Supporting Information

Photoisomerization Mechanism of Iminoguanidinium Receptors from Spectroscopic Methods and Quantum Chemical Calculations

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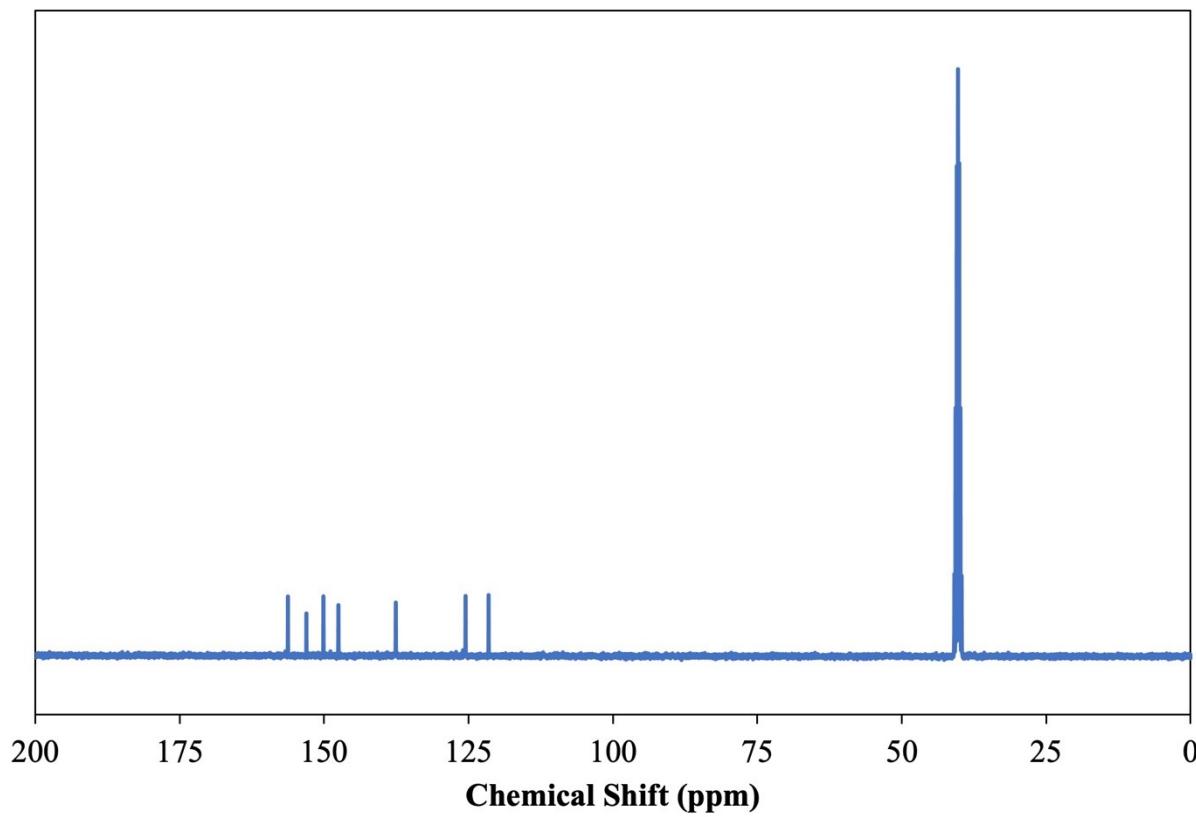
Figure S1. ^{13}C NMR (100 MHz) of 2PyMIG·HBr in DMSO-d_6.

Table S1. Crystallographic information for 2PyMIG·HBr.

	2PyMIG·HBr
Formula	$C_7H_{10}N_5Br$
FW	244.11
Crystal Class	Orthorhombic
Space Group	Pna2$_1$
a (Å)	11.057
b (Å)	10.978
c (Å)	7.917
α (deg)	90
β (deg)	90
γ (deg)	90
Z	4
Cell volume (Å^3)	961.0
Density (mg m^{-3})	1.687
μ (mm^{-1})	4.239
Temp (K)	100
Total Reflns	34281

R_{int}	0.0193
$R_1{}^a$	0.0183
$wR_2{}^a$	0.0427
GOF	1.077

$$^aR1 = \sum \frac{||F_O| - |F_C||}{|F_O|} ; wR2 = \left(\frac{\sum [w(F_O^2 - F_C^2)^2]}{\sum [w(F_O^2)^2]} \right)^{1/2}$$
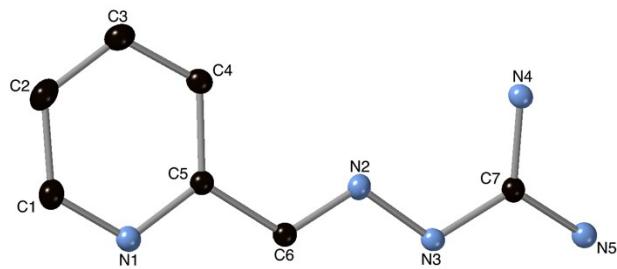

Figure S2. Thermal ellipsoid plot (50% probability level) of 2PyMIG·HBr. Hydrogen atoms have been omitted.
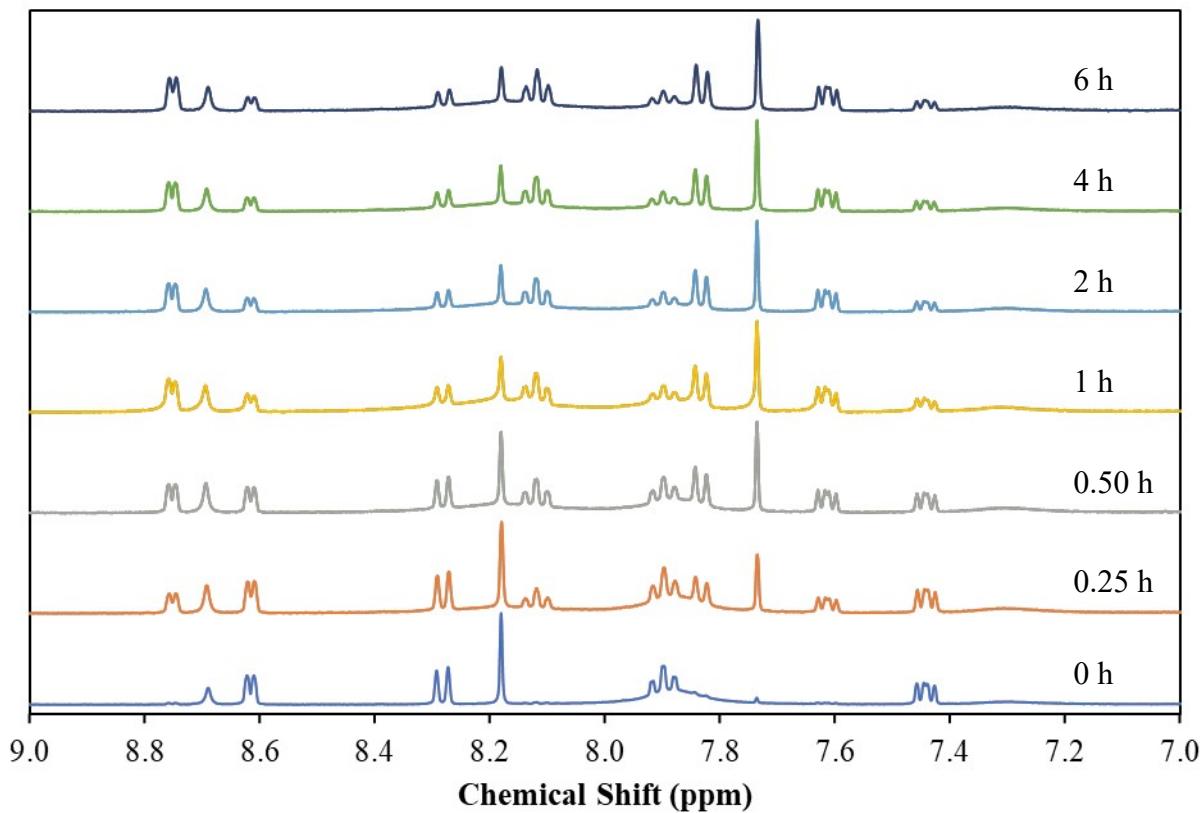
Figure S3. ^{1}H NMR (400 MHz) of 9.81 mM 2PyMIG·HBr in DMSO-d_6 during 6 h UV photoirradiation.
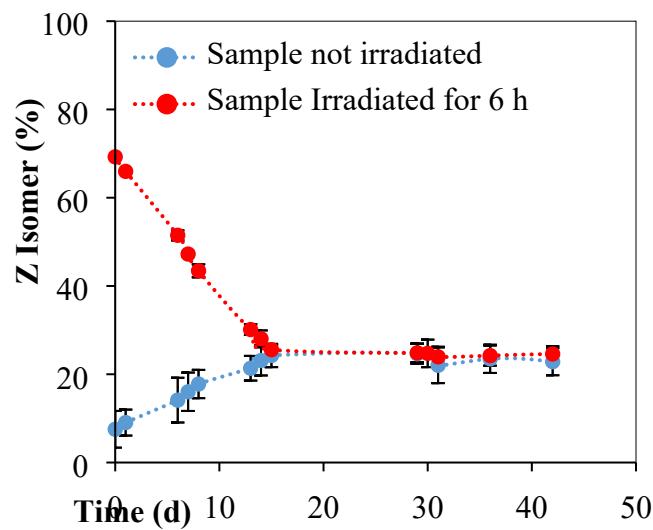
Figure S4. Thermal relaxation of 9.81 mM Z 2PyMIG·HCl in DMSO-d_6 after UV irradiation (red) and the untreated E isomer at (blue) converging at a thermal equilibrium. Dotted lines are for visual aid.

