# Supporting Information

# Revising Intramolecular Photoinduced Electron Transfer (PET) from First Principles

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## I. Computational Details.

Ground state geometry optimizations and analytical frequency calculations were performed with DFT (PBE0).[1-2] Excited-state geometry optimizations and numerical frequency calculations were carried out with TD-DFT. PBE0 is also used in the TD-DFT calculations, since this functional is found to provide a good balance between local excited (LE) and intramolecular charge transfer (ICT) states, with average absolute errors of ca. 0.14 eV for the low-lying excited states of conjugated organic compounds.[3] The def2-SVP basis sets were used for all atoms. These PBE0 and TD-PBE0 calculations were performed with the TURBOMOLE V6.6 program package.[4] For **7**-**8** the N-butyl chain is substituted by a N-methyl chain. In the case of the latter compounds, single-point ADC(2)/def2-TZVP calculations, as implemented in the TURBOMOLE V6.6 program package, were performed at all their stationary points along their photodeactivation pathways. The ADC(2)/def2-TZVP mean errors for the singlet excitation energies of organic compounds are ca. 0.22 eV,[5] and thus herein these results are considered our best theoretical estimators. The ($\pi\pi^*$/ $n\pi^*$) conical intersection of **7** was optimized with the complete active space self-consistent field (CASSCF)[6] method using the 6-31G basis set. In these calculations, the (4/3) active space, which includes all orbitals needed to describe both excited states simultaneously was chosen. Single-point CASPT2(4,3)/6-31G* calculations were performed at all the stationary points along the photodeactivation pathways of **7** to incorporate the effect of dynamic electron correlation. The conical intersection optimization and the single-point CASPT2 calculations were performed with the Gaussian09[7] and the MOLCAS 7.0[8] quantum chemistry packages, respectively.

For the rate calculations the MOMAP suite of programs was used.[9] The radiative and nonradiave rates are evaluated by using the thermal vibration correlation function (TVCF) theory. For the rate calculations, the difference between two electronic state PESs was considered by using $\underline{Q_e} = S\,\underline{Q_g} + \underline{D_e}$, where $S$ is the Duschinsky rotation matrix, $\underline{Q_e}$ and $\underline{Q_g}$ are the normal-mode coordinates of the ground and excited states, respectively; and $\underline{D_e}$ is the displacement between the minima of

the excited and ground state geometries. First-order perturbation theory was applied to compute the non-adiabatic electronic coupling, which required the evaluation of the transition electric field. Herein, the transition electric field was evaluated at the TD-PBE0/6-31G* level of theory with the Gaussian09 package. The derivatives of the transition dipole moments were calculated numerically around the equilibrium geometry of the ground state at the TD-PBE0/def2-SVP level of theory with the TURBOMOLE v6.6 program. The theoretical formalisms for calculating $k_r$ and $k_{nr}$ can be found below.

## II. Theoretical formalism to compute $k_{nr}$

According to the Fermi Golden Rule and the first-order perturbation theory, the nonradiative decay rate constant between two electronic states with same spin manifold can be written as

$$k_{nr} = \frac{2\pi}{\hbar}\sum_{kl} R_{kl}\, Z_i^{-1} \sum_{v,u} e^{-\beta E_{iv}} \langle \Theta_{fu} | \widehat{P_{fk}} | \Theta_{iv} \rangle \langle \Theta_{iv} | \widehat{P_{fl}} | \Theta_{fu} \rangle \delta(E_{iv} - E_{fu})$$

(S1),

where, $\hbar$ is the Planck constant, $\widehat{P_{fl}}$ is the normal momemtum operator of the *l*th normal mode in the final electronic state, $\Theta$ denotes the nuclear vibrational wave functions, v and u are the vibrational quantum numbers of the initial and final state, respectively, $Z_i$ is the partition function, $\beta = (k_B T)^{-1}$ and $R_{kl} = \langle \Phi_f | \widehat{P_{fk}} | \Phi_i \rangle \langle \Phi_i | \widehat{P_{fl}} | \Phi_f \rangle$ is the nonadiabatic electronic coupling. Applying the Fourier transform of the delta function, eq. S1 recasts into the following time-dependent form

$$k_{nr} = \sum_{kl} \frac{1}{\hbar^2} R_{kl} \int_{-\infty}^{\infty} dt \left[ e^{i w_{if} t} Z_i^{-1} \rho_{nr,kl}(t,T) \right]$$

(S2),

where $\rho_{nr,kl}(t,T)$ is the thermal vibration correlation function. More details of the correlation function part can be found somewhere else.[10]

**Theoretical formalism to compute $k_r$**

The radiative decay rate is obtained by integrating the light emission spectrum:

$$k_r = \int_0^\infty \sigma_{em}(\omega)d\omega = \int_0^\infty \sigma_{em}^{FC}(\omega)d\omega + \sum_k \sigma_{em,k}^{FC/HT}(\omega)d\omega + \sum_{k,l} \sigma_{em,kl}^{HT}(\omega)d\omega$$

(S3),

where these terms correspond to the Franck-Condon (FC), Franck-Condon-Herzberg-Teller (FCHT) and Herzberg-Teller (HT) contributions to the emission spectrum. According to the TVCF theory these terms have the following form

$$\sigma_{em}^{FC}(\omega) = \frac{2\omega^3}{3\pi\hbar c^3}|\overrightarrow{\mu_0}|^2 \int_{-\infty}^{\infty} e^{-i(\omega-\omega_{if})t} Z_{iv}^{-1}\, \rho_{em,0}^{FC}(t,T)dt$$

(S4),

$$\sigma_{em}^{FC/HT}(\omega) = \frac{2\omega^3}{3\pi\hbar c^3}\sum_k \overrightarrow{\mu_k}\,\overrightarrow{\mu_0} \int_{-\infty}^{\infty} e^{-i(\omega-\omega_{if})t} Z_{iv}^{-1}\, \rho_{em,k}^{FC/HT}(t,T)dt$$

(S5),

$$\sigma_{em}^{HT}(\omega) = \frac{2\omega^3}{3\pi\hbar c^3}\sum_{k,l} \overrightarrow{\mu_k}\,\overrightarrow{\mu_l} \int_{-\infty}^{\infty} e^{-i(\omega-\omega_{if})t} Z_{iv}^{-1}\, \rho_{em,kl}^{HT}(t,T)dt$$

(S6).

For strongly dipole-allowed transition, the spectrum is dominated by the zero-order term, i.e. FC, while for forbidden (or weakly dipole-allowed transitions), the other terms are necessary (HT approximation). More details can be found somewhere else.[10]

## III. Absorption and emission properties of compounds 1-6.

Table S1. Theoretical (PCM-TD-PBE0) and experimental absorption and emission maxima (in nm) for compounds 1-6.

| Compound | $\lambda_{absorption}$ (nm) [PCM-TD-PBE0/6-31G(d)] | $\lambda_{absorption}$ (nm) [Exp.] | $\lambda_{emission}$ (nm) [PCM-TD-PBE0/6-31G(d)][a] | $\lambda_{emission}$ (nm) [Exp.] |
|---|---|---|---|---|
| **1** | 374.4 | -[e] | - | -[e] |
| **2** | 362.1 | -[e] | 427.8 | 450[b] |
| **3** | 390.6 | -[e] | - | -[e] |
| **4** | 383.9 | 368[c] | 453.4 | 414[c] |
| **5** | 503.6 | 568[d] | 533.3 | 591[d] |
| **6** | 522.3 | -[e] | - | -[e] |

[a] Obtained vertically at the optimized excited state geometries. [b] Values obtained from Ref. 11 in acetonitrile. [c] Values obtained from Ref. 12 in methanol. [d] Values obtained from Ref. 13 in acetonitrile. [e] Values not determined experimentally.

## IV. Absorption and emission properties of compounds 7-8

Exemplarily for **7**, its excitation energy at the ADC(2)/def2-TZVP level of theory (3.54 eV, see Table S1) is in good agreement with the experimental absorption maxima, which peaks at 3.40 eV.[14] TD-PBE0 is also in reasonable agreement with the experiment (excitation energies within 0.2 eV). Exemplarily for **7**, the computed fluorescence emission energy at the ADC(2)/def2-TZVP level of theory (3.11 eV, see Table 1) is also in good agreement with the experiment, which shows a vibronically resolved spectrum peaking at 2.99 and 3.16 eV. Again, TD-PBE0 is in reasonable agreement with the experiment (within 0.2 eV).

Table S2. Lowest vertical (at the $S_0$ optimized geometry) and vertical relaxed (at the $\pi\pi^*$ and $n\pi^*$ optimized geometries) singlet electronic transition energies (in eV) and oscillator strengths (in parenthesis) of 7 and 8 calculated at different levels of theory.

| | | $(S_0)_{min}$ | | $(\pi\pi^*)_{min}$ | | $(n\pi^*)_{min}$ | |
|---|---|---|---|---|---|---|---|
| Compound | States | ADC(2)/ def2-TZVP | TD-PBE0/ def2-SVP | ADC(2)/ def2-TZVP | TD-PBE0/ def2-SVP | ADC(2)/ def2-TZVP | TD-PBE0/ def2-SVP |
| **7** | $\pi\pi^*$ | 3.54 (0.122) | 3.26 (0.109) | 3.11 (0.127) | 2.83 (0.116) | 3.25 (0.122) | 2.97 (0.110) |
| | $n\pi^*$ | 3.82 (0.001) | 3.60 (0.000) | 3.67 (0.000) | 3.33 (0.000) | 3.00 (0.000) | 2.11 (0.000) |
| **8** | $\pi\pi^*$ | 3.42 (0.122) | 3.19 (0.107) | 2.94 (0.116) | 2.77 (0.104) | - | - |

## V. Kohn-Sham orbitals (PBE0/def2-SVP) involved in the electronic excitations of 1-6.

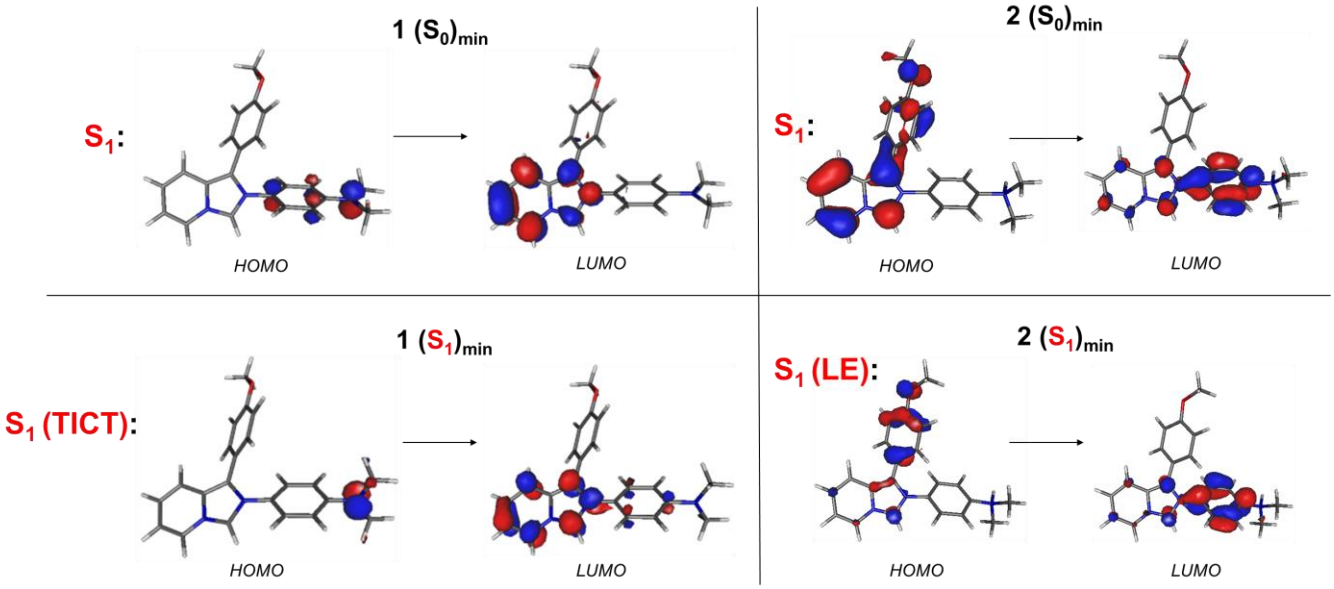


Figure S1. Kohn-Sham orbitals (PBE0/def2-SVP) involved in the electronic excitations of 1-2.

