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

Supporting Information

Photophysical Characterization of New and Efficient Synthetic Sunscreens

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Contents

• Computational Section

1.- Active space selection

Two different active spaces were checked to model compound **3** (14,13) and (6,5). The core chromophore was considered to be formed by the π density (orbitals π and π* of bonds C=C, C=N and n N_{imine}) and, in the extended active space, four π and π* orbitals of the phenyl rings, as seen below. The selected active orbitals are shown in figure S1 for the selected (14,13) active space. In case of using a (6,5) active space, the orbitals present are 1, 2, 5, 8 and 13, excluding all the phenyl orbitals. In both cases the involved transition is a π - π* between orbitals 5 and 8.

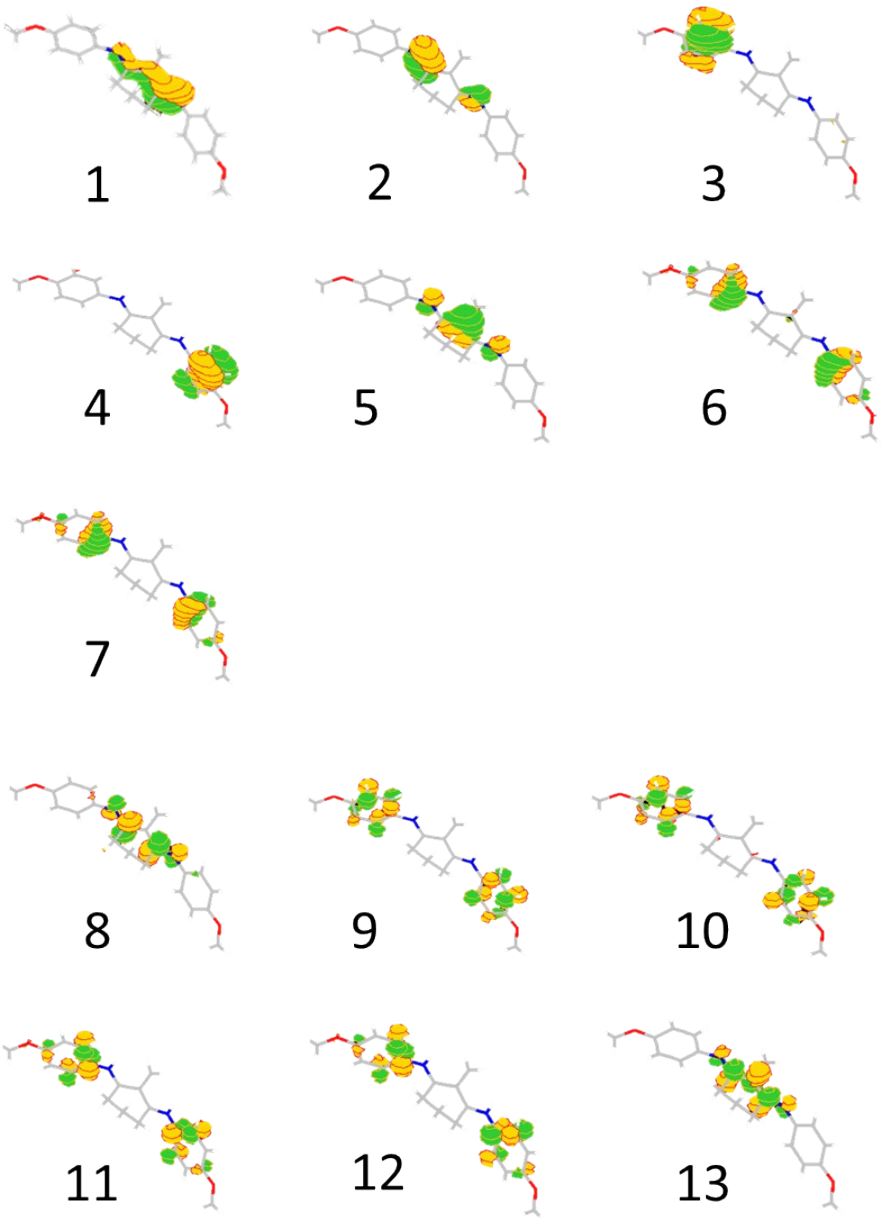

Figure S1. Orbitals involved in the (14,13) active space of **3**.

Absorption spectra were computed for both active spaces (14,13) and (6,5) to check for differences. In both cases, a transition between S_0-S_1 was observed at 326 nm and 327 nm, respectively. The oscillator strength values changed from f = 1.1066305 to f=0.82943528 due to lack of the phenyl ring contribution in the smaller active space. To ensure the ability of the (6,5) active space to reproduce the PES, the MEP was also computed for both active spaces.

2.- Minimum energy paths

The MEP was computed for both active spaces obtaining the same energetic profile as shown in Figure S2. A different, new deactivation channel consisting of the imine isomerization competing with the out-of-plane movement of the substituents of the cycle was found.[6]
The new deactivation path involving a C=N isomerization leads to the formation of a minimum in the PES followed by a conical intersection (CI) only 8 kcal/mol higher in energy. This barrier is low enough to allow for a fast deactivation to the ground state in agreement with the experimental data.

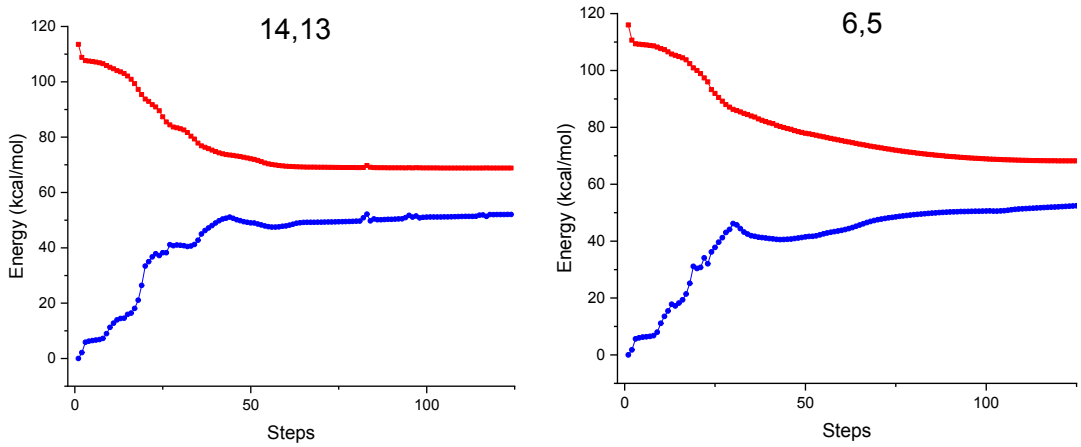

Figure S2. Comparison of MEP (CASSCF) with both active spaces for **3**.

