Supporting Information

Dynamic Stability for the Modification of a Blue Multi-Resonance Thermally Activated Delayed Fluorescence Molecule without Damaging Luminescent Properties

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Theory Background

Rate constants can be described by Fermi's Golden Rule, as follows:

$$k_{if} = \frac{2\pi}{\hbar}\left|\langle \Psi_f \left| H' \right| \Psi_i \rangle\right|^2 \delta(E_{fv'} - E_{iv}) \quad (1)$$

where i and f represent the initial and final states, v and v' represents vibrational states of the initial state and final state. H' is Hamiltonian perturbation operator ◦ E_{iv} and $E_{fv'}$ are the energies of initial and final state. The wavefunction is expressed as: $|\Psi_i\rangle = |\Phi_i\rangle|\Theta_v\rangle$ and $|\Psi_f\rangle = |\Phi_f\rangle|\Theta_{v'}\rangle$, Φ and Θ electron wavefunction and vibration wavefunction. The perturbation matrix element $\langle \Psi_f \left| H' \right| \Psi_i \rangle$ can be expressed in different formation for different natures of transition processes.

The spectrum of a radiative transition is expressed as[1-3]:

$$\sigma_{emi}(\omega,T) = \frac{4\omega^3}{3\hbar c^3}\sum_{v,v'} P_{iv}(T)\left|\langle \Theta_{v'} \left| \mu_0 \right| \Theta_v \rangle\right|^2 \delta(\omega_{iv,fv'} - \omega) \quad (2)$$

where ω is the circular frequency, $\mu_0 = \left|\langle \Phi_f \left| \vec{\mu}_0 \right| \Phi_i \rangle\right|$ is the transition dipole moment, $P_{iv}(T)$ is the Boltzmann distribution. The integral form of this emission rate constant k_r is expressed as follows[1-3]:

$$k_r(T) = \int_0^{+\infty} \sigma_{emi}(\omega,T)d\omega \quad (3)$$

The rate constant of internal conversion (IC) is expressed as[4-6]:

$$k_{IC} = \frac{2\pi}{\hbar}\sum_{v,v'} P_{iv}\left|\left\langle \Phi_f \Theta_{fv'} \left| \hat{H}_{BO} \right| \Phi_i \Theta_{iv} \right\rangle\right|^2 \delta(E_{fv'} - E_{iv}) \quad (4)$$

Where, $\hat{H}_{BO}$ is Born-Oppenheimer operator.

The rate constant of intersystem crossing (ISC) is expressed as[7]:

$$k_{ISC} = \frac{2\pi}{\hbar}\sum_{v,v'} P_{iv}\left|\left\langle \Phi_f \Theta_{fv'} \left| \hat{H}_{SO} \right| \Phi_i \Theta_{iv} \right\rangle\right|^2 \delta(E_{fv'} - E_{iv}) \quad (5)$$

where, $\left\langle \Phi_f \left| \hat{H}_{SO} \right| \Phi_i \right\rangle$ is electron spin-orbit coupling constant.

The calculation of reaction rate constant based on the transitional state theory (TST) using Eyring's equation[8-9]:

$$k_{reaction} = \kappa\frac{k_b T}{\hbar}\exp\left[-\frac{\Delta G^{\ddagger}}{RT}\right] \quad (6)$$

Where, $\kappa = 1 + \frac{1}{24}\left(\frac{\hbar v^{\ddagger}}{k_b T}\right)^2$ which is Wigner's expression for quantum tunneling[9], k_b is Boltzmann distribution coefficient, T is temperature, $\Delta G^{\ddagger}$ is activation free energy, R is the ideal gas constant, $v^{\ddagger}$ is the imaginal frequency at the transition state.

Supplemented Data

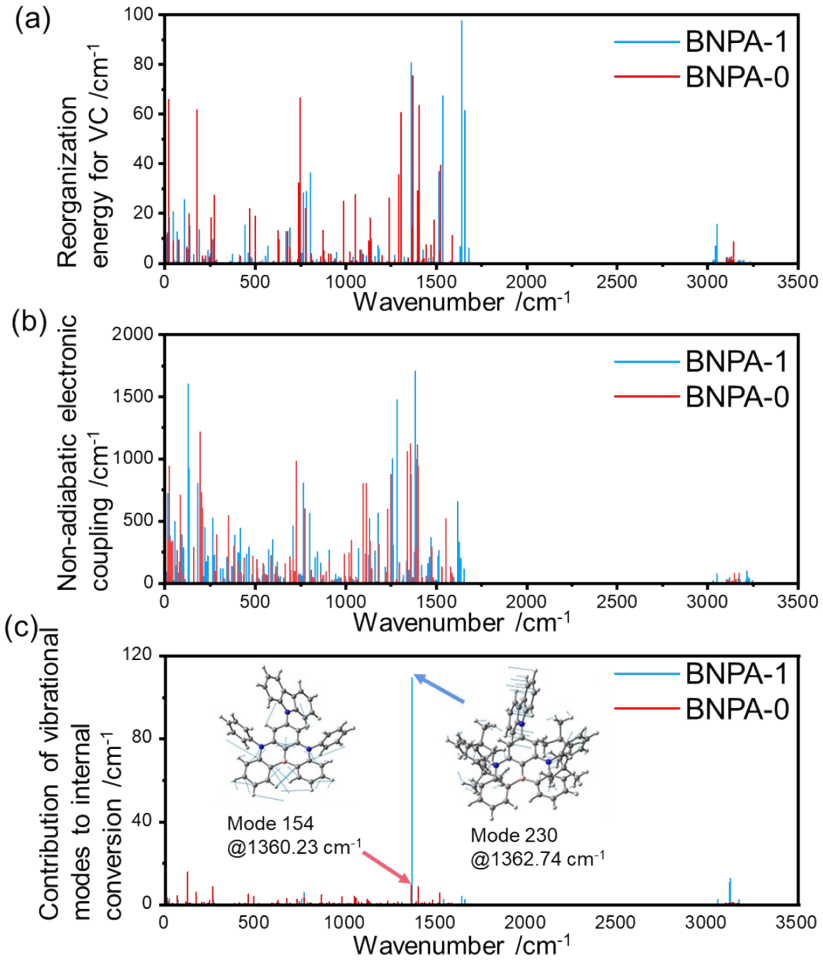

Figure S1. More details of the internal conversions of BNPA-0 and BNPA-1, (a) reorganization energies for vibronic coupling, (b) electronic couplings, (c) contributions of the vibrational modes to the internal conversions.

The k_{IC} of BNPA-1 is several orders of magnitude higher than that of BNPA-0. The details are shown in Figure S1. Figure S1 (a) shows the vibronic couplings and (b) shows the electronic couplings. Both the couplings shows no significant difference. However, the rate constant is consist of both the vibronic and the electronic couplings. Figure S1 (c) shows the total contribution of vibronic and electronic couplings to the rate constant at the energy of each vibrational modes. A significant difference is observed than at around 1360 cm^{-1} the intensity of BNPA-1 is about 100 cm^{-1} while for BNPA-0 the intensity is no larger than 20 cm^{-1}. For BNPA-1 the mode at 1362.74 cm^{-1} distributes almost on the entire molecule including the tert-butyl groups while for BNPA-0 the mode at 1360.23 cm^{-1} mainly distributes on the resonance core moiety.

Table S1. The calculated reaction rate constants evaluated at 298.15 K.

Transition state	$\Delta G^{\ddagger}$ /kcal mol^{-1}	Imaginary frequency /cm^{-1}	Rate constant /s^{-1}
$^3TS_{1\text{-}1}$*	32.05	-381.70	2.19×10^{-11}

$^3TS_{2\text{-}1}$*	28.44	-612.65	1.17×10^{-8}
$^3TS_{1\text{-}2}$*	12.77	-212.25	2.78×10^{3}
$^3TS_{2\text{-}2}$*	2.09	-77.65	1.83×10^{11}
$^3TS_3$*	30.08	-666.64	7.66×10^{-10}

For both Path 1 and Path 2 of BNPA-0, the first elementary reaction is the rate-limiting step with highest $\Delta G^{\ddagger}$. For Path 2 the $\Delta G^{\ddagger}$ (28.44 kcal mol^{-1}) is lower than that of Path 1 (32.05 kcal mol^{-1}). Therefore, Path 2 is the main reaction path. Then quantum yields of both the reaction paths can be calculated using the following equation.

$$\Phi_{reaction} = \frac{k_{reaction}}{k_{rISC} + k_{Phos.} + k_{ISC} + k_{reaction}}$$

The $\Phi_{reaction}$ for Path 2 and Path 1 are calculated to be 8.93×10^{-13} and 1.67×10^{-15} (the rate constant for the potential energy surface crossing through conical intersection is difficult to evaluate and it is ignored here). Both the $\Phi_{reaction}$ are tiny. However, the OLED emitters are expected to endure thousands, hundreds of thousand hours, or even longer operation time before the luminescent intensity decrease to 80% of the initial brightness. To evaluate the t_{80} and t_{50} (the time consumed when the brightness descends to 80% and 50%) the reaction kinetics were derived for Path 2. The reaction equations are listed as the follows:

(1) $^1R \underset{k_{-1}}{\overset{k_1}{\longleftrightarrow}} {}^3R^*$

(2) $^3R^* \xrightarrow{k_2} {}^3IM_{2\text{-}1}^*$ (slow)

(3) $^3IM_{2\text{-}1}^* \xrightarrow{k_3} P$ (fast)

For ^1R, its reaction rate is expressed as

$dc(^1R)/dt = - k_1\, c(^1R) + k_{-1}\, c(^3R^*)$.

For $^3R^*$ as an active specie in excited state, its concentration approximately keeps as a constant.

$dc(^3R^*)/dt = k_1\, c(^1R) - k_{-1}\, c(^3R^*) - k_2\, c(^3R^*) = 0$.

Then, $c(^3R^*) = [k_1/(k_{-1} + k_2)\,]\, c(^1R)$.

$dc(^1R)/dt = - k_1\, c(^1R) + k_{-1}\, c(^3R^*) = - k_1\, c(^1R) + [k_1 k_{-1}/(k_{-1} + k_2)\,]\, c(^1R) = - k_1 k_2/(k_{-1} + k_2)\, c(^1R)$

Considering that $k_2 << k_{-1}$ (k_{-1} represent the total rate constant for the reactant to decay from the excited state), $dc(^1R)/dt \approx - k_1 k_2/k_{-1}\, c(^1R)$.

This equation describes the consumption rate of the reactant and it is a first order reaction. Now, the k_1 representing the rate constant to generate $^3R^*$ containing the ISC and excitation is unknow. If we roughly make $k_1 \approx k_{-1}$, then it is possible to make a coarse evaluation of the t_{80} and t_{50}. If the concentration of the reactant and the luminescence intensity L are approximately in a linear relation like $c(^1R) = k\, L$, the equation above can be converted into $dL/dt = - k_2\, L$.