4
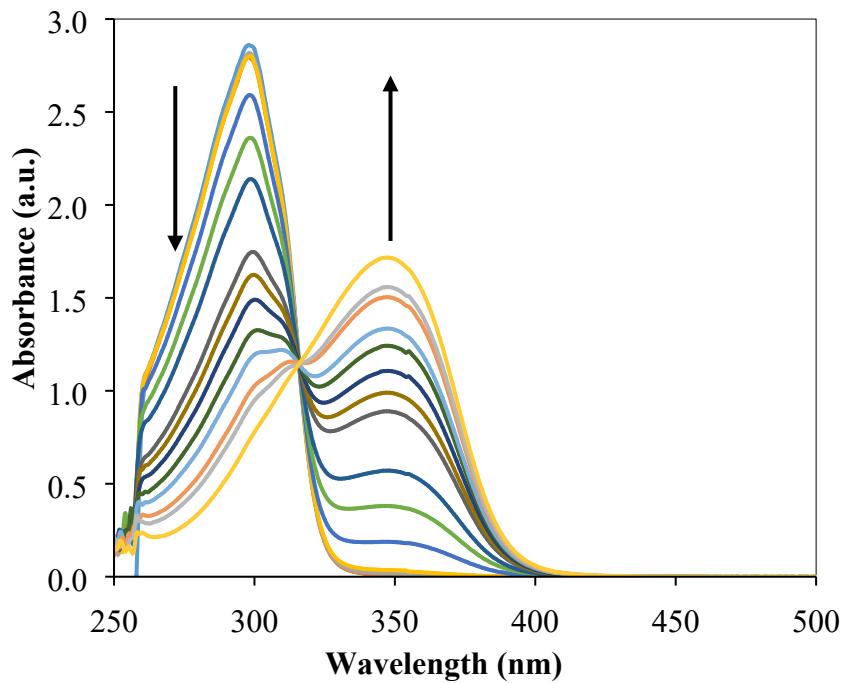
Figure S5. Titration of 2PyMIG·HBr with tetramethylammonium fluoride in DMSO. The protonated form decreases (303 nm) while the deprotonated form (352 nm) increases with the addition of the fluoride anion.
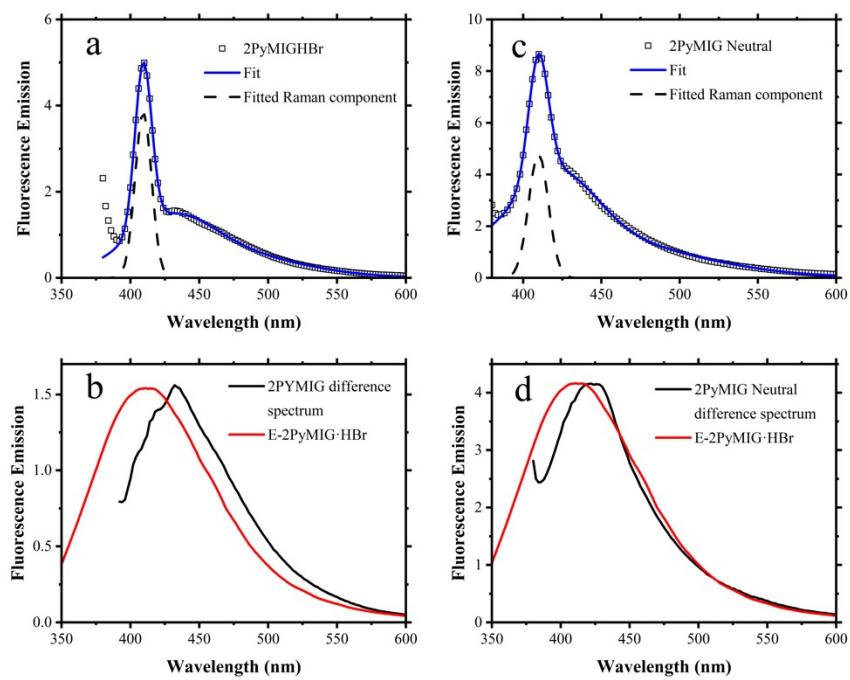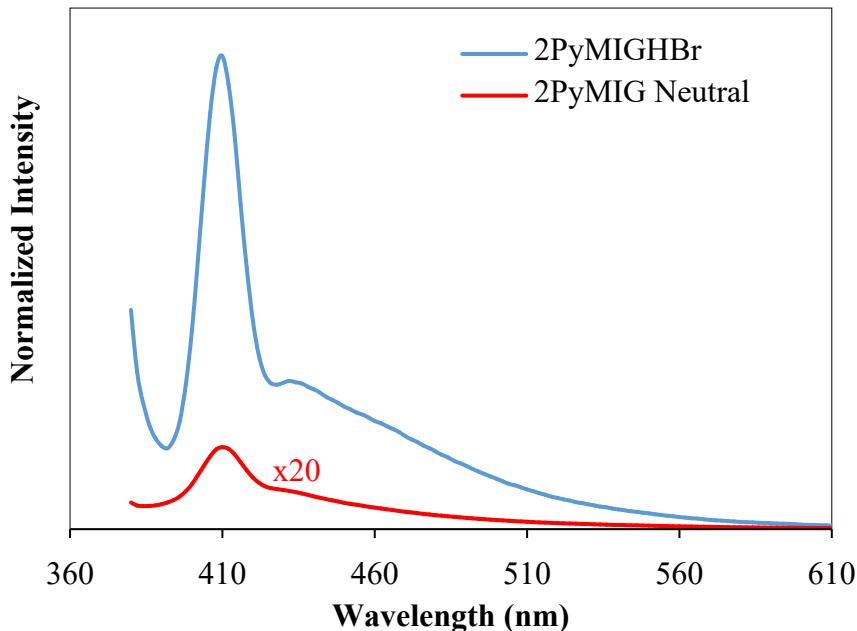
Figure S6. (Top) Emission spectra of 2PyMIG·HBr and 2PyMIG (λ_{exc} = 365 nm) normalized to the absorption of each species (cation = 0.011792; neutral = 0.102527). The neutral 2PyMIG emission data has been increased by a factor of 20 for easier viewing. The emission at 410 nm are

Raman bands from the DMSO solvent. (Bottom) To compare these spectra with the one shown in Figure 8, we fitted these spectra using three Gaussians and the resulting overall fit and the Raman component for each spectrum are shown by blue solid line and dash line, respectively, in the panel a and c. Upon subtracting the Raman component from the corresponding measured emission spectrum, the difference spectrum appears resemble the emission spectrum of *E*-2PyMIG·HBr (Figure 8) reasonably well, especially for the neutral form, which can be readily seen from the panel b and d. To ease comparison, the *E*-2PyMIG·HBr spectrum (red lines) was scaled.
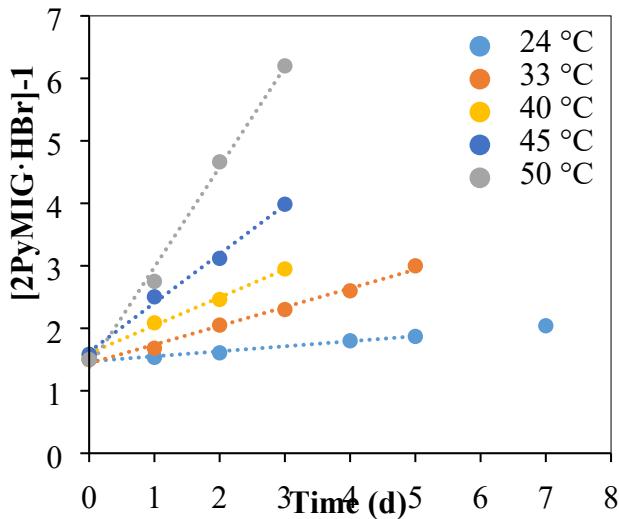
Figure S7. Second order thermal relaxation of 10 mM 2PyMIG·HBr $Z \rightarrow E$ in DMSO-d_6 at 24 (blue), 33 (orange), 40 (yellow), 45 (light blue), and 50 °C (gray).
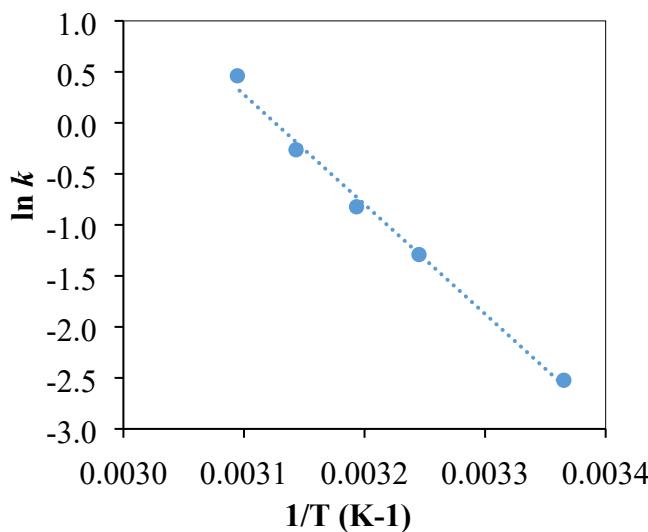
Figure S8. Arrhenius plot of the thermal isomerization of 2PyMIG·HBr Z → E in DMSO-d_6.
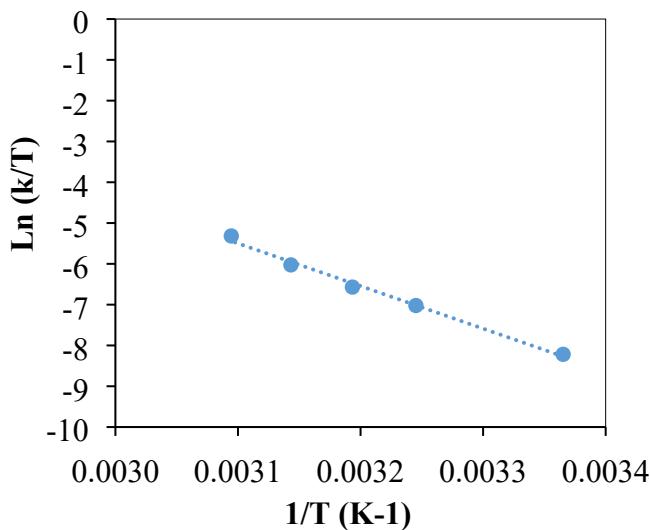
Figure S9. Eyring plot of the thermal isomerization of 2PyMIG·HBr Z → E in DMSO-d_6.
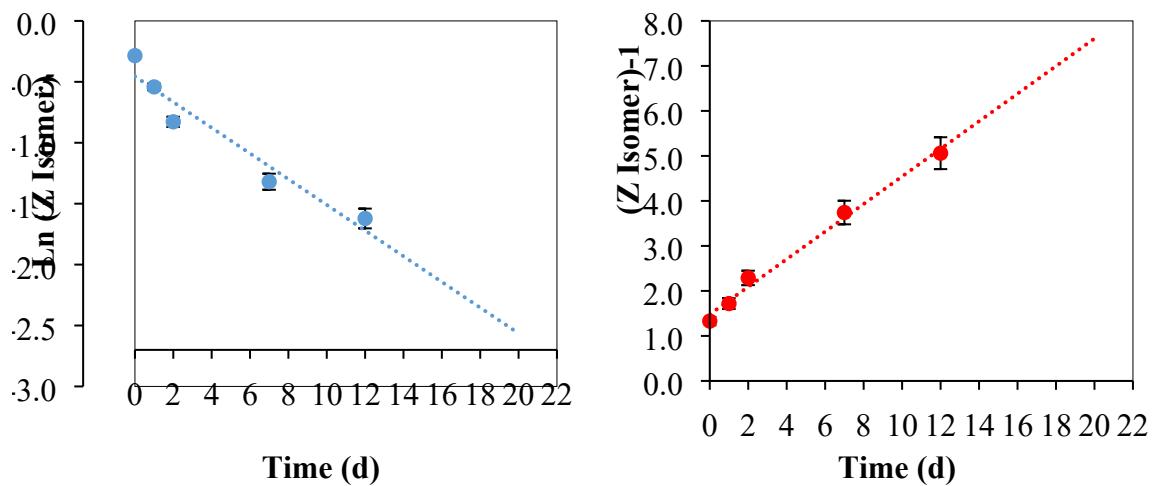
Figure S10. First (left) and second (right) order relaxation of *Z*-2PyMIG·HBr after photoirradiation at 24 °C
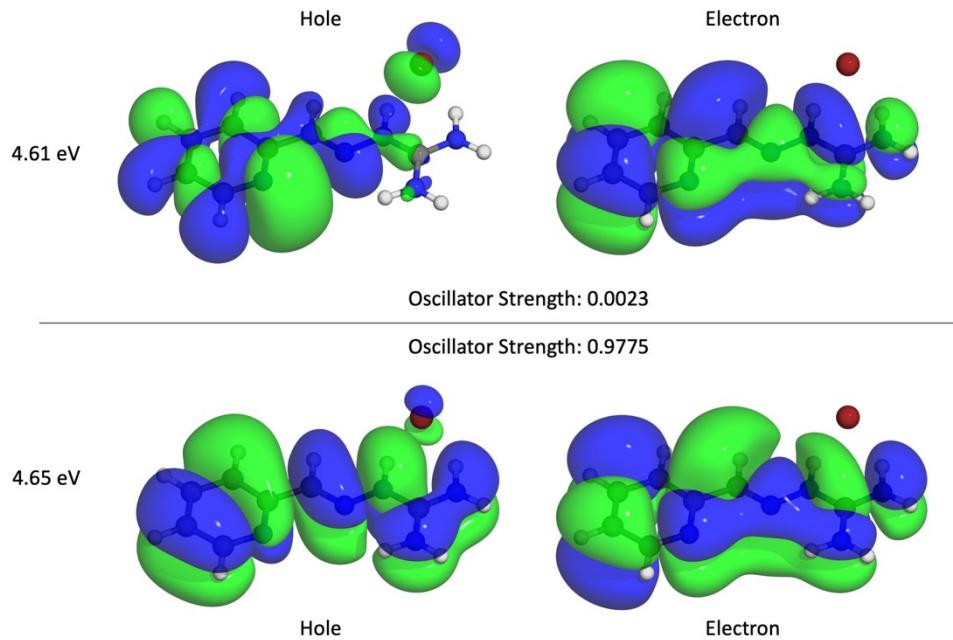
Figure S11. Natural transition orbitals (NTOs) (isovalue=0.02 a.u.) of the E_1 geometry for the first two excited states computed at the TD-ωB97XD/def2-TZVPP (PCM=DMSO) level of theory.
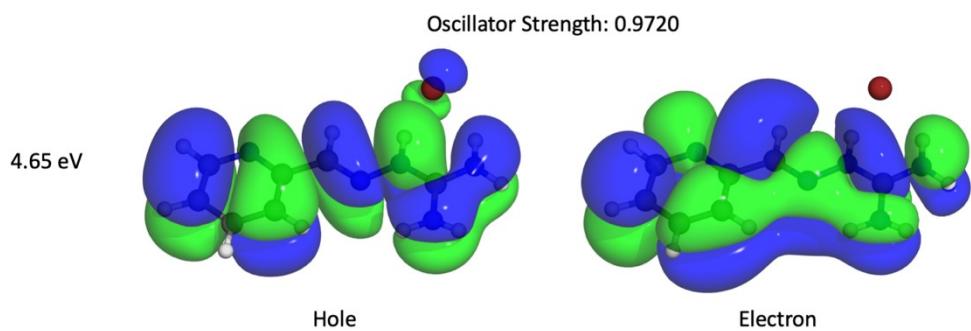
Figure S12. Natural Transition orbitals (NTOs) (isovalue=0.02 a.u.) of the E_2 geometry for the first excited state computed at the TD-ωB97XD/def2-TZVPP (PCM=DMSO) level of theory.

