Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information: Combined QM(MS-CASPT2)/MM Studies on Photocyclization and Photoisomerization of a Fulgide Derivative in Toluene Solution

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1. Two equilibrium conformers of the E-isomer

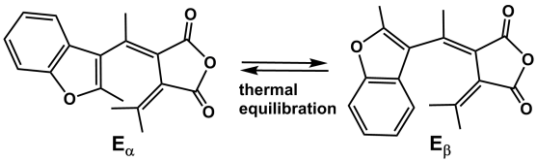

Figure S1. Two equilibrium conformers of the E-isomer (E_α and E_β).

2. The Choice of Active Spaces of E, Z and C Isomers of a Fulgide Derivative

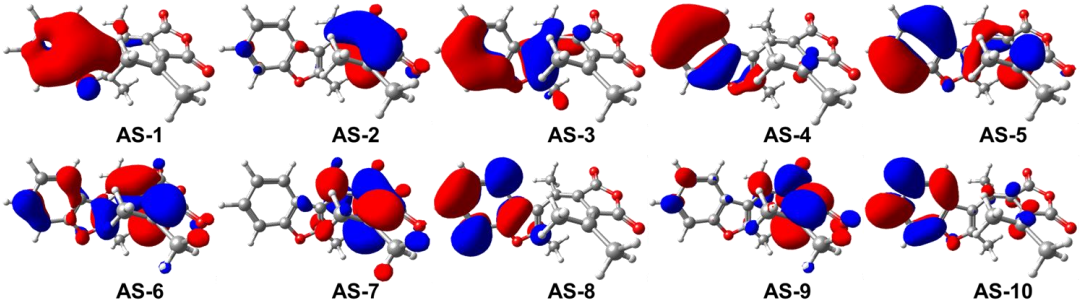

Figure S2. Molecular orbitals of E used as the active space in the CASSCF (12,10) optimizations.

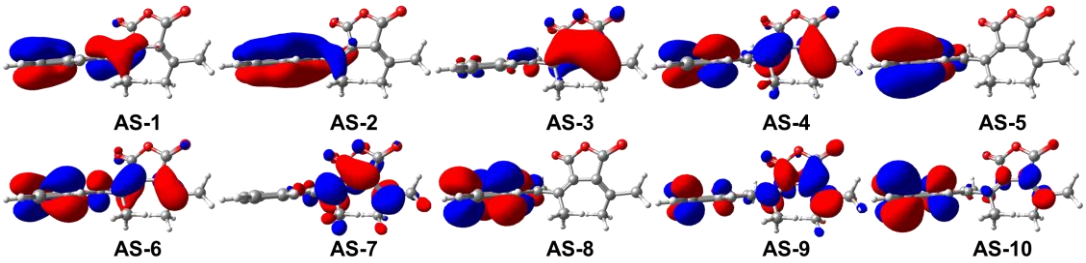

Figure S3. Molecular orbitals of Z used as the active space in the CASSCF (12,10) optimizations.

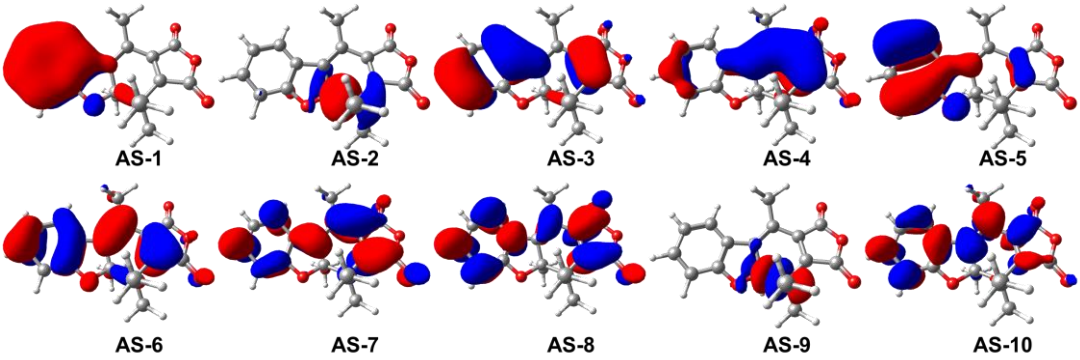

Figure S4. Molecular orbitals of C used as the active space in the CASSCF (12,10) optimizations.

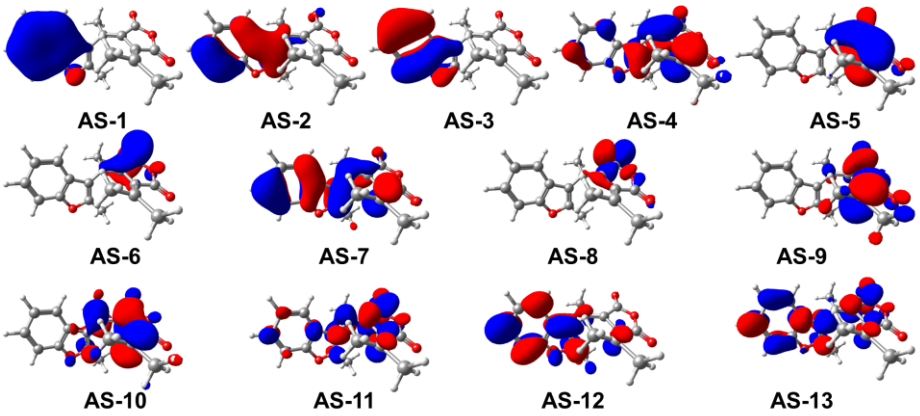

Figure S5. Molecular orbitals of E used as the active space in the MS-CASPT2 (16,13) refinements.