Then, this differential equation is resolved to give

$\ln(L_t/L_0) = - k_2\, t$,

where L_t is the luminescence intensity at time t and L_0 is the initial luminescence intensity.

Thus, when the luminescence intensity drops to its 80% the t_{80} is

$t_{80} = - \ln 0.8/k_2 = 5297.81$ hours.

t_{50} can also be calculated as $t_{50} = - \ln 0.5/k_2 = 16456.49$ hours.

Based on the same calculation, the $\Phi_{reaction}$ can be evaluated for BNPA-1. The rate constant

for the potential energy surface crossing through conical intersection is difficult to evaluate. If it is ignored the $\Phi_{reaction}$ is 1.09×10^{-15} which is much lower than that of BNPA-0. The conical intersection can make the difference even larger. The t_{50} and t_{80} of BNPA-1 can also be calculated to be 80919.48 hours and 251358.86 hours based on the same derivation and approximation of the reaction kinetics. Obviously the t_{50} and t_{80} of BNPA-1 are much improved comparing those of BNPA-0. The ignored conical intersection can enlarge the k_{-1} and make the consumption rate of the reactant slower according to the equation $dc(^1R)/dt \approx - k_1k_2/k_{-1}\, c(^1R)$. Both the $\Phi_{reaction}$ and t_{50} and t_{80} show BNPA-1 is more stable than BNPA-0 in triplet state.

These results indicate that to ensure a very long operation lifetime (like thousands of hours or even hundreds of thousand hours) for the requirement of industrialization of OLED, the reaction rate constant should be extremely small. On the other hand, it should be noticed that the estimated t_{50} and t_{80} are larger than most of the reported operation half lifetimes of OLEDs. They are over estimated which may be due to the coarse approximations we made during the calculation. The calculations above are rather ideal. Many factors in a real OLED device are neglected or difficult to be considered. However, it qualitatively indicates the modification of BNPA-0 can raise the stability in triplet state.

Table S2. The calculated geometries optimized in S_0 state

BNPA-0			
Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-1.25910600	0.00000000	0.00000000
C	-0.58038600	-1.20989400	-0.15719900
C	-0.58038600	1.20989400	0.15720000
C	0.82415100	-1.21186500	-0.13136700
H	-1.14613800	-2.12095600	-0.32072300
N	-2.67519900	0.00000000	0.00000100
C	0.82415100	1.21186500	0.13136600
H	-1.14613800	2.12095600	0.32072400
N	1.51438700	-2.42031900	-0.24265700
C	1.55635200	0.00000000	0.00000000
C	-3.49375700	0.88581000	-0.71514100
C	-3.49375700	-0.88581000	0.71514300
N	1.51438700	2.42031900	0.24265600
C	2.90641200	-2.51532200	-0.40327100
C	0.73218500	-3.62702000	-0.22715000
B	3.07083700	0.00000000	-0.00000100
C	-3.14512400	1.91646300	-1.59593200
C	-4.85336700	0.56357300	-0.45594900
C	-3.14512300	-1.91646300	1.59593400
C	-4.85336700	-0.56357300	0.45595200
C	2.90641200	2.51532200	0.40327000
C	0.73218500	3.62702000	0.22715000
C	3.47904000	-3.78794000	-0.62989000
C	3.73136300	-1.35381900	-0.35117300

C	0.40087100	-4.21174900	0.99719000
C	0.27964000	-4.18575800	-1.42481900
C	3.73136300	1.35381900	0.35117100
C	-4.17911400	2.63547100	-2.19643600
H	-2.10358300	2.15169200	-1.80934700
C	-5.87228100	1.30143700	-1.07177700
C	-4.17911300	-2.63547100	2.19643800
H	-2.10358200	-2.15169200	1.80934800
C	-5.87228100	-1.30143700	1.07178000
C	3.47904000	3.78794000	0.62988800
C	0.40087000	4.21174900	-0.99719100
C	0.27964000	4.18575800	1.42481900
C	4.83975900	-3.91145300	-0.87189700
H	2.85251800	-4.67746300	-0.63179300
C	5.10293200	-1.53370100	-0.64723100
C	-0.39221100	-5.36140900	1.02330500
H	0.76429600	-3.75462100	1.91873300
C	-0.51047300	-5.33731200	-1.39521700
H	0.54709300	-3.70849700	-2.36861400
C	5.10293300	1.53370200	0.64722900
C	-5.52979900	2.33906600	-1.93690700
H	-3.92919500	3.44633700	-2.88383000
H	-6.91964900	1.06109000	-0.87760500
C	-5.52979800	-2.33906700	1.93690900
H	-3.92919300	-3.44633800	2.88383200
H	-6.91964800	-1.06109100	0.87760800
C	4.83976000	3.91145300	0.87189400
H	2.85251800	4.67746300	0.63179100
C	-0.39221200	5.36140900	-1.02330500
H	0.76429500	3.75462100	-1.91873300
C	-0.51047200	5.33731200	1.39521700
H	0.54709400	3.70849700	2.36861400
C	5.66232300	-2.77711000	-0.90787600
H	5.26004400	-4.90334300	-1.05280800
H	5.74318700	-0.65412500	-0.69564700
C	-0.84891400	-5.92429500	-0.17215200
H	-0.65517200	-5.81754900	1.97963500
H	-0.86754900	-5.77385100	-2.32990800
C	5.66232300	2.77711100	0.90787300
H	5.74318700	0.65412500	0.69564400
H	-6.31339400	2.92428700	-2.42166900
H	-6.31339200	-2.92428700	2.42167200
H	5.26004400	4.90334300	1.05280600
C	-0.84891500	5.92429500	0.17215300

H	-0.65517300	5.81754900	-1.97963500
H	-0.86754800	5.77385100	2.32990900
H	6.72576300	-2.87033900	-1.13546100
H	-1.47151200	-6.82077700	-0.15076200
H	6.72576300	2.87034000	1.13545800
H	-1.47151200	6.82077700	0.15076200

BNPA-1

C	-0.00001300	-1.48626900	0.00000700
C	1.22048700	-0.81593100	-0.03837600
C	-1.22050400	-0.81591400	0.03838100
C	1.22031700	0.58989200	-0.04593800
H	2.14229800	-1.38880800	-0.06002900
N	-0.00002300	-2.90690900	0.00001900
C	-1.22031600	0.58990800	0.04592300
H	-2.14232300	-1.38877900	0.06004200
N	2.42907400	1.27401000	-0.07520500
C	0.00000500	1.31881300	-0.00001300
C	0.47809400	-3.71801800	-1.02890300
C	-0.47813300	-3.71799400	1.02896500
N	-2.42906300	1.27404300	0.07518100
C	2.53826000	2.66615800	-0.16925400
C	3.64015300	0.49071200	-0.05561100
B	0.00001500	2.83405700	-0.00002400
C	1.01633400	-3.34934200	-2.26519200
C	0.30583400	-5.08015400	-0.65822100
C	-1.01637200	-3.34928700	2.26524400
C	-0.30586700	-5.08013800	0.65831800
C	-2.53823100	2.66619300	0.16921000
C	-3.64015300	0.49076100	0.05560200
C	3.82925100	3.24015500	-0.23340600
C	1.38090900	3.49586300	-0.21415700
C	4.18686700	0.12634800	1.20131300
C	4.23083500	0.10836200	-1.28980600
C	-1.38086900	3.49588300	0.21409800
C	1.40645200	-4.37239300	-3.12994000
H	1.12121500	-2.30027500	-2.54041200
C	0.70582700	-6.08684600	-1.54719800
C	-1.40648400	-4.37231700	3.13002100
H	-1.12125600	-2.30021400	2.54043700
C	-0.70585500	-6.08680900	1.54732200
C	-3.82921500	3.24020800	0.23335400
C	-4.18687600	0.12638800	-1.20131500
C	-4.23083800	0.10843800	1.28980400
C	3.98265400	4.60573900	-0.42305600

H	4.70946800	2.60738600	-0.14813800
C	1.59566900	4.87363000	-0.45691200
C	5.36012200	-0.64611100	1.18360100
C	5.42332900	-0.62940600	-1.21765900
C	-1.59561200	4.87365800	0.45683200
C	1.25826400	-5.72722200	-2.77620200
H	1.83340700	-4.11292500	-4.10091200
H	0.58270000	-7.13862300	-1.28039600
C	-1.25829100	-5.72715400	2.77631700
H	-1.83343800	-4.11282500	4.10098600
H	-0.58272400	-7.13859200	1.28054700
C	-3.98259900	4.60579700	0.42298300
H	-4.70944000	2.60744900	0.14809700
C	-5.36014400	-0.64605100	-1.18358900
C	-5.42334300	-0.62931300	1.21767100
C	2.86050200	5.43349900	-0.56800600
H	4.98945300	5.02576900	-0.47730700
H	0.72976400	5.52021400	-0.58634700
C	5.97935400	-1.01000600	-0.00357800
C	-2.86043700	5.43354500	0.56791900
H	-0.72969700	5.52023300	0.58625700
H	1.57523900	-6.50292500	-3.47567700
H	-1.57526200	-6.50284000	3.47581300
H	-4.98939300	5.02584100	0.47722800
C	-5.97937900	-1.00991900	0.00359700
H	2.97958900	6.50134600	-0.75950800
H	6.89934600	-1.59783500	0.01624400
H	-2.97951000	6.50139600	0.75940400
H	-6.89938100	-1.59773300	-0.01621400
H	5.80439700	-0.96933600	2.12355100
H	5.93101100	-0.92066000	-2.13492000
H	-5.80442800	-0.96928000	-2.12353300
H	-5.93102800	-0.92054500	2.13493700
C	-3.74773800	0.44464500	2.73240300
C	-3.63539200	0.44771800	-2.62134300
C	3.74774400	0.44455500	-2.73241100
C	3.63538200	0.44770500	2.62133500
C	2.43458700	1.40464100	2.74362400
H	2.63378900	2.39263000	2.31081700
H	1.51610900	1.00190200	2.30379500
H	2.23719600	1.55290800	3.81695800
C	3.21140400	-0.89030500	3.27132000
H	4.04023500	-1.61185100	3.32024000
H	2.85513600	-0.71319500	4.29908800