Excited states from time dependent density functional theory

To select the active space, initial TD-DFT calculations were run at TD-ωB97XD/def2-TZVPP (PCM=DMSO) level of theory for the E_1 and E_2 geometries. In E_1, the two lowest singlet excited states were found to be close together in energy, at 4.61 and 4.65 eV (Figure S11). However, the lower state has an oscillator strength of 0.0023, while the higher state has one of 0.9775. This indicates the latter state is initially populated in this photoisomerization, though the darker state can also be populated by internal conversion. Furthermore, the NTOs indicate that this state at 4.65 eV is also a π-π^* state and is likely to be well-described by the choice of active space shown in Figure 3. Since the active space selected for CASSCF is chosen to describe the π-π^* state, it becomes the S_1 state for CASSCF. In E_2, the lowest energy excited state is at 4.65 eV and is π-π^* state as indicated by the NOs (Figure S12). This state has a similarly large oscillator strength at 0.9720. Thus, the S_1 state for both E_1 and E_2 can be characterized as π-π^* states and indicate the active space for CASSCF was chosen appropriately.

Excited states from Equation-of-Motion Coupled-Cluster Calculations with Single and Double excitations

TD-DFT calculations show that the n-π^* and a π-π^* states are nearly degenerate, with the n-π^* state being 0.04 eV lower in energy. This prompts questions about the role of the n-π^* state in the photochemical behavior of 2PyMIG·HBr on the S_1 surface. We analyzed the state ordering for these systems using EOM-CCSD calculations, with solvent effects included using the PCM model beyond the linear response using the PTED formalism. The results shown in Table S1 show that the π-π^* transitions are lower in energy and have a much larger oscillation strength compared to the n-π^* transitions for both the Franck-Condon geometries and the S_1 minima. Therefore, the lowest S_1 excited state near the Franck-Condon geometries has π-π^* character, justifying the choice of the active space for CASSCF that includes only the π orbitals.

Table S1. Excitation energies (ΔE, eV) and oscillator strengths for the lowest energy π-π^* and n-π^* transitions of 2PyMIG·HBr in DMSO computed with the EOM-CCSD-PCM method using the PTED scheme.

system[a]	ΔE π-π^*	π-π^* oscillator strength	ΔE n-π^*	n-π^* oscillator strength
E_1, Franck-Condon	4.81	0.478	4.87	0.0026
E_2, Franck-Condon	5.00	0.394	5.15	0.0037
E_1, minimum	4.46	0.320	4.71	0.0014
E_2, minimum	4.58	0.249	4.97	0.0021
Z_1, minimum	4.97	0.464	5.11	0.0020
Z_2, minimum	4.83	0.454	5.17	0.0018

XYZ coordinates and CASSCF S_0 and S_1 energies for 2PyMIGHBr and 2PyMIGH$^+$

For the geometries below, the CCNN and CNNC dihedral angles are listed with each XYZ coordinate as well as the CASSCF S_0 and S_1 energies.

2PyMIG·HBr E_1 geometries:

Geometries from E_1 to MECI$_1$ on the S$_1$ surface.
23
CCNN: 180.23 CNNC: 183.45 E(S0): -3115.40216 E(S1): -3115.22237
```
C      1.925479     1.404628     -2.066415
H      1.158082     1.248694     -0.194130
H      3.209070     1.873619     -0.594029
H      0.829637     1.008091     -3.700228
H      2.470055     1.376439     -4.012454
H      3.762866     2.223110     -2.182125
N     -0.235167     0.679039     -1.700404
H     -0.909658     0.591622      0.246084
N      0.973682     1.085369     -1.218216
N      3.110608     1.760211     -1.591611
N      1.703222     1.366519     -3.380058
C     -1.135835     0.451365     -0.798645
C     -2.489615     0.001870     -1.154891
C     -3.420915    -0.210584     -0.137528
N     -2.777565    -0.186327     -2.448081
C     -4.691670    -0.631033     -0.472230
C     -3.998943    -0.589318     -2.757247
C     -4.997278    -0.827470     -1.809170
H     -3.146612    -0.047048      0.888633
H     -4.199502    -0.731042     -3.804088
H     -5.971614    -1.153668     -2.120164
H     -5.427521    -0.801674      0.291671
Br     2.092310     1.813759      1.682018
```
23
CCNN: 180.27 CNNC: 183.16 E(S0): -3115.40141 E(S1): -3115.23195
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C      1.936511     1.410727     -2.069930
H      1.161655     1.254865     -0.208285
H      3.216041     1.876536     -0.590762
H      0.845883     1.016237     -3.706721
H      2.488319     1.380061     -4.013657
H      3.777466     2.225358     -2.176300
N     -0.236323     0.683892     -1.711843
H     -0.903736     0.598148      0.237179
N      0.981240     1.094841     -1.223701
N      3.121309     1.764119     -1.589011
N      1.719200     1.372759     -3.384241
C     -1.132419     0.456492     -0.807112
C     -2.475110     0.008324     -1.155967
C     -3.416931    -0.208071     -0.120376
N     -2.770077    -0.183215     -2.461547
C     -4.708311    -0.636820     -0.451724
C     -4.012632    -0.594183     -2.767369
C     -5.015188    -0.834603     -1.806180
```

H	-3.137846	-0.043365	0.903670
H	-4.218334	-0.736916	-3.812220
H	-5.989071	-1.161797	-2.115946
H	-5.441686	-0.808235	0.313384
Br	2.090076	1.811816	1.682169

23
CCNN: 180.17 CNNC: 183.05 E(S0): -3115.39857 E(S1): -3115.23445

C	1.935716	1.410760	-2.068226
H	1.140332	1.248869	-0.219130
H	3.207169	1.877138	-0.582015
H	0.850757	1.013619	-3.707117
H	2.494772	1.376565	-4.010447
H	3.777117	2.226037	-2.165304
N	-0.249586	0.678116	-1.733109
H	-0.913990	0.593384	0.218915
N	0.975881	1.095182	-1.225438
N	3.118439	1.763959	-1.581347
N	1.723496	1.371068	-3.383692
C	-1.143812	0.451576	-0.825000
C	-2.472754	0.007886	-1.170973
C	-3.426403	-0.213003	-0.118973
N	-2.772193	-0.184009	-2.490467
C	-4.737773	-0.647589	-0.443979
C	-4.035809	-0.600986	-2.785070
C	-5.041158	-0.843632	-1.814304
H	-3.139264	-0.047272	0.901882
H	-4.245938	-0.743576	-3.827894
H	-6.013854	-1.170753	-2.126894
H	-5.468053	-0.819406	0.322052
Br	2.100388	1.815963	1.687527

23
CCNN: 180.07 CNNC: 182.91 E(S0): -3115.39521 E(S1): -3115.23506

C	1.929552	1.408877	-2.069270
H	1.118501	1.243032	-0.228165
H	3.194980	1.875100	-0.578210
H	0.848834	1.009573	-3.709773
H	2.494430	1.370001	-4.009988
H	3.771144	2.223794	-2.159973
N	-0.263222	0.672669	-1.752016
H	-0.926202	0.588941	0.202276
N	0.965740	1.094512	-1.229458
N	3.110741	1.761000	-1.578380
N	1.721271	1.367281	-3.385538
C	-1.156782	0.446824	-0.841269
C	-2.477406	0.005564	-1.186149
C	-3.437117	-0.218966	-0.125050

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N      -2.779185     -0.185380     -2.513622
C      -4.759131     -0.656852     -0.444813
C      -4.054172     -0.605858     -2.798735
C      -5.059655     -0.850680     -1.823151
H      -3.143750     -0.052720      0.893490
H      -4.267024     -0.747818     -3.840382
H      -6.031384     -1.178009     -2.138154
H      -5.486913     -0.829508      0.322105
Br      2.111744      1.820624      1.694695
23
CCNN:  180.02 CNNC:  181.45 E(S0): -3115.39525 E(S1): -3115.23510
C       2.050402      0.990865     -1.988344
H       1.206413      0.869075     -0.158171
H       3.338992      1.303890     -0.477659
H       0.958735      0.709911     -3.644930
H       2.635290      0.900066     -3.918838
H       3.956294      1.641143     -2.046278
N      -0.199061      0.436398     -1.709434
H      -0.895033      0.376278      0.234633
N       1.049016      0.765307     -1.164136
N       3.254633      1.220362     -1.481082
N       1.855702      0.986546     -3.308205
C      -1.119808      0.264179     -0.813723
C      -2.462019     -0.078417     -1.186922
C      -3.451402     -0.261011     -0.145356
N      -2.753154     -0.218510     -2.523293
C      -4.794405     -0.600821     -0.493780
C      -4.049547     -0.544431     -2.835054
C      -5.084476     -0.742108     -1.880217
H      -3.160181     -0.137505      0.879847
H      -4.254065     -0.647510     -3.882930
H      -6.070174     -0.995135     -2.219428
H      -5.543685     -0.741028      0.258859
Br      2.253020      1.288035      1.783993
23
CCNN:  179.97 CNNC:  181.60 E(S0): -3115.39525 E(S1): -3115.23510
C       2.192440      0.534755     -1.930490
H       1.321826      0.451552     -0.110787
H       3.485891      0.714406     -0.402833
H       1.098147      0.380522     -3.602097
H       2.787653      0.436533     -3.857579
H       4.144585      1.029811     -1.958221
N      -0.098505      0.167191     -1.682565
H      -0.816343      0.123431      0.253965
N       1.167764      0.374887     -1.119721
N       3.406589      0.653151     -1.408284
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N	2.011627	0.573293	-3.251635
C	-1.039516	0.054938	-0.798480
C	-2.402633	-0.160995	-1.190263
C	-3.413997	-0.283336	-0.161065
N	-2.692011	-0.241588	-2.531915
C	-4.778078	-0.495776	-0.528044
C	-4.008911	-0.444487	-2.861564
C	-5.066200	-0.575235	-1.919803
H	-3.122912	-0.211945	0.869117
H	-4.211692	-0.502069	-3.913258
H	-6.066982	-0.732004	-2.272714
H	-5.543813	-0.589524	0.215195
Br	2.375375	0.765046	1.847089

23
CCNN: 179.80 CNNC: 182.05 E(S0): -3115.39521 E(S1): -3115.23506

C	2.345354	0.069060	-1.916657
H	1.458082	0.033903	-0.103920
H	3.637450	0.120974	-0.379774
H	1.252267	0.052644	-3.596865
H	2.943482	-0.024062	-3.843949
H	4.329363	0.408477	-1.923555
N	0.029372	-0.095806	-1.687765
H	-0.701529	-0.134783	0.243950
N	1.306224	-0.028050	-1.114212
N	3.562521	0.072935	-1.386347
N	2.176693	0.152509	-3.236678
C	-0.923557	-0.146849	-0.810890
C	-2.298758	-0.215596	-1.213928
C	-3.323344	-0.280851	-0.192650
N	-2.586523	-0.213749	-2.558341
C	-4.699469	-0.342862	-0.570741
C	-3.915080	-0.270341	-2.898635
C	-4.985757	-0.334415	-1.965129
H	-3.032826	-0.281075	0.840163
H	-4.116298	-0.262836	-3.952176
H	-5.995053	-0.375452	-2.326132
H	-5.475107	-0.392060	0.166488
Br	2.516355	0.284030	1.860413

23
CCNN: 179.32 CNNC: 181.63 E(S0): -3115.39493 E(S1): -3115.23475

C	2.490762	-0.441161	-1.929262
H	1.598256	-0.384358	-0.121585
H	3.775871	-0.485116	-0.390082
H	1.405818	-0.319767	-3.612373
H	3.088771	-0.531542	-3.858879
H	4.492177	-0.255357	-1.926858

N	0.170345	-0.377219	-1.708243
H	-0.574558	-0.455568	0.216803
N	1.444261	-0.471755	-1.129614
N	3.703332	-0.548593	-1.396222
N	2.333191	-0.327363	-3.246584
C	-0.788937	-0.382935	-0.837160
C	-2.160818	-0.279200	-1.244785
C	-3.195122	-0.312354	-0.231851
N	-2.435452	-0.145197	-2.585266
C	-4.566344	-0.190734	-0.613310
C	-3.758709	-0.020817	-2.928177
C	-4.837684	-0.035869	-2.002148
H	-2.915408	-0.426738	0.797606
H	-3.948508	0.095538	-3.977432
H	-5.841817	0.069491	-2.364500
H	-5.349023	-0.212423	0.117777
Br	2.675159	-0.089306	1.828686

23
CCNN: 177.98 CNNC: 174.50 E(S0): -3115.39326 E(S1): -3115.23301

C	2.539910	-1.011998	-1.875517
H	1.665541	-0.720794	-0.086429
H	3.816437	-1.080742	-0.336457
H	1.476545	-0.813307	-3.566922
H	3.128974	-1.218388	-3.800995
H	4.545626	-1.001727	-1.874167
N	0.244033	-0.666221	-1.671165
H	-0.556690	-0.914428	0.216057
N	1.494406	-0.914936	-1.076774
N	3.737667	-1.218995	-1.334958
N	2.392171	-0.941601	-3.194721
C	-0.735954	-0.699720	-0.824890
C	-2.083106	-0.426898	-1.239279
C	-3.147163	-0.507185	-0.260440
N	-2.304197	-0.084613	-2.552306
C	-4.487676	-0.194414	-0.642238
C	-3.596397	0.228947	-2.893008
C	-4.698850	0.193804	-1.995632
H	-2.912318	-0.797260	0.745472
H	-3.740365	0.518712	-3.915649
H	-5.675079	0.458639	-2.352683
H	-5.291016	-0.243791	0.064714
Br	2.812926	-0.224053	1.787813

23
CCNN: 174.88 CNNC: 159.06 E(S0): -3115.38879 E(S1): -3115.22833

| C | 2.487792 | -1.496503 | -1.738408 |
| H | 1.674224 | -0.856326 | -0.016544 |