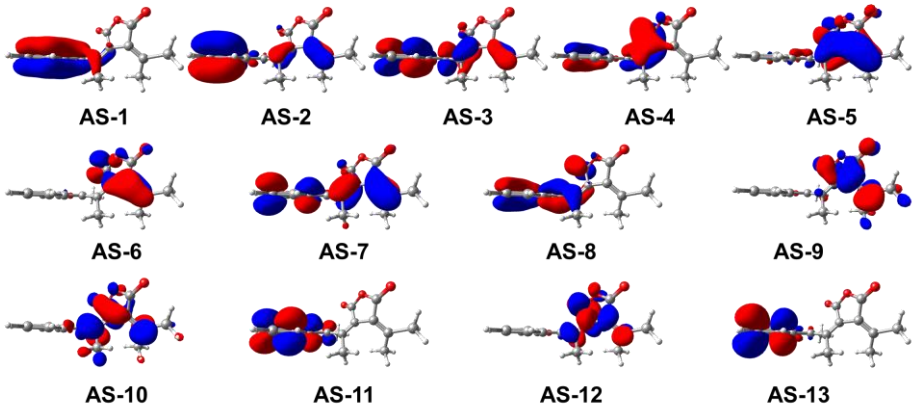

Figure S6. Molecular orbitals of Z used as the active space in the MS-CASPT2 (16,13) refinements.

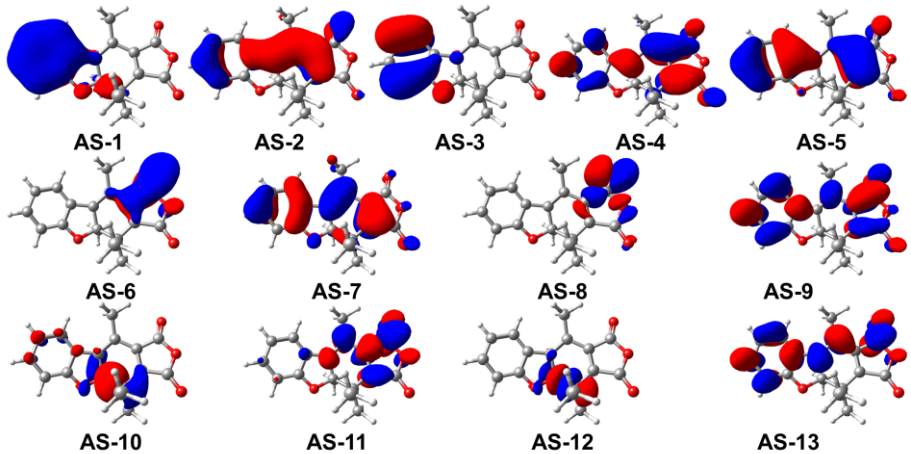

Figure S7. Molecular orbitals of C used as the active space in the MS-CASPT2 (16,13) refinements.

3. Relative Energies of the Optimized E, Z, and C Isomers in the S_1 State

Table S1. Relative energies of E, Z and C isomers in the S_0 and S_1 states using different basis sets relative to the corresponding S_0 minimum of C (unit: kcal/mol).

structures	environment	6-31G*/6-311G**/6-311++G**/def2-TZVP	
		S_0	S_1
C-isomer	MS-CASPT2(12,10)	0.0/0.0/0.0/0.0	55.3/48.1/46.7/44.8
	MS-CASPT2(12,10)/PCM	0.0/0.0/0.0/0.0	52.6/45.8/43.8/42.7
	MS-CASPT2(12,10)/MM	0.0/0.0/0.0/0.0	61.1/69.4/65.4/66.1
E-isomer	MS-CASPT2(12,10)	15.6/18.4/16.5/15.0	64.8/64.1/62.6/60.8
	MS-CASPT2(12,10)/PCM	14.3/16.8/15.0/14.0	65.2/61.7/60.1/58.8
	MS-CASPT2(12,10)/MM	40.0/41.7/41.0/39.7	84.5/83.8/82.4/80.8
Z-isomer	MS-CASPT2(12,10)	18.7/19.9/19.9/17.6	94.7/94.8/92.8/90.0
	MS-CASPT2(12,10)/PCM	16.6/24.8/17.4/22.7	95.2/94.6/86.2/90.4
	MS-CASPT2(12,10)/MM	27.9/30.8/31.0/28.0	101.0/103.4/104.5/97.9

For comparison, the triple-zeta basis sets of 6-311G**, 6-311++G** and def2-TZVP have been employed to evaluate the single-point energies of minima in the S_0 and S_1 states (Table S1). It is clear that the double-zeta 6-31G* basis set presents very similar results as those of the triple-zeta basis sets, except for some small deviations for the S_1 C-isomer.