H	2.39097700	-1.35406400	2.70172900
C	4.77191000	1.09721500	3.44806100
H	5.65756400	0.45447500	3.54559200
H	5.08952100	2.04546500	2.98591700
H	4.41034900	1.31888400	4.46451400
C	4.71282900	1.49987000	-3.31954800
H	4.64205800	2.44673000	-2.76402500
H	5.75869900	1.15849800	-3.28507400
H	4.45430600	1.70190200	-4.37191400
C	2.31329000	0.98061700	-2.90726500
H	1.55842800	0.28635000	-2.51616800
H	2.15694000	1.96433400	-2.45284300
H	2.12749500	1.09301500	-3.98678400
C	3.81955400	-0.84233600	-3.59334300
H	3.39742500	-0.64049100	-4.59000700
H	4.84565000	-1.20408700	-3.74556600
H	3.24099000	-1.65718600	-3.13275900
C	-4.71280500	1.49998400	3.31952500
H	-5.75868000	1.15862800	3.28505900
H	-4.45427600	1.70202800	4.37188800
H	-4.64202000	2.44683400	2.76398800
C	-2.31327500	0.98068600	2.90724600
H	-1.55842500	0.28640200	2.51615800
H	-2.15691000	1.96439400	2.45280900
H	-2.12747700	1.09309700	3.98676300
C	-3.81956700	-0.84223200	3.59335500
H	-3.39743300	-0.64037900	4.59001400
H	-4.84566900	-1.20396400	3.74558500
H	-3.24101900	-1.65709800	3.13278200
C	-2.43457100	1.40461800	-2.74365000
H	-2.63374100	2.39261800	-2.31085400
H	-1.51610200	1.00185700	-2.30382100
H	-2.23718100	1.55286700	-3.81698600
C	-4.77190900	1.09725300	-3.44806500
H	-4.41035200	1.31890200	-4.46452400
H	-5.65758300	0.45453800	-3.54557900
H	-5.08948800	2.04551700	-2.98592700
C	-3.21145600	-0.89030900	-3.27132100
H	-4.04030700	-1.61183200	-3.32023200
H	-2.85519000	-0.71321600	-4.29909300
H	-2.39103800	-1.35408600	-2.70173200

BNPA-2

C	0.00000200	1.47030900	0.00000100
C	1.22054300	0.79720600	0.03506700

C	-1.22054100	0.79720900	-0.03506600
C	1.22256300	-0.60600000	0.02427100
H	2.14531200	1.36270100	0.09040200
N	0.00000400	2.88786800	0.00000000
C	-1.22256600	-0.60599600	-0.02426900
H	-2.14530900	1.36270600	-0.09040100
N	2.44001500	-1.29055000	0.05923300
C	-0.00000200	-1.33345800	0.00000100
C	-0.70396500	3.70161400	0.89084100
C	0.70397700	3.70161000	-0.89084200
N	-2.44001800	-1.29054300	-0.05923200
C	2.53635600	-2.68551700	0.20306400
C	3.65110500	-0.51212300	0.04245800
B	-0.00000400	-2.84677600	0.00000100
C	-1.51216600	3.33545600	1.97160200
C	-0.44806000	5.06288400	0.57076100
C	1.51217600	3.33544700	-1.97160300
C	0.44807600	5.06288100	-0.57076600
C	-2.53636300	-2.68551000	-0.20306300
C	-3.65110700	-0.51211300	-0.04245800
C	3.81981000	-3.27143800	0.29942400
C	1.37385900	-3.50716100	0.24819000
C	4.08106200	0.09892900	-1.16470400
C	4.39125800	-0.37358400	1.24650500
C	-1.37386900	-3.50715700	-0.24818800
C	-2.08031100	4.36156800	2.72696500
H	-1.69095100	2.28638600	2.20310600
C	-1.03448300	6.07247600	1.34562600
C	2.08032600	4.36155500	-2.72696700
H	1.69095700	2.28637600	-2.20310500
C	1.03450300	6.07246900	-1.34563200
C	-3.81981900	-3.27142700	-0.29942300
C	-4.08106200	0.09894100	1.16470300
C	-4.39125800	-0.37357400	-1.24650500
C	3.95800000	-4.63298200	0.52204000
H	4.70605100	-2.64898500	0.20659300
C	1.56995500	-4.88206200	0.52484400
C	5.27502300	0.85066600	-1.13745200
C	5.59279200	0.36064400	1.21861100
C	-1.56996800	-4.88205800	-0.52484200
C	-1.85035000	5.71611300	2.41861400
H	-2.71439000	4.10593400	3.57876100
H	-0.84928600	7.12335400	1.11344900
C	1.85036900	5.71610100	-2.41861900

H	2.71440400	4.10591700	-3.57876200
H	0.84931000	7.12334900	-1.11345700
C	-3.95801200	-4.63297100	-0.52203800
H	-4.70605800	-2.64897200	-0.20659200
C	-5.27502100	0.85068100	1.13744900
C	-5.59279000	0.36065700	-1.21861300
C	2.82723800	-5.44935700	0.66983900
H	4.96055500	-5.05975800	0.60034600
H	0.69382100	-5.51614100	0.65056700
C	6.01182400	0.96400200	0.03750100
C	-2.82725300	-5.44935000	-0.66983700
H	-0.69383600	-5.51614000	-0.65056400
H	-2.31321200	6.49313100	3.02978600
H	2.31323400	6.49311700	-3.02979300
H	-4.96056900	-5.05974500	-0.60034400
C	-6.01182100	0.96401800	-0.03750500
H	2.93496800	-6.51360000	0.88754700
H	6.93780200	1.54333100	0.03069800
H	-2.93498500	-6.51359300	-0.88754400
H	-6.93779800	1.54335000	-0.03070300
H	-6.17281100	0.48747400	-2.13101600
H	-5.64518300	1.32159000	2.04462900
H	6.17281200	0.48746100	2.13101300
H	5.64518500	1.32157200	-2.04463200
N	-3.97669900	-1.01375800	-2.41503500
N	-3.33041400	-0.00342400	2.34188900
N	3.97669600	-1.01376300	2.41503600
N	3.33041200	-0.00343500	-2.34188900
C	-4.95793100	-1.33700500	-3.42828500
H	-5.20234000	-0.48759300	-4.10115900
H	-4.56693100	-2.15624500	-4.05180700
H	-5.88856800	-1.68731200	-2.95979800
C	-2.60874200	-0.89526500	-2.90623400
H	-2.04911300	-1.84444700	-2.82576100
H	-2.62763800	-0.59436300	-3.96824700
H	-2.05819200	-0.11959600	-2.36172200
C	-2.76780900	-1.29875300	2.74010900
H	-1.70068000	-1.39320300	2.48220600
H	-2.86559600	-1.40540000	3.83079200
H	-3.31134200	-2.13529700	2.27900500
C	-3.69520600	0.85123900	3.45834900
H	-4.61169300	0.51859200	3.98947800
H	-2.86661100	0.86029800	4.18118500
H	-3.84994300	1.88272600	3.11499300

C	2.60873900	-0.89526300	2.90623600
H	2.04910600	-1.84444300	2.82576500
H	2.62763700	-0.59435800	3.96824800
H	2.05819300	-0.11959300	2.36172200
C	4.95792700	-1.33701000	3.42828800
H	5.20233900	-0.48759700	4.10115900
H	4.56692400	-2.15624700	4.05181200
H	5.88856300	-1.68732200	2.95980200
C	2.76780300	-1.29876200	-2.74010700
H	1.70067400	-1.39321000	-2.48220200
H	2.86558800	-1.40541100	-3.83079000
H	3.31133500	-2.13530800	-2.27900300
C	3.69520500	0.85122700	-3.45835100
H	4.61169000	0.51857700	-3.98948000
H	2.86660900	0.86028600	-4.18118500
H	3.84994500	1.88271400	-3.11499500

BNPA-3

C	-1.47323600	0.00000000	0.00000000
C	-0.81053800	-1.22430200	-0.07762200
C	-0.81053800	1.22430200	0.07762200
C	0.58871900	-1.22574500	-0.01270200
H	-1.38064600	-2.13573700	-0.21082700
N	-2.92087800	0.00000000	0.00000000
C	0.58871900	1.22574500	0.01270200
H	-1.38064600	2.13573700	0.21082600
N	1.30024700	-2.43582100	0.00975800
C	1.34010700	0.00000000	0.00000000
C	-3.71562200	0.06730200	-1.12283300
C	-3.71562200	-0.06730200	1.12283400
N	1.30024700	2.43582000	-0.00975800
C	2.69271000	-2.48111600	-0.21672300
C	0.83632500	-3.76410500	0.10682900
B	2.87943800	0.00000000	0.00000000
C	-3.30638100	0.14766200	-2.46237800
C	-5.08846700	0.04335800	-0.73123800
C	-3.30638100	-0.14766100	2.46237800
C	-5.08846700	-0.04335800	0.73123800
C	2.69271000	2.48111600	0.21672300
C	0.83632500	3.76410500	-0.10682900
C	3.10936700	-3.81794200	-0.34941300
C	3.54551200	-1.36302200	-0.24755400
C	-0.41023100	-4.29669100	0.46482200
C	1.93809200	-4.64084100	-0.14670900
C	3.54551200	1.36302200	0.24755400

C	-4.31152500	0.20451400	-3.42877900
H	-2.24737500	0.16453800	-2.71453600
C	-6.06749600	0.10107700	-1.70745400
C	-4.31152500	-0.20451400	3.42877900
H	-2.24737500	-0.16453800	2.71453500
C	-6.06749600	-0.10107700	1.70745500
C	3.10936700	3.81794200	0.34941300
C	-0.41023100	4.29669100	-0.46482200
C	1.93809200	4.64084100	0.14670900
C	4.47201100	-4.08713900	-0.58595900
C	4.90340900	-1.68102300	-0.49959100
C	-0.56400100	-5.68579400	0.50055400
H	-1.24560000	-3.66956300	0.76263300
C	1.75633400	-6.02795900	-0.11113100
C	4.90340900	1.68102200	0.49959100
C	-5.66558500	0.18168400	-3.06133100
H	-4.04100600	0.26760300	-4.48267000
H	-7.12728500	0.08546600	-1.44994800
C	-5.66558500	-0.18168400	3.06133100
H	-4.04100600	-0.26760200	4.48267000
H	-7.12728500	-0.08546600	1.44994800
C	4.47201100	4.08713900	0.58595900
C	-0.56400100	5.68579400	-0.50055400
H	-1.24560000	3.66956300	-0.76263300
C	1.75633500	6.02795900	0.11113100
C	5.34763200	-3.00369600	-0.66937900
H	4.83125500	-5.11219400	-0.69315600
H	5.62971700	-0.87129200	-0.57611100
C	0.50111100	-6.54894300	0.19847700
H	-1.53363300	-6.10131600	0.78290900
H	2.60077000	-6.69098400	-0.31079600
C	5.34763200	3.00369600	0.66937900
H	5.62971700	0.87129100	0.57611200
H	-6.43024100	0.22737400	-3.83768100
H	-6.43024100	-0.22737400	3.83768100
H	4.83125500	5.11219300	0.69315600
C	0.50111100	6.54894300	-0.19847700
H	-1.53363200	6.10131600	-0.78290900
H	2.60077000	6.69098400	0.31079600
H	6.40816800	-3.18674500	-0.85929700
H	0.34975300	-7.62974800	0.22910500
H	6.40816800	3.18674400	0.85929700
H	0.34975300	7.62974800	-0.22910500