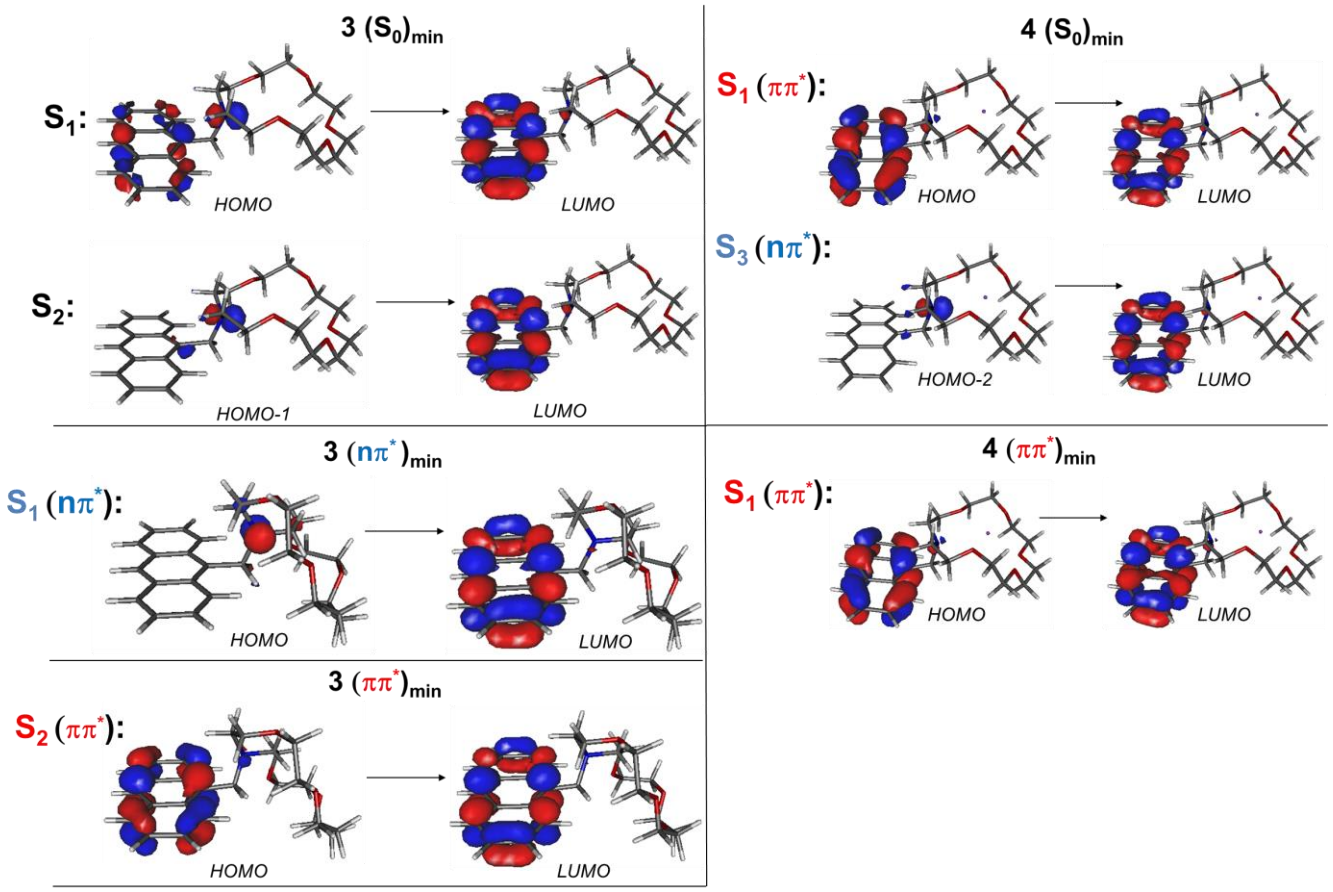


Figure S2. Kohn-Sham orbitals (PBE0/def2-SVP) involved in the electronic excitations of 3-4.

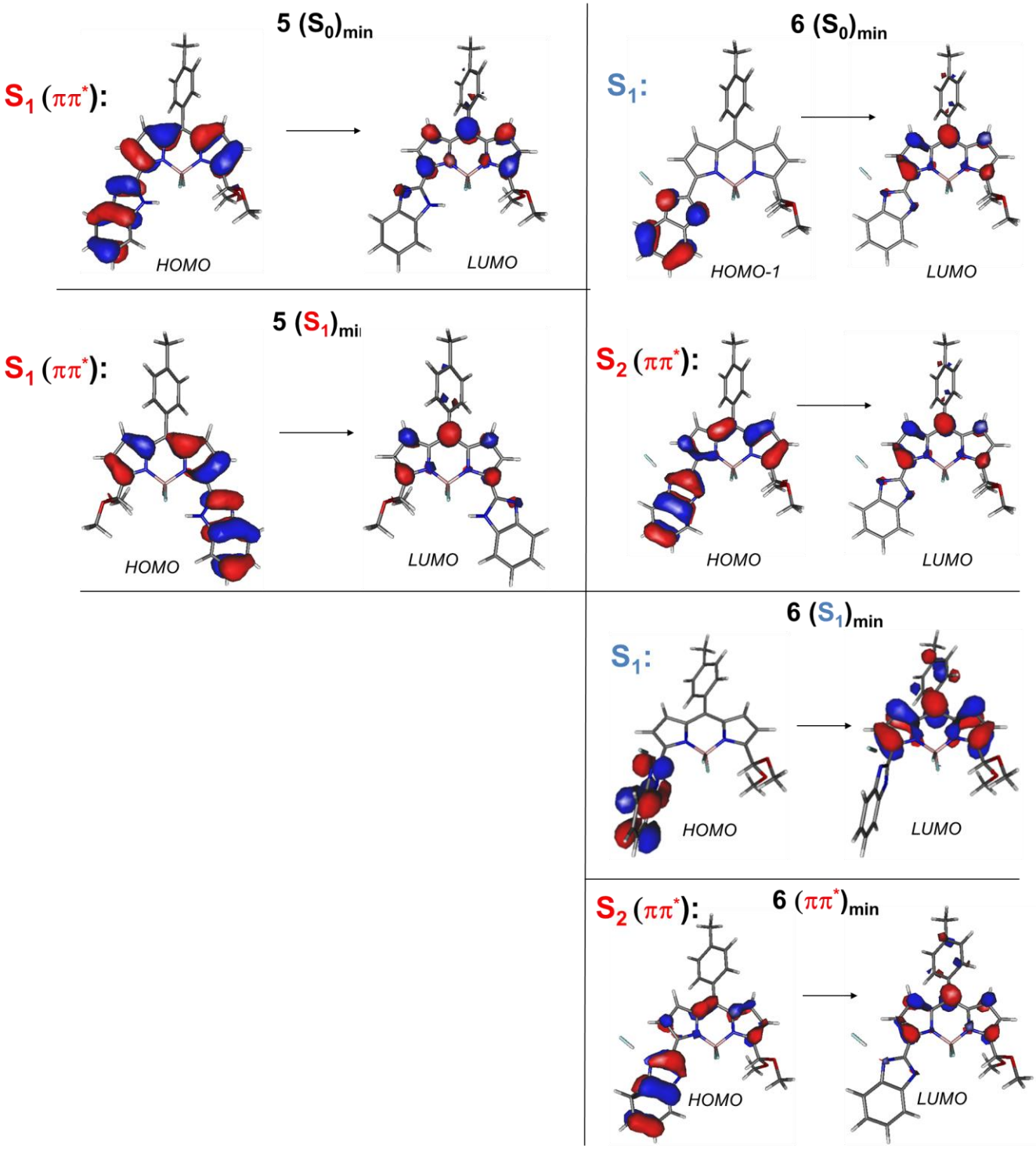


Figure S3. Kohn-Sham orbitals (PBE0/def2-SVP) involved in the electronic excitations of 5-6.

## VI. Cartesian coordinates of the optimized geometries of 1-8:

### 1 ($S_0$)$_{min}$

| | | | |
|---|---|---|---|
| C | -2.3789852 | 5.2546964 | -0.0986063 |
| C | -1.8378185 | 6.5648699 | -0.0717340 |
| C | -2.6815095 | 7.6365282 | -0.1537090 |
| C | -4.0917675 | 7.4344764 | -0.2646247 |
| C | -4.6210398 | 6.1840711 | -0.2668558 |
| C | -4.0554520 | 3.7907907 | -0.1302814 |
| C | -1.8315257 | 3.9742358 | -0.0149275 |
| H | -0.7576836 | 6.6829968 | 0.0224209 |
| H | -2.2856029 | 8.6529277 | -0.1299983 |
| H | -4.7667725 | 8.2880861 | -0.3417545 |
| H | -5.6860844 | 5.9616597 | -0.3372305 |
| N | -3.7676683 | 5.0998943 | -0.1709505 |
| N | -2.9046200 | 3.1071575 | -0.0363984 |
| C | -2.8636051 | 1.6774535 | 0.0071862 |
| C | -2.1080724 | 0.9620013 | -0.9243182 |
| C | -3.6090024 | 0.9920763 | 0.9678991 |
| C | -2.1011907 | -0.4210541 | -0.8979508 |
| H | -1.5259794 | 1.4900402 | -1.6820736 |
| C | -3.6096490 | -0.3925837 | 0.9975656 |
| H | -4.1837932 | 1.5450507 | 1.7153003 |
| C | -2.8549221 | -1.1469696 | 0.0622711 |
| H | -1.5074050 | -0.9483339 | -1.6431466 |
| H | -4.1968342 | -0.8939840 | 1.7653327 |
| H | -5.0439864 | 3.3478074 | -0.2087805 |
| C | 0.5314219 | 4.1683372 | -0.7327003 |
| C | 1.8833153 | 3.8609520 | -0.6110220 |
| C | 2.3045307 | 2.9515074 | 0.3695456 |
| C | 1.3474489 | 2.3611107 | 1.2155187 |
| C | 0.0077601 | 2.6743869 | 1.0883915 |
| C | -0.4268818 | 3.5895928 | 0.1097353 |
| H | 0.2173029 | 4.8588252 | -1.5196969 |
| H | 2.5987717 | 4.3260039 | -1.2893464 |
| H | 1.6938524 | 1.6606629 | 1.9776257 |
| H | -0.7134848 | 2.2133764 | 1.7663944 |
| O | 3.5728855 | 2.5894034 | 0.5700986 |
| C | 4.5901254 | 3.1455642 | -0.2281486 |
| H | 5.5330410 | 2.7081980 | 0.1204377 |
| H | 4.4511234 | 2.8959791 | -1.2936150 |
| H | 4.6399267 | 4.2417181 | -0.1146682 |
| N | -2.8526014 | -2.5071010 | 0.0852444 |
| C | -3.6416929 | -3.2166170 | 1.0654864 |
| H | -4.7163486 | -2.9815106 | 0.9771469 |
| H | -3.5245229 | -4.2956637 | 0.9141964 |
| H | -3.3239290 | -2.9865093 | 2.0972867 |
| C | -2.0637719 | -3.2483818 | -0.8717326 |
| H | -0.9897185 | -3.0076438 | -0.7937732 |

| | | | |
|---|---|---|---|
| **H** | **-2.1780332** | **-4.3216991** | **-0.6821721** |
| **H** | **-2.3843530** | **-3.0558227** | **-1.9103345** |

**1 $(S_1)_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-2.3656155** | **5.2075256** | **-0.2013588** |
| **C** | **-1.8219509** | **6.5119035** | **-0.3010156** |
| **C** | **-2.6733503** | **7.5982045** | **-0.3932097** |
| **C** | **-4.0687395** | **7.4124846** | **-0.3902377** |
| **C** | **-4.6000886** | **6.1432357** | **-0.2685943** |
| **C** | **-4.0667443** | **3.7668646** | **0.0171733** |
| **C** | **-1.8147570** | **3.9366669** | **-0.0771773** |
| **H** | **-0.7376680** | **6.6294769** | **-0.3019681** |
| **H** | **-2.2602373** | **8.6068583** | **-0.4699050** |
| **H** | **-4.7505972** | **8.2603586** | **-0.4757094** |
| **H** | **-5.6685029** | **5.9257568** | **-0.2386862** |
| **N** | **-3.7621378** | **5.0670674** | **-0.1572179** |
| **N** | **-2.8955730** | **3.0362125** | **0.0309267** |
| **C** | **-2.8686338** | **1.6462023** | **0.0294431** |
| **C** | **-1.8256362** | **0.9292641** | **-0.5908833** |
| **C** | **-3.9223257** | **0.9237236** | **0.6246597** |
| **C** | **-1.8356662** | **-0.4567886** | **-0.6077015** |
| **H** | **-1.0096039** | **1.4615070** | **-1.0789958** |
| **C** | **-3.9360926** | **-0.4637962** | **0.6035183** |
| **H** | **-4.7276080** | **1.4508705** | **1.1391908** |
| **C** | **-2.8905067** | **-1.1497675** | **-0.0108726** |
| **H** | **-1.0202928** | **-0.9917532** | **-1.1028605** |
| **H** | **-4.7610551** | **-1.0013999** | **1.0795985** |
| **H** | **-5.0588678** | **3.3502409** | **-0.1218129** |
| **C** | **0.5827188** | **4.0866421** | **-0.7319604** |
| **C** | **1.9369832** | **3.8309235** | **-0.5148507** |
| **C** | **2.3333897** | **3.0505750** | **0.5779415** |
| **C** | **1.3502106** | **2.5406017** | **1.4428642** |
| **C** | **0.0105985** | **2.8151349** | **1.2269031** |
| **C** | **-0.4071294** | **3.5952509** | **0.1296795** |
| **H** | **0.2904616** | **4.6790852** | **-1.6042526** |
| **H** | **2.6722194** | **4.2402386** | **-1.2102173** |
| **H** | **1.6769499** | **1.9478352** | **2.3010356** |
| **H** | **-0.7319431** | **2.4384762** | **1.9369032** |
| **O** | **3.6047369** | **2.7407700** | **0.8764879** |
| **C** | **4.6425606** | **3.2660872** | **0.0915360** |
| **H** | **5.5811002** | **2.9071498** | **0.5383354** |
| **H** | **4.5833935** | **2.9111258** | **-0.9547973** |
| **H** | **4.6389689** | **4.3723216** | **0.1012327** |
| **N** | **-2.9008006** | **-2.5930370** | **-0.0374453** |
| **C** | **-2.3087870** | **-3.3085912** | **1.0459061** |
| **H** | **-2.8601249** | **-3.0618985** | **1.9745862** |
| **H** | **-2.3210150** | **-4.3925439** | **0.8714212** |
| **H** | **-1.2779306** | **-2.9408328** | **1.1972169** |