Table S2. Single point energies of S_1 minima and conical intersections in the MS-CASPT2 (16,13) calculations (unit: kcal/mol).

structures	environment	S_0	S_1
C	MS-CASPT2(16,13)/6-31G*	0.0	52.8
E	MS-CASPT2(16,13)/6-31G*	16.4	62.5
Z	MS-CASPT2(16,13)/6-31G*	17.3	87.6
C	MS-CASPT2(16,13)/6-31G*/PCM	0.0	50.6
E	MS-CASPT2(16,13)/6-31G*/PCM	15.9	61.5
Z	MS-CASPT2(16,13)/6-31G*/PCM	19.0	84.7
C	MS-CASPT2(16,13)/6-31G*/MM	0.0	70.8
E	MS-CASPT2(16,13)/6-31G*/MM	30.7	82.3
Z	MS-CASPT2(16,13)/6-31G*/MM	27.5	96.7
S1S0-EC-MIN	MS-CASPT2(16,13)/6-31G*	67.3	73.5
S1S0-EZ-MIN	MS-CASPT2(16,13)/6-31G*	72.0	72.8
S1S0-EC-MIN	MS-CASPT2(16,13)/6-31G*/MM	82.2	83.7
S1S0-EZ-MIN	MS-CASPT2(16,13)/6-31G*/MM	88.0	94.3

Table S3. MS-CASPT2/6-31G* single point energies of Franck-Condon structures using different active spaces (unit: kcal/mol).

structures	active space for energies	S_0	S_1
C-FC	(12,10) π-space	0.0	61.9
C-FC	(16,13) n-space	0.0	60.1
E-FC	(12,10) π-space	15.6	105.5
E-FC	(16,13) n-space	16.4	100.9
Z-FC	(12,10) π-space	18.7	105.2
Z-FC	(16,13) n-space	17.3	105.9

Table S4. MS-CASPT2/6-31G* single point energies of S_1 minimum structures using different active spaces (unit: kcal/mol).

structures	active space for energies	S_0	S_1
C	(12,10) π-space	0.0	55.3
C	(16,13) n-space	0.0	52.8
E	(12,10) π-space	15.6	64.9
E	(16,13) n-space	16.4	62.5
Z	(12,10) π-space	18.7	94.7
Z	(16,13) n-space	17.3	87.6

We have assessed the effects of active spaces with or without n orbital on the single-point energies at the Franck-Condon points and S_1 minima (see Tables S3-S4). The S_1 vertical excitation energies of n-space, i.e., (16,13) are consistent with those of π-space, i.e., (12,10), except for the E isomer (100.9 vs. 105.5 kcal/mol). For the S_1 minima, the relative energies of n-space are a little lower than the energies of π-space, e.g. 52.8 vs. 55.3 kcal/mol for the C isomer. Nevertheless, the S_1 electronic state properties of C, Z and E for n-space and π-space are same with each other, which can be assigned as a π→π* type.

Table S5. The oscillator strengths of the C, E, Z isomers from the ground state to the S_1 state.

	C	**E**	**Z**
RASSCF(12,10)/6-31G*	0.451	0.187	0.125
RASSCF(12,10)/6-31G*/PCM	0.455	0.156	0.111
RASSCF(12,10)/6-31G*/MM	0.438	0.186	0.407
MS-CASPT2(12,10)/6-31G*	0.452	0.267	0.313
MS-CASPT2(12,10)/6-31G*/PCM	0.419	0.265	0.267
MS-CASPT2(12,10)/6-31G*/MM	0.433	0.251	0.365
MS-CASPT2(16,13)/6-31G*	0.376	0.292	0.178
MS-CASPT2(16,13)/6-31G*/PCM	0.370	0.264	0.158
MS-CASPT2(16,13)/6-31G*/MM	0.369	0.231	0.283

4. Cartesian Coordinates for Critical Structures

S0-C-MIN in Gas State

38

C	2.18390761	0.60307835	0.03957675
C	2.62209253	-0.72366383	0.00520866
C	3.93468022	-1.06832508	-0.16381432
C	4.86410646	-0.03204542	-0.30648553
C	4.46254981	1.30650703	-0.27123848
C	3.11749791	1.63699397	-0.10040373
C	0.73522747	0.55240908	0.19261939
C	0.43198477	-0.91238548	0.53579132
H	4.23266002	-2.09986219	-0.18586622
H	5.90312706	-0.27238856	-0.44074025
H	5.19441346	2.08671671	-0.37420153
H	2.81619104	2.66578499	-0.06567123
O	1.60816299	-1.61463592	0.14672982
C	0.31096784	-1.05083000	2.05978385
H	-0.59057961	-0.58481597	2.43992519
H	0.31518306	-2.09343784	2.34678902
H	1.16075700	-0.57216761	2.53124560
C	-0.24673835	1.48667862	0.06584857
C	0.00316594	2.95491534	-0.19713985
H	-0.91608075	3.48665550	-0.38940539
H	0.47974037	3.42667312	0.65574656
C	-1.59750181	0.91728585	0.06485296
O	-3.88992919	0.68690024	0.00138136
C	-2.91741112	1.62440193	0.14377219
C	-3.34328094	-0.54982225	-0.16034540
O	-3.99813886	-1.50364735	-0.34724154
O	-3.15844520	2.76013994	0.30516975
C	-1.86133194	-0.40023848	-0.06795969
C	-0.79230147	-1.46391131	-0.23911374
C	-1.23571370	-2.83870245	0.28704009
H	-0.38789067	-3.51378938	0.28987499
H	-1.63712287	-2.78958283	1.29163302
H	-2.00376792	-3.25670749	-0.34891007
C	-0.48825192	-1.58604915	-1.74673234
H	-1.39046999	-1.86061979	-2.28274062
H	-0.11606208	-0.65681340	-2.16246178
H	0.25433978	-2.35364131	-1.91653236
H	0.65386903	3.08312740	-1.05540301