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Table S3. Coordinates for $^{3}R^{*}$

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	1.274077	-0.000001	0.000000
C	0.566279	-1.196328	-0.190727
C	0.566282	1.196327	0.190726
C	-0.843614	-1.198541	-0.140940
H	1.123158	-2.111450	-0.372910
N	2.687996	-0.000003	-0.000001
C	-0.843611	1.198542	0.140940
H	1.123162	2.111447	0.372909
N	-1.526555	-2.414196	-0.261436
C	-1.592610	0.000001	0.000000
C	3.505154	0.840010	-0.764419
C	3.505153	-0.840016	0.764417
N	-1.526550	2.414199	0.261436
C	-2.924782	-2.557094	-0.145606
C	-0.730303	-3.605489	-0.407641
B	-3.101104	0.000003	0.000000
C	3.147687	1.824357	-1.692620
C	4.866588	0.538455	-0.485668
C	3.147684	-1.824363	1.692619
C	4.866587	-0.538463	0.485668
C	-2.924776	2.557099	0.145606
C	-0.730296	3.605490	0.407642
C	-3.467893	-3.856801	-0.178369
C	-3.759633	-1.397736	0.018850
C	-0.436610	-4.086940	-1.684122
C	-0.238450	-4.249928	0.729891
C	-3.759630	1.397743	-0.018850
C	4.176646	2.518989	-2.329278
H	2.102618	2.039293	-1.914910
C	5.879710	1.251565	-1.139182
C	4.176643	-2.518996	2.329277
H	2.102615	-2.039298	1.914908
C	5.879709	-1.251573	1.139182
C	-3.467884	3.856807	0.178369
C	-0.436601	4.086939	1.684122
C	-0.238442	4.249928	-0.729891
C	-4.840022	-4.054435	-0.013505
H	-2.819321	-4.718094	-0.322196
C	-5.133838	-1.664428	0.224190
C	0.362727	-5.224548	-1.822583
H	-0.833224	-3.563938	-2.555230
C	0.562146	-5.384793	0.585827

H	-0.485899	-3.853190	1.715456
C	-5.133834	1.664439	-0.224191
C	5.529391	2.242189	-2.055626
H	3.923637	3.292546	-3.057413
H	6.929211	1.029849	-0.934329
C	5.529388	-2.242197	2.055626
H	3.923633	-3.292553	3.057413
H	6.929210	-1.029859	0.934329
C	-4.840013	4.054445	0.013505
H	-2.819311	4.718098	0.322196
C	0.362738	5.224545	1.822583
H	-0.833216	3.563938	2.555230
C	0.562157	5.384791	-0.585826
H	-0.485892	3.853191	-1.715456
C	-5.671006	-2.952320	0.206701
H	-5.247356	-5.066331	-0.042683
H	-5.802120	-0.830533	0.429001
C	0.863793	-5.872203	-0.689625
H	0.598167	-5.602429	-2.819212
H	0.953788	-5.887575	1.471958
C	-5.670999	2.952331	-0.206701
H	-5.802117	0.830545	-0.429001
H	6.309205	2.806785	-2.569984
H	6.309202	-2.806794	2.569984
H	-5.247344	5.066341	0.042684
C	0.863806	5.872200	0.689626
H	0.598179	5.602425	2.819213
H	0.953800	5.887572	-1.471957
H	-6.742365	-3.095800	0.365472
H	1.492610	-6.757554	-0.800591
H	-6.742358	3.095814	-0.365473
H	1.492624	6.757549	0.800592

Table S4. Coordinates for $^{3}TS_{1\text{-}1}$*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-0.400085	-1.594680	-1.176629
C	0.922352	-1.797726	-0.795707
C	-0.954631	-0.309221	-1.301444
C	1.735562	-0.665613	-0.575908
H	1.304326	-2.805012	-0.641004
N	-1.706796	-2.337686	0.094635
C	-0.203193	0.796230	-0.837850
H	-1.968311	-0.182139	-1.675581
N	3.090951	-0.816283	-0.304000

C	1.177948	0.656906	-0.545675
C	-1.828578	-1.726068	1.341353
C	-2.992293	-2.548871	-0.365378
N	-0.822920	2.033905	-0.705347
C	3.999691	0.252405	-0.156125
C	3.606926	-2.158294	-0.231521
B	2.019356	1.860111	-0.216584
C	-0.806211	-1.246406	2.169083
C	-3.202807	-1.571167	1.704742
C	-3.376760	-3.081975	-1.603970
C	-3.967153	-2.112716	0.587881
C	-0.168263	3.188271	-0.251104
C	-2.261361	2.043072	-0.810428
C	5.376079	-0.042469	-0.040363
C	3.547548	1.603235	-0.148249
C	3.678734	-2.799239	1.006469
C	4.020893	-2.809332	-1.395372
C	1.232922	3.173655	0.020299
C	-1.168662	-0.604106	3.356704
H	0.237580	-1.359731	1.877315
C	-3.543291	-0.948284	2.904803
C	-4.742036	-3.182887	-1.878711
H	-2.617627	-3.397557	-2.320797
C	-5.324099	-2.230929	0.297992
C	-0.932894	4.357902	-0.031851
C	-2.880036	2.482406	-1.981334
C	-3.014531	1.552447	0.259345
C	6.310555	0.983214	0.027674
H	5.716276	-1.075448	-0.021622
C	4.542174	2.604966	-0.118473
C	4.171956	-4.104142	1.080646
H	3.346816	-2.269012	1.900281
C	4.513589	-4.113621	-1.317074
H	3.949360	-2.287982	-2.350676
C	1.781807	4.356779	0.567330
C	-2.517447	-0.460012	3.726091
H	-0.388796	-0.209296	4.010992
H	-4.589414	-0.829800	3.197270
C	-5.704531	-2.767390	-0.941048
H	-5.069644	-3.592372	-2.836427
H	-6.081840	-1.907161	1.015316
C	-0.333382	5.500909	0.473684
H	-1.999955	4.359459	-0.243197
C	-4.273007	2.427756	-2.082308

H	-2.266971	2.851237	-2.804883
C	-4.403857	1.490693	0.147388
H	-2.507423	1.199703	1.157225
C	5.900440	2.319945	-0.033245
H	7.370553	0.733243	0.110019
H	4.234988	3.647132	-0.191447
C	4.589597	-4.761682	-0.080163
H	4.227404	-4.608619	2.047124
H	4.837179	-4.626013	-2.225085
C	1.032563	5.503641	0.792014
H	2.831699	4.359057	0.854699
H	-2.767707	0.037414	4.665155
H	-6.764942	-2.863507	-1.182942
H	-0.940556	6.393301	0.640185
C	-5.034252	1.928053	-1.021187
H	-4.762907	2.764134	-2.998065
H	-4.989614	1.085246	0.973395
H	6.635138	3.127049	-0.015167
H	4.973448	-5.782030	-0.021310
H	1.498542	6.393197	1.219986
H	-6.120888	1.871484	-1.109140

Table S4. Coordinates for MECP

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	0.232495	-2.174402	-1.376006
C	-1.108052	-1.716059	-1.096151
C	1.121198	-1.063745	-1.240993
C	-1.574294	-0.404835	-0.878771
H	-1.880434	-2.502400	-1.175505
N	0.301932	-2.904713	0.843220
C	0.788580	0.275480	-1.017089
H	2.210777	-1.280299	-1.352836
N	-2.937272	-0.142249	-0.583081
C	-0.591704	0.582801	-0.682591
C	1.773057	-3.196839	0.861793
C	0.256352	-1.737696	1.654269
N	1.739735	1.304921	-0.867627
C	-3.358712	1.006056	0.071960
C	-3.899363	-1.151306	-0.937832
B	-0.992147	1.969023	-0.162311
C	2.333867	-4.305419	0.277404
C	2.478093	-2.238705	1.566556
C	-0.920844	-1.087447	2.102323
C	1.536711	-1.268112	2.093606

C	1.436211	2.646717	-0.563461
C	3.113487	0.969255	-1.136084
C	-4.717332	1.112851	0.474624
C	-2.435749	2.066703	0.364531
C	-4.424556	-1.166845	-2.229098
C	-4.293359	-2.117304	-0.003193
C	0.106899	3.050975	-0.241318
C	3.699322	-4.392099	0.274741
H	1.692834	-5.001481	-0.292418
C	3.908403	-2.350738	1.595054
C	-0.823022	0.070931	2.857307
H	-1.890409	-1.508407	1.825776
C	1.622904	-0.088182	2.852407
C	2.473562	3.608099	-0.598683
C	3.988450	0.660304	-0.094765
C	3.560277	0.944452	-2.459547
C	-5.144054	2.193881	1.219378
H	-5.418634	0.323643	0.213641
C	-2.927968	3.130272	1.168870
C	-5.357887	-2.143552	-2.587331
H	-4.092351	-0.412745	-2.943513
C	-5.223175	-3.093002	-0.364059
H	-3.866649	-2.103098	1.000252
C	-0.120469	4.435613	-0.060813
C	4.490816	-3.397476	0.929162
H	4.206420	-5.195900	-0.274084
H	4.505604	-1.593094	2.109473
C	0.445420	0.584891	3.195313
H	-1.719042	0.628090	3.126867
H	2.592273	0.320059	3.137876
C	2.198927	4.953392	-0.379060
H	3.492842	3.305205	-0.828351
C	5.316110	0.326829	-0.374101
H	3.617882	0.680431	0.929927
C	4.886888	0.608471	-2.737697
H	2.857099	1.180150	-3.258695
C	-4.240529	3.206395	1.600518
H	-6.191212	2.247388	1.523435
H	-2.227867	3.907293	1.473005
C	-5.759229	-3.105396	-1.656147
H	-5.770408	-2.150067	-3.597882
H	-5.526002	-3.846600	0.365443
C	0.892314	5.385214	-0.123120
H	-1.142920	4.772946	0.106182

H	5.576086	-3.480769	0.879839
H	0.502053	1.544679	3.718638
H	3.018967	5.674448	-0.430336
C	5.767082	0.298901	-1.695965
H	5.998673	0.080931	0.442689
H	5.232010	0.588479	-3.772845
H	-4.575541	4.041954	2.218001
H	-6.488706	-3.867555	-1.936333
H	0.669827	6.444531	0.014848
H	6.804024	0.035434	-1.914773