In order to ensure this differential effect of the aryl moieties on the shape of the PES, we also computed the MEP for the simplified compound **A** in which the phenyl substituents are changed by methyl groups (**A** has not been synthesized and it was studied only computationally, see Figures S3 and S4). As the more relevant feature, it should be noted that the shape of the PES clearly resembles that of palythine and related compound including the movement of substituents out of the plane of the cycle. In contrast, the minimum in the excited state related to the photoisomerization of a C=N bond is *ca.* 10 kcal/mol higher in energy and no conical intersection of isomerization was found.

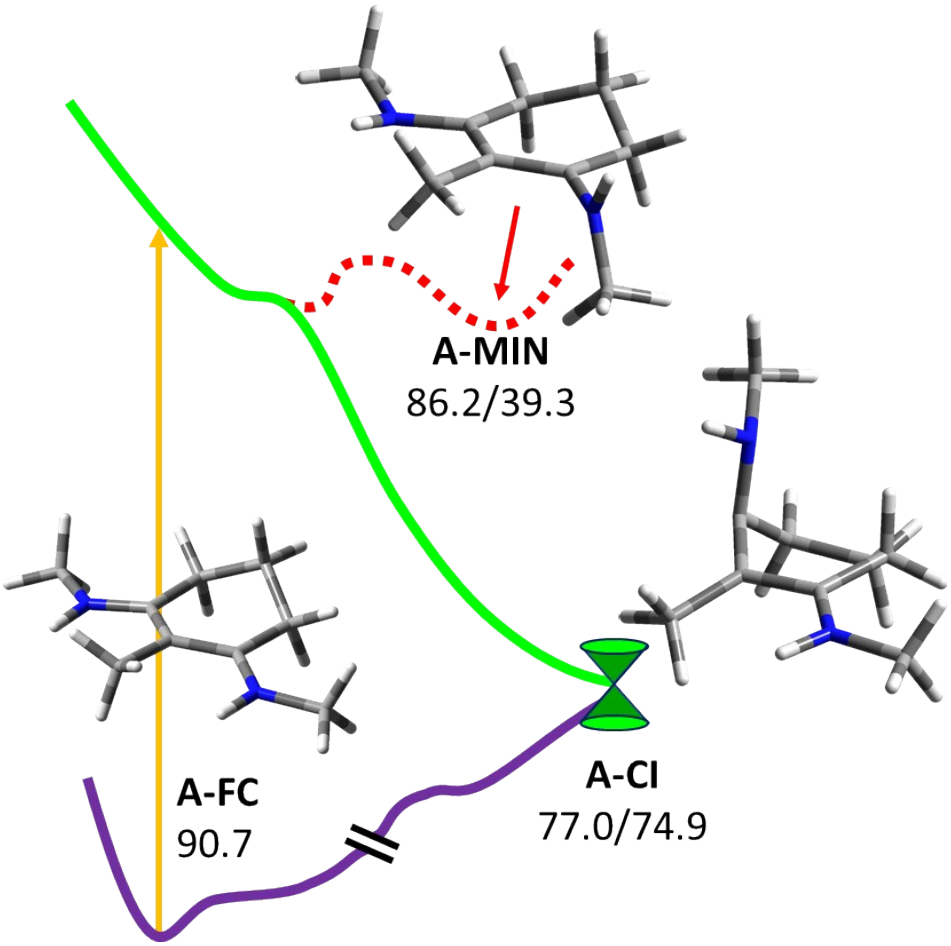

Figure S3. Critical points along the PES for **A** (CASPT2 energies relative to S_0).

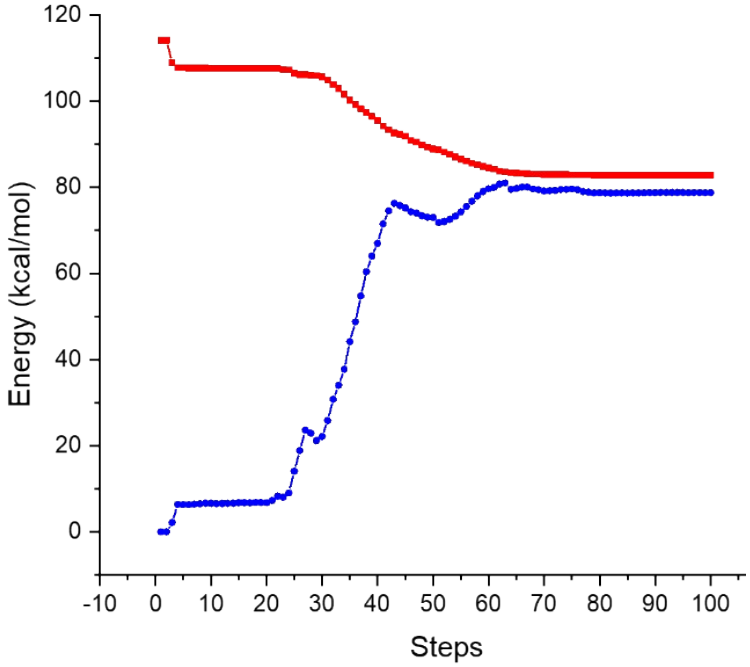

Figure S4. MEP (CASSCF) connecting FC to the CI (right) for **A**.