```
H     3.760013    -1.533161    -0.198592
H     1.453525    -1.334251    -3.454357
H     3.035443    -1.981070    -3.627236
H     4.481899    -1.691277    -1.729080
N     0.247943    -0.843701    -1.593195
H    -0.656697    -1.397124     0.176005
N     1.466410    -1.192666    -0.961414
N     3.660064    -1.779335    -1.174036
N     2.339024    -1.560084    -3.057501
C    -0.775382    -0.984173    -0.812391
C    -2.089519    -0.579358    -1.228474
C    -3.205355    -0.777433    -0.327084
N    -2.229172     0.000156    -2.466751
C    -4.506578    -0.321199    -0.698930
C    -3.483876     0.448368    -2.796322
C    -4.629843     0.319978    -1.964537
H    -3.037721    -1.257401     0.617843
H    -3.560389     0.925251    -3.754020
H    -5.571920     0.704109    -2.304293
H    -5.345752    -0.449078    -0.045357
Br    2.930843    -0.174014     1.731432
23
CCNN:  160.45 CNNC:  141.85 E(S0): -3115.35092 E(S1): -3115.23507
C     2.434351    -1.546657    -1.677481
H     1.734465    -0.510510    -0.085218
H     3.831817    -1.168191    -0.291921
H     1.235038    -1.906436    -3.258726
H     2.828355    -2.516133    -3.408719
H     4.430292    -1.661877    -1.815659
N     0.206849    -0.945708    -1.397855
H    -0.882035    -1.823824     0.116214
N     1.464944    -1.066099    -0.908889
N     3.663091    -1.623694    -1.181518
N     2.166030    -1.967339    -2.909590
C    -0.965812    -1.178869    -0.739427
C    -2.196068    -0.667389    -1.164307
C    -3.388979    -0.961601    -0.441454
N    -2.208469     0.114888    -2.282850
C    -4.584177    -0.405965    -0.860629
C    -3.359748     0.636811    -2.659052
C    -4.580452     0.421618    -1.992355
H    -3.343501    -1.596142     0.424088
H    -3.328494     1.259784    -3.535311
H    -5.480024     0.880752    -2.355526
H    -5.494719    -0.602797    -0.325687
Br    2.968815    -0.075492     1.712374
```

23

CCNN: 141.76 CNNC: 133.87 E(S0): -3115.32126 E(S1): -3115.24871

C	2.403171	-1.728836	-1.558215
H	1.641474	-0.408640	-0.220248
H	3.763278	-1.068181	-0.236365
H	1.221288	-2.471623	-3.004182
H	2.831140	-3.058989	-3.019059
H	4.403734	-1.825393	-1.644539
N	0.157468	-1.177469	-1.424641
H	-1.035248	-2.254921	-0.129837
N	1.404678	-1.106662	-0.927089
N	3.620659	-1.657157	-1.052913
N	2.157167	-2.418103	-2.666816
C	-1.037668	-1.430547	-0.821334
C	-2.235696	-0.775928	-1.170428
C	-3.451159	-1.116342	-0.519273
N	-2.190426	0.159076	-2.155949
C	-4.613989	-0.451965	-0.872085
C	-3.310643	0.774283	-2.481773
C	-4.553775	0.518368	-1.876962
H	-3.452481	-1.868253	0.247593
H	-3.235604	1.505803	-3.266251
H	-5.428370	1.055068	-2.191784
H	-5.543109	-0.679689	-0.383217
Br	2.970719	0.100529	1.648783

23

CCNN: 120.55 CNNC: 136.43 E(S0): -3115.28913 E(S1): -3115.26365

C	2.415430	-1.891965	-1.475167
H	1.533788	-0.427029	-0.382643
H	3.698291	-0.985930	-0.215050
H	1.312858	-2.933658	-2.786051
H	2.952490	-3.424922	-2.677228
H	4.420907	-1.899751	-1.494028
N	0.141014	-1.504723	-1.480192
H	-1.152570	-2.604347	-0.308550
N	1.363718	-1.230668	-0.980998
N	3.609216	-1.668456	-0.966527
N	2.239286	-2.767092	-2.459738
C	-1.061033	-1.691855	-0.872628
C	-2.212297	-0.894771	-1.127862
C	-3.439562	-1.193618	-0.491163
N	-2.100348	0.109964	-2.028215
C	-4.554361	-0.417302	-0.775116
C	-3.174495	0.828984	-2.297885
C	-4.429020	0.616387	-1.703717
H	-3.493117	-2.002506	0.213064

H	-3.049595	1.608063	-3.027707
H	-5.265223	1.234310	-1.970456
H	-5.494382	-0.612561	-0.293211
Br	2.916137	0.244104	1.567343

23

CCNN: 106.95 CNNC: 142.24 E(S0): -3115.27824 E(S1): -3115.27633

C	2.469682	-1.776199	-1.438969
H	1.396199	-0.372829	-0.448177
H	3.630640	-0.636441	-0.248622
H	1.531120	-3.079058	-2.644746
H	3.209387	-3.344787	-2.468910
H	4.466947	-1.554240	-1.454374
N	0.152061	-1.699342	-1.475307
H	-1.136828	-2.755693	-0.251187
N	1.348925	-1.211006	-1.020935
N	3.627681	-1.366094	-0.954952
N	2.422889	-2.748431	-2.350966
C	-1.005051	-1.838466	-0.804366
C	-2.144087	-0.989668	-1.018978
C	-3.351169	-1.249856	-0.341497
N	-2.018779	0.023419	-1.902633
C	-4.447626	-0.428110	-0.578836
C	-3.072762	0.785790	-2.131688
C	-4.314092	0.609701	-1.499451
H	-3.411020	-2.065725	0.355237
H	-2.939560	1.573041	-2.852512
H	-5.134599	1.262068	-1.730869
H	-5.377193	-0.595014	-0.066726
Br	2.651035	0.617465	1.445824

23

CCNN: 104.92 CNNC: 150.45 E(S0): -3115.28170 E(S1): -3115.28061

C	2.527297	-1.531519	-1.372322
H	1.359366	-0.312723	-0.258931
H	3.604543	-0.299401	-0.197176
H	1.703482	-2.897278	-2.600735
H	3.397509	-2.985228	-2.465789
H	4.479686	-1.057111	-1.473403
N	0.205145	-1.698733	-1.327441
H	-1.061353	-2.720445	-0.043823
N	1.379084	-1.113657	-0.894654
N	3.661545	-1.016115	-0.909461
N	2.559656	-2.466996	-2.331611
C	-0.929682	-1.831871	-0.645383
C	-2.095413	-1.014004	-0.898485
C	-3.298794	-1.290114	-0.227884
N	-1.976383	-0.003627	-1.781779

```
C    -4.406717    -0.482722    -0.472914
C    -3.036189     0.749405    -2.014268
C    -4.278565     0.557532    -1.388546
H    -3.352397    -2.106219     0.468983
H    -2.906518     1.541377    -2.729668
H    -5.104013     1.203421    -1.621163
H    -5.337690    -0.663421     0.031715
Br    2.330860     1.083295     1.310504
23
CCNN:  101.43 CNNC:  161.67 E(S0): -3115.28236 E(S1): -3115.28185
C     2.532350    -1.096652    -1.460759
H     1.319661    -0.096688    -0.193293
H     3.521436     0.228934    -0.319498
H     1.811820    -2.513639    -2.696634
H     3.502211    -2.399979    -2.646551
H     4.347093    -0.283738    -1.723492
N     0.263060    -1.578454    -1.226832
H    -0.953522    -2.538983     0.148715
N     1.389751    -0.859473    -0.879176
N     3.635536    -0.458918    -1.049545
N     2.619166    -1.974985    -2.474977
C    -0.857702    -1.707958    -0.537681
C    -2.062944    -0.962321    -0.845956
C    -3.252156    -1.250224    -0.159014
N    -1.979662     0.008509    -1.775125
C    -4.388477    -0.492365    -0.435473
C    -3.063078     0.718455    -2.032619
C    -4.295956     0.513402    -1.392067
H    -3.275844    -2.035566     0.573988
H    -2.960586     1.486284    -2.778125
H    -5.141404     1.125122    -1.644595
H    -5.311883    -0.683273     0.079152
Br    2.035518     1.450040     1.257460
23
CCNN:   96.81 CNNC:  179.37 E(S0): -3115.28329 E(S1): -3115.28229
C     2.422735    -0.646556    -1.643739
H     1.309955     0.080950    -0.125884
H     3.389101     0.722656    -0.540754
H     1.705958    -2.039587    -2.910237
H     3.364909    -1.733554    -3.047609
H     4.038537     0.447458    -2.081186
N     0.301852    -1.458579    -1.116247
H    -0.899500    -2.291324     0.344747
N     1.365323    -0.610693    -0.889597
N     3.500667     0.093281    -1.320735
N     2.469782    -1.422965    -2.743355
```