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119 **Table S5**. Coordinates for $^{1}IM_{1-1}$

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	0.948800	-3.293968	0.174409
C	2.008969	-2.457278	0.232393
C	-0.322103	-3.013744	-0.190020
C	1.801522	-1.155106	-0.369957
H	2.892231	-2.633712	0.847159
N	-2.489979	0.356755	2.000779
C	-0.611298	-1.609529	-0.421076
H	-1.030816	-3.770969	-0.526855
N	2.879157	-0.315827	-0.573282
C	0.481663	-0.705777	-0.602470
C	-2.484385	1.682651	1.619267
C	-1.195458	0.056160	2.294048
N	-1.889891	-1.206827	-0.696247
C	2.752848	1.065209	-0.822526
C	4.193254	-0.881522	-0.410735
B	0.226454	0.729658	-1.015570
C	-3.576469	2.449323	1.184131
C	-1.170668	2.265284	1.672374
C	-0.678530	-1.195985	2.691758
C	-0.304536	1.181576	2.112682
C	-2.218011	0.047038	-1.259413
C	-2.956078	-2.176636	-0.536951
C	3.921685	1.855470	-0.894423
C	1.468040	1.653905	-0.994189
C	4.901602	-0.679173	0.777286
C	4.737985	-1.649503	-1.441048
C	-1.219617	1.040262	-1.458617
C	-3.356204	3.777970	0.815944
H	-4.569832	2.000958	1.132351
C	-0.971748	3.596311	1.318015
C	0.691415	-1.314071	2.908412

H	-1.346213	-2.047269	2.830302
C	1.059386	1.038100	2.320948
C	-3.559556	0.287940	-1.624720
C	-3.244074	-3.039406	-1.598283
C	-3.681987	-2.221197	0.652439
C	3.825330	3.231257	-1.048710
H	4.903294	1.393497	-0.817808
C	1.426332	3.061255	-1.113283
C	6.165757	-1.251177	0.931900
H	4.457639	-0.071808	1.565988
C	6.001958	-2.222264	-1.280373
H	4.164067	-1.795176	-2.356963
C	-1.628142	2.226052	-2.110112
C	-2.073582	4.349569	0.882654
H	-4.194129	4.385138	0.466246
H	0.021669	4.047145	1.368715
C	1.554708	-0.222217	2.711992
H	1.107293	-2.277167	3.208860
H	1.743801	1.875364	2.167824
C	-3.911263	1.482996	-2.233492
H	-4.323236	-0.461157	-1.432186
C	-4.261937	-3.984293	-1.456210
H	-2.669793	-2.965035	-2.523341
C	-4.700880	-3.170311	0.781926
H	-3.463793	-1.476383	1.423542
C	2.570191	3.848965	-1.131162
H	4.738750	3.828235	-1.092154
H	0.455860	3.549470	-1.159491
C	6.716451	-2.023927	-0.095597
H	6.720415	-1.095390	1.859073
H	6.429192	-2.824568	-2.084201
C	-2.938736	2.454936	-2.500564
H	-0.880602	2.982422	-2.337387
H	-1.934190	5.394135	0.595647
H	2.624272	-0.349868	2.888397
H	-4.953582	1.653783	-2.510232
C	-4.988046	-4.053423	-0.262490
H	-4.489515	-4.664095	-2.279509
H	-5.278556	-3.211652	1.707523
H	2.492085	4.934339	-1.216568
H	7.704060	-2.472272	0.028150
H	-3.210554	3.386819	-2.999099
H	-5.784606	-4.792111	-0.151843

121 **Table S6**. Coordinates for $^{3}IM_{1\text{-}1}$*

Atom	X/Angstrom	Y/Angstrom	Z/Angstrom
C	0.630510	-3.349139	0.191203
C	1.781643	-2.626027	-0.006310
C	-0.669649	-2.947363	0.008843
C	1.595004	-1.288118	-0.426336
H	2.770961	-3.041548	0.171639
N	-1.797991	0.214101	2.245799
C	-0.839305	-1.620258	-0.455364
H	-1.516212	-3.607302	0.184746
N	2.704517	-0.460878	-0.618982
C	0.287441	-0.773973	-0.664960
C	-2.034978	1.481462	1.762419
C	-0.442028	0.162729	2.505458
N	-2.123061	-1.135754	-0.709251
C	2.615915	0.922763	-0.836186
C	4.007274	-1.070309	-0.607319
B	0.096875	0.652144	-1.138257
C	-3.260699	1.992726	1.308143
C	-0.845103	2.282590	1.717586
C	0.284778	-0.944643	2.960916
C	0.216178	1.403287	2.211201
C	-2.386267	0.099583	-1.316797
C	-3.233631	-2.006419	-0.416559
C	3.798005	1.696360	-0.781040
C	1.359125	1.544682	-1.080254
C	4.703989	-1.238213	0.591705
C	4.565927	-1.498239	-1.813914
C	-1.333244	1.018126	-1.594268
C	-3.289465	3.299689	0.814669
H	-4.155584	1.370323	1.326020
C	-0.892224	3.582317	1.244263
C	1.665883	-0.799473	3.137820
H	-0.219809	-1.892584	3.148396
C	1.583237	1.531993	2.381079
C	-3.721301	0.424308	-1.653248
C	-3.732305	-2.847835	-1.414555
C	-3.788851	-2.005386	0.864841
C	3.739362	3.077063	-0.907636
H	4.759378	1.214514	-0.615368
C	1.354690	2.953979	-1.181535
C	5.967027	-1.834699	0.581698
H	4.243618	-0.902146	1.519052
C	5.829954	-2.092420	-1.821250

H	4.002152	-1.358783	-2.737331
C	-1.681325	2.194708	-2.295123
C	-2.127874	4.084248	0.786882
H	-4.224690	3.711577	0.433065
H	0.005345	4.201245	1.204611
C	2.302149	0.418347	2.861290
H	2.255988	-1.649274	3.485155
H	2.102193	2.459623	2.133446
C	-4.010904	1.609730	-2.313352
H	-4.528728	-0.261624	-1.407524
C	-4.808730	-3.691203	-1.130809
H	-3.274017	-2.830830	-2.404554
C	-4.864989	-2.853942	1.141059
H	-3.351861	-1.349766	1.621247
C	2.508417	3.722180	-1.092705
H	4.663009	3.657294	-0.847579
H	0.399434	3.460305	-1.302711
C	6.531895	-2.261319	-0.623974
H	6.511380	-1.966574	1.518927
H	6.266847	-2.425927	-2.764551
C	-2.986161	2.499671	-2.659528
H	-0.886758	2.880525	-2.585093
H	-2.179082	5.101818	0.394319
H	3.379064	0.511315	3.015173
H	-5.048241	1.834913	-2.571541
C	-5.377154	-3.693480	0.147255
H	-5.202850	-4.348798	-1.908230
H	-5.303634	-2.859660	2.141127
H	2.458158	4.810101	-1.169061
H	7.519446	-2.726903	-0.630381
H	-3.209114	3.418487	-3.205002
H	-6.218328	-4.353831	0.368497

Table S6. Coordinates for $^{3}TS_{1\text{-}2}$*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	0.341231	-3.687735	0.718043
C	1.492179	-3.065263	0.297393
C	-0.955255	-3.242680	0.597834
C	1.306299	-1.793362	-0.306033
H	2.479584	-3.495593	0.450803
N	-0.532776	1.243313	0.657534
C	-1.114617	-1.990342	-0.046177
H	-1.807929	-3.818301	0.954337
N	2.427337	-1.028021	-0.681624

C	0.015443	-1.250007	-0.461827
C	-1.012719	2.542986	0.556030
C	0.460945	1.276829	1.645389
N	-2.392791	-1.452385	-0.265502
C	2.367360	0.271970	-1.208249
C	3.723341	-1.620976	-0.488961
B	-0.205679	0.195994	-0.976913
C	-2.092992	3.012280	-0.212743
C	-0.291251	3.436282	1.410773
C	1.171374	0.204452	2.200439
C	0.671140	2.604999	2.123672
C	-2.635740	-0.489596	-1.273653
C	-3.509010	-2.044256	0.410392
C	3.576592	0.922319	-1.558694
C	1.120834	0.936898	-1.382442
C	4.431249	-1.362095	0.687265
C	4.258499	-2.453379	-1.473956
C	-1.561777	0.291485	-1.768784
C	-2.401126	4.373702	-0.154879
H	-2.681557	2.335067	-0.824272
C	-0.614264	4.786785	1.457971
C	2.109395	0.478669	3.203068
H	0.986413	-0.817390	1.882649
C	1.614012	2.863136	3.112236
C	-3.935891	-0.314766	-1.785335
C	-4.167338	-3.156593	-0.124622
C	-3.932062	-1.490520	1.621224
C	3.557053	2.222392	-2.038025
H	4.529311	0.411480	-1.438915
C	1.157955	2.265428	-1.850853
C	5.687013	-1.943047	0.876677
H	3.990514	-0.702796	1.435594
C	5.514089	-3.033968	-1.278550
H	3.684194	-2.639752	-2.382406
C	-1.809405	1.102702	-2.887541
C	-1.669200	5.254205	0.657164
H	-3.234566	4.754964	-0.747783
H	-0.067255	5.472378	2.108608
C	2.343989	1.788161	3.644375
H	2.660335	-0.349336	3.654188
H	1.779507	3.879124	3.477025
C	-4.152536	0.555520	-2.853158
H	-4.773237	-0.870192	-1.365998
C	-5.251676	-3.714619	0.556546

H	-3.822119	-3.573413	-1.072028
C	-5.017353	-2.050157	2.299908
H	-3.399156	-0.623322	2.014179
C	2.342396	2.912419	-2.178097
H	4.500139	2.709799	-2.294727
H	0.217866	2.810233	-1.937540
C	6.228937	-2.779637	-0.104186
H	6.243727	-1.742125	1.794137
H	5.934925	-3.686079	-2.046319
C	-3.083866	1.241511	-3.438745
H	-0.979613	1.663549	-3.319951
H	-1.935087	6.312945	0.680869
H	3.087912	1.972477	4.421858
H	-5.165447	0.674325	-3.244764
C	-5.677557	-3.162096	1.768697
H	-5.765820	-4.582996	0.139608
H	-5.347666	-1.617124	3.246242
H	2.329981	3.943101	-2.537473
H	7.210168	-3.234019	0.046693
H	-3.247798	1.891968	-4.300223
H	-6.525456	-3.599506	2.299778