3.- Isomerization: CI and thermal reversion

The topology around the conical intersection is a key factor to understand any deactivation mechanism. In this case, we found according to MOLCAS descriptors,[3] a highly sloped funnel leading to the formation of a single product. This means a conical intersection that promotes an aborted geometrical transformation with stating material recovery and not the appearance of photoproducts. Thus, a low (if any) isomerization quantum yield for the photoisomerization is expected.

The shape of the PES around the CI was explored by applying geometrical distortions along the *x* and *y* vectors[3] shown in Figure S5. These vectors are a mathematical transformation of the classical descriptors (gradient difference (GD) and derivative coupling (DC) vector). The GD and DC vectors are also shown in Figure S5. Specifically, the movement related with the DC vector corresponds with an aborted isomerization.

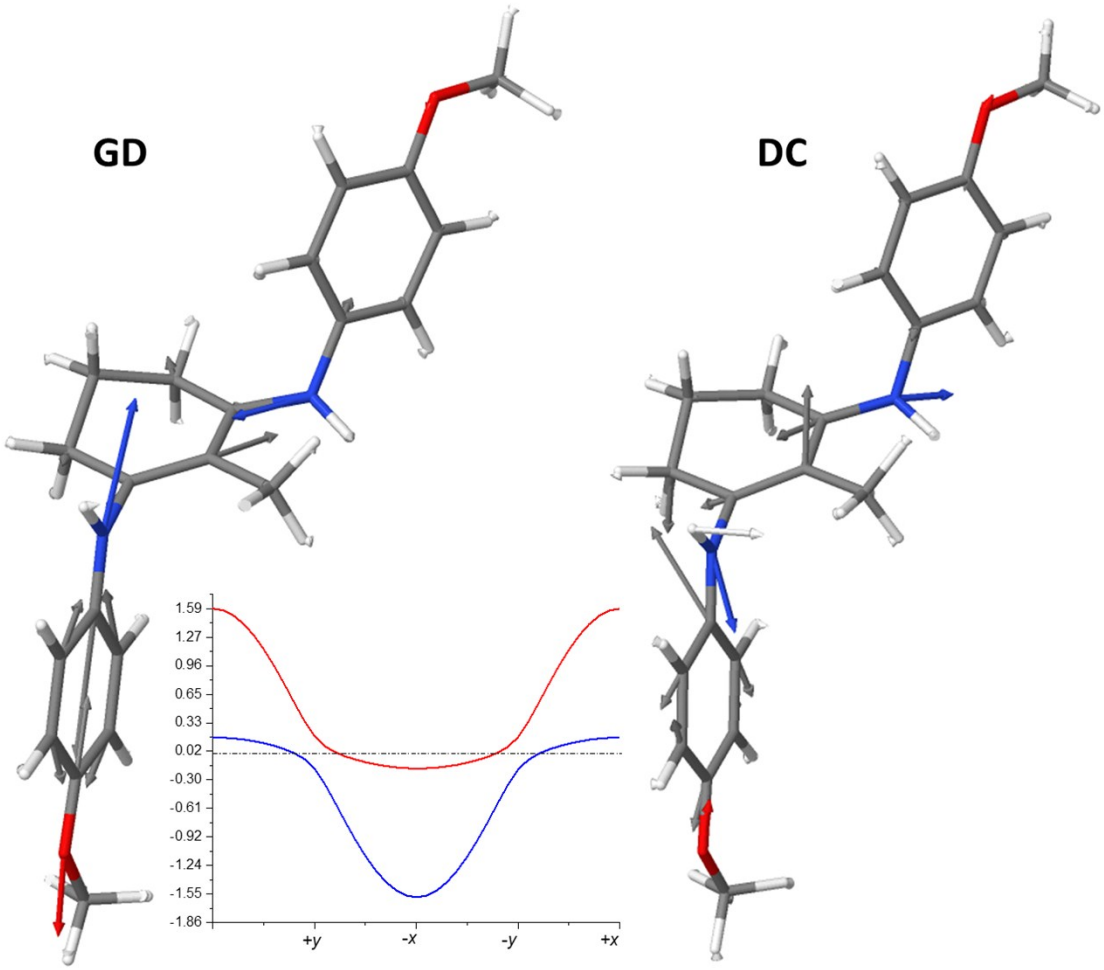

Figure S5. PES topology around the CI and S_1 (red) and S_0 (blue) energy difference (kcal/mol). CI isomerization vectors GD (left) and DC (right).

Even with a sloped CI topology, the formation of the *Z* isomer could still be possible. In fact, this feature has been also observed in natural MAAs as a complementary mechanism of photoprotection. In addition, both the starting isomer and the photoisomer contribute to the photoprotection as they absorb in a similar region of the spectrum (see computed

absorption in Figure S6). To explore the relative stability and UV capabilities of the *Z*-isomer, we computed both isomers at the MP2 level including methanol as solvent to reproduce the experimental data (Figure S5).
The *Z* photoisomer can be thermally converted to the starting isomer *E* through a transition state characterized by computing the intrinsic reaction coordinate. The obtained TS connects both isomers through a low energy barrier (13.7 kcal/mol, see Figure S6). This process should be fast enough to avoid the accumulation of the photoisomer at room temperature.