S1-C-MIN in Gas State

38

C	2.13145994	0.61308615	0.05661277
C	2.58375170	-0.74316079	0.11964802
C	3.91128365	-1.11357471	-0.14068353
C	4.77969473	-0.09927467	-0.45792621

C	4.38754730	1.23994962	-0.53452047
C	3.05153557	1.62161228	-0.28519902
C	0.74040837	0.55753341	0.31612211
C	0.39361890	-0.87401795	0.67155684
H	4.20849046	-2.14218730	-0.09131784
H	5.80746302	-0.34150829	-0.65999528
H	5.11565337	1.98662224	-0.78708479
H	2.75710724	2.64775206	-0.35378969
O	1.65288973	-1.57309830	0.42985988
C	0.13104667	-1.04116134	2.17136327
H	-0.82472398	-0.61034144	2.43131217
H	0.13128783	-2.08846482	2.43887921
H	0.90703031	-0.54202581	2.74093409
C	-0.27318035	1.51078473	0.14613346
C	0.00537970	2.98266877	-0.00461460
H	-0.90078154	3.55184236	0.13068361
H	0.73940527	3.32447285	0.71785452
C	-1.58269851	0.96488417	0.02984120
O	-3.82392699	0.66933320	-0.08365087
C	-2.87515966	1.63204292	0.04492308
C	-3.24905124	-0.58370644	-0.18359309
O	-3.93865222	-1.54991128	-0.32291751
O	-3.16927391	2.78930750	0.14994838
C	-1.83406961	-0.40905809	-0.10262336
C	-0.75078794	-1.44159651	-0.23661514
C	-1.19322038	-2.84422751	0.21044117
H	-0.34396233	-3.52103437	0.23319852
H	-1.66054088	-2.83546229	1.18560512
H	-1.92403547	-3.23201964	-0.48420262
C	-0.26886281	-1.53494341	-1.70157599
H	-1.09985446	-1.84617094	-2.32206997
H	0.07889702	-0.57957152	-2.07841776
H	0.52626669	-2.26626102	-1.81293714
H	0.38617081	3.20107116	-1.00060050

S0-E-MIN in Gas State

38

C	2.25057481	0.36913582	-0.06137159
C	2.94600440	-0.59178694	0.63680584
C	4.27208067	-0.92853095	0.38439268
C	4.90107300	-0.23404098	-0.64299611
C	4.21573981	0.74952088	-1.37874216
C	2.88874127	1.06029440	-1.10045705
C	0.91014290	0.36808548	0.51884607
C	0.94152494	-0.55267139	1.49471439
H	4.77381140	-1.68464913	0.95800038
H	5.92635256	-0.45321344	-0.87955854
H	4.72776343	1.26790499	-2.16906946

H	2.37248919	1.81134803	-1.67035493
O	2.15525643	-1.14813467	1.57987899
C	-0.05789952	-1.02006021	2.49604704
H	-0.92376414	-0.37348526	2.50946239
H	-0.38564311	-2.02992155	2.27051433
H	0.38774274	-1.02753287	3.48420855
C	-0.20061850	1.28582701	0.17914857
C	0.10761343	2.76724275	0.34668103
H	-0.43905204	3.17915247	1.18677254
H	1.16323074	2.90374473	0.53467316
C	-1.44347169	0.85042143	-0.17910202
O	-3.73210430	0.98483908	0.02489485
C	-2.63106741	1.75742791	-0.14188422
C	-3.45491370	-0.34735185	-0.01871486
O	-4.29439671	-1.14033186	0.20297524
O	-2.70695200	2.92938001	-0.19829865
C	-2.01622953	-0.49707418	-0.39695207
C	-1.52594550	-1.57979683	-1.05701795
C	-2.29578704	-2.86935038	-1.23318267
H	-1.64181768	-3.70439952	-0.99823954
H	-3.17615994	-2.93433466	-0.61819337
H	-2.58882412	-2.98203092	-2.27375916
C	-0.18082554	-1.58651724	-1.73810903
H	-0.27277184	-2.09267893	-2.69398093
H	0.20669963	-0.59550426	-1.91709523
H	0.55006288	-2.13477811	-1.15286729
H	-0.17275791	3.33922515	-0.52612815

S1-E-MIN in Gas State

38

C	2.20565259	0.45786510	0.02004321
C	2.61914380	-0.86073412	0.25823152
C	3.86352012	-1.33427001	-0.02965616
C	4.77303488	-0.42380932	-0.58397628
C	4.40889333	0.87861103	-0.83485353
C	3.11631235	1.33965662	-0.54637614
C	0.79476460	0.50276584	0.40253582
C	0.50317672	-0.82934546	0.92764494
H	4.12850906	-2.35646502	0.16438363
H	5.76922457	-0.75419059	-0.81578621
H	5.12382640	1.55825833	-1.26184781
H	2.85544144	2.35692128	-0.76226535
O	1.61608968	-1.59500220	0.81025309
C	-0.25749669	-1.15046901	2.18126932
H	-1.15737870	-0.56307493	2.27321886
H	-0.50992204	-2.20221481	2.20883598
H	0.38243031	-0.93564815	3.03333462
C	-0.19698926	1.43889903	0.07788941