Table S6. Coordinates for $^{3}P_{1\text{-}1}$*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	1.045118	-3.164597	1.161819
C	2.145724	-2.432525	0.806861
C	-0.269176	-2.908048	0.824318
C	1.880909	-1.236205	0.062237
H	3.158100	-2.730970	1.071888
N	-0.630087	1.379005	0.283625
C	-0.487979	-1.752522	0.030115
H	-1.091113	-3.555723	1.127831
N	2.947937	-0.416898	-0.324569
C	0.563702	-0.860998	-0.244901
C	-1.931028	1.890953	0.248502
C	-0.210837	1.428749	1.612269
N	-1.739197	-1.483260	-0.541874
C	2.800509	0.825789	-0.977890
C	4.280222	-0.851566	0.007983
B	0.178294	0.576044	-0.835325
C	-2.789193	2.129537	-0.840900
C	-2.371168	2.202111	1.572969
C	1.032177	1.088241	2.170385
C	-1.259828	1.905867	2.451540

C	-1.804324	-0.760274	-1.756341
C	-2.931983	-2.073823	-0.010945
C	3.966948	1.535718	-1.356350
C	1.510930	1.377915	-1.199824
C	4.878093	-0.400079	1.186778
C	4.955574	-1.722930	-0.848314
C	-0.791556	0.186059	-2.056733
C	-4.068767	2.620930	-0.586221
H	-2.478549	1.940556	-1.863480
C	-3.661251	2.688571	1.805810
C	1.195111	1.194019	3.552126
H	1.864825	0.777416	1.549686
C	-1.077842	2.005225	3.832675
C	-2.860379	-0.992868	-2.655915
C	-3.273807	-3.398953	-0.302710
C	-3.766816	-1.287016	0.789350
C	3.857463	2.800083	-1.914546
H	4.952398	1.102244	-1.199520
C	1.455438	2.679244	-1.725921
C	6.167103	-0.828450	1.510673
H	4.330659	0.283819	1.836690
C	6.244702	-2.148700	-0.518739
H	4.464215	-2.059439	-1.762122
C	-0.786036	0.745097	-3.343082
C	-4.515256	2.888305	0.720621
H	-4.738708	2.798833	-1.430019
H	-3.990042	2.911562	2.823339
C	0.153688	1.640184	4.383064
H	2.158595	0.929248	3.993696
H	-1.887161	2.364600	4.472249
C	-2.861301	-0.358738	-3.895189
H	-3.663652	-1.680398	-2.393959
C	-4.449248	-3.943117	0.221715
H	-2.619645	-3.989903	-0.945899
C	-4.943178	-1.834537	1.304723
H	-3.488359	-0.252982	0.993519
C	2.595717	3.389341	-2.091929
H	4.762677	3.337710	-2.203694
H	0.472341	3.139173	-1.850740
C	6.850639	-1.702408	0.659425
H	6.637539	-0.479472	2.431678
H	6.776208	-2.830957	-1.184703
C	-1.806869	0.490290	-4.259298
H	0.011429	1.442354	-3.607781

H	-5.527103	3.264855	0.882750
H	0.312260	1.711928	5.460723
H	-3.679510	-0.549812	-4.592997
C	-5.284372	-3.161610	1.025623
H	-4.715796	-4.977614	-0.004085
H	-5.594337	-1.218561	1.927945
H	2.511845	4.391287	-2.517816
H	7.857832	-2.036652	0.915414
H	-1.800181	0.968261	-5.241250
H	-6.204229	-3.587121	1.432037

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127 **Table S7**. Coordinates for $^{1}P_{1\text{-}1}$

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	0.836708	-3.169663	-0.614026
C	1.965621	-2.494890	-0.802613
C	-0.413054	-2.739699	-0.408540
C	1.783034	-1.019258	-0.610596
H	2.835146	-2.842646	-1.362673
N	-0.514310	1.195198	1.016571
C	-0.608526	-1.348000	-0.846406
H	-1.143069	-3.198140	0.264068
N	2.878026	-0.212835	-0.633690
C	0.487787	-0.487423	-0.678251
C	-1.865116	1.421151	1.313948
C	0.024498	0.529447	2.121991
N	-1.829122	-0.845846	-1.185659
C	2.804796	1.223647	-0.637339
C	4.168924	-0.841023	-0.500063
B	0.168659	1.069686	-0.422593
C	-2.841260	2.155194	0.614849
C	-2.205854	0.818883	2.565119
C	1.353876	0.155870	2.372671
C	-0.985376	0.245842	3.085823
C	-1.929838	0.445849	-1.788170
C	-2.999825	-1.670326	-1.077798
C	4.010622	1.952140	-0.679592
C	1.558006	1.874397	-0.479899
C	4.562432	-1.340016	0.742955
C	4.995168	-0.970389	-1.619267
C	-0.910134	1.402046	-1.574574
C	-4.135849	2.210433	1.130333
H	-2.605802	2.682901	-0.304516
C	-3.513689	0.884318	3.063352
C	1.645841	-0.525338	3.554429

H	2.151988	0.436571	1.692465
C	-0.673138	-0.443001	4.264744
C	-3.018436	0.702851	-2.637013
C	-3.164875	-2.782193	-1.908181
C	-3.961644	-1.336934	-0.118941
C	3.990088	3.337804	-0.559617
H	4.965823	1.442021	-0.780872
C	1.593782	3.269240	-0.318108
C	5.804391	-1.966747	0.866974
H	3.889795	-1.244742	1.595138
C	6.236130	-1.597228	-1.487373
H	4.659128	-0.579622	-2.580798
C	-0.974484	2.574154	-2.341972
C	-4.484406	1.569000	2.334500
H	-4.894530	2.773415	0.582090
H	-3.761763	0.412060	4.016831
C	0.644073	-0.838687	4.491674
H	2.681815	-0.803001	3.766107
H	-1.452521	-0.659173	4.999349
C	-3.076154	1.908037	-3.331527
H	-3.801899	-0.042447	-2.768454
C	-4.306692	-3.575852	-1.771365
H	-2.403848	-3.013528	-2.654390
C	-5.101364	-2.132867	0.004857
H	-3.810587	-0.465660	0.516972
C	2.776689	4.005395	-0.366398
H	4.929843	3.892261	-0.594623
H	0.650070	3.785404	-0.128053
C	6.642286	-2.093422	-0.244553
H	6.115916	-2.359184	1.836596
H	6.884818	-1.701640	-2.358982
C	-2.040311	2.840127	-3.203491
H	-0.182108	3.315989	-2.231431
H	-5.508527	1.632135	2.707859
H	0.905458	-1.372677	5.407309
H	-3.921428	2.106642	-3.993473
C	-5.275395	-3.251331	-0.817211
H	-4.440919	-4.445945	-2.416823
H	-5.852267	-1.876794	0.754519
H	2.757838	5.090318	-0.243058
H	7.612238	-2.584041	-0.143952
H	-2.073997	3.777888	-3.762426
H	-6.168037	-3.871631	-0.714380

129 **Table S8**. Coordinates for $^{3}TS_{1\text{-}2}$'*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	0.077238	-1.836538	1.996082
C	-1.248717	-1.612097	1.735703
C	1.161664	-1.063041	1.632010
C	-1.525877	-0.515334	0.875453
H	-2.042032	-2.236576	2.141393
N	0.736349	-3.472371	-1.596371
C	0.858282	0.063445	0.847010
H	2.177719	-1.301133	1.938143
N	-2.852660	-0.202793	0.544182
C	-0.455302	0.233965	0.316546
C	0.404670	-2.263561	-1.993159
C	2.088704	-3.384945	-1.210815
N	1.799592	1.071274	0.560516
C	-3.203969	0.906366	-0.242804
C	-3.901845	-1.043447	1.047606
B	-0.809059	0.930739	-1.002124
C	-0.862478	-1.841226	-2.530546
C	1.515174	-1.288935	-1.913088
C	2.872315	-4.406095	-0.669505
C	2.632052	-2.081504	-1.411464
C	1.300803	2.398320	0.303238
C	3.137340	1.072316	1.077851
C	-4.540474	1.355827	-0.283343
C	-2.222009	1.538859	-1.051433
C	-4.385543	-2.083346	0.250146
C	-4.430215	-0.823624	2.322433
C	1.102863	2.913921	-0.962820
C	-1.062152	-0.525421	-2.791154
H	-1.626172	-2.594261	-2.734929
C	1.317559	0.020535	-2.192943
C	4.198204	-4.116185	-0.330663
H	2.444239	-5.397753	-0.514515
C	3.956523	-1.806679	-1.073877
C	0.989310	3.257681	1.374446
C	3.425247	0.823029	2.427255
C	4.177917	1.426431	0.209594
C	-4.891310	2.427130	-1.097408
H	-5.299751	0.868363	0.326126
C	-2.621941	2.608833	-1.873118
C	-5.406929	-2.905952	0.730186
H	-3.948880	-2.238641	-0.737311
C	-5.451472	-1.648660	2.799924

H	-4.032664	-0.008219	2.928516
C	0.621804	4.173591	-1.258586
C	-0.057576	0.530234	-2.415407
H	-2.015736	-0.178669	-3.191030
H	2.132534	0.743843	-2.142076
C	4.736372	-2.833967	-0.530603
H	4.827172	-4.899655	0.098400
H	4.380638	-0.813058	-1.217976
C	0.499394	4.541385	1.135104
H	1.128016	2.892255	2.394020
C	4.744418	0.879061	2.882569
H	2.617287	0.588201	3.119146
C	5.492119	1.497252	0.671806
H	3.942734	1.654115	-0.830684
C	-3.934292	3.067648	-1.897630
H	-5.929086	2.767722	-1.107515
H	-1.868228	3.094076	-2.497622
C	-5.940754	-2.689136	2.004256
H	-5.783916	-3.720933	0.109338
H	-5.865469	-1.478908	3.795795
C	0.313302	5.006015	-0.172824
H	0.482987	4.513024	-2.287251
H	-0.099003	1.385832	-3.106194
H	5.774138	-2.634741	-0.255449
H	0.253904	5.188480	1.979135
C	5.782754	1.210504	2.008555
H	4.957919	0.673557	3.933552
H	6.292916	1.770587	-0.018200
H	-4.218957	3.907143	-2.534541
H	-6.738174	-3.333958	2.378945
H	-0.072827	6.011898	-0.351952
H	6.811967	1.255037	2.369576

Table S9. Coordinates for $^{3}IM_{1\text{-}2}$'*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-3.446819	2.691254	0.697053
C	-3.879671	1.414469	0.493709
C	-2.135937	3.122739	0.661604
C	-2.891749	0.431269	0.191247
H	-4.933209	1.149479	0.554565
N	4.235533	-2.392759	-2.103320
C	-1.176073	2.159294	0.335673
H	-1.828260	4.142408	0.894771
N	-3.321712	-0.882658	0.019618