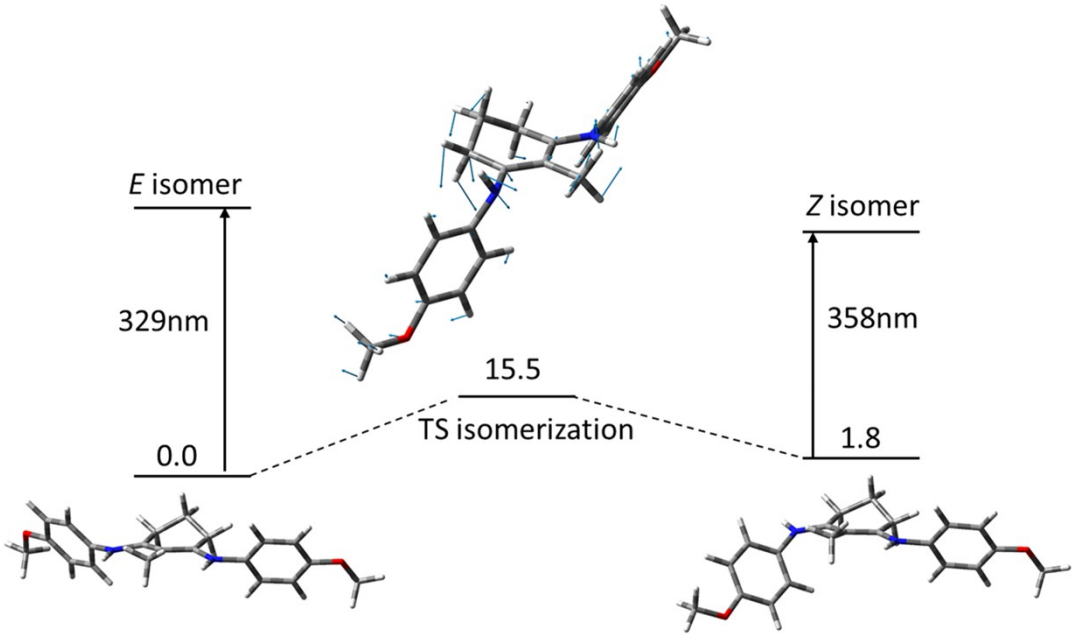

Figure S6. Schematic isomerization path and TS with displacement vectors. Energies in kcal/mol and absorption wavelength in nm.

4.- *Z*-isomer

Methanol solutions (5E-5M) of **3** were irradiated with different light sources and temperatures trying to find some experimental evidence for the *Z*-isomer formation. Irradiation with 400W medium pressure Hg lamp or a monochromatic light (340nm) at -20ºC did not allow the detection of the photoisomer. Both UV-Vis spectroscopy and NMR were used in these experiments.

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6.- Cartesian Coordinates

3-FC (Minimum S_0):

S_0 = -1068.33004984

S_1 = -1068.14914901

C	-0.000183	-0.876515	1.575765
C	-1.246992	-0.672208	0.731242
C	-1.207930	0.649164	-0.001976
C	0.000169	1.315775	-0.262872
C	1.207923	0.648574	-0.001735
C	1.246452	-0.673151	0.730760
N	-2.363798	1.142925	-0.421808
H	-2.341397	1.982321	-0.958646
C	-3.672257	0.582314	-0.220072
C	-4.456375	1.018934	0.857241
C	-5.727981	0.510337	1.026743
C	-6.242111	-0.438291	0.120717
C	-5.469710	-0.857560	-0.939724
C	-4.180589	-0.342705	-1.112763
O	-7.482624	-0.859043	0.385260
C	-8.110463	-1.788898	-0.461906
N	2.363849	1.142692	-0.420938
H	2.341510	1.982787	-0.956724
C	3.672266	0.581857	-0.219598
C	4.179433	-0.344808	-1.111248
C	5.468463	-0.859958	-0.938466
C	6.241997	-0.439240	0.120580
C	5.729077	0.511108	1.025483
C	4.457498	1.019893	0.856319
O	7.482569	-0.860073	0.384704
C	8.109268	-1.791583	-0.461489
H	-0.000513	-1.874203	1.997141
H	0.000264	-0.177550	2.405998
H	-2.136799	-0.716034	1.343062
H	-1.340464	-1.463492	-0.008444
H	2.136553	-0.718013	1.342084
H	1.338749	-1.464223	-0.009296
H	-4.068087	1.747362	1.545908
H	-6.349405	0.826633	1.842491
H	-5.838550	-1.573804	-1.646883
H	-3.588706	-0.666735	-1.949564
H	-9.090481	-1.956713	-0.044968
H	-8.209499	-1.396036	-1.467235
H	-7.565024	-2.725390	-0.486335
H	3.586709	-0.669916	-1.947033
H	5.836367	-1.577540	-1.644755
H	6.351350	0.828480	1.840165
H	4.070085	1.749533	1.544195
H	8.207534	-1.400432	-1.467560
H	9.089603	-1.959087	-0.045171
H	7.563443	-2.727901	-0.483859
C	0.001659	2.679985	-0.927717
H	-0.857541	3.268370	-0.629108
H	0.855575	3.270695	-0.618352
H	0.008301	2.623263	-2.013232

3-Minimum S_1 (14,13):

S_0 = -1068.24710157

S_1 = -1068.22038198

C	-0.443386	-0.998368	2.464876
C	-1.178578	-1.198214	1.143038
C	-0.941877	-0.052326	0.189034
C	0.240889	0.696024	0.241987
C	1.209170	0.358315	1.190153
C	1.041138	-0.720156	2.231180
N	-1.839728	0.086101	-0.857886
H	-1.569609	0.703322	-1.588848
C	-3.253405	-0.009709	-0.682736
C	-3.923962	0.717583	0.314202
C	-5.296293	0.625132	0.444649
C	-6.039258	-0.181608	-0.434522
C	-5.389097	-0.885954	-1.421748
C	-3.996616	-0.806414	-1.537657
O	-7.365942	-0.189717	-0.220976
C	-8.200978	-0.957057	-1.045915
N	2.440226	1.088552	1.253713
H	2.461683	1.892934	1.853585
C	3.578372	0.770291	0.666649
C	3.692145	-0.344588	-0.214398
C	4.885578	-0.645688	-0.807877
C	6.023327	0.137609	-0.564845
C	5.929503	1.262698	0.312276
C	4.748677	1.574571	0.911207
O	7.208131	-0.066380	-1.083594
C	7.458150	-1.143022	-1.973602
H	-0.557475	-1.873570	3.093942
H	-0.882679	-0.160932	2.998804
H	-2.237681	-1.316454	1.328258
H	-0.851019	-2.120864	0.664335
H	1.518917	-0.414824	3.158065
H	1.547149	-1.630968	1.912311
H	-3.365827	1.351985	0.980029
H	-5.822133	1.172837	1.203728
H	-5.929537	-1.509900	-2.106329
H	-3.493939	-1.372668	-2.300150
H	-9.205554	-0.800247	-0.685188
H	-8.137277	-0.634437	-2.079386
H	-7.957646	-2.011927	-0.979961
H	2.826753	-0.943991	-0.414154
H	4.939468	-1.489546	-1.466278
H	6.814687	1.845002	0.479391
H	4.678498	2.419505	1.571719
H	6.849592	-1.048122	-2.862824
H	8.499684	-1.065212	-2.234195
H	7.272109	-2.089675	-1.484481
C	0.464010	1.825436	-0.746093
H	-0.419422	2.448211	-0.820396
H	1.281869	2.470839	-0.457049
H	0.688380	1.447490	-1.739661