```
C    -0.822798    -1.547636    -0.437179
C    -2.049371    -0.881541    -0.840688
C    -3.239578    -1.135517    -0.144209
N    -1.977757    -0.003108    -1.858030
C    -4.391906    -0.439311    -0.505782
C    -3.075371     0.649949    -2.194382
C    -4.311232     0.473833    -1.551334
H    -3.252752    -1.847079     0.660584
H    -2.982215     1.346912    -3.007540
H    -5.167844     1.037429    -1.869640
H    -5.317521    -0.606172     0.013123
Br    1.879829     1.640445     1.301106
23
CCNN:   93.06 CNNC:  199.37 E(S0): -3115.28495 E(S1): -3115.28328
C     2.183271    -0.268797    -1.787230
H     1.299376     0.184851    -0.029436
H     3.203265     1.071903    -0.703233
H     1.344967    -1.552088    -3.090348
H     2.943090    -1.109015    -3.450394
H     3.610032     1.012039    -2.343655
N     0.287853    -1.371851    -0.987190
H    -0.945822    -2.042471     0.532967
N     1.279989    -0.422138    -0.863293
N     3.240105     0.530546    -1.553454
N     2.098213    -0.913289    -2.963057
C    -0.866643    -1.405679    -0.335983
C    -2.088802    -0.826580    -0.858636
C    -3.300959    -1.017651    -0.178817
N    -1.993252    -0.076838    -1.974155
C    -4.448715    -0.393242    -0.663071
C    -3.088006     0.509299    -2.425460
C    -4.343443     0.389148    -1.808567
H    -3.332762    -1.626327     0.705729
H    -2.976152     1.103849    -3.314187
H    -5.195971     0.894106    -2.222050
H    -5.390359    -0.514177    -0.160685
Br    1.872727     1.759077     1.377163
23
CCNN:   91.21 CNNC:  215.06 E(S0): -3115.28596 E(S1): -3115.28424
C     1.896594     0.149780    -1.858528
H     1.276013     0.347648     0.054434
H     2.960944     1.490363    -0.816453
H     0.895922    -1.013451    -3.163144
H     2.409714    -0.450000    -3.718690
H     3.159807     1.559028    -2.499757
N     0.258640    -1.217210    -0.894281
```

H	-0.986127	-1.829703	0.635662
N	1.167900	-0.173441	-0.824623
N	2.910943	1.013185	-1.704714
N	1.666289	-0.390858	-3.061447
C	-0.915926	-1.253224	-0.273891
C	-2.139138	-0.774640	-0.884441
C	-3.360492	-0.885487	-0.201256
N	-2.038360	-0.192052	-2.096142
C	-4.508673	-0.356084	-0.785626
C	-3.134838	0.305031	-2.641765
C	-4.397108	0.255585	-2.030679
H	-3.397260	-1.362419	0.760620
H	-3.018438	0.765084	-3.606515
H	-5.250217	0.681351	-2.524119
H	-5.456369	-0.419158	-0.283930
Br	1.919639	1.959468	1.437668

23
CCNN: 89.31 CNNC: 224.60 E(S0): -3115.28596 E(S1): -3115.28594

C	1.717569	0.400744	-1.838752
H	1.281141	0.555263	0.130999
H	2.817468	1.769723	-0.878219
H	0.593075	-0.742767	-3.054528
H	1.976143	-0.040416	-3.798470
H	2.829617	1.893503	-2.568962
N	0.294475	-1.084505	-0.723044
H	-0.972820	-1.627344	0.834897
N	1.127026	0.020017	-0.730361
N	2.693572	1.313059	-1.771136
N	1.380226	-0.133717	-3.009468
C	-0.900046	-1.120569	-0.113067
C	-2.112270	-0.729014	-0.791055
C	-3.352893	-0.823459	-0.136587
N	-1.992435	-0.227350	-2.038597
C	-4.494252	-0.362160	-0.785800
C	-3.085433	0.202372	-2.646748
C	-4.362404	0.165440	-2.067799
H	-3.406009	-1.232942	0.854993
H	-2.953012	0.596352	-3.638410
H	-5.210499	0.536401	-2.611556
H	-5.453856	-0.412542	-0.305810
Br	1.971569	2.235229	1.438391

Geometries from MECI$_1$ to E_1 on the S$_0$ surface.
23
CCNN: 89.31 CNNC: 224.60 E(S0): -3115.28596 E(S1): -3115.28594

C	1.717569	0.400744	-1.838752

H	1.281141	0.555263	0.130999
H	2.817468	1.769723	-0.878219
H	0.593075	-0.742767	-3.054528
H	1.976143	-0.040416	-3.798470
H	2.829617	1.893503	-2.568962
N	0.294475	-1.084505	-0.723044
H	-0.972820	-1.627344	0.834897
N	1.127026	0.020017	-0.730361
N	2.693572	1.313059	-1.771136
N	1.380226	-0.133717	-3.009468
C	-0.900046	-1.120569	-0.113067
C	-2.112270	-0.729014	-0.791055
C	-3.352893	-0.823459	-0.136587
N	-1.992435	-0.227350	-2.038597
C	-4.494252	-0.362160	-0.785800
C	-3.085433	0.202372	-2.646748
C	-4.362404	0.165440	-2.067799
H	-3.406009	-1.232942	0.854993
H	-2.953012	0.596352	-3.638410
H	-5.210499	0.536401	-2.611556
H	-5.453856	-0.412542	-0.305810
Br	1.971569	2.235229	1.438391

23

CCNN: 119.34 CNNC: 221.17 E(S0): -3115.33011 E(S1): -3115.23421

C	1.786415	0.512003	-1.829710
H	1.454236	0.378095	0.161628
H	3.092487	1.531583	-0.718941
H	0.451052	-0.238115	-3.122852
H	1.883043	0.401137	-3.846878
H	3.087293	1.931158	-2.361108
N	0.161376	-0.869787	-0.946166
H	-0.975020	-1.137080	0.786462
N	1.183046	0.035872	-0.758850
N	2.888115	1.245792	-1.666109
N	1.320557	0.247425	-3.042800
C	-0.949654	-0.850468	-0.254474
C	-2.232546	-0.664327	-0.928454
C	-3.405928	-0.688051	-0.164947
N	-2.231872	-0.392918	-2.245293
C	-4.620404	-0.395830	-0.782653
C	-3.391249	-0.123159	-2.824334
C	-4.615600	-0.103651	-2.141742
H	-3.358325	-0.909813	0.884932
H	-3.356155	0.094515	-3.876550
H	-5.521082	0.134022	-2.667086
H	-5.534493	-0.394500	-0.218563

| Br | 2.030619 | 2.197601 | 1.478255 |

23

CCNN: 146.96 CNNC: 212.63 E(S0): -3115.37645 E(S1): -3115.20061

C	1.922235	0.679095	-1.897573
H	1.385307	0.412551	0.028294
H	3.189153	1.486769	-0.587018
H	0.674144	0.161772	-3.388652
H	2.213747	0.743170	-3.897564
H	3.403775	1.986773	-2.182947
N	0.027331	-0.538765	-1.320675
H	-0.886877	-0.498072	0.531033
N	1.169195	0.186928	-0.938935
N	3.069192	1.277364	-1.569057
N	1.559432	0.566708	-3.171497
C	-0.993517	-0.465549	-0.542219
C	-2.365308	-0.519019	-1.076521
C	-3.434898	-0.495150	-0.176019
N	-2.535598	-0.490195	-2.404910
C	-4.735898	-0.413508	-0.674669
C	-3.774373	-0.416512	-2.871801
C	-4.910347	-0.369077	-2.053557
H	-3.249604	-0.516867	0.881021
H	-3.875483	-0.385359	-3.941257
H	-5.887397	-0.294265	-2.491453
H	-5.577753	-0.383635	-0.006470
Br	2.063747	2.107998	1.532253

23

CCNN: 168.07 CNNC: 200.77 E(S0): -3115.39680 E(S1): -3115.21922

C	1.970143	0.928879	-2.004673
H	1.223481	0.693782	-0.152809
H	3.178492	1.564635	-0.550883
H	0.838532	0.521862	-3.614281
H	2.448957	1.010847	-3.970475
H	3.638308	2.026887	-2.120625
N	-0.104253	-0.018110	-1.620086
H	-0.898853	0.104531	0.287517
N	1.070523	0.498551	-1.139292
N	3.125130	1.391047	-1.548764
N	1.719354	0.877481	-3.309070
C	-1.085422	-0.025270	-0.766708
C	-2.470737	-0.299510	-1.184900
C	-3.465061	-0.355249	-0.207234
N	-2.732048	-0.405566	-2.491669
C	-4.779022	-0.516518	-0.590023
C	-4.020438	-0.563486	-2.851594
C	-5.073604	-0.617360	-1.940045

H	-3.201853	-0.271104	0.831281
H	-4.204210	-0.636388	-3.907430
H	-6.083630	-0.733040	-2.285286
H	-5.559494	-0.553151	0.147564
Br	2.102613	1.976083	1.588618

23
CCNN: 179.91 CNNC: 182.77 E(S0): -3115.40214 E(S1): -3115.22430

C	1.878198	1.241754	-2.075009
H	1.047863	1.139451	-0.241507
H	3.123737	1.750792	-0.582640
H	0.786494	0.827161	-3.708444
H	2.428427	1.210714	-4.027334
H	3.752979	1.972965	-2.179045
N	-0.310838	0.576493	-1.745486
H	-1.036588	0.512424	0.192067
N	0.895142	0.963044	-1.233649
N	3.046682	1.601085	-1.584634
N	1.671909	1.152696	-3.387434
C	-1.238565	0.375772	-0.858265
C	-2.595707	-0.043388	-1.251663
C	-3.538387	-0.293971	-0.252827
N	-2.869858	-0.164358	-2.553736
C	-4.810240	-0.684844	-0.608909
C	-4.117844	-0.546791	-2.889547
C	-5.116886	-0.816783	-1.953973
H	-3.268096	-0.180633	0.781037
H	-4.310466	-0.634566	-3.943238
H	-6.095382	-1.117766	-2.278228
H	-5.549305	-0.882793	0.145096
Br	2.184014	1.827535	1.646746

Geometries from $MECI_1$ to Z_1 on the S_0 surface.
23
CCNN: 89.31 CNNC: 224.60 E(S0): -3115.28596 E(S1): -3115.28594

C	1.717569	0.400744	-1.838752
H	1.281141	0.555263	0.130999
H	2.817468	1.769723	-0.878219
H	0.593075	-0.742767	-3.054528
H	1.976143	-0.040416	-3.798470
H	2.829617	1.893503	-2.568962
N	0.294475	-1.084505	-0.723044
H	-0.972820	-1.627344	0.834897
N	1.127026	0.020017	-0.730361
N	2.693572	1.313059	-1.771136
N	1.380226	-0.133717	-3.009468
C	-0.900046	-1.120569	-0.113067

```
C    -2.112270    -0.729014    -0.791055
C    -3.352893    -0.823459    -0.136587
N    -1.992435    -0.227350    -2.038597
C    -4.494252    -0.362160    -0.785800
C    -3.085433     0.202372    -2.646748
C    -4.362404     0.165440    -2.067799
H    -3.406009    -1.232942     0.854993
H    -2.953012     0.596352    -3.638410
H    -5.210499     0.536401    -2.611556
H    -5.453856    -0.412542    -0.305810
Br    1.971569     2.235229     1.438391
23
CCNN:  41.64 CNNC:  222.87 E(S0): -3115.36208 E(S1): -3115.21579
C     1.836796     0.080804    -1.754768
H     0.931632     0.607048    -0.034342
H     2.443731     1.874748    -1.084321
H     1.364177    -1.642383    -2.709999
H     2.693315    -0.795460    -3.367164
H     2.771820     1.562000    -2.730573
N     0.541894    -1.427132    -0.449823
H    -0.926645    -2.288810     0.558590
N     1.074263    -0.134373    -0.720112
N     2.563018     1.200568    -1.826640
N     1.928370    -0.824635    -2.734554
C    -0.698180    -1.456333    -0.084109
C    -1.847735    -0.694755    -0.605127
C    -3.116413    -0.935158    -0.067479
N    -1.645747     0.151009    -1.624751
C    -4.214606    -0.264212    -0.604478
C    -2.694251     0.779272    -2.135659
C    -4.001752     0.610652    -1.663501
H    -3.237621    -1.630616     0.741902
H    -2.494705     1.440832    -2.958886
H    -4.812753     1.146602    -2.119225
H    -5.201151    -0.427830    -0.211837
Br    1.751420     2.325405     1.279264
23
CCNN:  12.05 CNNC:  201.38 E(S0): -3115.39056 E(S1): -3115.20945
C     2.361611    -0.353511    -1.377124
H     0.876511     0.517342    -0.297047
H     2.751403     1.568847    -0.918145
H     2.302507    -2.304374    -1.841030
H     3.777419    -1.530475    -2.202493
H     3.702751     0.902404    -2.198071
N     0.665082    -1.620018    -0.394218
H    -0.899070    -2.642054     0.204045
```

