08359795
C	-4.25559778	2.97974331	0.20393463
C	-3.32876104	1.95222063	0.14453063

C	-3.74445071	0.60914556	0.12606482
C	-5.13631897	0.32615002	0.16961239
C	-6.06521320	1.39116351	0.23002019
C	-5.62883010	2.69716700	0.24680556
H	-3.91914103	4.02227327	0.21777668
H	-2.25972683	2.19947482	0.11183527
C	-2.80764571	-0.48351926	0.06467665
C	-5.60747049	-1.02092326	0.15307120
H	-7.13808294	1.16202662	0.26330869
H	-6.34738716	3.52259615	0.29357394
C	-4.73159442	-2.07568936	0.09484239
C	-3.33414142	-1.82221032	0.05035770
H	-6.69002386	-1.20028228	0.18796411
H	-5.06718000	-3.11058833	0.08117345
C	-1.39930778	-0.29369022	0.01819169
H	-0.98973101	0.73294700	0.02894038
N	-0.62346979	-1.39666972	-0.03758887
O	-2.56244573	-2.89022378	-0.00440191
H	-1.54256021	-2.60174900	-0.03427925
H	1.59817983	-2.59244647	-0.14835802

S1-CIS-KETO

C	5.52483000	2.82055000	-0.15511000
C	6.01025000	1.53028000	-0.20421000
C	5.12325000	0.43082000	-0.19938000
C	3.71701000	0.65512000	-0.14340000
C	3.25241000	1.98786000	-0.09398000
C	4.13777000	3.04623000	-0.09978000
H	6.73212000	-1.03416000	-0.29310000
H	6.21005000	3.67392000	-0.15875000
H	7.09112000	1.34477000	-0.24753000
C	5.64440000	-0.89505000	-0.25065000
C	2.82435000	-0.47466000	-0.13909000
H	2.17479000	2.19363000	-0.05024000
H	3.76449000	4.07593000	-0.06109000
C	3.40266000	-1.78030000	-0.19191000
C	4.80658000	-1.98119000	-0.24725000
H	5.17850000	-3.00328000	-0.28570000
C	1.40780000	-0.32356000	-0.08450000
H	0.98244000	0.69654000	-0.04419000
O	2.69451000	-2.90624000	-0.19412000
N	0.65187000	-1.42667000	-0.08439000

C	-4.26270000	2.99238000	0.20077000
C	-3.33848000	1.96457000	0.14225000
C	-3.75506000	0.61492000	0.12402000
C	-5.15259000	0.33798000	0.16740000
C	-6.07370000	1.40064000	0.22665000
C	-5.63476000	2.71136000	0.24316000
H	-3.92531000	4.03485000	0.21431000
H	-2.26783000	2.21082000	0.10983000
C	-2.83304000	-0.47307000	0.06417000
C	-5.63099000	-1.01429000	0.15133000
H	-7.14815000	1.17789000	0.25977000
H	-6.35423000	3.53611000	0.28935000
C	-4.76680000	-2.06874000	0.09440000
C	-3.34748000	-1.84261000	0.04900000
H	-6.71653000	-1.18000000	0.18622000
H	-5.10838000	-3.10287000	0.08125000
C	-1.42508000	-0.28253000	0.01829000
H	-0.99189000	0.72820000	0.02753000
N	-0.62948000	-1.39358000	-0.03754000
O	-2.54564000	-2.82984000	-0.00403000
H	-1.24009000	-2.36088000	-0.03936000
H	1.69330000	-2.71009000	-0.15332000

S1S0-TRANS-ENOL

C	-7.98036547	1.18640152	-1.20171098
C	-6.77527600	0.59632614	-0.89089152
C	-5.79209971	1.30329792	-0.15981933
C	-6.07988116	2.63681955	0.24413915
C	-7.32570673	3.22125571	-0.08726486
C	-8.26093914	2.50755142	-0.79846257
H	-8.73604539	0.63022425	-1.76840362
H	-6.58429379	-0.43332826	-1.21685921
C	-4.52062712	0.72752917	0.18491464
C	-5.12103765	3.39253893	0.98292513
H	-7.53241311	4.25087676	0.23184828
H	-9.22669190	2.95397328	-1.05756929
C	-3.90944074	2.85240909	1.31549028
C	-3.60716970	1.51743894	0.91477898
H	-5.37475990	4.41835142	1.28066358
H	-3.15600139	3.40149767	1.87809399
O	-2.38779561	1.11747556	1.29833246
N	-2.98262456	-1.09837553	0.15008299
N	-2.67245903	-2.28117515	-0.20605567