3-CI Isomerization S_1/S_0 (14,13):

S_0 = -1068.21609300

S_1 = -1068.21603983

C	-0.346060	-1.275977	2.478879
C	-1.039935	-1.666659	1.176477
C	-0.910374	-0.596146	0.120760
C	0.158513	0.301059	0.124853
C	1.153172	0.152600	1.103558
C	1.102659	-0.852957	2.225599

N	-1.838601	-0.669540	-0.937273
H	-1.511471	-0.324395	-1.811261
C	-3.220069	-0.397413	-0.714038
C	-3.668389	0.465285	0.296066
C	-5.021657	0.699239	0.473466
C	-5.963184	0.097227	-0.372241
C	-5.529897	-0.742069	-1.375035
C	-4.165566	-0.999321	-1.533336
O	-7.250252	0.405044	-0.117363
C	-8.266726	-0.154292	-0.901927
N	2.282296	1.047736	1.120817
H	2.176488	1.900131	1.641788
C	3.455908	0.844566	0.585787
C	3.747313	-0.327413	-0.185865
C	4.980759	-0.512147	-0.726417
C	5.997530	0.445345	-0.541921
C	5.726633	1.629288	0.220927
C	4.501957	1.829373	0.767857
O	7.207344	0.358382	-1.015983
C	7.642503	-0.753154	-1.791077
H	-0.366081	-2.099523	3.183106
H	-0.879492	-0.449483	2.939066
H	-2.089038	-1.861577	1.363943
H	-0.626734	-2.598503	0.792075
H	1.534168	-0.428043	3.127771
H	1.706960	-1.725449	1.979650
H	-2.959533	0.951116	0.942783
H	-5.374290	1.353188	1.248856
H	-6.224939	-1.222516	-2.035725
H	-3.840035	-1.679001	-2.300145
H	-9.195770	0.232321	-0.512159
H	-8.168530	0.136487	-1.942423
H	-8.272347	-1.236582	-0.828805
H	2.976376	-1.054872	-0.335666
H	5.171197	-1.397654	-1.299029
H	6.520694	2.340320	0.341305
H	4.295503	2.714039	1.341614
H	7.059043	-0.829968	-2.697882
H	8.670642	-0.546892	-2.032618
H	7.575225	-1.663741	-1.212364
C	0.256826	1.380951	-0.936112
H	-0.726987	1.752480	-1.189296
H	0.840230	2.231614	-0.605985
H	0.715207	1.009397	-1.848677

3-CI S_1/S_0 (14,13):

S_0 = -1068.19275993

S_1 = -1068.19275245

C	-0.447722	-1.390969	-0.179482
C	-1.455283	-0.671545	-1.097470
C	-1.328980	0.806567	-0.812446
C	0.002923	1.325819	-1.164762
C	1.117979	0.634185	-0.558777
C	0.990617	-0.857949	-0.306377
N	-1.705768	1.211158	0.485409
H	-1.592215	2.195535	0.609720
C	-2.949358	0.763821	1.051757
C	-2.951131	0.219381	2.343046
C	-4.134076	-0.184278	2.932945
C	-5.349569	-0.059207	2.239489

C	-5.355375	0.476764	0.971135
C	-4.157469	0.895497	0.382971
O	-6.434064	-0.490299	2.902658
C	-7.703475	-0.386291	2.314380
N	2.251026	1.230005	-0.384945
H	2.284798	2.207774	-0.612202
C	3.497874	0.644402	0.068418
C	4.358975	0.079960	-0.849102
C	5.578701	-0.449146	-0.416016
C	5.916671	-0.399970	0.919195
C	5.029734	0.187912	1.847044
C	3.825888	0.713289	1.427778
O	7.045255	-0.871360	1.443861
C	8.020555	-1.472539	0.623569
H	-0.426965	-2.451186	-0.402900
H	-0.776660	-1.289818	0.845359
H	-2.452977	-1.040925	-0.903932
H	-1.230352	-0.861636	-2.142263
H	1.583804	-1.144626	0.551213
H	1.467325	-1.309648	-1.174027
H	-2.023011	0.127699	2.877312
H	-4.151045	-0.598653	3.922992
H	-6.268741	0.590642	0.420733
H	-4.180679	1.325578	-0.602697
H	-8.401344	-0.781322	3.035744
H	-7.954809	0.646865	2.101794
H	-7.763343	-0.969676	1.402219
H	4.104771	0.045506	-1.892938
H	6.235830	-0.885791	-1.141054
H	5.317767	0.216958	2.880150
H	3.152438	1.164530	2.133659
H	8.391972	-0.771890	-0.114544
H	8.823748	-1.759868	1.282106
H	7.624571	-2.353160	0.131997
C	0.180529	2.421666	-2.173941
H	-0.005755	3.404577	-1.740194
H	1.167457	2.436932	-2.625555
H	-0.547871	2.299012	-2.968995

3-Minimum S_1 (6,5):

S_0 = -1068.15857300

S_1 = -1068.13623018

C	-0.413995	-0.997229	2.487036
C	-1.146627	-1.247732	1.172829
C	-0.933593	-0.122685	0.190885
C	0.230427	0.657694	0.223439
C	1.214845	0.367883	1.175231
C	1.062487	-0.690240	2.239882
N	-1.832278	-0.041345	-0.868897
H	-1.552252	0.533639	-1.630410
C	-3.246837	-0.084347	-0.683064
C	-3.883418	0.650385	0.316054
C	-5.251263	0.606650	0.459680
C	-6.026655	-0.157989	-0.411712
C	-5.403864	-0.882151	-1.416598
C	-4.019788	-0.847747	-1.534850
O	-7.352077	-0.126522	-0.195980
C	-8.215118	-0.855852	-1.026054
N	2.425572	1.131432	1.222710
H	2.433062	1.941006	1.811672