```
N      1.217918     -0.368190     -0.729927
N      3.066936      0.764589     -1.446150
N      2.808518     -1.459227     -1.984457
C     -0.593760     -1.676098     -0.155820
C     -1.684503     -0.706569     -0.377830
C     -2.952091     -1.002278      0.126836
N     -1.444881      0.368971     -1.128822
C     -3.995293     -0.146929     -0.154213
C     -2.450596      1.186568     -1.396835
C     -3.749567      0.973888     -0.936211
H     -3.106172     -1.881710      0.722934
H     -2.216352      2.040047     -2.004474
H     -4.533081      1.664563     -1.186765
H     -4.981438     -0.347841      0.222054
Br     1.402984      2.461159      0.882036
23
CCNN:    1.81 CNNC:  176.98 E(S0): -3115.39561 E(S1): -3115.21457
C      2.674344     -0.702882     -0.750404
H      0.886517      0.219861     -0.494750
H      2.840852      1.288083     -0.483549
H      2.794110     -2.700849     -0.801059
H      4.296776     -1.901325     -0.753290
H      4.297406      0.465986     -0.962323
N      0.730888     -1.887121     -0.390575
H     -0.918858     -2.897278      0.016938
N      1.355367     -0.692434     -0.620195
N      3.326322      0.435614     -0.755838
N      3.317942     -1.862109     -0.927576
C     -0.548719     -1.911493     -0.199172
C     -1.536780     -0.808204     -0.216965
C     -2.723400     -0.919515      0.513331
N     -1.250839      0.253605     -0.968496
C     -3.619230      0.124291      0.478374
C     -2.109843      1.268066     -0.993442
C     -3.316581      1.246936     -0.284955
H     -2.923931     -1.801369      1.093483
H     -1.821551      2.115449     -1.581599
H     -3.982012      2.087455     -0.329534
H     -4.535132      0.073993      1.037452
Br     1.116991      2.574763      0.377035
23
CCNN:    0.52 CNNC:  182.50 E(S0): -3115.39996 E(S1): -3115.21559
C      2.491317     -0.929358     -0.400404
H      0.658849     -0.004050     -0.147296
H      2.683476      1.093954     -0.337964
H      2.589370     -2.933845     -0.375141
```

H	4.102596	-2.147421	-0.472480
H	4.127387	0.197745	-0.690454
N	0.529019	-2.129800	-0.067830
H	-1.135106	-3.161926	0.176404
N	1.176399	-0.898196	-0.205064
N	3.155473	0.196382	-0.481410
N	3.112581	-2.103975	-0.541979
C	-0.745701	-2.166021	0.074479
C	-1.759882	-1.060984	0.116681
C	-3.112086	-1.353640	0.269861
N	-1.310629	0.186473	0.001782
C	-4.006476	-0.296731	0.297040
C	-2.156802	1.187842	0.034579
C	-3.528446	0.994263	0.177957
H	-3.450019	-2.369056	0.363746
H	-1.724585	2.166320	-0.051146
H	-4.191821	1.837444	0.196528
H	-5.059166	-0.480962	0.411279
Br	1.332348	2.827097	0.071603

2PyMIGHBr E$_2$ geometries:
Geometries from E_2 to MECI$_2$ on the S$_1$ surface.
23
CCNN: 179.68 CNNC: 182.73 E(S0): -3115.40299 E(S1): -3115.22124

C	-1.971684	-3.802363	2.653184
H	-1.057310	-3.884981	0.867333
H	-0.515197	-5.181232	2.548474
H	-3.485209	-2.529118	2.994997
H	-3.004460	-3.444036	4.353212
H	-1.481313	-5.241255	3.970202
N	-2.551533	-2.401270	0.897094
H	-1.473193	-2.545321	-0.880289
N	-1.741788	-3.372522	1.430408
N	-1.184697	-4.736720	3.166247
N	-2.981785	-3.301314	3.369478
C	-2.277734	-2.086321	-0.330437
C	-3.077249	-1.046251	-1.056459
C	-4.234694	-0.471456	-0.535033
N	-2.582088	-0.725884	-2.255780
C	-4.896081	0.478468	-1.296851
C	-3.224530	0.188084	-2.974393
C	-4.388721	0.818071	-2.532857
H	-4.600019	-0.766181	0.427890
H	-2.801248	0.423889	-3.932554
H	-4.874295	1.548880	-3.153602
H	-5.794971	0.940543	-0.928160

```
Br      0.452428    -5.496450    0.326878
23
CCNN:  178.45 CNNC:  182.27 E(S0): -3115.39887 E(S1): -3115.23380
C      -1.967861    -3.805166    2.651428
H      -1.070311    -3.906037    0.856227
H      -0.545646    -5.213862    2.528609
H      -3.453785    -2.502984    3.005685
H      -2.979864    -3.427748    4.359650
H      -1.493415    -5.254785    3.962960
N      -2.544812    -2.386349    0.894294
H      -1.459943    -2.527058   -0.875042
N      -1.739205    -3.380591    1.426050
N      -1.194867    -4.755315    3.156530
N      -2.962094    -3.284852    3.375993
C      -2.269262    -2.072029   -0.328842
C      -3.059255    -1.055281   -1.046036
C      -4.245959    -0.484972   -0.522586
N      -2.552511    -0.720087   -2.259137
C      -4.929229     0.476542   -1.295278
C      -3.214222     0.204227   -2.986823
C      -4.402145     0.827258   -2.548234
H      -4.612319    -0.788432    0.436906
H      -2.787603     0.448492   -3.940774
H      -4.888649     1.553024   -3.172343
H      -5.834736     0.926389   -0.932383
Br      0.453036    -5.495342    0.328598
23
CCNN:  179.10 CNNC:  182.07 E(S0): -3115.39702 E(S1): -3115.23447
C      -1.977712    -3.815205    2.648327
H      -1.061863    -3.896109    0.855367
H      -0.525853    -5.198324    2.542534
H      -3.485311    -2.535628    2.989397
H      -3.004264    -3.447730    4.349524
H      -1.486851    -5.252471    3.966938
N      -2.568604    -2.390238    0.888575
H      -1.469532    -2.534886   -0.868727
N      -1.745550    -3.388885    1.423868
N      -1.191153    -4.750565    3.160822
N      -2.984162    -3.308785    3.365447
C      -2.282360    -2.074204   -0.332564
C      -3.046814    -1.075484   -1.039877
C      -4.241206    -0.477676   -0.504612
N      -2.541585    -0.748320   -2.277454
C      -4.938340     0.502596   -1.279916
C      -3.217542     0.191837   -3.002076
C      -4.402763     0.837478   -2.555541
```

H	-4.597482	-0.775674	0.459958
H	-2.797782	0.426793	-3.960601
H	-4.880504	1.563910	-3.183814
H	-5.833513	0.962670	-0.910923
Br	0.456299	-5.493452	0.329520

23

CCNN: 179.44 CNNC: 181.90 E(S0): -3115.39579 E(S1): -3115.23462

C	-1.986174	-3.823168	2.645007
H	-1.058978	-3.890996	0.855512
H	-0.516483	-5.188744	2.548204
H	-3.508211	-2.558988	2.978500
H	-3.022058	-3.463243	4.341973
H	-1.484479	-5.253238	3.967388
N	-2.580947	-2.397566	0.885459
H	-1.472723	-2.538338	-0.865755
N	-1.752031	-3.394332	1.421746
N	-1.191025	-4.748799	3.162013
N	-3.000471	-3.326303	3.357657
C	-2.288222	-2.077357	-0.333960
C	-3.045945	-1.080520	-1.039920
C	-4.235064	-0.469146	-0.499156
N	-2.546374	-0.762698	-2.285765
C	-4.933511	0.515173	-1.273374
C	-3.224060	0.181411	-3.007444
C	-4.401446	0.839128	-2.555803
H	-4.585752	-0.761557	0.469111
H	-2.809279	0.409358	-3.969733
H	-4.876319	1.566401	-3.185041
H	-5.822309	0.982933	-0.899963
Br	0.458885	-5.491800	0.330762

23

CCNN: 178.79 CNNC: 179.11 E(S0): -3115.39511 E(S1): -3115.23409

C	-1.817773	-3.714869	2.694143
H	-0.975640	-3.841021	0.868230
H	-0.473251	-5.196394	2.526131
H	-3.287497	-2.393061	3.068422
H	-2.861535	-3.385224	4.402004
H	-1.341568	-5.162787	4.008376
N	-2.419029	-2.278072	0.947238
H	-1.254410	-2.338072	-0.771114
N	-1.584650	-3.280798	1.469639
N	-1.066125	-4.694069	3.175713
N	-2.765814	-3.153402	3.441019
C	-2.095238	-1.910489	-0.251357
C	-2.855851	-0.912940	-0.950739
C	-4.070928	-0.340681	-0.423724

N	-2.335684	-0.554108	-2.177451
C	-4.777167	0.642693	-1.191967
C	-3.018517	0.393322	-2.890069
C	-4.222627	1.010318	-2.452466
H	-4.438831	-0.672197	0.525358
H	-2.584111	0.656613	-3.834515
H	-4.698737	1.740430	-3.077445
H	-5.690245	1.072191	-0.831593
Br	0.286774	-5.629705	0.253195

23

CCNN: 178.05 CNNC: 174.92 E(S0): -3115.39421 E(S1): -3115.23302

C	-1.576831	-3.573270	2.734325
H	-0.874804	-3.792945	0.861835
H	-0.356939	-5.152933	2.513350
H	-2.988040	-2.199993	3.144107
H	-2.590126	-3.229280	4.459419
H	-1.062440	-4.987259	4.074396
N	-2.251914	-2.181663	0.978967
H	-1.058754	-2.157543	-0.719708
N	-1.386778	-3.169075	1.489452
N	-0.856791	-4.586352	3.188227
N	-2.433895	-2.933083	3.524602
C	-1.925015	-1.776481	-0.205903
C	-2.719705	-0.800932	-0.900077
C	-3.987301	-0.325832	-0.401093
N	-2.178945	-0.366318	-2.092626
C	-4.727139	0.637880	-1.162347
C	-2.893083	0.564459	-2.796716
C	-4.150096	1.087600	-2.385748
H	-4.369919	-0.719348	0.518061
H	-2.441059	0.891009	-3.712729
H	-4.648764	1.808794	-3.003441
H	-5.681138	0.991254	-0.826091
Br	0.128817	-5.739852	0.210797

23

CCNN: 177.28 CNNC: 165.89 E(S0): -3115.39254 E(S1): -3115.23109

C	-1.302430	-3.423320	2.724347
H	-0.801511	-3.777607	0.812315
H	-0.188217	-5.076675	2.485694
H	-2.651124	-2.002891	3.164771
H	-2.207328	-2.996599	4.486517
H	-0.697576	-4.764553	4.102851
N	-2.115386	-2.123075	0.955720
H	-0.860418	-1.936483	-0.686179
N	-1.200970	-3.084453	1.448582
N	-0.590922	-4.444853	3.167770

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N    -2.054363   -2.699270    3.551160
C    -1.771149   -1.640906   -0.193873
C    -2.609015   -0.693404   -0.878777
C    -3.937856   -0.358798   -0.427360
N    -2.046003   -0.143095   -2.011210
C    -4.718751    0.582614   -1.174887
C    -2.800427    0.767057   -2.700648
C    -4.118974    1.155344   -2.334583
H    -4.332784   -0.842225    0.442442
H    -2.330539    1.187524   -3.568114
H    -4.645827    1.868108   -2.938469
H    -5.717914    0.829540   -0.876950
Br   -0.026851   -5.850296    0.201615
23
CCNN:  176.61 CNNC:  152.41 E(S0): -3115.38973 E(S1): -3115.22793
C    -1.035808   -3.279484    2.647959
H    -0.776048   -3.799101    0.729236
H    -0.002577   -4.987284    2.427692
H    -2.316954   -1.807284    3.113019
H    -1.763499   -2.713760    4.449260
H    -0.306033   -4.520193    4.061382
N    -2.030798   -2.103743    0.876519
H    -0.692310   -1.683880   -0.650853
N    -1.059494   -3.036005    1.347447
N    -0.312452   -4.290348    3.094538
N    -1.673544   -2.466239    3.491153
C    -1.655989   -1.505505   -0.205575
C    -2.531351   -0.579660   -0.877128
C    -3.913389   -0.406280   -0.500872
N    -1.948319    0.113737   -1.916210
C    -4.729092    0.520407   -1.228673
C    -2.738817    1.007732   -2.586834
C    -4.110569    1.242568   -2.291537
H    -4.316511   -0.996809    0.296095
H    -2.254036    1.541376   -3.380778
H    -4.661782    1.953467   -2.875457
H    -5.765299    0.648780   -0.988140
Br   -0.166991   -5.964696    0.227040
23
CCNN:  175.81 CNNC:  137.19 E(S0): -3115.38644 E(S1): -3115.22426
C    -0.808664   -3.158782    2.527482
H    -0.791090   -3.848576    0.647736
H     0.156422   -4.911658    2.348780
H    -2.008455   -1.621413    3.005699
H    -1.327557   -2.428440    4.340819
H     0.053547   -4.292477    3.958505
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N      -1.987979    -2.114035     0.772107
H      -0.578564    -1.447113    -0.593174
N      -0.970870    -3.023173     1.223594
N      -0.068598    -4.153979     2.982174
N      -1.326683    -2.253251     3.362534
C      -1.585842    -1.390147    -0.217843
C      -2.487744    -0.476813    -0.875343
C      -3.902514    -0.450670    -0.593657
N      -1.895586     0.353364    -1.801871
C      -4.742298     0.469066    -1.301764
C      -2.711984     1.236519    -2.455935
C      -4.116570     1.332146    -2.249653
H      -4.306520    -1.141085     0.118134
H      -2.220934     1.876276    -3.162879
H      -4.685549     2.045645    -2.812864
H      -5.799879     0.491580    -1.131241
Br     -0.279310    -6.067655     0.270860
23
CCNN:  166.46 CNNC:  126.30 E(S0): -3115.35077 E(S1): -3115.23989
C      -0.763869    -3.145947     2.511499
H      -0.954317    -3.946123     0.660376
H      -0.092976    -5.032116     2.349247
H      -1.633038    -1.388138     2.927116
H      -1.019792    -2.215537     4.286104
H      -0.014864    -4.345124     3.941223
N      -1.796359    -2.087726     0.715942
H      -0.459048    -1.096036    -0.530407
N      -0.994249    -3.065941     1.184569
N      -0.178213    -4.225044     2.966943
N      -1.069215    -2.121070     3.297157
C      -1.496389    -1.172652    -0.269539
C      -2.455337    -0.367045    -0.895079
C      -3.857261    -0.506178    -0.685154
N      -1.947961     0.570637    -1.748243
C      -4.725333     0.330191    -1.370758
C      -2.793350     1.358485    -2.381671
C      -4.192862     1.290814    -2.238376
H      -4.224072    -1.267514    -0.023123
H      -2.352926     2.084410    -3.041692
H      -4.823403     1.961483    -2.790400
H      -5.787840     0.232022    -1.245096
Br     -0.301302    -6.101580     0.291977
23
CCNN:  152.68 CNNC:  121.05 E(S0): -3115.33087 E(S1): -3115.24894
C      -0.601688    -3.101088     2.489255
H      -1.035938    -3.898037     0.670813
```