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|---|---|---|---|
| **C** | **-3.4991963** | **-3.2577893** | **-1.1488670** |
| **H** | **-2.9449188** | **-2.9789015** | **-2.0666602** |
| **H** | **-3.4989447** | **-4.3480117** | **-1.0188707** |
| **H** | **-4.5260563** | **-2.8729710** | **-1.2858938** |

**2 $(S_0)_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-2.3791625** | **5.1990295** | **-0.2007592** |
| **C** | **-1.8688144** | **6.5200344** | **-0.1308106** |
| **C** | **-2.7268160** | **7.5708959** | **-0.2941840** |
| **C** | **-4.1163256** | **7.3352479** | **-0.5286899** |
| **C** | **-4.6184608** | **6.0743057** | **-0.5731193** |
| **C** | **-4.0192001** | **3.6979159** | **-0.3702492** |
| **C** | **-1.8043105** | **3.9340544** | **-0.0680411** |
| **H** | **-0.8042371** | **6.6632859** | **0.0588885** |
| **H** | **-2.3588393** | **8.5970082** | **-0.2416069** |
| **H** | **-4.8004218** | **8.1742217** | **-0.6680784** |
| **H** | **-5.6681879** | **5.8286923** | **-0.7363542** |
| **N** | **-3.7512256** | **5.0089954** | **-0.3961753** |
| **N** | **-2.8554572** | **3.0410087** | **-0.1788242** |
| **C** | **-2.7727783** | **1.6154554** | **-0.1661234** |
| **C** | **-1.8758533** | **0.9650341** | **-1.0138777** |
| **C** | **-3.6144692** | **0.8876641** | **0.6764873** |
| **C** | **-1.8279805** | **-0.4258310** | **-1.0190168** |
| **H** | **-1.2197760** | **1.5383175** | **-1.6704949** |
| **C** | **-3.5739511** | **-0.5040555** | **0.6651334** |
| **H** | **-4.2955999** | **1.4031560** | **1.3568265** |
| **C** | **-2.6783212** | **-1.1460609** | **-0.1846306** |
| **H** | **-1.1258782** | **-0.9322310** | **-1.6879877** |
| **H** | **-4.2394222** | **-1.0580046** | **1.3307886** |
| **H** | **-4.9910714** | **3.2404755** | **-0.5333979** |
| **C** | **0.6038124** | **4.1516795** | **-0.6090713** |
| **C** | **1.9451564** | **3.8778001** | **-0.3685175** |
| **C** | **2.3059703** | **3.0135707** | **0.6789051** |
| **C** | **1.2926846** | **2.4327400** | **1.4687735** |
| **C** | **-0.0371395** | **2.7132808** | **1.2239629** |
| **C** | **-0.4097328** | **3.5799121** | **0.1758105** |
| **H** | **0.3423744** | **4.8139913** | **-1.4385588** |
| **H** | **2.7045813** | **4.3375740** | **-1.0008988** |
| **H** | **1.5950883** | **1.7838633** | **2.2926946** |
| **H** | **-0.7986833** | **2.2839324** | **1.8799037** |
| **O** | **3.5521000** | **2.6902669** | **0.9966149** |
| **C** | **4.6369610** | **3.2665130** | **0.2969863** |
| **H** | **5.5472165** | **2.8662331** | **0.7572627** |
| **H** | **4.6193143** | **2.9880285** | **-0.7692492** |
| **H** | **4.6364319** | **4.3641310** | **0.3947446** |
| **N** | **-2.6129206** | **-2.6206084** | **-0.2127014** |
| **C** | **-2.1272706** | **-3.2062258** | **1.0779810** |
| **H** | **-2.8705503** | **-3.0123080** | **1.8604476** |
| **H** | **-2.0004758** | **-4.2885151** | **0.9470550** |

| | | | |
|---|---|---|---|
| **H** | **-1.1714666** | **-2.7379155** | **1.3418297** |
| **C** | **-3.8889762** | **-3.2545441** | **-0.6755256** |
| **H** | **-4.1734765** | **-2.8162362** | **-1.6395611** |
| **H** | **-3.7266483** | **-4.3351185** | **-0.7790981** |
| **H** | **-4.6718352** | **-3.0685277** | **0.0692718** |
| **H** | **-1.9044400** | **-2.8539051** | **-0.9187371** |

**2 ($S_1$)$_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-2.3804060** | **5.2153310** | **-0.4502863** |
| **C** | **-1.9671523** | **6.5621503** | **-0.5346717** |
| **C** | **-2.9232434** | **7.5532489** | **-0.5896482** |
| **C** | **-4.3050771** | **7.2374255** | **-0.5582270** |
| **C** | **-4.7045371** | **5.9359748** | **-0.4441739** |
| **C** | **-3.9168076** | **3.6147302** | **-0.2702945** |
| **C** | **-1.7283861** | **3.9735471** | **-0.3320481** |
| **H** | **-0.9058656** | **6.8072975** | **-0.5397940** |
| **H** | **-2.6142324** | **8.5986278** | **-0.6535731** |
| **H** | **-5.0599765** | **8.0231438** | **-0.6107656** |
| **H** | **-5.7441940** | **5.6110120** | **-0.3861325** |
| **N** | **-3.7476082** | **4.9535213** | **-0.3848609** |
| **N** | **-2.7324826** | **3.0104534** | **-0.1976836** |
| **C** | **-2.6116047** | **1.6020937** | **-0.0666455** |
| **C** | **-1.7508301** | **0.8610115** | **-0.9381800** |
| **C** | **-3.4452533** | **0.9183112** | **0.8513652** |
| **C** | **-1.7551790** | **-0.5162691** | **-0.8661809** |
| **H** | **-1.1394073** | **1.3606366** | **-1.6886495** |
| **C** | **-3.4404342** | **-0.4550685** | **0.9206794** |
| **H** | **-4.0781599** | **1.4816201** | **1.5413199** |
| **C** | **-2.5825690** | **-1.1893720** | **0.0487952** |
| **H** | **-1.1165877** | **-1.0804876** | **-1.5537706** |
| **H** | **-4.0728706** | **-0.9502838** | **1.6595732** |
| **H** | **-4.8752287** | **3.1017070** | **-0.3058457** |
| **C** | **0.5753446** | **4.5321640** | **-1.0459515** |
| **C** | **1.9370918** | **4.4440232** | **-0.8995272** |
| **C** | **2.4932008** | **3.5560711** | **0.0668465** |
| **C** | **1.6341508** | **2.7369551** | **0.8452289** |
| **C** | **0.2709766** | **2.8230794** | **0.6732558** |
| **C** | **-0.2980673** | **3.7478524** | **-0.2468650** |
| **H** | **0.1644941** | **5.1956566** | **-1.8086679** |
| **H** | **2.6237439** | **5.0331269** | **-1.5106192** |
| **H** | **2.0443659** | **2.0436343** | **1.5798096** |
| **H** | **-0.3828068** | **2.1979562** | **1.2810321** |
| **O** | **3.7956213** | **3.5602430** | **0.1486829** |
| **C** | **4.5124247** | **2.7482106** | **1.0740646** |
| **H** | **5.5699929** | **2.9878032** | **0.9232644** |
| **H** | **4.2174540** | **2.9918013** | **2.1055546** |
| **H** | **4.3382422** | **1.6827244** | **0.8625693** |
| **N** | **-2.6616855** | **-2.6542886** | **-0.0022488** |
| **C** | **-2.3470014** | **-3.3208674** | **1.2969934** |

| | | | |
|---|---|---|---|
| **H** | **-3.1159088** | **-3.0517899** | **2.0302539** |
| **H** | **-2.3414101** | **-4.4091543** | **1.1537552** |
| **H** | **-1.3675201** | **-2.9709054** | **1.6414574** |
| **C** | **-3.9526233** | **-3.1559715** | **-0.5719242** |
| **H** | **-4.0951236** | **-2.7046909** | **-1.5605985** |
| **H** | **-3.9189450** | **-4.2507402** | **-0.6468122** |
| **H** | **-4.7686261** | **-2.8509481** | **0.0935608** |
| **H** | **-1.9277813** | **-2.9440780** | **-0.6573913** |

**3 ($S_0$) $_{min}$**

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|---|---|---|---|
| **C** | **3.3364653** | **-3.7183770** | **-0.8791058** |
| **C** | **2.6787698** | **-2.5172856** | **-0.8553838** |
| **C** | **3.3527030** | **-1.2873254** | **-0.5632213** |
| **C** | **4.7743652** | **-1.3700043** | **-0.3265608** |
| **C** | **5.4225629** | **-2.6429909** | **-0.3383539** |
| **C** | **4.7279463** | **-3.7900801** | **-0.6031107** |
| **C** | **2.6952515** | **-0.0300748** | **-0.5290479** |
| **C** | **5.5025919** | **-0.2031208** | **-0.0967639** |
| **C** | **4.8942068** | **1.0511441** | **-0.1341719** |
| **C** | **3.4728791** | **1.1463938** | **-0.3684283** |
| **C** | **2.9248753** | **2.4672418** | **-0.4549013** |
| **H** | **1.8652272** | **2.5952325** | **-0.6698325** |
| **C** | **3.6976081** | **3.5867222** | **-0.2945799** |
| **C** | **5.0878183** | **3.4771859** | **-0.0245528** |
| **C** | **5.6644856** | **2.2402521** | **0.0491098** |
| **H** | **2.7852185** | **-4.6316877** | **-1.1161592** |
| **H** | **1.6144675** | **-2.5043010** | **-1.0831443** |
| **H** | **6.4968815** | **-2.6763319** | **-0.1383981** |
| **H** | **5.2369630** | **-4.7567203** | **-0.6135488** |
| **H** | **6.5772000** | **-0.2718112** | **0.0939796** |
| **H** | **3.2398222** | **4.5755736** | **-0.3777756** |
| **H** | **5.6891009** | **4.3787454** | **0.1133143** |
| **H** | **6.7355769** | **2.1356212** | **0.2417550** |
| **C** | **1.1751017** | **0.0533086** | **-0.6382767** |
| **H** | **0.8076968** | **-0.7456077** | **-1.2973586** |
| **H** | **0.8926280** | **0.9788495** | **-1.1595731** |
| **N** | **0.4204970** | **-0.0088498** | **0.6099035** |
| **C** | **-3.9722583** | **-3.1176885** | **1.2148164** |
| **H** | **-4.5185407** | **-4.0688044** | **1.0410750** |
| **H** | **-3.8736852** | **-2.9821226** | **2.3033937** |
| **C** | **-2.5792415** | **-3.2563453** | **0.6349596** |
| **H** | **-2.1849412** | **-4.2559808** | **0.9233492** |
| **H** | **-2.6159524** | **-3.2470960** | **-0.4751545** |
| **C** | **-0.4352843** | **-2.3608969** | **0.6639470** |
| **H** | **-0.4060546** | **-2.3023873** | **-0.4445670** |
| **H** | **-0.0260514** | **-3.3580563** | **0.9354829** |
| **C** | **0.4432422** | **-1.2887175** | **1.2887010** |
| **H** | **0.0585722** | **-1.1428951** | **2.3085992** |
| **H** | **1.4706736** | **-1.6928885** | **1.3993086** |