C	3.572309	0.810400	0.643538
C	3.688597	-0.321696	-0.215991
C	4.876186	-0.635325	-0.805159
C	6.010954	0.166837	-0.569810
C	5.909489	1.305180	0.282816
C	4.736149	1.617245	0.867788
O	7.187993	-0.041957	-1.079830
C	7.459965	-1.135399	-1.950791
H	-0.506031	-1.857478	3.139756
H	-0.871491	-0.156587	3.000296
H	-2.203638	-1.382529	1.359435
H	-0.800743	-2.176272	0.718229
H	1.538250	-0.355721	3.157067
H	1.585201	-1.599473	1.941745
H	-3.298937	1.261158	0.981467
H	-5.746813	1.167354	1.229866
H	-5.970037	-1.481950	-2.101774
H	-3.537837	-1.426561	-2.301885
H	-9.212477	-0.667764	-0.660421
H	-8.143791	-0.525035	-2.056348
H	-8.009200	-1.919207	-0.971596
H	2.822237	-0.924465	-0.399897
H	4.937181	-1.490775	-1.447307
H	6.793134	1.893543	0.438307
H	4.660995	2.474144	1.512011
H	6.856787	-1.061074	-2.844855
H	8.502666	-1.046240	-2.201706
H	7.280644	-2.072649	-1.442762
C	0.416040	1.771083	-0.790293
H	-0.488129	2.361818	-0.877059
H	1.213462	2.446128	-0.513585
H	0.651440	1.380315	-1.776721

3-CI isomerization S_1/S_0 (6,5):

S_0 = -1068.13304316

S_1 = -1068.13304286

C	-0.339966	-1.221785	2.516047
C	-1.036906	-1.631313	1.221613
C	-0.910077	-0.571249	0.156050
C	0.160591	0.327499	0.144220
C	1.167387	0.193415	1.113666
C	1.105824	-0.797858	2.250715
N	-1.833824	-0.655375	-0.903891
H	-1.502115	-0.330465	-1.784515
C	-3.216050	-0.398681	-0.696658
C	-3.686602	0.405507	0.338619
C	-5.037903	0.625043	0.505658
C	-5.959258	0.066007	-0.374467
C	-5.499853	-0.725518	-1.417244
C	-4.139774	-0.963664	-1.558538
O	-7.253842	0.350876	-0.135022
C	-8.250332	-0.183660	-0.961931
N	2.288860	1.093112	1.118890
H	2.190078	1.945517	1.634871
C	3.467498	0.868156	0.579174
C	3.734498	-0.315499	-0.183489
C	4.957339	-0.532812	-0.731423
C	5.987824	0.420140	-0.555671
C	5.737308	1.609764	0.197412
C	4.527805	1.828150	0.742578

O	7.184782	0.310711	-1.033982
C	7.610908	-0.811096	-1.807951
H	-0.355983	-2.036484	3.231133
H	-0.874504	-0.390965	2.967300
H	-2.084986	-1.828266	1.411872
H	-0.620468	-2.565229	0.845162
H	1.541929	-0.361509	3.144836
H	1.709637	-1.675277	2.015683
H	-2.991332	0.865326	1.018149
H	-5.401749	1.241144	1.306999
H	-6.180006	-1.176736	-2.113560
H	-3.795048	-1.604920	-2.350298
H	-9.189717	0.175724	-0.571153
H	-8.138597	0.155401	-1.986477
H	-8.245689	-1.268173	-0.937454
H	2.946850	-1.028127	-0.321001
H	5.133754	-1.424571	-1.297844
H	6.544831	2.307774	0.306962
H	4.339296	2.720756	1.309853
H	7.022498	-0.883248	-2.711520
H	8.639624	-0.611168	-2.050848
H	7.535787	-1.716234	-1.222635
C	0.241273	1.393934	-0.932099
H	-0.745100	1.777340	-1.157232
H	0.850558	2.235103	-0.628156
H	0.662131	1.005382	-1.856019

3-CI S_1/S_0 (6,5):

S_0 = -1068.10960675

S_1 = -1068.10960332

C	-0.451846	-1.390474	-0.185942
C	-1.455487	-0.670733	-1.108962
C	-1.328332	0.805085	-0.817935
C	0.003657	1.328183	-1.165815
C	1.115781	0.636989	-0.556482
C	0.985856	-0.853763	-0.301080
N	-1.712295	1.210240	0.476508
H	-1.588141	2.192192	0.609228
C	-2.952217	0.761221	1.047010
C	-2.949959	0.215340	2.326550
C	-4.122717	-0.189468	2.923761
C	-5.335212	-0.064622	2.247114
C	-5.348920	0.477923	0.969567
C	-4.159877	0.893038	0.385303
O	-6.420066	-0.492772	2.907618
C	-7.691420	-0.388400	2.321889
N	2.252756	1.232635	-0.383191
H	2.286479	2.209625	-0.612241
C	3.498999	0.644962	0.069715
C	4.356603	0.071508	-0.842221
C	5.565766	-0.455390	-0.414854
C	5.906991	-0.395700	0.931961
C	5.027120	0.198313	1.843794
C	3.831185	0.720393	1.416607
O	7.035973	-0.868255	1.449205
C	8.008000	-1.476619	0.629014
H	-0.427861	-2.450096	-0.411815
H	-0.789380	-1.291949	0.836096
H	-2.454202	-1.038552	-0.919125
H	-1.225327	-0.859019	-2.152833