H	-0.074184	-5.030836	2.282625
H	-1.235533	-1.252738	2.927561
H	-0.549031	-2.099980	4.246394
H	0.187923	-4.342665	3.858522
N	-1.687550	-1.956949	0.792596
H	-0.387395	-0.768515	-0.309717
N	-0.979195	-3.020479	1.191223
N	-0.071576	-4.220470	2.905657
N	-0.728207	-2.038616	3.270214
C	-1.425044	-1.003668	-0.169361
C	-2.420270	-0.298726	-0.860198
C	-3.810521	-0.572628	-0.739929
N	-1.956502	0.693028	-1.673834
C	-4.709065	0.184057	-1.476149
C	-2.828806	1.396331	-2.364890
C	-4.220816	1.194576	-2.309793
H	-4.146596	-1.363496	-0.096917
H	-2.420807	2.163264	-2.998999
H	-4.878486	1.806012	-2.897888
H	-5.763951	-0.009070	-1.410857
Br	-0.387386	-6.128946	0.304872

23

CCNN: 137.22 CNNC: 123.77 E(S0): -3115.31327 E(S1): -3115.25716

C	-0.442460	-3.077304	2.515174
H	-1.073019	-3.801935	0.722670
H	-0.028325	-5.027464	2.227814
H	-0.898443	-1.195970	3.023907
H	-0.143470	-2.106423	4.266638
H	0.388229	-4.388077	3.792459
N	-1.566829	-1.805356	0.949122
H	-0.335814	-0.515729	-0.119903
N	-0.933791	-2.947476	1.261349
N	0.047960	-4.235059	2.870243
N	-0.429313	-2.023868	3.318189
C	-1.342550	-0.884022	-0.052706
C	-2.359945	-0.289690	-0.823778
C	-3.726450	-0.666422	-0.752535
N	-1.937392	0.708915	-1.647589
C	-4.646946	-0.004545	-1.552228
C	-2.827009	1.318026	-2.404504
C	-4.199647	1.011005	-2.400936
H	-4.031719	-1.453295	-0.089862
H	-2.449826	2.092119	-3.048752
H	-4.875207	1.551821	-3.036157
H	-5.687035	-0.271223	-1.519202
Br	-0.489570	-6.107044	0.296569

23
CCNN: 122.36 CNNC: 129.39 E(S0): -3115.29399 E(S1): -3115.26725
C	-0.322996	-3.065965	2.554199
H	-1.105605	-3.693251	0.785465
H	-0.029011	-5.028715	2.190768
H	-0.614715	-1.172482	3.134280
H	0.167089	-2.163411	4.300255
H	0.506590	-4.455854	3.745151
N	-1.435222	-1.657122	1.109504
H	-0.290544	-0.317632	0.013124
N	-0.886047	-2.870307	1.342755
N	0.115036	-4.260982	2.851893
N	-0.191045	-2.039073	3.381674
C	-1.254092	-0.791688	0.050014
C	-2.286895	-0.309804	-0.789546
C	-3.626301	-0.766024	-0.731944
N	-1.902920	0.669524	-1.650152
C	-4.564224	-0.201571	-1.586182
C	-2.805400	1.184056	-2.461823
C	-4.155511	0.794347	-2.474934
H	-3.903652	-1.530549	-0.031893
H	-2.457299	1.946366	-3.135604
H	-4.845286	1.262101	-3.151598
H	-5.587920	-0.525504	-1.560373
Br	-0.581669	-6.061987	0.278658

23
CCNN: 109.90 CNNC: 136.90 E(S0): -3115.28006 E(S1): -3115.27899
C	-0.305173	-3.074412	2.653609
H	-1.108564	-3.577791	0.856852
H	-0.087838	-5.033141	2.211827
H	-0.468121	-1.185165	3.310756
H	0.293457	-2.263823	4.413472
H	0.425234	-4.553668	3.802144
N	-1.314367	-1.525581	1.269944
H	-0.228294	-0.198119	0.101280
N	-0.856000	-2.800090	1.461835
N	0.078872	-4.301719	2.904882
N	-0.133400	-2.095860	3.532546
C	-1.148190	-0.752658	0.143466
C	-2.190485	-0.400697	-0.759511
C	-3.500700	-0.925941	-0.686560
N	-1.840629	0.523492	-1.687930
C	-4.450706	-0.484694	-1.599526
C	-2.751231	0.919831	-2.556404
C	-4.076744	0.456064	-2.559545
H	-3.752701	-1.641471	0.072573

H	-2.429366	1.643267	-3.283938
H	-4.776525	0.829246	-3.282978
H	-5.456736	-0.859344	-1.561692
Br	-0.646141	-5.954133	0.236670

23
CCNN: 106.29 CNNC: 143.53 E(S0): -3115.28615 E(S1): -3115.28179

C	-0.251051	-3.120672	2.776466
H	-0.905771	-3.558070	0.909228
H	-0.038485	-5.070848	2.308515
H	-0.396684	-1.241368	3.488265
H	0.321818	-2.361133	4.568915
H	0.323916	-4.655878	3.949838
N	-1.144760	-1.508667	1.353692
H	-0.081602	-0.244473	0.076434
N	-0.712891	-2.808411	1.576111
N	0.111770	-4.366101	3.023181
N	-0.148835	-2.178115	3.713631
C	-0.976241	-0.833925	0.192573
C	-2.044968	-0.573969	-0.731765
C	-3.316978	-1.168377	-0.625255
N	-1.736563	0.300303	-1.714515
C	-4.285296	-0.844876	-1.569938
C	-2.662241	0.588736	-2.611774
C	-3.957394	0.050002	-2.587047
H	-3.528172	-1.849672	0.175925
H	-2.376302	1.280506	-3.383456
H	-4.671557	0.331059	-3.337758
H	-5.266908	-1.277142	-1.513153
Br	-0.754336	-5.777430	0.176438

23
CCNN: 103.41 CNNC: 152.91 E(S0): -3115.28847 E(S1): -3115.28257

C	-0.395462	-3.184330	2.911512
H	-0.793704	-3.573164	0.968391
H	-0.134553	-5.119394	2.427101
H	-0.612768	-1.327045	3.656715
H	0.046217	-2.459285	4.745725
H	-0.106164	-4.774785	4.109881
N	-1.047115	-1.528296	1.401547
H	0.030168	-0.360205	0.053639
N	-0.691631	-2.841034	1.680129
N	-0.051187	-4.442772	3.174099
N	-0.437160	-2.277264	3.896225
C	-0.877427	-0.918711	0.224041
C	-1.954143	-0.683247	-0.710408
C	-3.221818	-1.274430	-0.577869
N	-1.639709	0.137313	-1.732798