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|---|---|---|---|
| **C** | **0.5565360** | **1.1441682** | **1.4768038** |
| **H** | **1.6152456** | **1.4381812** | **1.6302979** |
| **H** | **0.1637775** | **0.8771259** | **2.4686899** |
| **C** | **-0.2294238** | **2.3687424** | **1.0370376** |
| **H** | **0.2498458** | **3.2735279** | **1.4690815** |
| **H** | **-0.1807288** | **2.4846385** | **-0.0653227** |
| **C** | **-2.3347354** | **3.3982447** | **1.1955456** |
| **H** | **-1.7474299** | **4.3294369** | **1.3344568** |
| **H** | **-3.1589835** | **3.4088155** | **1.9267040** |
| **C** | **-2.9507422** | **3.4099206** | **-0.1898427** |
| **H** | **-3.3135760** | **4.4378567** | **-0.4125032** |
| **H** | **-2.1824480** | **3.1747197** | **-0.9560467** |
| **O** | **-1.7511776** | **-2.2440678** | **1.1144398** |
| **O** | **-4.7057402** | **-2.0295684** | **0.7394258** |
| **O** | **-3.9971698** | **2.4926568** | **-0.2345325** |
| **O** | **-1.5528374** | **2.2741344** | **1.4741295** |
| **C** | **-5.2853211** | **-2.2089482** | **-0.5165153** |
| **C** | **-6.0231010** | **-0.9547185** | **-0.9076943** |
| **H** | **-6.0006024** | **-3.0595633** | **-0.5028949** |
| **H** | **-4.5302949** | **-2.4264717** | **-1.2972662** |
| **H** | **-6.6877082** | **-1.1790431** | **-1.7697679** |
| **H** | **-6.6702330** | **-0.6459322** | **-0.0622076** |
| **C** | **-4.5723562** | **2.3363329** | **-1.4931277** |
| **C** | **-5.6674645** | **1.3040017** | **-1.4143210** |
| **H** | **-3.8187536** | **2.0096625** | **-2.2389426** |
| **H** | **-5.0048994** | **3.2924264** | **-1.8590555** |
| **H** | **-6.2704613** | **1.3411659** | **-2.3471218** |
| **H** | **-6.3418711** | **1.5680139** | **-0.5748569** |
| **O** | **-5.1047764** | **0.0443566** | **-1.2236906** |

**3 ($n\pi^*$)$_{min}$**

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|---|---|---|---|
| **C** | **-3.0857880** | **3.8061286** | **0.3651713** |
| **C** | **-2.1955852** | **2.7547151** | **0.1543719** |
| **C** | **-2.6362900** | **1.4621961** | **-0.2278002** |
| **C** | **-4.0597746** | **1.2615427** | **-0.3783916** |
| **C** | **-4.9343431** | **2.3537466** | **-0.1538383** |
| **C** | **-4.4622120** | **3.6063713** | **0.2111548** |
| **C** | **-1.7622499** | **0.3514323** | **-0.4487748** |
| **C** | **-4.5375086** | **-0.0137356** | **-0.7389720** |
| **C** | **-3.6869325** | **-1.1113374** | **-0.9654035** |
| **C** | **-2.2580035** | **-0.9331192** | **-0.8244102** |
| **C** | **-1.4392178** | **-2.0648702** | **-1.0686554** |
| **H** | **-0.3553409** | **-1.9702270** | **-0.9908923** |
| **C** | **-1.9654467** | **-3.3061842** | **-1.4282132** |
| **C** | **-3.3489606** | **-3.4711113** | **-1.5539020** |
| **C** | **-4.1876316** | **-2.3884878** | **-1.3260840** |
| **H** | **-2.7017118** | **4.7890146** | **0.6504615** |
| **H** | **-1.1292728** | **2.9566557** | **0.2766224** |
| **H** | **-6.0081238** | **2.1854686** | **-0.2760565** |

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|---|---|---|---|
| **H** | **-5.1614644** | **4.4298518** | **0.3771757** |
| **H** | **-5.6163250** | **-0.1562405** | **-0.8491449** |
| **H** | **-1.2911478** | **-4.1460698** | **-1.6187322** |
| **H** | **-3.7669023** | **-4.4415704** | **-1.8331683** |
| **H** | **-5.2706101** | **-2.5042831** | **-1.4257200** |
| **C** | **-0.2915137** | **0.5529994** | **-0.2934468** |
| **H** | **0.0504647** | **1.5532494** | **-0.6175077** |
| **H** | **0.3173446** | **-0.1332759** | **-0.9055774** |
| **N** | **0.2407416** | **0.4246485** | **1.0601133** |
| **C** | **4.1041497** | **3.1370243** | **-0.3124909** |
| **H** | **4.6663407** | **3.7641191** | **-1.0350591** |
| **H** | **4.6404631** | **3.2127506** | **0.6459856** |
| **C** | **2.6865649** | **3.7074210** | **-0.1909949** |
| **H** | **2.7234977** | **4.6214268** | **0.4341901** |
| **H** | **2.3019204** | **4.0124084** | **-1.1751335** |
| **C** | **2.0100191** | **2.0919415** | **1.4685664** |
| **H** | **1.4387998** | **2.5283670** | **2.3092021** |
| **H** | **3.0768359** | **2.1091586** | **1.7381511** |
| **C** | **1.6450498** | **0.6137595** | **1.2805611** |
| **H** | **2.2033133** | **0.2236948** | **0.4165531** |
| **H** | **1.9248202** | **0.0433712** | **2.1760409** |
| **C** | **-0.5942933** | **0.1142330** | **2.1833477** |
| **H** | **-1.6197508** | **0.4237632** | **1.9522124** |
| **H** | **-0.2133682** | **0.6620620** | **3.0595802** |
| **C** | **-0.5755042** | **-1.3845508** | **2.4941919** |
| **H** | **-1.3132721** | **-1.5613441** | **3.2988642** |
| **H** | **-0.9117514** | **-1.9374125** | **1.6020035** |
| **C** | **1.0969189** | **-3.0801260** | **2.7107923** |
| **H** | **0.3778124** | **-3.7734699** | **3.1886840** |
| **H** | **2.0595029** | **-3.1845171** | **3.2335487** |
| **C** | **1.2711043** | **-3.4917346** | **1.2631575** |
| **H** | **1.6071303** | **-4.5498655** | **1.2548407** |
| **H** | **0.3066320** | **-3.4643928** | **0.7199827** |
| **O** | **1.7434254** | **2.7856632** | **0.2873876** |
| **O** | **4.1448705** | **1.7848406** | **-0.6552027** |
| **O** | **2.2123849** | **-2.6608376** | **0.6406493** |
| **O** | **0.7148364** | **-1.7414480** | **2.8999192** |
| **C** | **3.6934455** | **1.4512536** | **-1.9397941** |
| **C** | **3.9632328** | **-0.0132176** | **-2.1744405** |
| **H** | **4.2353140** | **2.0376259** | **-2.7091646** |
| **H** | **2.6124163** | **1.6539893** | **-2.0598006** |
| **H** | **3.8427663** | **-0.2397276** | **-3.2528482** |
| **H** | **5.0176315** | **-0.2154015** | **-1.9040862** |
| **C** | **2.4545186** | **-3.0076979** | **-0.6932091** |
| **C** | **3.5268832** | **-2.1349067** | **-1.2902259** |
| **H** | **1.5319342** | **-2.9227145** | **-1.2997925** |
| **H** | **2.7966620** | **-4.0606429** | **-0.7665240** |
| **H** | **3.7771389** | **-2.5498394** | **-2.2870126** |
| **H** | **4.4416565** | **-2.1893765** | **-0.6672904** |
| **O** | **3.0962840** | **-0.8048478** | **-1.4073184** |

**3 ($\pi\pi^*$)$_{min}$**

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|---|---|---|---|
| **C** | **-2.6345437** | **3.8340451** | **0.2118304** |
| **C** | **-1.9199472** | **2.6267456** | **0.0878039** |
| **C** | **-2.5727887** | **1.4121851** | **-0.1978102** |
| **C** | **-3.9986820** | **1.4435253** | **-0.3832041** |
| **C** | **-4.6910507** | **2.6626909** | **-0.2416831** |
| **C** | **-4.0144079** | **3.8551510** | **0.0564030** |
| **C** | **-1.8700123** | **0.1673756** | **-0.3267568** |
| **C** | **-4.6657906** | **0.2488928** | **-0.7186866** |
| **C** | **-3.9891541** | **-0.9700085** | **-0.9320910** |
| **C** | **-2.5558793** | **-1.0161144** | **-0.7574713** |
| **C** | **-1.9169173** | **-2.2460210** | **-1.0259114** |
| **H** | **-0.8321988** | **-2.3192776** | **-0.9495684** |
| **C** | **-2.6338766** | **-3.3933768** | **-1.4212163** |
| **C** | **-4.0129901** | **-3.3439671** | **-1.5574614** |
| **C** | **-4.6846485** | **-2.1342943** | **-1.3133001** |
| **H** | **-2.0914006** | **4.7548903** | **0.4367224** |
| **H** | **-0.8373015** | **2.6339652** | **0.2134771** |
| **H** | **-5.7761747** | **2.6681307** | **-0.3749158** |
| **H** | **-4.5727672** | **4.7882775** | **0.1606081** |
| **H** | **-5.7510528** | **0.2741308** | **-0.8562643** |
| **H** | **-2.0905996** | **-4.3202946** | **-1.6195772** |
| **H** | **-4.5760387** | **-4.2309101** | **-1.8562908** |
| **H** | **-5.7710765** | **-2.0807753** | **-1.4211562** |
| **C** | **-0.3999685** | **0.1387668** | **-0.0101551** |
| **H** | **0.1199532** | **0.8610749** | **-0.6623153** |
| **H** | **0.0415784** | **-0.8423651** | **-0.2662958** |
| **N** | **-0.0852144** | **0.5174493** | **1.3605812** |
| **C** | **3.8006865** | **3.4224108** | **-0.4692247** |
| **H** | **4.2548766** | **4.1169203** | **-1.2080534** |
| **H** | **4.1938302** | **3.7107867** | **0.5174808** |
| **C** | **2.2753557** | **3.5970415** | **-0.5176337** |
| **H** | **2.0105086** | **4.5306108** | **0.0225375** |
| **H** | **1.9323947** | **3.7248947** | **-1.5562663** |
| **C** | **1.7925285** | **2.1557093** | **1.3212760** |
| **H** | **1.2424364** | **2.8640828** | **1.9737028** |
| **H** | **2.8659465** | **2.2123402** | **1.5742636** |
| **C** | **1.3359211** | **0.7345329** | **1.5783150** |
| **H** | **1.9553988** | **0.0493987** | **0.9692260** |
| **H** | **1.5724903** | **0.4974853** | **2.6245663** |
| **C** | **-0.7820289** | **-0.2182289** | **2.3926740** |
| **H** | **-1.8693620** | **-0.0946802** | **2.2488549** |
| **H** | **-0.5433489** | **0.2453214** | **3.3644928** |
| **C** | **-0.4935847** | **-1.7105381** | **2.4856567** |
| **H** | **-1.1410428** | **-2.1616098** | **3.2675728** |
| **H** | **-0.7649793** | **-2.2013661** | **1.5323631** |
| **C** | **1.3613461** | **-3.1890062** | **2.6017159** |
| **H** | **0.6833117** | **-3.9556852** | **3.0294893** |
| **H** | **2.3136172** | **-3.2411169** | **3.1527529** |
| **C** | **1.6290192** | **-3.5423209** | **1.1522553** |

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|---|---|---|---|
| **H** | **1.9524742** | **-4.6046789** | **1.1051268** |
| **H** | **0.6955412** | **-3.4742493** | **0.5565842** |
| **O** | **1.5798197** | **2.4910634** | **-0.0302458** |
| **O** | **4.2216405** | **2.1075586** | **-0.6675563** |
| **O** | **2.6100107** | **-2.6974211** | **0.6292293** |
| **O** | **0.8615646** | **-1.9007959** | **2.7957883** |
| **C** | **3.9457074** | **1.5624937** | **-1.9257132** |
| **C** | **4.4292905** | **0.1352201** | **-1.9658149** |
| **H** | **4.4652910** | **2.1385640** | **-2.7199945** |
| **H** | **2.8631968** | **1.5714311** | **-2.1488696** |
| **H** | **4.5470071** | **-0.1773450** | **-3.0250560** |
| **H** | **5.4322789** | **0.0914450** | **-1.4957478** |
| **C** | **2.8826773** | **-2.9334794** | **-0.7182346** |
| **C** | **3.9777791** | **-2.0240169** | **-1.2128513** |
| **H** | **1.9771809** | **-2.7780277** | **-1.3408986** |
| **H** | **3.2099655** | **-3.9834240** | **-0.8733395** |
| **H** | **4.3050279** | **-2.3987948** | **-2.2055927** |
| **H** | **4.8494841** | **-2.0967700** | **-0.5311087** |
| **O** | **3.5262225** | **-0.7073375** | **-1.3106132** |