C	-1.510266	0.796768	0.046497
C	3.185200	-1.636348	-1.868719
C	4.831615	-2.614690	-0.843036
N	0.184176	2.607838	0.358603
C	-2.470662	-1.950424	-0.284017
C	-4.724528	-1.169960	0.182242
B	-0.536572	-0.286947	-0.464646
C	2.237821	-1.125994	-2.827921
C	3.005869	-1.309085	-0.437678
C	5.984065	-3.356819	-0.575986
C	4.123856	-1.976808	0.216757
C	0.525942	3.692718	-0.475671
C	1.029843	2.206664	1.419923
C	-2.995686	-3.263141	-0.343001
C	-1.095627	-1.710821	-0.542811
C	-5.228479	-1.464239	1.450916
C	-5.564096	-1.160596	-0.933265
C	1.416185	4.695429	-0.109169
C	1.203838	-0.362254	-2.399167
H	2.378688	-1.366472	-3.883489
C	1.976682	-0.545754	-0.007600
C	6.418813	-3.451132	0.750886
H	6.522708	-3.843179	-1.390967
C	4.566854	-2.073015	1.535296
C	-0.028363	3.807933	-1.769264
C	2.426990	2.331587	1.307394
C	0.490883	1.609724	2.572108
C	-2.162241	-4.327501	-0.647860
H	-4.049631	-3.445485	-0.146166
C	-0.288807	-2.835749	-0.853819
C	-6.587357	-1.748700	1.603802
H	-4.550953	-1.467530	2.305882
C	-6.922382	-1.446126	-0.776040
H	-5.145092	-0.930776	-1.913882
C	1.809314	5.748457	-0.902247
C	0.977001	0.013215	-0.966516
H	0.490644	0.038023	-3.125140
H	1.851899	-0.324555	1.052986
C	5.723066	-2.818454	1.794916
H	7.318657	-4.026435	0.980857
H	4.027047	-1.576151	2.345140
C	0.314480	4.879074	-2.595430
H	-0.731163	3.046553	-2.113356
C	3.258820	1.865302	2.324475

H	2.864867	2.752268	0.403744
C	1.335214	1.133591	3.576045
H	-0.588469	1.508774	2.675311
C	-0.796065	-4.122093	-0.904283
H	-2.581575	-5.335467	-0.684924
H	0.768934	-2.678349	-1.047994
C	-7.434632	-1.739612	0.491432
H	-6.984841	-1.978954	2.594005
H	-7.581846	-1.439232	-1.645854
C	1.229070	5.851779	-2.179468
H	2.529229	6.491191	-0.550219
H	1.061061	1.112265	-0.919921
H	6.090561	-2.909892	2.819216
H	-0.132463	4.944802	-3.589241
C	2.723058	1.255863	3.462436
H	4.340414	1.953970	2.207413
H	0.897177	0.666486	4.460606
H	-0.144056	-4.964541	-1.140104
H	-8.496437	-1.962331	0.612589
H	1.493932	6.683712	-2.835190
H	3.378831	0.880338	4.249633

Table S10. Coordinates for $^{3}P_{1\text{-}2}$'*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-3.051026	2.783451	1.086161
C	-3.726000	1.641801	0.765528
C	-1.689290	2.982111	0.994722
C	-2.952219	0.552945	0.269719
H	-4.806202	1.564273	0.869020
N	4.841710	-0.832671	-1.691937
C	-0.933414	1.916370	0.488525
H	-1.193690	3.899990	1.311542
N	-3.628173	-0.628437	-0.043132
C	-1.535891	0.681234	0.080491
C	3.485355	-0.685135	-1.556528
C	5.204710	-1.760076	-0.725470
N	0.477165	2.126768	0.423990
C	-3.016505	-1.762354	-0.583451
C	-5.047119	-0.686581	0.199349
B	-0.785546	-0.501301	-0.559449
C	2.650365	0.183059	-2.283928
C	2.934323	-1.507313	-0.515149
C	6.497181	-2.224336	-0.452930
C	4.084849	-2.224225	0.039004

C	0.908000	3.320672	-0.214512
C	1.336557	1.418048	1.298085
C	-3.790375	-2.917697	-0.847555
C	-1.627622	-1.747209	-0.873702
C	-5.518256	-1.095476	1.448492
C	-5.937788	-0.342482	-0.819639
C	0.384213	3.643437	-1.477657
C	1.298102	0.240448	-1.947984
H	3.070736	0.805720	-3.075579
C	1.588795	-1.449081	-0.212087
C	6.666022	-3.149097	0.586047
H	7.341356	-1.861232	-1.041464
C	4.264654	-3.134856	1.068036
C	1.815386	4.204192	0.392072
C	2.718515	1.360546	1.042875
C	0.822646	0.724076	2.405138
C	-3.194018	-4.036337	-1.408634
H	-4.852875	-2.935550	-0.615598
C	-1.071127	-2.911472	-1.462156
C	-6.894336	-1.158006	1.680016
H	-4.801698	-1.359755	2.227387
C	-7.313093	-0.406736	-0.584297
H	-5.544264	-0.027890	-1.787194
C	0.770184	4.816664	-2.123499
C	0.743329	-0.547558	-0.914956
H	0.649990	0.926179	-2.495288
H	1.173995	-2.059588	0.592850
C	5.569130	-3.596878	1.335453
H	7.664509	-3.524728	0.818253
H	3.420851	-3.483816	1.667003
C	2.208173	5.369298	-0.268283
H	2.211358	3.974549	1.380952
C	3.556425	0.616866	1.868207
H	3.127096	1.865737	0.169907
C	1.671260	-0.033735	3.216067
H	-0.243977	0.766485	2.622782
C	-1.825709	-4.041720	-1.728207
H	-3.806051	-4.919322	-1.606445
H	-0.009128	-2.903046	-1.710083
C	-7.792052	-0.813889	0.664746
H	-7.265941	-1.476552	2.655739
H	-8.012047	-0.137665	-1.378444
C	1.691711	5.683729	-1.528206
H	0.353032	5.049952	-3.105453

H	-0.339104	2.971740	-1.940438
H	5.728173	-4.314929	2.142747
H	2.916506	6.044272	0.217003
C	3.041460	-0.094049	2.957124
H	4.621061	0.562976	1.633456
H	1.249178	-0.574887	4.066053
H	-1.367759	-4.923068	-2.180493
H	-8.867252	-0.863069	0.847269
H	2.000510	6.597326	-2.039329
H	3.701420	-0.693089	3.586495

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135 **Table S11**. Coordinates for $^{3}TS_{1\text{-}3}$'*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-3.150155	3.033945	0.242298
C	-3.748444	1.809913	0.168778
C	-1.788887	3.281039	0.241814
C	-2.894712	0.674688	0.039466
H	-4.830157	1.695602	0.210488
N	4.044147	-2.937622	-1.754053
C	-0.963826	2.164545	0.089205
H	-1.353692	4.269945	0.388041
N	-3.477134	-0.591436	0.022721
C	-1.478237	0.845755	-0.087316
C	2.988868	-2.153700	-1.693209
C	4.724391	-2.752899	-0.529816
N	0.450044	2.387732	0.199617
C	-2.741801	-1.780538	-0.053542
C	-4.909068	-0.689537	0.140651
B	-0.651982	-0.385562	-0.500723
C	1.966398	-1.974693	-2.692341
C	2.893783	-1.396229	-0.428319
C	5.909487	-3.368740	-0.124901
C	4.066767	-1.822207	0.325562
C	1.066489	3.075679	-0.879615
C	1.085072	2.254621	1.448161
C	-3.399477	-3.021357	0.113454
C	-1.347072	-1.737151	-0.316846
C	-5.502173	-0.709525	1.405206
C	-5.690585	-0.771240	-1.013366
C	1.138536	2.470997	-2.125961
C	0.937394	-1.127333	-2.443396
H	2.039211	-2.535874	-3.626043
C	1.881441	-0.529306	-0.192736
C	6.426476	-3.045565	1.135904

H	6.410086	-4.080129	-0.783787
C	4.588586	-1.504920	1.578405
C	1.609105	4.368990	-0.766419
C	2.488365	2.353596	1.547764
C	0.346538	1.945097	2.605593
C	-2.674502	-4.201486	0.048242
H	-4.470077	-3.056958	0.303230
C	-0.652544	-2.971610	-0.375132
C	-6.890999	-0.809350	1.513946
H	-4.869328	-0.646452	2.291559
C	-7.079308	-0.871853	-0.900177
H	-5.202994	-0.756117	-1.989086
C	1.693358	3.039529	-3.252181
C	0.807213	-0.316803	-1.195295
H	0.157710	-0.987111	-3.197007
H	1.832162	0.021959	0.745550
C	5.778493	-2.127219	1.977792
H	7.353140	-3.516521	1.472039
H	4.083819	-0.789762	2.232525
C	2.192101	4.979889	-1.879394
H	1.576969	4.877781	0.199512
C	3.124280	2.143968	2.769860
H	3.080087	2.564065	0.657810
C	1.000241	1.729420	3.819931
H	-0.737916	1.863133	2.550946
C	-1.289316	-4.186580	-0.188101
H	-3.195356	-5.151380	0.188343
H	0.420338	-2.954633	-0.559218
C	-7.679951	-0.890437	0.362212
H	-7.357749	-0.824926	2.500587
H	-7.693266	-0.935392	-1.800487
C	2.234674	4.330022	-3.118338
H	1.732341	2.509063	-4.206231
H	0.884684	0.766667	-1.571608
H	6.208201	-1.897051	2.954971
H	2.614283	5.981724	-1.779570
C	2.389948	1.827101	3.917466
H	4.213034	2.216161	2.817463
H	0.406018	1.484211	4.703030
H	-0.725213	-5.119743	-0.227751
H	-8.765361	-0.968679	0.448907
H	2.694052	4.818324	-3.980779
H	2.893820	1.658088	4.870346