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C     -4.185026    -1.007339    -1.545839
C     -2.561790     0.378514    -2.649397
C     -3.853251    -0.165088    -2.604948
H     -3.431353    -1.919360     0.252840
H     -2.273371     1.031622    -3.452961
H     -4.562763     0.070343    -3.375605
H     -5.163068    -1.445467    -1.476359
Br    -0.748562    -5.655815     0.115141
23
CCNN:  100.11 CNNC:  163.46 E(S0): -3115.28783 E(S1): -3115.28292
C     -0.753320    -3.263102     3.004844
H     -0.780551    -3.590767     1.009529
H     -0.395239    -5.180719     2.515156
H     -1.055706    -1.421939     3.754229
H     -0.581186    -2.582429     4.895538
H     -0.752179    -4.904907     4.164638
N     -1.089602    -1.555148     1.449135
H      0.034255    -0.473012     0.066207
N     -0.838338    -2.884179     1.756577
N     -0.455040    -4.535035     3.289973
N     -0.965929    -2.383210     3.999992
C     -0.897508    -0.981166     0.263551
C     -1.958121    -0.733236    -0.690292
C     -3.252330    -1.257016    -0.541580
N     -1.597606     0.023606    -1.744345
C     -4.194649    -0.991337    -1.529916
C     -2.500932     0.265233    -2.680345
C     -3.815454    -0.215817    -2.623590
H     -3.495922    -1.850700     0.317445
H     -2.175959     0.866499    -3.509680
H     -4.507853     0.014535    -3.411190
H     -5.192659    -1.379176    -1.451118
Br    -0.597112    -5.592681     0.074288
23
CCNN:   97.87 CNNC:  176.99 E(S0): -3115.28710 E(S1): -3115.28305
C     -1.062802    -3.305248     2.983274
H     -0.739527    -3.632552     1.016667
H     -0.624996    -5.218828     2.563453
H     -1.486365    -1.468766     3.682651
H     -1.148831    -2.620044     4.869916
H     -1.328106    -4.955085     4.088501
N     -1.052700    -1.589165     1.402551
H      0.066562    -0.632703    -0.062431
N     -0.932331    -2.926382     1.744528
N     -0.814212    -4.580616     3.321911
N     -1.441267    -2.430990     3.937271
```

C	-0.888576	-1.063881	0.196689
C	-1.982122	-0.757470	-0.705161
C	-3.298006	-1.191643	-0.480337
N	-1.628577	-0.044643	-1.790696
C	-4.271827	-0.880771	-1.424701
C	-2.561305	0.242102	-2.683996
C	-3.899988	-0.150209	-2.551154
H	-3.536472	-1.753154	0.401730
H	-2.241347	0.807482	-3.540125
H	-4.615295	0.112861	-3.307380
H	-5.287738	-1.200928	-1.286918
Br	-0.434508	-5.582500	0.072696

23
CCNN: 94.13 CNNC: 190.35 E(S0): -3115.28489 E(S1): -3115.28395

C	-1.353976	-3.311902	2.871146
H	-0.729004	-3.644846	0.979257
H	-0.888260	-5.231562	2.516083
H	-1.799099	-1.464786	3.525123
H	-1.742964	-2.648568	4.725683
H	-1.780872	-4.953286	3.939417
N	-1.038374	-1.595013	1.322013
H	0.033235	-0.727179	-0.232585
N	-1.037659	-2.937099	1.663368
N	-1.173714	-4.587820	3.239353
N	-1.853798	-2.431448	3.760121
C	-0.926649	-1.093998	0.096200
C	-2.057168	-0.740505	-0.739269
C	-3.375081	-1.110097	-0.427246
N	-1.739868	-0.057501	-1.854922
C	-4.390941	-0.765906	-1.313793
C	-2.712703	0.262592	-2.692455
C	-4.057314	-0.066424	-2.471758
H	-3.584060	-1.649291	0.476088
H	-2.421367	0.803379	-3.574487
H	-4.805713	0.220301	-3.186146
H	-5.409887	-1.037402	-1.108767
Br	-0.247123	-5.604528	0.113576

23
CCNN: 92.49 CNNC: 198.54 E(S0): -3115.28409 E(S1): -3115.28409

C	-1.534444	-3.318416	2.748480
H	-0.698144	-3.642522	0.936824
H	-1.026208	-5.237504	2.443092
H	-2.040830	-1.469640	3.350803
H	-2.108531	-2.651557	4.555300
H	-2.034980	-4.956988	3.795427
N	-1.055745	-1.596166	1.249276

H	-0.025329	-0.749759	-0.343138
N	-1.105033	-2.941816	1.573517
N	-1.393773	-4.591659	3.126756
N	-2.116473	-2.436266	3.583049
C	-0.980324	-1.093622	0.020092
C	-2.135355	-0.711274	-0.767612
C	-3.450456	-1.030873	-0.393250
N	-1.846630	-0.054309	-1.906583
C	-4.493205	-0.662793	-1.238214
C	-2.844834	0.288637	-2.704461
C	-4.188882	0.009971	-2.420142
H	-3.637919	-1.549843	0.525602
H	-2.574933	0.807847	-3.605954
H	-4.958499	0.313761	-3.104484
H	-5.510742	-0.895510	-0.983559
Br	-0.112847	-5.631911	0.163269

Geometries from MECI$_2$ to E_2 on the S$_0$ surface.
23
CCNN: 92.49 CNNC: 198.54 E(S0): -3115.28409 E(S1): -3115.28409

C	-1.534444	-3.318416	2.748480
H	-0.698144	-3.642522	0.936824
H	-1.026208	-5.237504	2.443092
H	-2.040830	-1.469640	3.350803
H	-2.108531	-2.651557	4.555300
H	-2.034980	-4.956988	3.795427
N	-1.055745	-1.596166	1.249276
H	-0.025329	-0.749759	-0.343138
N	-1.105033	-2.941816	1.573517
N	-1.393773	-4.591659	3.126756
N	-2.116473	-2.436266	3.583049
C	-0.980324	-1.093622	0.020092
C	-2.135355	-0.711274	-0.767612
C	-3.450456	-1.030873	-0.393250
N	-1.846630	-0.054309	-1.906583
C	-4.493205	-0.662793	-1.238214
C	-2.844834	0.288637	-2.704461
C	-4.188882	0.009971	-2.420142
H	-3.637919	-1.549843	0.525602
H	-2.574933	0.807847	-3.605954
H	-4.958499	0.313761	-3.104484
H	-5.510742	-0.895510	-0.983559
Br	-0.112847	-5.631911	0.163269

23
CCNN: 120.64 CNNC: 195.53 E(S0): -3115.33093 E(S1): -3115.23501

C	-1.545536	-3.402099	2.762602

H	-0.502204	-3.574303	1.044580
H	-0.634624	-5.168596	2.531099
H	-2.491474	-1.706303	3.246007
H	-2.419025	-2.856644	4.484674
H	-1.769733	-5.098999	3.805561
N	-1.347758	-1.647385	1.241860
H	-0.204624	-1.182578	-0.453948
N	-1.097209	-2.962365	1.608086
N	-1.170627	-4.607038	3.180599
N	-2.374217	-2.659510	3.510031
C	-1.183963	-1.279131	-0.012980
C	-2.279908	-0.729049	-0.796353
C	-3.615798	-0.765574	-0.371956
N	-1.913179	-0.237809	-1.991741
C	-4.599340	-0.283373	-1.230773
C	-2.856000	0.215602	-2.803321
C	-4.216418	0.216515	-2.473873
H	-3.864224	-1.170667	0.588702
H	-2.523098	0.594396	-3.752377
H	-4.939444	0.594235	-3.171843
H	-5.633783	-0.304970	-0.941911
Br	-0.048261	-5.638941	0.183182

23

CCNN: 146.66 CNNC: 189.95 E(S0): -3115.37782 E(S1): -3115.20176

C	-1.601816	-3.534974	2.806775
H	-0.585381	-3.576491	1.070525
H	-0.419897	-5.131718	2.588381
H	-2.843249	-2.030409	3.259656
H	-2.545007	-3.113054	4.528865
H	-1.500687	-5.211374	3.901821
N	-1.789732	-1.825268	1.209480
H	-0.592098	-1.702152	-0.482788
N	-1.258686	-3.057542	1.634296
N	-1.010326	-4.642041	3.248557
N	-2.541087	-2.934077	3.549989
C	-1.556646	-1.537655	-0.028316
C	-2.516012	-0.781047	-0.845447
C	-3.835402	-0.543051	-0.445954
N	-2.040691	-0.410158	-2.039364
C	-4.692183	0.096368	-1.338807
C	-2.861584	0.200885	-2.886008
C	-4.198288	0.476190	-2.587168
H	-4.174030	-0.871455	0.516711
H	-2.442445	0.478328	-3.835537
H	-4.822938	0.964388	-3.311204
H	-5.716472	0.281300	-1.073866

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Br      0.059115    -5.621244    0.208730
23
CCNN:  168.01 CNNC:  184.69 E(S0): -3115.39838 E(S1): -3115.21683
C      -1.804359    -3.693445    2.773546
H      -0.843338    -3.722799    1.012521
H      -0.460911    -5.165119    2.593881
H      -3.224115    -2.338295    3.179439
H      -2.793180    -3.330302    4.488149
H      -1.490200    -5.289944    3.943575
N      -2.229222    -2.142974    1.091088
H      -1.039562    -2.204676   -0.616720
N      -1.532736    -3.222134    1.579210
N      -1.082128    -4.705755    3.247987
N      -2.800925    -3.178982    3.504791
C      -1.930518    -1.838276   -0.134930
C      -2.756216    -0.875290   -0.929859
C      -4.022439    -0.450780   -0.534576
N      -2.196373    -0.518550   -2.091234
C      -4.734736     0.372318   -1.394846
C      -2.885480     0.275853   -2.899237
C      -4.163594     0.742312   -2.592414
H      -4.436923    -0.777559    0.398852
H      -2.408728     0.544816   -3.823681
H      -4.686575     1.371319   -3.288238
H      -5.722472     0.705352   -1.133716
Br      0.227282    -5.574068    0.257224
23
CCNN:  179.68 CNNC:  182.73 E(S0): -3115.40299 E(S1): -3115.22124
C      -1.971684    -3.802363    2.653184
H      -1.057310    -3.884981    0.867333
H      -0.515197    -5.181232    2.548474
H      -3.485209    -2.529118    2.994997
H      -3.004460    -3.444036    4.353212
H      -1.481313    -5.241255    3.970202
N      -2.551533    -2.401270    0.897094
H      -1.473193    -2.545321   -0.880289
N      -1.741788    -3.372522    1.430408
N      -1.184697    -4.736720    3.166247
N      -2.981785    -3.301314    3.369478
C      -2.277734    -2.086321   -0.330437
C      -3.077249    -1.046251   -1.056459
C      -4.234694    -0.471456   -0.535033
N      -2.582088    -0.725884   -2.255780
C      -4.896081     0.478468   -1.296851
C      -3.224530     0.188084   -2.974393
C      -4.388721     0.818071   -2.532857
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H	-4.600019	-0.766181	0.427890
H	-2.801248	0.423889	-3.932554
H	-4.874295	1.548880	-3.153602
H	-5.794971	0.940543	-0.928160
Br	0.452428	-5.496450	0.326878

Geometries from MECI$_2$ to Z_2 on the S$_0$ surface.
23
CCNN: 92.49 CNNC: 198.54 E(S0): -3115.28409 E(S1): -3115.28409

C	-1.534444	-3.318416	2.748480
H	-0.698144	-3.642522	0.936824
H	-1.026208	-5.237504	2.443092
H	-2.040830	-1.469640	3.350803
H	-2.108531	-2.651557	4.555300
H	-2.034980	-4.956988	3.795427
N	-1.055745	-1.596166	1.249276
H	-0.025329	-0.749759	-0.343138
N	-1.105033	-2.941816	1.573517
N	-1.393773	-4.591659	3.126756
N	-2.116473	-2.436266	3.583049
C	-0.980324	-1.093622	0.020092
C	-2.135355	-0.711274	-0.767612
C	-3.450456	-1.030873	-0.393250
N	-1.846630	-0.054309	-1.906583
C	-4.493205	-0.662793	-1.238214
C	-2.844834	0.288637	-2.704461
C	-4.188882	0.009971	-2.420142
H	-3.637919	-1.549843	0.525602
H	-2.574933	0.807847	-3.605954
H	-4.958499	0.313761	-3.104484
H	-5.510742	-0.895510	-0.983559
Br	-0.112847	-5.631911	0.163269

23
CCNN: 56.17 CNNC: 198.13 E(S0): -3115.34848 E(S1): -3115.22138

C	-1.385932	-3.205814	2.790181
H	-1.036031	-3.457420	0.812111
H	-1.427452	-5.148853	2.262910
H	-1.224102	-1.386385	3.607187
H	-1.363351	-2.652269	4.716352
H	-2.063379	-4.789493	3.817052
N	-0.721275	-1.440722	1.398340
H	0.033369	-0.297312	-0.055064
N	-1.121953	-2.783698	1.574994
N	-1.515238	-4.504155	3.036505
N	-1.522692	-2.320804	3.790825
C	-0.804236	-0.917348	0.207512

C	-1.970708	-0.803374	-0.679900
C	-3.214416	-1.404044	-0.437296
N	-1.748461	-0.023448	-1.747417
C	-4.253185	-1.175863	-1.335646
C	-2.740871	0.182550	-2.602929
C	-4.015849	-0.366621	-2.444110
H	-3.368064	-2.011236	0.432522
H	-2.518210	0.813626	-3.443809
H	-4.786343	-0.161201	-3.163142
H	-5.219683	-1.614973	-1.172052
Br	-0.284474	-5.572893	0.121269

23

CCNN: 25.91 CNNC: 201.45 E(S0): -3115.38713 E(S1): -3115.20800

C	-0.952387	-3.081239	2.906371
H	-0.888724	-3.372031	0.912554
H	-1.211614	-5.014306	2.400494
H	-0.517457	-1.288307	3.678493
H	-0.618900	-2.542048	4.811710
H	-1.582003	-4.619916	4.037909
N	-0.304107	-1.381981	1.427764
H	0.053650	0.040642	0.121819
N	-0.848618	-2.675544	1.658673
N	-1.164679	-4.361904	3.172283
N	-0.858457	-2.196816	3.909437
C	-0.573425	-0.810222	0.312374
C	-1.692845	-0.922136	-0.654226
C	-2.776944	-1.803965	-0.579852
N	-1.606348	0.023370	-1.602079
C	-3.805070	-1.675064	-1.514581
C	-2.579161	0.129197	-2.496929
C	-3.708495	-0.692772	-2.494806
H	-2.840344	-2.553187	0.179985
H	-2.461239	0.900460	-3.235940
H	-4.476455	-0.559477	-3.233358
H	-4.657166	-2.326785	-1.470117
Br	-0.644181	-5.513086	0.081072

23

CCNN: 7.31 CNNC: 189.68 E(S0): -3115.39553 E(S1): -3115.21561

C	-0.416228	-3.047239	2.958908
H	-0.800270	-3.209918	0.979545
H	-0.767993	-4.942746	2.369489
H	0.150773	-1.289860	3.716747
H	0.320755	-2.611068	4.781877
H	-0.563730	-4.711717	4.078812
N	-0.216916	-1.230493	1.525941
H	-0.118752	0.353588	0.366255

N	-0.667929	-2.540728	1.753637
N	-0.552523	-4.337187	3.157580
N	-0.079628	-2.230281	3.955049
C	-0.581156	-0.610222	0.465864
C	-1.541906	-0.898214	-0.625935
C	-2.501138	-1.915075	-0.648592
N	-1.443643	0.013665	-1.607294
C	-3.375657	-1.982872	-1.734715
C	-2.271561	-0.062691	-2.639276
C	-3.260950	-1.043600	-2.752711
H	-2.586902	-2.635902	0.135179
H	-2.148575	0.685365	-3.401215
H	-3.911813	-1.059466	-3.606582
H	-4.118377	-2.756925	-1.774509
Br	-1.035673	-5.455125	0.117820

23

CCNN: 0.34 CNNC: 180.36 E(S0): -3115.39695 E(S1): -3115.21543

C	-0.159305	-3.037706	2.929648
H	-0.785818	-3.085868	1.008897
H	-0.564219	-4.907447	2.283591
H	0.435636	-1.300656	3.739092
H	0.688508	-2.678668	4.733899
H	0.079615	-4.789798	3.891048
N	-0.319862	-1.092100	1.665747
H	-0.406404	0.552269	0.597564
N	-0.610122	-2.466647	1.812963
N	-0.239700	-4.340479	3.063938
N	0.314405	-2.274124	3.907403
C	-0.725062	-0.473295	0.624641
C	-1.501670	-0.890546	-0.569504
C	-2.457565	-1.905491	-0.600873
N	-1.217171	-0.130871	-1.637346
C	-3.111023	-2.167404	-1.806527
C	-1.840633	-0.384926	-2.779510
C	-2.793882	-1.398288	-2.920076
H	-2.695308	-2.484626	0.265952
H	-1.577418	0.241151	-3.612047
H	-3.265636	-1.567104	-3.869554
H	-3.831859	-2.960369	-1.862513
Br	-1.257133	-5.388257	0.145743