C	0.15314248	2.87512907	-0.21466541
H	-0.68990556	3.52218898	-0.02867639
H	0.98727656	3.20486135	0.39126499
C	-1.54607974	0.97368062	-0.04993626
O	-3.81248250	0.88196800	0.26972577
C	-2.75570322	1.74966622	0.25067926
C	-3.42028865	-0.38632333	0.00658377
O	-4.17758587	-1.28667392	0.00083925
O	-2.91007242	2.89618250	0.48282828
C	-1.95214757	-0.36168829	-0.29095131
C	-1.18951110	-1.48623533	-0.72425133
C	-1.72427994	-2.88829763	-0.53258647
H	-0.89395221	-3.58823377	-0.53131165
H	-2.27085480	-3.00681539	0.39212711
H	-2.39287092	-3.17496503	-1.34060022
C	-0.25135993	-1.34426469	-1.90644549
H	-0.77966694	-1.62799454	-2.81491731
H	0.11298480	-0.33698179	-2.04748398
H	0.60087945	-2.00822995	-1.81157208
H	0.43014696	2.98064733	-1.26158841

S0-Z-MIN in Gas State

38

C	2.63655486	0.69975615	0.38756837
C	3.54801702	0.27159557	1.34235656
C	4.77106136	0.90157788	1.57492186
C	5.05641085	1.99687483	0.81060046
C	4.14235679	2.46843423	-0.16230355
C	2.94926484	1.84431110	-0.37572397
C	1.50932327	-0.21344958	0.50905221
C	1.84820365	-1.09664397	1.50449996
H	5.44691809	0.53610255	2.32597491
H	5.98644389	2.51732319	0.95259496
H	4.39701369	3.34179378	-0.73569139
H	2.26117275	2.23112237	-1.10657524
O	3.07234116	-0.81667636	2.00224413
C	1.15713540	-2.26744903	2.11459535
H	1.82044339	-3.12508847	2.13598866
H	0.85664831	-2.04064139	3.13077901
H	0.27060429	-2.53052934	1.55247410
C	0.30418699	-0.26144619	-0.35127679
C	0.58926446	-0.43370321	-1.82759746
H	-0.26130191	-0.19161746	-2.44734962
H	1.41474742	0.20497494	-2.10993458
C	-0.95601974	-0.13697275	0.13224172
O	-2.41761628	1.13858747	1.35894351
C	-1.27628735	0.41256133	1.49491386
C	-3.01923094	0.97552102	0.14973781

O	-3.97526986	1.59307658	-0.14048453
O	-0.73032542	0.31547067	2.52558976
C	-2.25437349	-0.08035686	-0.58512536
C	-2.79997127	-0.93533456	-1.47966535
C	-4.18395980	-0.76395142	-2.06241762
H	-4.82240240	-1.57843656	-1.73226003
H	-4.64651414	0.17131574	-1.79852132
H	-4.12252930	-0.82846141	-3.14492671
C	-2.09863040	-2.19011348	-1.94172397
H	-1.78115927	-2.09962934	-2.97584567
H	-1.23835402	-2.44052050	-1.33885052
H	-2.79524990	-3.02075644	-1.89509574
H	0.89698512	-1.45324716	-2.03176668

S1-Z-MIN in Gas State

38

C	2.53077695	0.57601619	0.38773885
C	3.39844369	0.38056133	1.46025103
C	4.44601966	1.22252719	1.78343025
C	4.58981405	2.31788983	0.96165817
C	3.72696437	2.56576428	-0.13095389
C	2.70142594	1.71798829	-0.42676013
C	1.61256580	-0.50920231	0.40140790
C	2.01645496	-1.27993665	1.53531866
H	5.09115731	1.03956041	2.62085268
H	5.38263490	3.01546693	1.16069403
H	3.88583465	3.44691449	-0.72393357
H	2.03017954	1.90596785	-1.24278269
O	3.04645417	-0.76158773	2.12929717
C	1.39412895	-2.48980626	2.11408410
H	2.12731464	-3.08178717	2.64509966
H	0.62682596	-2.15991100	2.80685508
H	0.92048872	-3.06736922	1.33356997
C	0.43749160	-0.78409104	-0.43747097
C	0.74130868	-1.05242163	-1.90053078
H	-0.00078148	-0.59215009	-2.53956350
H	1.70753502	-0.64129821	-2.18728625
C	-0.77329433	-0.19231600	0.03818685
O	-2.00203581	1.11920073	1.45085861
C	-0.81747737	0.44759178	1.30625082
C	-2.77299849	0.95946585	0.35039208
O	-3.80214728	1.53181406	0.25138419
O	-0.01133284	0.48954329	2.20720252
C	-2.09826694	-0.03143848	-0.54643387
C	-2.78862825	-0.71778596	-1.51797357
C	-4.16587552	-0.32665167	-2.00793750
H	-4.93114187	-0.95236591	-1.55186317
H	-4.41491213	0.70069995	-1.80478359