**4 $(S_0)_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-3.3773285** | **3.7120397** | **-1.0154840** |
| **C** | **-2.7116574** | **2.5146707** | **-0.9965518** |
| **C** | **-3.3571850** | **1.2911257** | **-0.6277528** |
| **C** | **-4.7680983** | **1.3738517** | **-0.3341717** |
| **C** | **-5.4218784** | **2.6439269** | **-0.3319437** |
| **C** | **-4.7485381** | **3.7887317** | **-0.6543782** |
| **C** | **-2.6941357** | **0.0359923** | **-0.5807263** |
| **C** | **-5.4838008** | **0.2075353** | **-0.0652563** |
| **C** | **-4.8827105** | **-1.0480583** | **-0.1469566** |
| **C** | **-3.4716918** | **-1.1439041** | **-0.4362210** |
| **C** | **-2.9441556** | **-2.4650776** | **-0.5984605** |
| **H** | **-1.9066060** | **-2.5944272** | **-0.9030441** |
| **C** | **-3.7192294** | **-3.5834833** | **-0.4379993** |
| **C** | **-5.0912243** | **-3.4746236** | **-0.0878412** |
| **C** | **-5.6528761** | **-2.2358402** | **0.0448094** |
| **H** | **-2.8527642** | **4.6179709** | **-1.3291350** |
| **H** | **-1.6727997** | **2.4962508** | **-1.3220492** |
| **H** | **-6.4852812** | **2.6759227** | **-0.0818929** |
| **H** | **-5.2618164** | **4.7526693** | **-0.6601031** |
| **H** | **-6.5470356** | **0.2770132** | **0.1795554** |
| **H** | **-3.2817669** | **-4.5723901** | **-0.5958969** |
| **H** | **-5.6924466** | **-4.3755301** | **0.0511209** |
| **H** | **-6.7136836** | **-2.1290108** | **0.2851444** |
| **C** | **-1.1740242** | **-0.0389027** | **-0.6414813** |
| **H** | **-0.7768051** | **0.7756846** | **-1.2618454** |
| **H** | **-0.8578907** | **-0.9560617** | **-1.1576362** |
| **N** | **-0.4539711** | **0.0060260** | **0.6562912** |
| **C** | **3.7222186** | **3.2106342** | **1.1405324** |
| **H** | **4.3061335** | **4.1230631** | **0.9190336** |

| | | | |
|---|---|---|---|
| **H** | **3.7896510** | **3.0270241** | **2.2240098** |
| **C** | **2.2736632** | **3.4395788** | **0.7668498** |
| **H** | **1.9085486** | **4.3346671** | **1.3073465** |
| **H** | **2.1680106** | **3.6552904** | **-0.3156468** |
| **C** | **0.1397832** | **2.4507551** | **0.8590871** |
| **H** | **-0.0170928** | **2.6050699** | **-0.2234271** |
| **H** | **-0.2418897** | **3.3571012** | **1.3660076** |
| **C** | **-0.6398487** | **1.2620741** | **1.3839046** |
| **H** | **-0.3112384** | **1.1047506** | **2.4229946** |
| **H** | **-1.7056632** | **1.5558482** | **1.4423976** |
| **C** | **-0.7284839** | **-1.1490440** | **1.5128916** |
| **H** | **-1.8110176** | **-1.3646103** | **1.5870421** |
| **H** | **-0.3967178** | **-0.9065432** | **2.5343961** |
| **C** | **-0.0164088** | **-2.4293866** | **1.1241650** |
| **H** | **-0.4857256** | **-3.2683144** | **1.6712969** |
| **H** | **-0.1329872** | **-2.6444475** | **0.0468765** |
| **C** | **2.0996315** | **-3.5175811** | **1.2025327** |
| **H** | **1.4952699** | **-4.4228948** | **1.3926055** |
| **H** | **2.9393696** | **-3.5235158** | **1.9156595** |
| **C** | **2.6550109** | **-3.5640578** | **-0.2049835** |
| **H** | **3.1889478** | **-4.5231352** | **-0.3517454** |
| **H** | **1.8399858** | **-3.5276128** | **-0.9558176** |
| **O** | **1.5202915** | **2.3048191** | **1.1147654** |
| **O** | **4.2921373** | **2.0845258** | **0.5137150** |
| **O** | **3.5290857** | **-2.4754019** | **-0.3735777** |
| **O** | **1.3530811** | **-2.3501273** | **1.4614017** |
| **C** | **4.7315047** | **2.2747253** | **-0.8097725** |
| **C** | **5.4410443** | **1.0294496** | **-1.2728095** |
| **H** | **5.4348999** | **3.1269441** | **-0.8672106** |
| **H** | **3.8856895** | **2.4913453** | **-1.4903654** |
| **H** | **5.8706553** | **1.2120430** | **-2.2766636** |
| **H** | **6.2774965** | **0.8052549** | **-0.5830468** |
| **C** | **4.0852984** | **-2.3598842** | **-1.6595451** |
| **C** | **5.1279372** | **-1.2726385** | **-1.6529179** |
| **H** | **3.2979484** | **-2.1286351** | **-2.4038794** |
| **H** | **4.5679911** | **-3.3069425** | **-1.9673615** |
| **H** | **5.5902838** | **-1.2158995** | **-2.6571028** |
| **H** | **5.9261352** | **-1.5292631** | **-0.9295619** |
| **O** | **4.5336145** | **-0.0456577** | **-1.3055750** |
| **K** | **2.6413596** | **-0.1113597** | **0.7384978** |

**4 $(\pi\pi^*)_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-3.1568197** | **3.7412520** | **-1.2349980** |
| **C** | **-2.5358488** | **2.4763295** | **-1.2272922** |
| **C** | **-3.1800033** | **1.3268195** | **-0.7326152** |
| **C** | **-4.5521464** | **1.4711376** | **-0.3125912** |
| **C** | **-5.1428727** | **2.7494789** | **-0.2988218** |
| **C** | **-4.4497290** | **3.8826422** | **-0.7519801** |
| **C** | **-2.5590517** | **0.0338791** | **-0.6375243** |
| **C** | **-5.2779272** | **0.3190149** | **0.0536124** |

| | | | |
|---|---|---|---|
| **C** | **-4.7523180** | **-0.9817432** | **-0.0886906** |
| **C** | **-3.3793481** | **-1.1383195** | **-0.5007410** |
| **C** | **-2.9286105** | **-2.4480602** | **-0.7512106** |
| **H** | **-1.9297569** | **-2.6053880** | **-1.1606234** |
| **C** | **-3.7437820** | **-3.5772807** | **-0.5388665** |
| **C** | **-5.0413115** | **-3.4182770** | **-0.0733945** |
| **C** | **-5.5407051** | **-2.1249341** | **0.1456765** |
| **H** | **-2.6158099** | **4.6046395** | **-1.6285416** |
| **H** | **-1.5402981** | **2.3919677** | **-1.6662670** |
| **H** | **-6.1683032** | **2.8488223** | **0.0661441** |
| **H** | **-4.9353853** | **4.8604527** | **-0.7382460** |
| **H** | **-6.3219822** | **0.4321099** | **0.3589466** |
| **H** | **-3.3491820** | **-4.5740957** | **-0.7473546** |
| **H** | **-5.6776953** | **-4.2864699** | **0.1091278** |
| **H** | **-6.5660133** | **-1.9908523** | **0.4996437** |
| **C** | **-1.0536843** | **-0.0810048** | **-0.6013106** |
| **H** | **-0.5878498** | **0.7338837** | **-1.1729927** |
| **H** | **-0.7168094** | **-1.0033357** | **-1.0971064** |
| **N** | **-0.4395281** | **-0.0676882** | **0.7538830** |
| **C** | **3.6051295** | **3.2027364** | **1.2054490** |
| **H** | **4.1702742** | **4.1269145** | **0.9834816** |
| **H** | **3.7038671** | **3.0029987** | **2.2837148** |
| **C** | **2.1439968** | **3.4165862** | **0.8736356** |
| **H** | **1.7780846** | **4.2890651** | **1.4495280** |
| **H** | **2.0061140** | **3.6620526** | **-0.1987648** |
| **C** | **0.0282412** | **2.3942857** | **1.0230606** |
| **H** | **-0.1909645** | **2.6147621** | **-0.0361756** |
| **H** | **-0.3469699** | **3.2569859** | **1.6057253** |
| **C** | **-0.7011011** | **1.1596278** | **1.5060474** |
| **H** | **-0.3842274** | **0.9855030** | **2.5463885** |
| **H** | **-1.7816122** | **1.4013024** | **1.5492932** |
| **C** | **-0.7661473** | **-1.2454415** | **1.5587898** |
| **H** | **-1.8548175** | **-1.4423141** | **1.5933777** |
| **H** | **-0.4593311** | **-1.0396824** | **2.5964364** |
| **C** | **-0.0674878** | **-2.5235320** | **1.1461186** |
| **H** | **-0.5258743** | **-3.3630359** | **1.7018945** |
| **H** | **-0.2151413** | **-2.7355403** | **0.0724348** |
| **C** | **2.0569205** | **-3.5964068** | **1.1308251** |
| **H** | **1.4644895** | **-4.5132681** | **1.3018499** |
| **H** | **2.9148147** | **-3.6223314** | **1.8216983** |
| **C** | **2.5746410** | **-3.5829854** | **-0.2911305** |
| **H** | **3.1167562** | **-4.5280532** | **-0.4895675** |
| **H** | **1.7389144** | **-3.5289987** | **-1.0175625** |
| **O** | **1.4212399** | **2.2587879** | **1.2068834** |
| **O** | **4.1742053** | **2.0948113** | **0.5465789** |
| **O** | **3.4287308** | **-2.4764183** | **-0.4414131** |
| **O** | **1.3096166** | **-2.4448824** | **1.4496521** |
| **C** | **4.5657445** | **2.3102445** | **-0.7876228** |
| **C** | **5.2752559** | **1.0821496** | **-1.2932890** |
| **H** | **5.2559507** | **3.1723780** | **-0.8557419** |
| **H** | **3.6948966** | **2.5257012** | **-1.4365298** |

| | | | |
|---|---|---|---|
| **H** | **5.6690384** | **1.2861196** | **-2.3076138** |
| **H** | **6.1371503** | **0.8581239** | **-0.6351691** |
| **C** | **3.9495671** | **-2.3098907** | **-1.7361641** |
| **C** | **4.9797965** | **-1.2116974** | **-1.7189994** |
| **H** | **3.1402922** | **-2.0622534** | **-2.4512492** |
| **H** | **4.4341781** | **-3.2400563** | **-2.0891743** |
| **H** | **5.4139367** | **-1.1149811** | **-2.7326036** |
| **H** | **5.8009184** | **-1.4836028** | **-1.0272005** |
| **O** | **4.3818681** | **-0.0044274** | **-1.3149260** |
| **K** | **2.5857089** | **-0.1527163** | **0.8189203** |

**5 $(S_0)_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-1.1573807** | **-1.5916300** | **-0.0363161** |
| **C** | **-0.5610079** | **-2.8735932** | **-0.0924624** |
| **C** | **0.8047573** | **-2.6829778** | **-0.0863435** |
| **C** | **1.0331436** | **-1.2838204** | **-0.0211175** |
| **N** | **-0.1948512** | **-0.6405463** | **-0.0026060** |
| **C** | **2.2438936** | **-0.5738008** | **-0.0168872** |
| **C** | **2.2299638** | **0.8306844** | **-0.0285610** |
| **C** | **3.2921364** | **1.7656558** | **0.0466408** |
| **N** | **1.0398666** | **1.5354619** | **-0.0857237** |
| **C** | **2.7242725** | **3.0290889** | **0.0169794** |
| **C** | **1.3306537** | **2.8474058** | **-0.0689643** |
| **B** | **-0.3715108** | **0.9007284** | **-0.1240871** |
| **F** | **-1.1207227** | **1.3773446** | **0.9731333** |
| **F** | **-1.0321282** | **1.2242992** | **-1.2892987** |
| **C** | **3.5324021** | **-1.2950849** | **-0.0029968** |
| **C** | **4.5114105** | **-1.0313914** | **-0.9737310** |
| **C** | **3.8135587** | **-2.2559094** | **0.9794263** |
| **C** | **5.7244763** | **-1.7105423** | **-0.9601716** |
| **H** | **4.3016658** | **-0.3059171** | **-1.7627344** |
| **C** | **5.0357576** | **-2.9210583** | **0.9919777** |
| **H** | **3.0737123** | **-2.4640730** | **1.7555750** |
| **C** | **6.0151218** | **-2.6634155** | **0.0251339** |
| **H** | **6.4625815** | **-1.4996169** | **-1.7388861** |
| **H** | **5.2355527** | **-3.6570280** | **1.7756083** |
| **C** | **7.3424697** | **-3.3630697** | **0.0555492** |
| **H** | **7.7174378** | **-3.5595376** | **-0.9594515** |
| **H** | **8.0998605** | **-2.7455354** | **0.5672860** |
| **H** | **7.2835957** | **-4.3207142** | **0.5918401** |
| **H** | **1.5804501** | **-3.4435436** | **-0.1347216** |
| **H** | **4.3468526** | **1.5127649** | **0.1277090** |
| **H** | **3.2233394** | **3.9942759** | **0.0538712** |
| **H** | **-1.1269407** | **-3.8004674** | **-0.1320578** |
| **C** | **0.3019340** | **3.9470768** | **-0.1166880** |
| **H** | **-0.7196212** | **3.5143617** | **-0.1613494** |
| **O** | **0.4079907** | **4.7734684** | **1.0101624** |
| **O** | **0.5722432** | **4.7012731** | **-1.2366015** |
| **C** | **-0.3964601** | **5.6796400** | **-1.5168197** |