H	1.571854	-1.135394	0.563020
H	1.473165	-1.308807	-1.160894
H	-2.018436	0.119881	2.854647
H	-4.128061	-0.606809	3.912963
H	-6.265177	0.592497	0.424786
H	-4.184650	1.325331	-0.599730
H	-8.386638	-0.785102	3.044903
H	-7.944094	0.644899	2.112096
H	-7.753406	-0.971120	1.409512
H	4.099905	0.030900	-1.885581
H	6.222743	-0.899698	-1.135208
H	5.310776	0.237941	2.877796
H	3.160656	1.180114	2.119988
H	8.379269	-0.781091	-0.113838
H	8.811900	-1.761065	1.287760
H	7.609369	-2.359686	0.144381
C	0.181845	2.427405	-2.171879
H	-0.002733	3.407775	-1.731866
H	1.169719	2.442551	-2.620557
H	-0.546744	2.307924	-2.966711

3-TS MP2-MeOH:

S_0 = -1068.24764811

Freq = *i*42.8402 cm^{-1}

C	-0.485488	-1.141712	2.229964
C	-1.323939	-1.038664	0.960144
C	-1.118375	0.297174	0.322248
C	0.159620	0.979893	0.396099
C	1.157936	0.384579	1.114722
C	0.977010	-0.884716	1.900068
N	-2.092998	0.869706	-0.345319
H	-1.918131	1.803488	-0.722844
N	2.457921	0.986453	1.114174
H	2.692756	1.300994	2.059295
H	-0.614869	-2.134390	2.671163
H	-0.836461	-0.406767	2.962901
H	-2.387572	-1.195854	1.159150
H	-1.009024	-1.814322	0.247911
H	1.579842	-0.811848	2.813316
H	1.395344	-1.722605	1.323684
C	0.347144	2.278049	-0.338485
H	-0.316012	3.056213	0.056091
H	1.376131	2.609857	-0.208635
H	0.150202	2.162441	-1.410005
C	3.482372	0.125850	0.615637
C	3.307900	-0.510802	-0.624436
C	4.694143	-0.026586	1.293505
C	4.317155	-1.309688	-1.147764
H	2.378180	-0.383547	-1.175509
C	5.723575	-0.809100	0.758756
H	4.842930	0.462463	2.254894
C	5.534572	-1.458008	-0.466326
H	4.189689	-1.812714	-2.102975
H	6.650981	-0.902524	1.313462
C	-3.395251	0.330994	-0.604456
C	-4.509129	1.087639	-0.244596
C	-3.533210	-0.887700	-1.279073
C	-5.789719	0.606112	-0.518035
H	-4.384182	2.037107	0.270214
C	-4.807761	-1.365558	-1.549644

H	-2.658740	-1.444035	-1.604794
C	-5.940743	-0.624875	-1.173324
H	-6.646813	1.200436	-0.223407
H	-4.949963	-2.306516	-2.073074
O	6.461149	-2.258908	-1.084708
O	-7.135691	-1.191859	-1.493864
C	-8.321240	-0.466335	-1.136054
H	-9.148396	-1.085132	-1.478584
H	-8.384013	-0.329682	-0.052880
H	-8.351704	0.504718	-1.637979
C	7.710159	-2.433000	-0.408924
H	7.568047	-2.902525	0.569415
H	8.296816	-3.089996	-1.049362
H	8.229913	-1.477728	-0.286231

3-*E* isomer MP2-MeOH:

S_0 = -1068.27254679

C	-3.295090	-0.629501	1.829206
C	-3.499235	0.873406	1.729336
C	-2.231854	1.547059	1.285379
C	-1.224004	0.857493	0.592540
C	-1.529450	-0.419995	0.096568
C	-2.774367	-1.156797	0.502103
N	-2.087438	2.845557	1.576186
H	-1.236597	3.312657	1.272086
C	-3.040322	3.659896	2.265826
C	-2.708433	4.183567	3.521308
C	-3.612553	5.006628	4.180303
C	-4.849270	5.316525	3.591318
C	-5.174482	4.798252	2.330669
C	-4.257792	3.980361	1.665500
O	-5.658413	6.128827	4.332341
C	-6.931927	6.467609	3.768120
N	-0.704142	-1.027655	-0.764328
H	0.137120	-0.533180	-1.051327
C	-0.905030	-2.318600	-1.347256
C	-1.934857	-2.524003	-2.265190
C	-2.111058	-3.779043	-2.853021
C	-1.228584	-4.820130	-2.535256
C	-0.181000	-4.599911	-1.626147
C	-0.015918	-3.354141	-1.034595
O	-1.296339	-6.083214	-3.048760
C	-2.353483	-6.350892	-3.979215
H	-4.239771	-1.119850	2.082403
H	-2.579167	-0.855879	2.626555
H	-3.811152	1.299156	2.688325
H	-4.300563	1.095970	1.011730
H	-2.552247	-2.227263	0.556622
H	-3.539820	-1.034376	-0.276171
H	-1.754452	3.932983	3.978746
H	-3.381728	5.422286	5.157191
H	-6.116198	5.032273	1.847119
H	-4.491045	3.601214	0.673677
H	-7.412986	7.104782	4.508133
H	-6.812363	7.016361	2.829500
H	-7.537764	5.572354	3.600658
H	-2.596679	-1.703804	-2.531902
H	-2.919818	-3.917667	-3.561617
H	0.492004	-5.421561	-1.397412
H	0.787542	-3.182881	-0.322384

H	-2.263571	-5.719976	-4.868199
H	-2.233332	-7.396683	-4.256548
H	-3.332485	-6.201267	-3.514748
C	0.084575	1.526657	0.258307
H	0.387893	2.215746	1.051619
H	0.895095	0.795171	0.193535
H	0.048555	2.083481	-0.684832

3-*Z*-isomer MP2-MeOH:

S_0 = -1068.26639260

C	-0.077213	-0.917354	1.467639
C	-1.282702	-0.672484	0.571581
C	-1.341901	0.778714	0.191536
C	-0.185994	1.583703	0.114314
C	1.051753	0.938903	0.225556
C	1.175146	-0.473533	0.735670
N	-2.538876	1.316363	-0.060220
H	-2.574871	2.306444	-0.295865
C	-3.793867	0.631892	-0.049987
C	-4.788819	1.053894	0.840424
C	-6.026147	0.423679	0.831459
C	-6.281713	-0.625224	-0.067048
C	-5.286889	-1.037565	-0.963740
C	-4.047555	-0.393145	-0.961251
O	-7.528874	-1.172627	0.018668
C	-7.830382	-2.248190	-0.880049
N	2.223933	1.504970	-0.108682
H	3.058525	0.998058	0.182059
C	2.449934	2.577556	-1.018747
C	3.396545	3.553050	-0.706579
C	3.678582	4.576588	-1.614608
C	3.007481	4.613534	-2.844295
C	2.065287	3.620419	-3.157711
C	1.797628	2.596132	-2.259446
O	3.192636	5.564875	-3.806894
C	4.149804	6.594005	-3.526204
H	-0.010212	-1.978580	1.724564
H	-0.188530	-0.355174	2.401005
H	-2.215222	-0.951313	1.070874
H	-1.208850	-1.292204	-0.332313
H	2.058699	-0.537817	1.382694
H	1.365927	-1.132865	-0.122912
H	-4.584165	1.858023	1.543086
H	-6.813595	0.728017	1.515261
H	-5.462230	-1.833999	-1.678088
H	-3.284459	-0.685734	-1.677910
H	-8.852907	-2.539045	-0.645939
H	-7.768714	-1.918843	-1.921219
H	-7.158028	-3.095562	-0.717481
H	3.903286	3.527098	0.255448
H	4.415695	5.325658	-1.348094
H	1.571141	3.657764	-4.124761
H	1.089769	1.811414	-2.515408
H	5.148800	6.172620	-3.380852
H	4.145888	7.237016	-4.404642
H	3.858577	7.171399	-2.643890
C	-0.328392	3.073397	-0.069088
H	-1.127745	3.446091	0.581488
H	0.584035	3.588353	0.231114
H	-0.553455	3.368023	-1.100156

A-FC-Min S_0:

S_0 = -459.45255680

S_1 = -459.27059318

C	0.000068	2.066073	0.499135
C	1.247987	1.436588	-0.098666
C	1.208916	-0.071141	-0.005659
C	0.000006	-0.770419	0.139247
C	-1.208850	-0.071036	-0.005642
C	-1.247806	1.436673	-0.098845
N	2.360702	-0.708180	-0.100081
N	-2.360643	-0.708074	-0.099966
C	-0.000243	-2.275713	0.324018
C	3.689679	-0.114899	-0.243670
C	-3.689580	-0.114818	-0.244039
H	0.000121	3.132844	0.313187
H	-0.000013	1.926196	1.574841
H	2.129164	1.810246	0.405668
H	1.347258	1.707613	-1.147769
H	-2.129053	1.810478	0.405258
H	-1.346817	1.707588	-1.147999
H	-2.336819	-1.703328	-0.096535
H	0.855576	-2.605749	0.901711
H	-0.855681	-2.605202	0.902612
H	-0.000878	-2.824876	-0.615060
H	4.386609	-0.916015	-0.435273
H	3.718488	0.572897	-1.076289
H	3.988104	0.394480	0.662535
H	-4.386468	-0.915973	-0.435627
H	-3.988222	0.394767	0.661979
H	-3.718184	0.572789	-1.076821
H	2.336898	-1.703430	-0.096592

A-CI S_1/S_0:

S_0 = -459.31917383

S_1 = -459.31917134

C	0.191395	1.805495	-0.716309
C	1.479286	0.931073	-0.819324
C	1.351771	-0.313335	0.031069
C	0.106825	-1.045527	-0.272362
C	-1.091946	-0.269549	-0.064798
C	-0.903527	1.205434	0.194917
N	1.566121	-0.183021	1.425511
N	-2.260897	-0.815511	-0.134447
C	0.098986	-2.438192	-0.829850
C	2.694399	0.617163	1.888771
C	-3.575847	-0.158297	0.005719
H	0.429228	2.786834	-0.326672
H	-0.222861	1.961590	-1.705856
H	2.352287	1.506233	-0.546311
H	1.622753	0.625536	-1.849192
H	-0.607944	1.289955	1.233599
H	-1.829067	1.748624	0.065535
H	-2.286334	-1.804280	-0.300555
H	-0.029057	-3.183203	-0.043814
H	-0.679079	-2.600183	-1.571507
H	1.050062	-2.642845	-1.303166
H	2.797663	0.464355	2.954302
H	3.635878	0.357761	1.410893

H	2.505618	1.671112	1.731388
H	-4.327970	-0.930279	0.007878
H	-3.610290	0.384898	0.936041
H	-3.737328	0.504991	-0.829874
H	1.602793	-1.087546	1.848562

A-MIN S_1:

S_0 = -459.38297013

S_1 = -459.29521969

C	-0.419956	-0.912681	2.509802
C	-1.190387	-1.117667	1.206601
C	-0.961529	0.005408	0.222975
C	0.216892	0.752654	0.249121
C	1.181236	0.453961	1.213298
C	1.061852	-0.639362	2.253014
N	-1.875165	0.170600	-0.795903
H	-1.796636	1.011964	-1.316873
N	2.412617	1.145917	1.221520
H	2.504487	1.966851	1.801517
H	-0.519082	-1.787459	3.141429
H	-0.844533	-0.074194	3.052343
H	-2.243785	-1.196230	1.441336
H	-0.908568	-2.063160	0.745229
H	1.555807	-0.345339	3.175031
H	1.560908	-1.539887	1.899186
C	0.442401	1.846019	-0.777263
H	-0.332520	2.602599	-0.717136
H	1.386597	2.360513	-0.646697
H	0.435827	1.439151	-1.782611
C	-3.225245	-0.358689	-0.758547
H	-3.709533	-0.095632	-1.688408
H	-3.215397	-1.438222	-0.692205
H	-3.821365	0.037827	0.059902
C	3.624088	0.674800	0.573809
H	4.263495	1.516835	0.355236
H	4.130344	0.008931	1.267629
H	3.354983	0.132544	-0.318289