C	-4.17919293	-0.61672866	-0.19177635
H	-4.91431522	-1.23054537	-0.74762840
C	-1.46726140	-2.85202975	0.09360654
C	-2.29988517	-4.86842489	3.18092701
C	-1.06456595	-5.33512601	3.54095627
C	0.09171496	-5.02684003	2.76000870
C	-0.01324417	-4.21227324	1.60462639
C	-1.30470819	-3.68738571	1.22918706
C	-2.41577850	-4.05003266	2.02434259
H	1.42095244	-6.16375921	4.04802309
H	-3.20131728	-5.09402243	3.74811454
H	-0.94510862	-5.96109407	4.43425135
C	1.35329736	-5.53629834	3.15066732
C	1.16023684	-3.91697774	0.87588148
C	2.37983937	-4.42974411	1.27213194
C	2.47945737	-5.24298174	2.41363668
H	1.11101641	-3.27959720	-0.01463879
H	3.28442557	-4.19964182	0.69728090
H	3.45789501	-5.63335564	2.71329299
H	-0.66586203	-2.79365780	-0.66996420
H	-2.22328055	0.15448041	1.03617534
O	-3.68543674	-3.69348669	1.75186703
H	-3.76859610	-3.39448124	0.79899055

S1S0-TRANS-KETO

C	-8.06080061	1.15294481	1.25967905
C	-6.80470218	0.62322673	1.04066935
C	-5.82199941	1.38910653	0.35394663
C	-6.14946629	2.67047640	-0.12832328
C	-7.44875874	3.20094656	0.12364911
C	-8.38385133	2.44417161	0.80272240
H	-8.81790630	0.56017508	1.77916599
H	-6.59251878	-0.38673331	1.38650424
C	-4.48057792	0.87345589	0.08527636
C	-5.21127135	3.47436510	-0.84768418
H	-7.69587006	4.21102602	-0.24118670
H	-9.38929230	2.84612450	0.99670774
C	-3.96566072	2.97978137	-1.12741276
C	-3.62172133	1.67763417	-0.65544713
H	-5.50666404	4.47623832	-1.18003773
H	-3.23084276	3.55055223	-1.68376566
O	-2.36224325	1.33857088	-1.01821433

N	-2.90498650	-0.90217161	0.26869837
N	-2.52838175	-2.02839697	0.82503210
C	-4.07475283	-0.42007038	0.61293073
H	-4.74642885	-0.95150930	1.32028722
C	-1.36795832	-2.65121533	0.36836428
C	-1.41668484	-6.48857660	0.66656972
C	-0.54278062	-6.66594615	1.68040124
C	0.10206477	-5.54686101	2.32269182
C	-0.18063426	-4.22542195	1.88217204
C	-1.09196514	-4.00792250	0.83664009
C	-1.74587486	-5.13148676	0.18484247
H	1.23337116	-6.77148750	3.70890414
H	-1.91964452	-7.32181410	0.15353328
H	-0.29676504	-7.67342777	2.04453183
C	1.01463331	-5.75151637	3.37424216
C	0.46659371	-3.13299044	2.51622279
C	1.35785512	-3.36134407	3.54437353
C	1.63247618	-4.66942970	3.97480535
H	0.24272190	-2.11742432	2.16564529
H	1.86226293	-2.52060959	4.03441013
H	2.34292155	-4.83013681	4.78984796
H	-0.94266656	-2.33192450	-0.59381403
H	-2.13935444	0.42178697	-0.70944362
O	-2.56583891	-4.97657079	-0.73777591
H	-3.14663949	-2.57566890	1.45983197