| | | | |
|---|---|---|---|
| **H** | **-0.4674909** | **6.4229991** | **-0.7064638** |
| **H** | **-0.0918945** | **6.1813936** | **-2.4446644** |
| **H** | **-1.3929015** | **5.2236276** | **-1.6696742** |
| **C** | **-0.1083988** | **4.2320540** | **2.1938231** |
| **H** | **-1.1695426** | **3.9420744** | **2.0860366** |
| **H** | **0.4506751** | **3.3376623** | **2.5246014** |
| **H** | **-0.0240135** | **5.0054935** | **2.9689762** |
| **C** | **-2.5913204** | **-1.3922455** | **-0.0218106** |
| **C** | **-4.5685390** | **-0.4511744** | **0.1759261** |
| **C** | **-4.6735903** | **-1.8326262** | **-0.1397397** |
| **C** | **-5.6915839** | **0.3634830** | **0.3494848** |
| **C** | **-5.9410561** | **-2.4202029** | **-0.2874552** |
| **C** | **-6.9308824** | **-0.2423887** | **0.1969810** |
| **H** | **-5.6010581** | **1.4247408** | **0.5899064** |
| **C** | **-7.0543700** | **-1.6139713** | **-0.1161738** |
| **H** | **-6.0274135** | **-3.4807341** | **-0.5309219** |
| **H** | **-7.8360813** | **0.3571345** | **0.3205308** |
| **H** | **-8.0531948** | **-2.0427352** | **-0.2261042** |
| **N** | **-3.2261583** | **-0.2088336** | **0.2434527** |
| **N** | **-3.4309860** | **-2.3846709** | **-0.2500701** |
| **H** | **-2.7516814** | **0.6507601** | **0.5118422** |

**5 $(\pi\pi^*)_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-1.0494188** | **-1.9307854** | **-0.0443964** |
| **C** | **-0.3191592** | **-3.1248980** | **-0.0454297** |
| **C** | **1.0332715** | **-2.7797225** | **-0.0578128** |
| **C** | **1.0976026** | **-1.3718220** | **-0.0332463** |
| **N** | **-0.1775659** | **-0.8641438** | **-0.0408942** |
| **C** | **2.2601827** | **-0.5043136** | **-0.0413702** |
| **C** | **2.0608270** | **0.8807064** | **-0.0512996** |
| **C** | **2.9932188** | **1.9596237** | **0.0068217** |
| **N** | **0.7824551** | **1.4311674** | **-0.0568366** |
| **C** | **2.2608349** | **3.1333009** | **0.0198369** |
| **C** | **0.8974261** | **2.7740944** | **-0.0193656** |
| **B** | **-0.5285992** | **0.6356828** | **0.0101172** |
| **F** | **-1.2418574** | **0.9373308** | **1.1634360** |
| **F** | **-1.3441362** | **0.9828856** | **-1.0988783** |
| **C** | **3.6064267** | **-1.0772364** | **-0.0592356** |
| **C** | **4.5826902** | **-0.6127421** | **-0.9619645** |
| **C** | **3.9796884** | **-2.1087356** | **0.8250347** |
| **C** | **5.8631918** | **-1.1514570** | **-0.9739118** |
| **H** | **4.3123805** | **0.1552283** | **-1.6898682** |
| **C** | **5.2659739** | **-2.6324332** | **0.8128320** |
| **H** | **3.2557352** | **-2.4765344** | **1.5551192** |
| **C** | **6.2368359** | **-2.1682126** | **-0.0854153** |
| **H** | **6.5899469** | **-0.7833481** | **-1.7038108** |
| **H** | **5.5267833** | **-3.4211127** | **1.5244106** |
| **C** | **7.6303299** | **-2.7235232** | **-0.0790989** |
| **H** | **8.1022559** | **-2.6432310** | **-1.0691497** |

| | | | |
|---|---|---|---|
| H | 8.2705193 | -2.1742757 | 0.6324642 |
| H | 7.6429164 | -3.7809168 | 0.2230831 |
| H | 1.8838013 | -3.4535318 | -0.1008497 |
| H | 4.0737514 | 1.8524087 | 0.0586010 |
| H | 2.6292389 | 4.1556544 | 0.0626131 |
| H | -0.7660069 | -4.1159827 | -0.0541702 |
| C | -0.2648855 | 3.7264157 | 0.0175712 |
| H | -1.2221767 | 3.1649125 | -0.0029036 |
| O | -0.2200602 | 4.5233648 | 1.1712133 |
| O | -0.1515394 | 4.5512314 | -1.0820202 |
| C | -1.2505202 | 5.4034441 | -1.2763890 |
| H | -1.3779196 | 6.1024894 | -0.4338876 |
| H | -1.0611723 | 5.9737770 | -2.1955012 |
| H | -2.1874605 | 4.8276411 | -1.4032949 |
| C | -0.6422750 | 3.8901270 | 2.3475754 |
| H | -1.6633915 | 3.4781702 | 2.2499776 |
| H | 0.0253714 | 3.0593341 | 2.6387563 |
| H | -0.6330874 | 4.6461913 | 3.1445295 |
| C | -2.4891565 | -1.8692582 | -0.0561658 |
| C | -4.5241962 | -2.4995696 | 0.0776446 |
| C | -4.5420679 | -1.1129773 | -0.2930354 |
| C | -5.7452318 | -3.1933780 | 0.2484638 |
| C | -5.7241829 | -0.4133111 | -0.4953579 |
| C | -6.9198581 | -2.4950919 | 0.0475316 |
| H | -5.7353928 | -4.2471956 | 0.5314448 |
| C | -6.9118080 | -1.1267054 | -0.3189674 |
| H | -5.7316375 | 0.6414525 | -0.7760303 |
| H | -7.8801330 | -3.0003216 | 0.1723269 |
| H | -7.8652419 | -0.6136503 | -0.4665910 |
| N | -3.2565227 | -2.9341347 | 0.2133791 |
| N | -3.2230865 | -0.7622859 | -0.3668669 |
| H | -2.8064921 | 0.1209820 | -0.6736426 |

**6 ($S_0$)$_{min}$**

| | | | |
|---|---|---|---|
| C | -1.1697782 | -1.5219189 | -0.0732528 |
| C | -0.5570533 | -2.8171170 | -0.1413309 |
| C | 0.7959396 | -2.6217567 | -0.1280697 |
| C | 1.0254018 | -1.2115705 | -0.0462184 |
| N | -0.2100943 | -0.5701150 | -0.0291930 |
| C | 2.2360488 | -0.5300648 | -0.0276387 |
| C | 2.2565407 | 0.8877754 | -0.0356512 |
| C | 3.3302387 | 1.8034888 | 0.0268581 |
| N | 1.0807638 | 1.5962191 | -0.0847084 |
| C | 2.7714650 | 3.0795880 | 0.0015828 |
| C | 1.3799340 | 2.9100452 | -0.0682544 |
| B | -0.3782736 | 0.9923938 | -0.0269450 |
| F | -0.9458695 | 1.4320755 | 1.1542977 |
| F | -1.0572097 | 1.4219517 | -1.1445029 |
| C | 3.5131296 | -1.2778047 | -0.0045248 |
| C | 4.5087930 | -1.0374897 | -0.9640706 |

| | | | |
|---|---|---|---|
| **C** | **3.7686900** | **-2.2480172** | **0.9752450** |
| **C** | **5.7053079** | **-1.7471332** | **-0.9459178** |
| **H** | **4.3245130** | **-0.2975335** | **-1.7459034** |
| **C** | **4.9697521** | **-2.9525587** | **0.9889460** |
| **H** | **3.0155256** | **-2.4401462** | **1.7424544** |
| **C** | **5.9619789** | **-2.7171546** | **0.0312162** |
| **H** | **6.4563927** | **-1.5487136** | **-1.7167147** |
| **H** | **5.1407980** | **-3.7032900** | **1.7663751** |
| **C** | **7.2688959** | **-3.4576112** | **0.0634980** |
| **H** | **7.6433030** | **-3.6599416** | **-0.9513724** |
| **H** | **8.0454505** | **-2.8721231** | **0.5848775** |
| **H** | **7.1764604** | **-4.4186538** | **0.5903021** |
| **H** | **1.5745179** | **-3.3790190** | **-0.1872625** |
| **H** | **4.3837163** | **1.5403950** | **0.0930650** |
| **H** | **3.2827374** | **4.0390574** | **0.0280887** |
| **H** | **-1.1190016** | **-3.7495196** | **-0.1985312** |
| **C** | **0.3410859** | **3.9960054** | **-0.0977573** |
| **H** | **-0.6686470** | **3.5438083** | **-0.1588052** |
| **O** | **0.4180719** | **4.8184857** | **1.0417125** |
| **O** | **0.5899380** | **4.7925240** | **-1.2035869** |
| **C** | **-0.4259907** | **5.7184813** | **-1.4693236** |
| **H** | **-0.5440039** | **6.4450306** | **-0.6471737** |
| **H** | **-0.1496866** | **6.2559500** | **-2.3878124** |
| **H** | **-1.3983537** | **5.2154972** | **-1.6333573** |
| **C** | **-0.0693566** | **4.2315953** | **2.2158046** |
| **H** | **-1.1077025** | **3.8729536** | **2.1006555** |
| **H** | **0.5388323** | **3.3649655** | **2.5324557** |
| **H** | **-0.0316616** | **4.9990493** | **3.0028258** |
| **C** | **-2.5995065** | **-1.3406076** | **-0.0478394** |
| **C** | **-4.5317541** | **-0.5030494** | **0.0567978** |
| **C** | **-4.6493042** | **-1.9296313** | **-0.0640682** |
| **C** | **-5.6909415** | **0.2967472** | **0.1453321** |
| **C** | **-5.9132123** | **-2.5537256** | **-0.0966076** |
| **C** | **-6.9218204** | **-0.3330038** | **0.1115659** |
| **H** | **-5.6003504** | **1.3817823** | **0.2368376** |
| **C** | **-7.0312309** | **-1.7441128** | **-0.0081266** |
| **H** | **-5.9919140** | **-3.6398964** | **-0.1884626** |
| **H** | **-7.8369780** | **0.2627310** | **0.1779118** |
| **H** | **-8.0275753** | **-2.1961225** | **-0.0302874** |
| **N** | **-3.2273052** | **-0.1634369** | **0.0649806** |
| **N** | **-3.4053590** | **-2.4430880** | **-0.1275034** |
| **H** | **-3.0991458** | **-3.9177395** | **-0.2333111** |
| **F** | **-2.8609589** | **-4.8845902** | **-0.2943220** |

**6 ($S_1$)$_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-1.0475809** | **-1.8570573** | **0.4918464** |
| **C** | **-0.4376408** | **-3.0959265** | **0.5577804** |
| **C** | **0.9516027** | **-2.8690210** | **0.4665205** |
| **C** | **1.1389572** | **-1.4824844** | **0.3535886** |
| **N** | **-0.1004011** | **-0.8839336** | **0.3709363** |