H	-4.22360029	-0.49212795	-3.08158445
C	-2.28732554	-2.01067929	-2.11498904
H	-1.95592136	-1.89323637	-3.14423082
H	-1.48155125	-2.44613140	-1.54213804
H	-3.10425535	-2.72826591	-2.13215842
H	0.77362865	-2.11103829	-2.14921729

S0-C-MIN in QM

38

C	30.295636180	28.185010029	27.898294006
C	30.711848210	26.851792930	27.846631003
C	31.922563295	26.471174907	27.339770968
C	32.770638359	27.476048979	26.861239935
C	32.391314333	28.820143073	26.904236936
C	31.147497243	29.186742101	27.420450972
C	28.962631086	28.176228026	28.490419048
C	28.801058073	26.754537925	29.050553092
H	32.208792316	25.436797832	27.323289965
H	33.733008428	27.206667956	26.466526905
H	33.063064380	29.577938128	26.544339911
H	30.866483222	30.220052174	27.467150975
O	29.788777146	25.997044872	28.358791038
C	29.190495100	26.747464926	30.534027197
H	28.476134051	27.286175965	31.145704243
H	29.270204106	25.733275853	30.898782222
H	30.158350171	27.217546957	30.649376206
C	27.974436013	29.107694096	28.576947058
C	28.066195020	30.521313195	28.054535017
H	27.088018951	30.957274226	27.919255008
H	28.608393056	31.164625245	28.736296065
C	26.715334924	28.575263057	29.102760095
O	24.562480767	28.410045046	29.901489153
C	25.518583838	29.326078111	29.600283130
C	25.017224802	27.147353955	29.661707136
O	24.340636753	26.202502886	29.810502147
O	25.362602827	30.478058194	29.749769141
C	26.431485904	27.260172962	29.194454103
C	27.393736972	26.161262881	28.775436073
C	27.158005954	24.853877786	29.547603127
H	27.965922012	24.161652740	29.346138110
H	27.099927952	25.008947798	30.617233202
H	26.230904888	24.394348757	29.237329102
C	27.194479957	25.892383862	27.269836961
H	26.170628884	25.589304842	27.080763946
H	27.406812973	26.769784924	26.670355922
H	27.849540006	25.096407805	26.943362941
H	28.576703055	30.536222198	27.100670949

S1-C-MIN in QM

38

C	30.461520950	28.128512568	28.057856949
C	30.899993985	26.761299641	28.089978267
C	32.112802897	26.307760125	27.546889340
C	32.928956138	27.256968027	26.932950972
C	32.519998937	28.610474543	26.868894081
C	31.302244123	29.059298143	27.417560050
C	29.198594936	28.149065934	28.675749885
C	28.954345921	26.758308165	29.248685510
H	32.371084729	25.268373949	27.602318328
H	33.867653685	26.964247165	26.503748143
H	33.160293677	29.323979193	26.385750268
H	31.036127758	30.092677120	27.341591634
O	30.027746638	25.981190483	28.675049397
C	29.194466909	26.712288663	30.761700612
H	28.413919137	27.239491107	31.292937980
H	29.226260719	25.688403665	31.105094006
H	30.145941684	27.173544398	30.991298344
C	28.208726954	29.113104700	28.732258512
C	28.410559655	30.534854306	28.287736330
H	27.617783353	31.167187908	28.652879284
H	29.359680380	30.923926994	28.629243248
C	26.923453515	28.638063040	29.137245084
O	24.762412759	28.478920629	29.807323379
C	25.732105688	29.391057199	29.523033819
C	25.216932459	27.197875407	29.632394399
O	24.507129965	26.265346124	29.810885975
O	25.534086868	30.556232210	29.615954127
C	26.607101349	27.285623038	29.216252157
C	27.558789002	26.179804294	28.842032321
C	27.249631693	24.852286714	29.554798933
H	28.054847306	24.144443970	29.386941496
H	27.112501119	24.975760632	30.620321618
H	26.336000055	24.428636569	29.164347934
C	27.505383190	25.933451213	27.319570912
H	26.505398520	25.625923008	27.038754634
H	27.751574978	26.824622928	26.755484507
H	28.192124886	25.143165367	27.037439697
H	28.404189747	30.580442185	27.201700332

S0-E-MIN in QM

38

C	30.250198820	28.680329348	28.421044604
C	31.159893718	27.675806972	28.659180266
C	32.387175617	27.568372899	28.012197541
C	32.680523755	28.554526861	27.076899979