S1S0-CIS-ENOL

C	4.49875000	2.68138000	-1.36974000
C	5.18486000	1.51058000	-1.15850000
C	4.53712000	0.39443000	-0.57491000
C	3.16555000	0.48374000	-0.20287000
C	2.48758000	1.70485000	-0.43687000
C	3.13862000	2.77493000	-1.00560000
H	6.32138000	-0.85127000	-0.66393000
H	4.99371000	3.54797000	-1.82081000
H	6.24255000	1.42326000	-1.44022000
C	5.26522000	-0.81241000	-0.36738000
C	2.52511000	-0.65823000	0.38662000
H	1.42945000	1.80670000	-0.16609000
H	2.60387000	3.71549000	-1.18355000
C	3.28646000	-1.82641000	0.56680000
C	4.65840000	-1.90477000	0.19126000

H	5.18475000	-2.84319000	0.36239000
C	1.13640000	-0.61423000	0.78631000
H	0.57001000	0.33330000	0.66598000
O	2.83275000	-2.97404000	1.10265000
N	0.57111000	-1.69219000	1.31705000
C	-4.25249000	2.72870000	1.41690000
C	-3.38099000	1.66143000	1.51619000
C	-3.36593000	0.65200000	0.52730000
C	-4.24656000	0.76768000	-0.57597000
C	-5.12373000	1.87610000	-0.66294000
C	-5.12726000	2.84007000	0.32271000
H	-4.26501000	3.50135000	2.19352000
H	-2.70830000	1.59763000	2.37902000
C	-2.46229000	-0.47461000	0.58714000
C	-4.25092000	-0.22156000	-1.60898000
H	-5.79549000	1.95879000	-1.52618000
H	-5.80214000	3.69943000	0.25823000
C	-3.42171000	-1.30708000	-1.55308000
C	-2.52272000	-1.43159000	-0.45258000
H	-4.94265000	-0.09547000	-2.45219000
H	-3.41226000	-2.08175000	-2.31617000
C	-1.53685000	-0.64296000	1.65788000
H	-1.71202000	-0.07338000	2.60512000
N	-0.64810000	-1.65474000	1.66516000
O	-1.80558000	-2.55893000	-0.48294000
H	-1.35611000	-2.73162000	0.40293000
H	1.87017000	-2.89132000	1.37189000

S1S0-CIS-KETO

C	-7.95561791	1.68394923	0.08319662
C	-6.91821245	0.83238256	0.41150664
C	-5.58146499	1.29666485	0.34806981
C	-5.31742884	2.63527317	-0.05395874
C	-6.39584992	3.47833068	-0.38351198
C	-7.69417119	3.00423557	-0.31448053
H	-8.99172235	1.33361067	0.13256261
H	-7.10521532	-0.19868623	0.72547084
C	-4.50001610	0.44591573	0.67011553
C	-3.96086012	3.11780862	-0.12299781
H	-6.19888157	4.51075243	-0.69505339
H	-8.53179671	3.66280222	-0.57117181
C	-2.91053388	2.31752348	0.18665262

C	-3.12480373	0.93218262	0.60192224
H	-3.80528927	4.15900246	-0.43582449
H	-1.87734017	2.66302731	0.14276787
O	-2.17582248	0.17616656	0.89035912
N	-4.58468098	-1.95828299	0.22490244
N	-3.80483016	-3.03255659	0.47772823
C	-4.67495148	-0.92619774	1.12482436
H	-4.53809482	-1.13737363	2.19222050
C	-2.63116132	-2.77461157	0.99363382
C	-1.38721371	-6.32121176	1.54834547
C	-0.13895875	-6.09406848	2.05626806
C	0.35849606	-4.76466985	2.21673835
C	-0.43807345	-3.64984302	1.85823037
C	-1.75814397	-3.88081563	1.33843816
C	-2.19779239	-5.20398400	1.18074419
H	2.26650695	-5.43954644	3.01059190
H	-1.79357079	-7.32128872	1.40807128
H	0.50522274	-6.93521439	2.34744628
C	1.66281913	-4.56472028	2.73569328
C	0.10137837	-2.34744423	2.01651631
C	1.37112966	-2.18225314	2.52203866
C	2.15914585	-3.29226749	2.88770422
H	-0.48076250	-1.46742442	1.73066438
H	1.78483573	-1.17366597	2.64245797
H	3.16537729	-3.12909447	3.28819908
H	-2.28220981	-1.74187256	1.20815606
H	-4.68779820	-1.70984483	-0.77616675
O	-3.39486923	-5.55852147	0.69282324
H	-3.95248885	-4.74415405	0.47212736