| | | | |
|---|---|---|---|
| **C** | **2.3291129** | **-0.7077320** | **0.1394197** |
| **C** | **2.2003768** | **0.6839861** | **-0.1249326** |
| **C** | **3.1797223** | **1.6850345** | **-0.3295667** |
| **N** | **0.9626440** | **1.2962217** | **-0.1596961** |
| **C** | **2.5051322** | **2.8993574** | **-0.4980066** |
| **C** | **1.1434196** | **2.6273336** | **-0.3851606** |
| **B** | **-0.3696242** | **0.6293559** | **0.2592203** |
| **F** | **-0.7930901** | **1.1593123** | **1.4832546** |
| **F** | **-1.3695147** | **0.8553846** | **-0.6922622** |
| **C** | **3.6411185** | **-1.3505912** | **0.1699748** |
| **C** | **4.6373305** | **-1.0635794** | **-0.7885829** |
| **C** | **3.9767894** | **-2.3002195** | **1.1581030** |
| **C** | **5.8825682** | **-1.6786538** | **-0.7518411** |
| **H** | **4.4028132** | **-0.3688177** | **-1.5969506** |
| **C** | **5.2262567** | **-2.9090956** | **1.1892240** |
| **H** | **3.2410368** | **-2.5374632** | **1.9287466** |
| **C** | **6.2118246** | **-2.6129106** | **0.2393810** |
| **H** | **6.6174740** | **-1.4383166** | **-1.5272281** |
| **H** | **5.4471411** | **-3.6306813** | **1.9824914** |
| **C** | **7.5725831** | **-3.2473267** | **0.2927574** |
| **H** | **7.9603101** | **-3.4588817** | **-0.7162464** |
| **H** | **8.3086229** | **-2.5897297** | **0.7882673** |
| **H** | **7.5546187** | **-4.1943309** | **0.8528910** |
| **H** | **1.7350883** | **-3.6219147** | **0.4398121** |
| **H** | **4.2554304** | **1.5290578** | **-0.3269192** |
| **H** | **2.9337547** | **3.8820724** | **-0.6824909** |
| **H** | **-0.9452232** | **-4.0538859** | **0.6481083** |
| **C** | **0.0118882** | **3.6058021** | **-0.4619101** |
| **H** | **-0.9443029** | **3.0833125** | **-0.2586594** |
| **O** | **0.1611214** | **4.6664962** | **0.4590019** |
| **O** | **-0.0114120** | **4.1718736** | **-1.7295921** |
| **C** | **-1.1563334** | **4.9306877** | **-1.9835027** |
| **H** | **-1.2378785** | **5.7963696** | **-1.3029719** |
| **H** | **-1.0904010** | **5.2943626** | **-3.0194234** |
| **H** | **-2.0766280** | **4.3222501** | **-1.8831627** |
| **C** | **0.0136320** | **4.2840031** | **1.7949349** |
| **H** | **-0.9455419** | **3.7648059** | **1.9763752** |
| **H** | **0.8177485** | **3.5998647** | **2.1223233** |
| **H** | **0.0542121** | **5.1990811** | **2.4049118** |
| **C** | **-2.4977335** | **-1.5444438** | **0.5090915** |
| **C** | **-4.4496839** | **-0.9760966** | **1.1123390** |
| **C** | **-4.4669481** | **-1.2079808** | **-0.3096699** |
| **C** | **-5.5958394** | **-0.5859331** | **1.7595309** |
| **C** | **-5.6516236** | **-1.0573173** | **-1.0809418** |
| **C** | **-6.7689293** | **-0.4252528** | **0.9778676** |
| **H** | **-5.6050372** | **-0.4026351** | **2.8348372** |
| **C** | **-6.7964941** | **-0.6575114** | **-0.4093505** |
| **H** | **-5.6053639** | **-1.2583266** | **-2.1524682** |
| **H** | **-7.6881704** | **-0.1065753** | **1.4749669** |
| **H** | **-7.7305638** | **-0.5138132** | **-0.9554440** |
| **N** | **-3.1677784** | **-1.2289146** | **1.5775834** |

| | | | |
|---|---|---|---|
| **N** | **-3.2580332** | **-1.5794877** | **-0.6864455** |
| **H** | **-3.2987917** | **-1.9223960** | **-2.3055759** |
| **F** | **-3.6835840** | **-2.0764476** | **-3.1718061** |

**6 ($S_2$) min**

| | | | |
|---|---|---|---|
| **C** | **-1.1505172** | **-1.5763954** | **-0.0737117** |
| **C** | **-0.5624356** | **-2.8392799** | **-0.2282213** |
| **C** | **0.8194551** | **-2.6444723** | **-0.2132999** |
| **C** | **1.0427751** | **-1.2603421** | **-0.0465469** |
| **N** | **-0.1776575** | **-0.6211333** | **0.0278308** |
| **C** | **2.2906290** | **-0.5461988** | **-0.0312752** |
| **C** | **2.2742754** | **0.8611294** | **-0.0780843** |
| **C** | **3.3255111** | **1.8217917** | **-0.0212474** |
| **N** | **1.0770222** | **1.5475128** | **-0.1420435** |
| **C** | **2.7330732** | **3.0747123** | **-0.0721190** |
| **C** | **1.3405083** | **2.8663818** | **-0.1432574** |
| **B** | **-0.3600548** | **0.9264992** | **0.0395525** |
| **F** | **-0.8318627** | **1.3870926** | **1.2568705** |
| **F** | **-1.1421647** | **1.3375880** | **-1.0218504** |
| **C** | **3.5530788** | **-1.2798929** | **0.0235270** |
| **C** | **4.6543539** | **-0.9225278** | **-0.7861322** |
| **C** | **3.7273014** | **-2.3830036** | **0.8860204** |
| **C** | **5.8522037** | **-1.6202957** | **-0.7252711** |
| **H** | **4.5402001** | **-0.1081150** | **-1.5040093** |
| **C** | **4.9350734** | **-3.0672110** | **0.9478004** |
| **H** | **2.9032014** | **-2.6807558** | **1.5373475** |
| **C** | **6.0265999** | **-2.7056851** | **0.1470858** |
| **H** | **6.6737057** | **-1.3254937** | **-1.3860545** |
| **H** | **5.0358198** | **-3.9064446** | **1.6430147** |
| **C** | **7.3347491** | **-3.4380179** | **0.2207031** |
| **H** | **7.7149385** | **-3.6894325** | **-0.7826647** |
| **H** | **8.1124159** | **-2.8291602** | **0.7140659** |
| **H** | **7.2407665** | **-4.3746074** | **0.7895926** |
| **H** | **1.5914124** | **-3.3980979** | **-0.3477093** |
| **H** | **4.3852561** | **1.5964069** | **0.0680003** |
| **H** | **3.2167478** | **4.0490692** | **-0.0531697** |
| **H** | **-1.1230621** | **-3.7638791** | **-0.3570825** |
| **C** | **0.2762351** | **3.9251264** | **-0.1837820** |
| **H** | **-0.7234137** | **3.4494460** | **-0.1487324** |
| **O** | **0.4056337** | **4.8266682** | **0.8896127** |
| **O** | **0.4362455** | **4.6463689** | **-1.3557973** |
| **C** | **-0.6418227** | **5.4935063** | **-1.6422146** |
| **H** | **-0.7824490** | **6.2559039** | **-0.8566784** |
| **H** | **-0.4221969** | **5.9959205** | **-2.5950169** |
| **H** | **-1.5841207** | **4.9232903** | **-1.7515345** |
| **C** | **-0.0150643** | **4.3184314** | **2.1249851** |
| **H** | **-1.0501924** | **3.9342948** | **2.0841109** |
| **H** | **0.6248995** | **3.4880384** | **2.4742388** |
| **H** | **0.0414037** | **5.1420586** | **2.8518564** |

| | | | |
|---|---|---|---|
| **C** | **-2.5956321** | **-1.3400000** | **-0.0142619** |
| **C** | **-4.4865889** | **-0.4810914** | **0.3461002** |
| **C** | **-4.6657989** | **-1.8337067** | **-0.1511817** |
| **C** | **-5.6078054** | **0.3095432** | **0.6604720** |
| **C** | **-5.9550817** | **-2.3805486** | **-0.3174469** |
| **C** | **-6.8634962** | **-0.2471894** | **0.4869709** |
| **H** | **-5.4730770** | **1.3283869** | **1.0309036** |
| **C** | **-7.0345593** | **-1.5787676** | **0.0035453** |
| **H** | **-6.0781612** | **-3.4017882** | **-0.6857014** |
| **H** | **-7.7539225** | **0.3418376** | **0.7253582** |
| **H** | **-8.0503340** | **-1.9676693** | **-0.1132747** |
| **N** | **-3.1676102** | **-0.2140573** | **0.4239299** |
| **N** | **-3.4473318** | **-2.3510308** | **-0.3754118** |
| **H** | **-3.1702517** | **-3.8247149** | **-0.7472039** |
| **F** | **-2.9846426** | **-4.7756592** | **-0.9262276** |

**7 $(S_0)_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-6.8000810** | **-0.8697649** | **0.0840536** |
| **C** | **-5.4971436** | **-0.7177796** | **-0.2990721** |
| **C** | **-4.8441233** | **0.5505427** | **-0.2198631** |
| **C** | **-5.5669392** | **1.6963371** | **0.2828799** |
| **C** | **-6.9304341** | **1.4817769** | **0.6689785** |
| **C** | **-7.5241344** | **0.2520378** | **0.5707686** |
| **C** | **-3.5165201** | **0.6945439** | **-0.6225818** |
| **C** | **-4.9196810** | **2.9517068** | **0.3628565** |
| **C** | **-3.5851771** | **3.0831516** | **-0.0902393** |
| **C** | **-2.8696131** | **1.9308593** | **-0.5733242** |
| **C** | **-1.5107232** | **2.0708981** | **-0.9888047** |
| **H** | **-0.9840264** | **1.1819894** | **-1.3463173** |
| **C** | **-0.8815173** | **3.2842627** | **-0.9426668** |
| **C** | **-1.5883734** | **4.4305120** | **-0.4882424** |
| **C** | **-2.8924678** | **4.3354612** | **-0.0797828** |
| **H** | **-2.9718778** | **-0.1802875** | **-0.9892932** |
| **H** | **-7.2880334** | **-1.8449899** | **0.0159951** |
| **H** | **-4.9257884** | **-1.5685650** | **-0.6801135** |
| **H** | **-7.5219855** | **2.3178018** | **1.0412270** |
| **H** | **-8.5686730** | **0.1312650** | **0.8686433** |
| **H** | **0.1591472** | **3.3789738** | **-1.2620904** |
| **H** | **-1.0863922** | **5.4013126** | **-0.4762684** |
| **H** | **-3.4386227** | **5.2322394** | **0.2107419** |
| **C** | **-5.6109587** | **4.1633845** | **0.9530704** |
| **H** | **-4.9463149** | **4.5904088** | **1.7228118** |
| **H** | **-6.5211765** | **3.8444798** | **1.4965529** |
| **N** | **-5.8777710** | **5.2070030** | **-0.0194057** |
| **H** | **-6.1439532** | **6.0593256** | **0.4664120** |
| **C** | **-6.8622696** | **4.8706636** | **-1.0188251** |
| **H** | **-7.8581970** | **4.5905552** | **-0.6100300** |
| **H** | **-6.5085498** | **4.0198217** | **-1.6223084** |
| **H** | **-7.0044857** | **5.7199496** | **-1.7038605** |

**7 ($\pi\pi^*$)$_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-6.8563678** | **-0.8500422** | **0.0393975** |
| **C** | **-5.4936677** | **-0.7126432** | **-0.2748743** |
| **C** | **-4.8401414** | **0.5323434** | **-0.1952570** |
| **C** | **-5.5752720** | **1.6986626** | **0.2335891** |
| **C** | **-6.9426847** | **1.5225950** | **0.5327196** |
| **C** | **-7.5761820** | **0.2675898** | **0.4370340** |
| **C** | **-3.4763542** | **0.6664784** | **-0.5287039** |
| **C** | **-4.8908017** | **2.9535707** | **0.3283518** |
| **C** | **-3.5292468** | **3.0800463** | **-0.1003210** |
| **C** | **-2.8031214** | **1.9046308** | **-0.5020831** |
| **C** | **-1.4448963** | **2.0175306** | **-0.8579733** |
| **H** | **-0.8989194** | **1.1114187** | **-1.1389436** |
| **C** | **-0.7879812** | **3.2594377** | **-0.8538928** |
| **C** | **-1.4920295** | **4.4016355** | **-0.4964322** |
| **C** | **-2.8491072** | **4.3136178** | **-0.1264539** |
| **H** | **-2.9251668** | **-0.2250491** | **-0.8469398** |
| **H** | **-7.3392898** | **-1.8286718** | **-0.0336133** |
| **H** | **-4.9163451** | **-1.5871984** | **-0.5909018** |
| **H** | **-7.5470484** | **2.3782268** | **0.8384019** |
| **H** | **-8.6395874** | **0.1856576** | **0.6796365** |
| **H** | **0.2665430** | **3.3200907** | **-1.1376440** |
| **H** | **-1.0013835** | **5.3793486** | **-0.5042625** |
| **H** | **-3.4053468** | **5.2262845** | **0.0934654** |
| **C** | **-5.5658814** | **4.1639258** | **0.9232153** |
| **H** | **-4.8916726** | **4.5817856** | **1.6952334** |
| **H** | **-6.4846667** | **3.8547235** | **1.4633654** |
| **N** | **-5.8163073** | **5.2268989** | **-0.0378475** |
| **H** | **-6.0802340** | **6.0755131** | **0.4604029** |
| **C** | **-6.7925162** | **4.9111110** | **-1.0530578** |
| **H** | **-7.7991219** | **4.6388582** | **-0.6574983** |
| **H** | **-6.4356949** | **4.0598035** | **-1.6588712** |
| **H** | **-6.9129646** | **5.7733965** | **-1.7308399** |