C	31.770717804	29.593932521	26.811261927
C	30.551104033	29.668224546	27.474607797
C	29.106811835	28.373075268	29.275753170
C	29.447635819	27.260197564	29.944106157
H	33.061293996	26.761416235	28.227393491
H	33.614657164	28.520061837	26.546356701
H	32.019926564	30.339314814	26.078761814
H	29.860583683	30.462864081	27.263768161
O	30.678709194	26.822534037	29.588701895
C	28.761848029	26.440700145	30.981498987
H	27.903384670	26.964944287	31.375382563
H	28.428056959	25.495764630	30.566441891
H	29.442849379	26.222871548	31.794993069
C	27.871064524	29.175490967	29.418773651
C	28.076144156	30.625009059	29.834739026
H	27.774036891	30.772696037	30.865338008
H	29.121484232	30.885595262	29.752195853
C	26.621908443	28.647677979	29.258345821
O	24.439313551	28.422799652	29.951758261
C	25.402584237	29.354136105	29.758582165
C	24.809279569	27.180213407	29.541023025
O	24.099290889	26.259101663	29.713810208
O	25.213889298	30.488390252	30.004699079
C	26.138874026	27.302726153	28.869704528
C	26.563050269	26.442363402	27.904877177
C	25.911228313	25.104787872	27.633380943
H	26.688549708	24.352407152	27.532792423
H	25.224085739	24.794733085	28.400882845
H	25.381080003	25.137884189	26.685297845
C	27.693147089	26.759205623	26.958267594
H	27.409779430	26.442608422	25.959532602
H	27.931131253	27.810747440	26.921940206
H	28.593483048	26.215339298	27.224033781
H	27.494277522	31.305578749	29.230895481

S1-E-MIN in QM

38

C	30.200374443	28.862432427	28.604826957
C	30.788627114	27.606068364	28.522180922
C	31.957158342	27.326959666	27.871186023
C	32.589937357	28.400052687	27.232407725
C	32.017222055	29.671546155	27.258552738
C	30.820617429	29.919293084	27.937691596
C	28.926048343	28.657851576	29.304612237
C	28.899694517	27.232079683	29.613485801
H	32.353767615	26.329988427	27.843735419
H	33.512443573	28.236305624	26.707007765
H	32.495468121	30.478400021	26.738280833

H	30.402898551	30.905542562	27.931823348
O	30.022348876	26.673105215	29.163653690
C	28.407719005	26.550295124	30.855730007
H	27.494438339	26.982761743	31.223612591
H	28.269112286	25.495951768	30.667252099
H	29.174013869	26.654225610	31.615940804
C	27.811112271	29.454421570	29.373165610
C	27.870607992	30.950275275	29.325520766
H	27.267493452	31.349549426	30.130103933
H	28.877834898	31.324400504	29.416523880
C	26.537775208	28.793073900	29.444788756
O	24.436920537	28.262178645	30.142929623
C	25.361673782	29.279893759	30.132805076
C	24.914644803	27.163567718	29.529771039
O	24.294761123	26.166866831	29.448006894
O	25.120258385	30.314993150	30.654950093
C	26.280567744	27.492946551	28.976482697
C	27.063146911	26.612234987	28.183054163
C	26.711955503	25.138443810	28.119893133
H	27.585636016	24.579144665	27.797022969
H	26.390499549	24.740384909	29.071872542
H	25.916794433	24.938016286	27.406532726
C	27.705706148	27.118922923	26.901467137
H	27.031537661	26.938492537	26.067482777
H	27.923168872	28.177006170	26.911032529
H	28.624007082	26.582880996	26.686334069
H	27.427150028	31.304995067	28.401074566

S0-Z-MIN in QM

38

C	30.637085207	28.528105051	28.643878063
C	31.777678289	28.215239031	29.345883110
C	33.031090379	28.736303066	29.062725089
C	33.099288383	29.654520136	28.024151015
C	31.939319301	30.035262161	27.315760963
C	30.709255210	29.480415122	27.613992989
C	29.575057129	27.740210997	29.275578107
C	30.171787172	27.072513946	30.276343177
H	33.896368440	28.447366049	29.625853133
H	34.046202449	30.085554167	27.759427000
H	32.018378302	30.771374216	26.537483912
H	29.831387149	29.785104142	27.077182951
O	31.489932265	27.335655969	30.334862184
C	29.684310138	26.101191881	31.292763251
H	28.690505067	25.751796855	31.052351232
H	30.357793186	25.253850817	31.343091257
H	29.649583135	26.574614914	32.266642322
C	28.200808028	27.562824984	28.772654072

C	28.113877023	27.210253958	27.303699966
H	28.790157070	27.834353006	26.739651926
H	28.429541047	26.184570884	27.145094956
C	27.077608949	27.697941991	29.541023126
O	25.823188856	29.019458086	30.940611228
C	27.052639948	28.453171050	30.834522218
C	24.963202795	28.602193057	29.972673156
O	23.881070718	29.053741088	29.892219153
O	27.871469006	28.616728058	31.657964277
C	25.654469845	27.545416984	29.177555097
C	25.004006801	26.553592909	28.505324050
C	23.521920690	26.572483912	28.213844029
H	23.045545658	25.697315851	28.641388062
H	23.022757655	27.452489977	28.579209058
H	23.374171683	26.509759908	27.138530951
C	25.703971848	25.314033822	28.005424014
H	25.806013858	25.327040825	26.924343935
H	26.683605922	25.178746812	28.439665044
H	25.105358807	24.444356758	28.251334031
H	27.119678953	27.338111966	26.904145938