**7 ($n\pi^*$)$_{min}$**

| | | | |
|---|---|---|---|
| **C** | **3.6890980** | **-1.4029434** | **0.1055971** |
| **C** | **2.4699567** | **-2.0482095** | **0.2535780** |
| **C** | **1.2378101** | **-1.3731502** | **0.0664085** |
| **C** | **1.2532918** | **0.0262600** | **-0.2964981** |
| **C** | **2.5199176** | **0.6494721** | **-0.4260174** |
| **C** | **3.7132522** | **-0.0466676** | **-0.2360463** |
| **C** | **-0.0000231** | **-2.0248798** | **0.2258684** |
| **C** | **0.0000041** | **0.6877168** | **-0.4851588** |
| **C** | **-1.2533203** | **0.0262859** | **-0.2964912** |
| **C** | **-1.2378330** | **-1.3731397** | **0.0664164** |
| **C** | **-2.4700011** | **-2.0481701** | **0.2535866** |
| **H** | **-2.4382344** | **-3.1076005** | **0.5222368** |
| **C** | **-3.6891231** | **-1.4029038** | **0.1056162** |

| | | | |
|---|---|---|---|
| **C** | **-3.7132686** | **-0.0466072** | **-0.2360288** |
| **C** | **-2.5199119** | **0.6494937** | **-0.4259981** |
| **H** | **-0.0000246** | **-3.0845120** | **0.4956888** |
| **H** | **4.6227628** | **-1.9502317** | **0.2564668** |
| **H** | **2.4381872** | **-3.1076309** | **0.5222294** |
| **H** | **2.5928698** | **1.7051106** | **-0.6997191** |
| **H** | **4.6667605** | **0.4738814** | **-0.3561433** |
| **H** | **-4.6228031** | **-1.9501703** | **0.2564850** |
| **H** | **-4.6667637** | **0.4739395** | **-0.3561156** |
| **H** | **-2.5928668** | **1.7051553** | **-0.6996991** |
| **C** | **0.0000017** | **2.1179062** | **-0.8952314** |
| **H** | **-0.8697509** | **2.4007466** | **-1.5161688** |
| **H** | **0.8697489** | **2.4007290** | **-1.5161878** |
| **N** | **0.0000300** | **3.0754288** | **0.1958871** |
| **H** | **0.0000057** | **4.0665275** | **-0.0416843** |
| **C** | **0.0000825** | **2.7138313** | **1.5662907** |
| **H** | **0.8748118** | **2.0702968** | **1.7557170** |
| **H** | **-0.8747218** | **2.0704260** | **1.7558124** |
| **H** | **0.0001749** | **3.6014776** | **2.2068120** |

**7 ($n\pi^*/\pi\pi^*$)$_{CI}$**

| | | | |
|---|---|---|---|
| **C** | **3.566550** | **-1.721105** | **0.251812** |
| **C** | **2.334065** | **-2.370973** | **0.109650** |
| **C** | **1.141606** | **-1.654218** | **-0.023700** |
| **C** | **1.200879** | **-0.221898** | **-0.038065** |
| **C** | **2.445036** | **0.398238** | **0.121479** |
| **C** | **3.626508** | **-0.343207** | **0.267933** |
| **C** | **-0.111329** | **-2.282660** | **-0.130347** |
| **C** | **-0.012779** | **0.508400** | **-0.217711** |
| **C** | **-1.281325** | **-0.125374** | **-0.211042** |
| **C** | **-1.322087** | **-1.571862** | **-0.202646** |
| **C** | **-2.568130** | **-2.209779** | **-0.267160** |
| **H** | **-2.601088** | **-3.282192** | **-0.286705** |
| **C** | **-3.756034** | **-1.478213** | **-0.303108** |
| **C** | **-3.731675** | **-0.095468** | **-0.272346** |
| **C** | **-2.502981** | **0.571056** | **-0.223685** |
| **H** | **-0.150460** | **-3.355762** | **-0.116250** |
| **H** | **4.461437** | **-2.304257** | **0.352813** |
| **H** | **2.299487** | **-3.443716** | **0.105483** |
| **H** | **2.501492** | **1.465042** | **0.161082** |
| **H** | **4.562321** | **0.164832** | **0.388706** |
| **H** | **-4.693599** | **-1.998960** | **-0.349326** |
| **H** | **-4.643511** | **0.468300** | **-0.285236** |
| **H** | **-2.508654** | **1.640877** | **-0.181350** |
| **C** | **0.075641** | **1.998647** | **-0.404646** |
| **H** | **-0.798514** | **2.348746** | **-0.959749** |
| **H** | **0.924221** | **2.245938** | **-1.038492** |
| **N** | **0.235194** | **2.679335** | **0.853637** |
| **H** | **-0.258933** | **2.283972** | **1.620864** |

| | | | |
|---|---|---|---|
| **C** | **0.357635** | **4.117791** | **0.850030** |
| **H** | **-0.524738** | **4.628980** | **0.456411** |
| **H** | **1.204278** | **4.416593** | **0.241817** |
| **H** | **0.529610** | **4.470765** | **1.857356** |

**8 ($S_0$)$_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-6.8216159** | **-0.8222173** | **0.0630050** |
| **C** | **-5.5326077** | **-0.6615866** | **-0.3626344** |
| **C** | **-4.8713773** | **0.5985723** | **-0.2482146** |
| **C** | **-5.5693398** | **1.7233422** | **0.3271142** |
| **C** | **-6.9153672** | **1.5048445** | **0.7566509** |
| **C** | **-7.5154707** | **0.2789392** | **0.6300322** |
| **C** | **-3.5596759** | **0.7592652** | **-0.6985598** |
| **C** | **-4.8911215** | **2.9616992** | **0.4341827** |
| **C** | **-3.5507297** | **3.1044375** | **-0.0024706** |
| **C** | **-2.8818476** | **1.9770582** | **-0.5970764** |
| **C** | **-1.5431270** | **2.1178940** | **-1.0688848** |
| **H** | **-1.0566190** | **1.2475043** | **-1.5159660** |
| **C** | **-0.8772834** | **3.3090671** | **-0.9636971** |
| **C** | **-1.5183292** | **4.4189669** | **-0.3568925** |
| **C** | **-2.8065812** | **4.3223844** | **0.1086994** |
| **H** | **-3.0467326** | **-0.0958830** | **-1.1471614** |
| **H** | **-7.3197753** | **-1.7896230** | **-0.0259476** |
| **H** | **-4.9819098** | **-1.4986547** | **-0.7986646** |
| **H** | **-7.4915114** | **2.3109341** | **1.2139821** |
| **H** | **-8.5424410** | **0.1442152** | **0.9777552** |
| **H** | **0.1471781** | **3.4065170** | **-1.3280681** |
| **H** | **-0.9712468** | **5.3577048** | **-0.2417466** |
| **H** | **-3.2279167** | **5.1935617** | **0.6193301** |
| **C** | **-5.5837741** | **4.1738330** | **0.9683867** |
| **H** | **-4.9615745** | **4.7306622** | **1.6832103** |
| **H** | **-6.5372093** | **3.9537731** | **1.4606619** |
| **N** | **-5.8938796** | **5.1467377** | **-0.1549575** |
| **H** | **-6.1658557** | **6.0549365** | **0.2401619** |
| **C** | **-6.9259365** | **4.6885077** | **-1.1170325** |
| **H** | **-7.8852964** | **4.5969443** | **-0.5932990** |
| **H** | **-6.6234010** | **3.7110615** | **-1.5116325** |
| **H** | **-7.0111497** | **5.4184008** | **-1.9313837** |
| **H** | **-5.0076304** | **5.3085756** | **-0.6558815** |

**8 ($\pi\pi^*$)$_{min}$**

| | | | |
|---|---|---|---|
| **C** | **-6.8709766** | **-0.8585174** | **0.1200011** |
| **C** | **-5.5655886** | **-0.6587033** | **-0.3622501** |
| **C** | **-4.9143060** | **0.5845285** | **-0.2505949** |
| **C** | **-5.6055526** | **1.6868912** | **0.3591175** |
| **C** | **-6.9122658** | **1.4514509** | **0.8362223** |
| **C** | **-7.5407901** | **0.1973619** | **0.7192751** |
| **C** | **-3.6007220** | **0.7659721** | **-0.7349085** |

| | | | |
|---|---|---|---|
| **C** | **-4.9283708** | **2.9446336** | **0.4498427** |
| **C** | **-3.5606149** | **3.0959085** | **0.0391258** |
| **C** | **-2.9058816** | **1.9869406** | **-0.6073335** |
| **C** | **-1.5865711** | **2.1441530** | **-1.0756934** |
| **H** | **-1.1037225** | **1.3014277** | **-1.5761090** |
| **C** | **-0.8871690** | **3.3492425** | **-0.9070303** |
| **C** | **-1.4952579** | **4.4131505** | **-0.2577621** |
| **C** | **-2.8203329** | **4.2847480** | **0.2124501** |
| **H** | **-3.0900284** | **-0.0827384** | **-1.1973311** |
| **H** | **-7.3445812** | **-1.8372485** | **0.0230161** |
| **H** | **-5.0357960** | **-1.4858668** | **-0.8418387** |
| **H** | **-7.4690761** | **2.2444406** | **1.3396024** |
| **H** | **-8.5518671** | **0.0647542** | **1.1088440** |
| **H** | **0.1360981** | **3.4394499** | **-1.2768435** |
| **H** | **-0.9524382** | **5.3461613** | **-0.0945346** |
| **H** | **-3.2232327** | **5.1133384** | **0.8046126** |
| **C** | **-5.6331020** | **4.1716922** | **0.9059319** |
| **H** | **-5.0971363** | **4.7029233** | **1.7099466** |
| **H** | **-6.6597962** | **3.9972383** | **1.2465335** |
| **N** | **-5.7250945** | **5.1706694** | **-0.2408536** |
| **H** | **-6.0044232** | **6.0922785** | **0.1167138** |
| **C** | **-6.6105539** | **4.7647839** | **-1.3553349** |
| **H** | **-7.6447009** | **4.7132920** | **-0.9925633** |
| **H** | **-6.2889978** | **3.7771051** | **-1.7076873** |
| **H** | **-6.5338605** | **5.4985906** | **-2.1672624** |
| **H** | **-4.7552466** | **5.2755229** | **-0.5883026** |

## VII. References:


[1] Ernzerhof, M.; Scuseria, G. E. Assessment of the Perdew-Burke-Ernzerhof Exchange-correlation Functional. *J. Chem. Phys.* **1999**, *110*, 5029.

[2] Adamo, C.; Barone, V. Toward Reliable Density Functional Methods Without Adjustable Parameters: The PBE0 Model. *J. Chem. Phys.* **1999**, *110*, 6158.

[3] Jacquemin, D.; Perpète, E. A.; Scuseria, G. E.; Ciofini, I.; Adamo, C. TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids. *J. Chem. Theory and Comput.* **2008**, *4*, 123-135.

[4] TURBOMOLE V6.6 2014, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1987-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.

[5] Harbach, P. H.; Wormit, M.; Dreuw, A. The Third-Order Algebraic Diagrammatic Construction Method (ADC(3)) for the Polarization Propagator for Closed-shell Molecules: Efficient Implementation and Benchmarking. *J. Chem. Phys.* **2014**, *141*, 064113-1-064113-17.

[6] Roos, B. O. In *Ab Initio Methods in Quantum Chemistry II*; Lawley, K. P., Eds., Wiley: Chichester, 1987.

[7] Gaussian 09, Revision A.1, Gaussian, Inc., Wallingford CT, 2009.

[8] Aquilante, F.; De Vico, L.; Ferré, N.; Ghigo, G.; Malmqvist, P. A.; Neogrády, P.; Pedersen, T. B.; Pitonak, M.; Reiher, M.; Roos, B. O.; Serrano-Andrés, L.; Urban, M.; Veryazov, V.; Lindh, R. MOLCAS 7. The Next Generation. *J. Comput. Chem.* **2010**, *31*, 224-227.

[9] Shuai, Z. G.; Peng, Q.; Niu, Y. L.; Geng, H. MOMAP, a free and open-source molecular materials property prediction package, Revision 0.2.004, Shuai group, Beijing, CN, 2014, http://www.shuaigroup.net/.

[10] Niu, Y.; Peng, Q.; Deng, C.; Gao, X.; Shuai, Z. Theory of Excited State Decays and Optical Spectra: Application to Polyatomic Molecules. *J. Phys. Chem. A* **2010**, *114*, 7817-7831.

[11] Hutt, J. T.; Jo, J.; Olassz, A.; Chen, C.-H.; Lee, D.; Aron, Z. D. Fluorescence Switching of Imidazo[1,5-a]pyridinium Ions: pH-Sensors with Dual Emission Pathways. *Org. Lett.* **2012**, *14*, 3162-3165.

[12] Prassana de Silva, A.; de Silva, S. A. Fluorescent Signaling Crown Ethers; "Switching On" of Fluorescence by Alkali Metal Ion Recognition and Binding in situ. *J. Chem. Soc., Chem. Commun.* **1986**, 1709-1710.

[13] Madhu, S.; Ravikanth, M. Boron-Dipyrromethene Based Reversible and Reusable Selective Chemosensor for Fluoride Detection. *Inorg. Chem.* **2014**, *53*, 1646-1653.

[14] Xu, K.; Zhao, J.; Escudero, D.; Mahmood, Z.; Jacquemin, D. Controlling Triplet-Triplet Annihilation Upconversion by Tuning the PET in Aminomethyleneanthracenes Derivatives. *J. Phys. Chem. C* **2015**, *119*, 23801-23812.