S1-Z-MIN in QM

38

C	30.674668328	28.422355312	28.689996892
C	31.890536397	28.311971499	29.354272157
C	33.021634521	29.001773845	29.019860282
C	32.893389542	29.898024921	27.948104635
C	31.671811819	30.071556296	27.270438287
C	30.550214380	29.337175948	27.621055727
C	29.791258865	27.498947220	29.290383391
C	30.563663128	26.923183719	30.340161709
H	33.946262473	28.875850790	29.546770012
H	33.750499673	30.464301760	27.640186930
H	31.621157840	30.783098889	26.469615565
H	29.611531718	29.453783658	27.115330598
O	31.781593301	27.399132701	30.373774392
C	30.153369956	25.960961254	31.379173641
H	29.189872835	25.545813706	31.128843322
H	30.897064449	25.180522762	31.483699695
H	30.070529878	26.498833028	32.317600551
C	28.391798274	27.161559591	28.966129736
C	28.230080468	26.440410764	27.641281374
H	29.089148412	26.616386642	26.999085364
H	28.133822523	25.360722687	27.735910686
C	27.401392140	27.931385677	29.644692928
O	26.742721487	29.528143258	31.148652765
C	27.801998654	28.785072042	30.710965722
C	25.626447354	29.201321860	30.457546744

O	24.624169700	29.801375141	30.629079740
O	28.877910533	28.928555352	31.240803490
C	25.946211703	28.028270966	29.575544088
C	24.967716471	27.204465050	29.080020586
C	23.486675967	27.501511369	29.138932545
H	23.005614583	26.838407360	29.854704646
H	23.256253841	28.516995668	29.407309423
H	23.037378786	27.282992376	28.172616063
C	25.260061114	25.842601618	28.498252877
H	25.287419683	25.854183646	27.411372560
H	26.188857495	25.428662896	28.860555646
H	24.465266012	25.159664738	28.777011857
H	27.360623748	26.798831167	27.106527131

S1S0-EC-MIN in QM

38

C	29.83323097	28.41336384	28.72291635
C	30.53533433	27.26270481	29.05089070
C	31.75098365	26.93950464	28.47444103
C	32.25773565	27.84565642	27.55862203
C	31.56716962	29.01924413	27.21125386
C	30.34841456	29.30133215	27.77136676
C	28.62028703	28.39864762	29.52223461
C	28.72828042	27.20296162	30.29673755
H	32.27074597	26.03839906	28.73622662
H	33.20738871	27.64541914	27.09775612
H	32.00056464	29.69581969	26.49931119
H	29.80795469	30.18500536	27.49850570
O	29.88679959	26.52577257	29.95407311
C	28.18149837	26.96480195	31.65536548
H	27.09842788	26.97784405	31.63438125
H	28.52742329	26.01438974	32.03722399
H	28.49504208	27.75403380	32.32903660
C	27.65062389	29.46892025	29.67444956
C	28.03150830	30.93042158	29.56484139
H	27.32538227	31.52188542	30.13116260
H	29.02118859	31.12402651	29.96095026
C	26.36194783	29.00373233	29.72672075
O	24.15449582	28.68252828	30.17645993
C	25.07267082	29.65488112	30.11843706
C	24.69482256	27.43310714	29.79785952
O	23.98612983	26.47550925	29.78522442
O	24.84778746	30.78800780	30.36421911
C	26.04088381	27.67420187	29.46756478
C	27.07436699	26.81874841	28.92223952
C	27.02789252	25.35598454	29.30508178
H	27.88763334	24.80696261	28.94827784
H	26.88393302	25.19547688	30.35966572

H	26.13822857	24.97647451	28.80868802
C	27.43403742	26.98601465	27.45561550
H	26.66821003	26.44364783	26.90843150
H	27.41135701	28.01609556	27.13771303
H	28.39277387	26.54498583	27.21080827
H	28.00611931	31.30128851	28.54289134

S1S0-EZ-MIN in QM

38

C	30.57828029	28.56633535	28.66870695
C	31.38596075	27.77598183	29.46520995
C	32.73194463	27.61736322	29.40000459
C	33.35345305	28.35293770	28.40777920
C	32.59816471	29.16959754	27.56041071
C	31.22405767	29.27710146	27.66383468
C	29.19992277	28.31450355	29.13191282
C	29.35279841	27.35672514	30.23914751
H	33.26636755	26.97329937	30.06834572
H	34.41759177	28.29551958	28.28823413
H	33.10628088	29.73426858	26.80223411
H	30.69166365	29.89521134	26.97147625
O	30.55157040	27.11293900	30.41511699
C	28.42121963	26.76268581	31.20784655
H	27.95396678	27.60557577	31.71814086
H	27.64729267	26.23076809	30.68306927
H	28.97543787	26.13063452	31.88499279
C	28.00242357	28.90076754	28.88397272
C	27.99014954	30.16522168	28.08542920
H	27.50846925	30.87303924	28.75041365
H	28.94735286	30.54557669	27.77096602
C	26.74526368	28.42679809	29.38373320
O	25.08804081	28.27247207	30.86682681
C	26.36132814	28.83716473	30.57503112
C	24.68615123	27.51249772	29.86085950
O	23.62885333	26.96526437	29.86674709
O	26.92699055	29.48400345	31.48713040
C	25.76444260	27.48966629	28.79515423
C	25.72462821	26.72068676	27.68728116
C	24.63051935	25.73000498	27.35069395
H	25.03630479	24.71844756	27.32395070
H	23.81671847	25.75248493	28.05315908
H	24.23240926	25.92520910	26.35650864
C	26.80902455	26.74905189	26.63271091
H	26.38664696	26.97350009	25.65526383
H	27.58400940	27.48334052	26.81384113
H	27.29836129	25.77996505	26.54041985
H	27.32478356	30.02587551	27.24409521