137 **Table S12**. Coordinates for $^{3}TS_{2\text{-}1}$*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-1.218222	0.006146	-0.309582
C	-0.582529	-1.199024	-0.586086
C	-0.469176	1.146496	0.031070
C	0.838910	-1.275655	-0.510352
H	-1.153714	-2.079744	-0.869245
N	-2.627150	0.098849	-0.349665
C	0.950554	1.090464	0.038183
H	-0.994027	2.057601	0.300316
N	1.404689	-2.499872	-0.700962
C	1.629448	-0.116381	-0.231459
C	-3.524787	-0.808251	0.237197
C	-3.362398	1.132413	-0.947321
N	1.674030	2.238895	0.324986
C	2.767736	-2.640999	-0.887252
C	0.586177	-3.877739	0.262885
B	3.136448	-0.186828	-0.258367
C	-3.266573	-1.972097	0.968318
C	-4.849521	-0.348748	0.011574
C	-2.919902	2.238708	-1.681500
C	-4.746971	0.886184	-0.742133
C	3.075718	2.271832	0.434689
C	0.933826	3.459463	0.527165
C	3.212799	-3.936818	-1.255134
C	3.697861	-1.556630	-0.737146
C	0.375202	-3.600434	1.613592
C	-0.274746	-4.709373	-0.452602
C	3.858370	1.098156	0.188492
C	-4.362858	-2.682902	1.457208
H	-2.254272	-2.324773	1.157502
C	-5.932254	-1.081854	0.514201
C	-3.884141	3.111117	-2.188474
H	-1.860059	2.416093	-1.860166
C	-5.693997	1.777142	-1.262128
C	3.692973	3.489763	0.799597
C	0.601913	4.246901	-0.577027
C	0.525882	3.822614	1.811949
C	4.546565	-4.164353	-1.543665
H	2.480157	-4.740416	-1.318973
C	5.040270	-1.840246	-1.061909
C	-0.672335	-4.244031	2.282293
H	1.032552	-2.908740	2.149179
C	-1.322792	-5.344737	0.222263

H	-0.127296	-4.870398	-1.525127
C	5.253817	1.220280	0.406367
C	-5.682575	-2.249815	1.232832
H	-4.180558	-3.598205	2.022743
H	-6.955138	-0.738549	0.346085
C	-5.257368	2.890179	-1.979227
H	-3.560609	3.982132	-2.762118
H	-6.760086	1.596494	-1.110014
C	5.068342	3.556452	0.965166
H	3.090891	4.381343	0.961146
C	-0.152419	5.408024	-0.392761
H	0.933173	3.939099	-1.569845
C	-0.225850	4.986218	1.991238
H	0.795275	3.187618	2.657006
C	5.466189	-3.104277	-1.463501
H	4.879595	-5.161575	-1.837855
H	5.777514	-1.039760	-1.015019
C	-1.521132	-5.118933	1.590702
H	-0.827096	-4.064601	3.350191
H	-1.989594	-6.020096	-0.320979
C	5.857872	2.409431	0.784444
H	5.876267	0.334220	0.293333
H	-6.516339	-2.833608	1.627322
H	-5.985157	3.593550	-2.387889
H	5.528103	4.504700	1.250539
C	-0.567176	5.777504	0.890118
H	-0.419486	6.023070	-1.253994
H	-0.550832	5.271776	2.993340
H	6.517146	-3.272714	-1.708181
H	-2.340687	-5.615060	2.114107
H	6.937260	2.453741	0.942189
H	-1.160422	6.682705	1.032032

Table S12. Coordinates for $^{3}IM_{2\text{-}1}$*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-1.515796	-0.868868	-0.608875
C	-0.818642	-2.063641	-0.814045
C	-0.840834	0.349983	-0.526981
C	0.594756	-2.044893	-0.892774
H	-1.336321	-3.017328	-0.905102
N	-2.923971	-0.883724	-0.465193
C	0.570095	0.385914	-0.664839
H	-1.409268	1.253551	-0.328293
N	1.202653	-3.253577	-1.018346

C	1.306328	-0.805367	-0.827163
C	-3.637493	-1.673806	0.445440
C	-3.825566	-0.047588	-1.135966
N	1.232045	1.603103	-0.573439
C	2.562999	-3.336300	-0.989017
C	2.200486	-0.096687	2.095220
B	2.822228	-0.801378	-0.848179
C	-3.168257	-2.613865	1.368802
C	-5.017725	-1.350239	0.348242
C	-3.588700	0.894578	-2.142415
C	-5.137927	-0.315820	-0.661719
C	2.621130	1.739964	-0.690220
C	0.440969	2.774699	-0.291887
C	3.077647	-4.662949	-1.055757
C	3.465494	-2.217257	-0.857468
C	0.943511	-0.464545	2.530481
C	2.970255	0.919352	2.623320
C	3.466257	0.600863	-0.866840
C	-4.108369	-3.246135	2.183842
H	-2.106990	-2.847028	1.451811
C	-5.940446	-2.001599	1.176522
C	-4.688264	1.580189	-2.660168
H	-2.582184	1.085363	-2.513835
C	-6.224316	0.386014	-1.199371
C	3.175427	3.040775	-0.625110
C	-0.113545	3.505926	-1.343935
C	0.213299	3.140240	1.036071
C	4.434921	-4.907932	-0.950296
H	2.352380	-5.469904	-1.171303
C	4.831541	-2.522883	-0.719670
C	0.416671	0.251868	3.618426
H	0.373218	-1.261550	2.049198
C	2.425773	1.620762	3.713956
H	3.947940	1.179140	2.212478
C	4.848570	0.857887	-1.034999
C	-5.480634	-2.950346	2.088590
H	-3.767109	-3.986215	2.910417
H	-7.003946	-1.762997	1.110379
C	-5.993090	1.334672	-2.194279
H	-4.528965	2.321440	-3.445971
H	-7.237663	0.188156	-0.844007
C	4.540591	3.227912	-0.762281
H	2.529166	3.902032	-0.471523
C	-0.910070	4.618671	-1.062511

H	0.080024	3.194210	-2.371444
C	-0.582319	4.255037	1.309930
H	0.652441	2.547909	1.837690
C	5.318550	-3.830663	-0.763782
H	4.815992	-5.930415	-0.994256
H	5.547023	-1.719425	-0.548604
C	1.158034	1.285303	4.204294
H	-0.577175	0.002845	3.999140
H	2.994047	2.434286	4.172479
C	5.391145	2.132297	-0.983748
H	5.512163	0.018101	-1.231796
H	-6.188947	-3.466517	2.739107
H	-6.830435	1.890216	-2.620396
H	4.948253	4.239797	-0.710594
C	-1.144940	4.993269	0.263994
H	-1.350657	5.191287	-1.880717
H	-0.767352	4.542976	2.346569
H	6.389122	-4.015214	-0.650664
H	0.741040	1.838188	5.048774
H	6.463650	2.283922	-1.118398
H	-1.770757	5.860716	0.482500

Table S13. Coordinates for $^{3}TS_{2\text{-}2}$*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-1.668018	-0.749754	-0.561987
C	-0.988250	-1.944681	-0.830302
C	-0.977982	0.457823	-0.444810
C	0.423243	-1.942142	-0.936334
H	-1.521682	-2.887095	-0.946336
N	-3.074467	-0.756047	-0.402415
C	0.427360	0.481362	-0.633518
H	-1.529034	1.360556	-0.197247
N	1.022360	-3.154348	-1.096455
C	1.141301	-0.711419	-0.854955
C	-3.792062	-1.592511	0.462748
C	-3.974870	0.107084	-1.040410
N	1.115983	1.686238	-0.534109
C	2.385488	-3.245380	-1.090106
C	2.659788	-0.301570	1.570663
B	2.662086	-0.716652	-0.874860
C	-3.326696	-2.577710	1.339688
C	-5.172257	-1.267154	0.373366
C	-3.736379	1.091970	-2.004722
C	-5.289058	-0.185410	-0.585978

C	2.481034	1.823400	-0.821523
C	0.410190	2.818568	0.010433
C	2.896879	-4.569404	-1.201224
C	3.295986	-2.137280	-0.942274
C	1.615571	-0.880089	2.268666
C	3.531742	0.633869	2.097353
C	3.300089	0.678448	-1.065404
C	-4.270677	-3.253307	2.114274
H	-2.265073	-2.809903	1.420323
C	-6.098948	-1.961341	1.161431
C	-4.835243	1.796906	-2.497614
H	-2.729138	1.298601	-2.365562
C	-6.374557	0.537502	-1.096686
C	3.039909	3.122455	-0.849287
C	-0.297178	3.681805	-0.827611
C	0.430200	3.012347	1.393869
C	4.256759	-4.818367	-1.125242
H	2.170018	-5.373381	-1.327841
C	4.662409	-2.442623	-0.834209
C	1.434207	-0.484553	3.603519
H	0.946276	-1.605905	1.803712
C	3.335145	1.016403	3.434867
H	4.333314	1.072884	1.500943
C	4.650013	0.917647	-1.407970
C	-5.642968	-2.955342	2.025845
H	-3.932585	-4.029139	2.804118
H	-7.162441	-1.721267	1.100930
C	-6.141354	1.529496	-2.047900
H	-4.674419	2.570609	-3.251191
H	-7.389013	0.321467	-0.755369
C	4.378881	3.298444	-1.158599
H	2.417953	3.989578	-0.637119
C	-0.997999	4.755553	-0.272083
H	-0.296252	3.502776	-1.903881
C	-0.270293	4.089231	1.941259
H	0.989049	2.317266	2.022216
C	5.147103	-3.749914	-0.923964
H	4.634111	-5.840228	-1.203582
H	5.375455	-1.638796	-0.647036
C	2.287907	0.463040	4.179433
H	0.617419	-0.915799	4.188173
H	4.001518	1.754882	3.888552
C	5.193559	2.193031	-1.458026
H	5.281629	0.063985	-1.650981

H	-6.354236	-3.505656	2.644365
H	-6.978093	2.101459	-2.452936
H	4.792930	4.308633	-1.182741
C	-0.984489	4.959241	1.110998
H	-1.557955	5.431385	-0.920982
H	-0.261822	4.245503	3.021592
H	6.218698	-3.940821	-0.833007
H	2.136466	0.771040	5.216226
H	6.241344	2.338565	-1.727476
H	-1.534890	5.797112	1.543250

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143 **Table S14**. Coordinates for $^3P_2$*

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-1.687710	-0.665667	-0.418266
C	-0.950737	-1.796326	-0.822610
C	-1.049521	0.542776	-0.161245
C	0.462125	-1.750758	-0.881850
H	-1.454670	-2.720683	-1.103647
N	-3.093851	-0.749438	-0.314959
C	0.360899	0.616887	-0.318911
H	-1.632334	1.403971	0.150707
N	1.103167	-2.886433	-1.281234
C	1.137754	-0.536834	-0.575504
C	-3.798929	-1.747470	0.373093
C	-4.016376	0.151247	-0.866999
N	1.011001	1.836614	-0.206261
C	2.471140	-2.915433	-1.357733
C	2.811506	-0.569956	1.323709
B	2.702413	-0.506615	-0.360659
C	-3.313385	-2.824289	1.121836
C	-5.190173	-1.488883	0.254790
C	-3.798149	1.280824	-1.662624
C	-5.329082	-0.280132	-0.535787
C	2.349009	2.049500	-0.601911
C	0.252973	2.962627	0.283606
C	3.010893	-4.140585	-1.844044
C	3.349897	-1.853432	-0.947245
C	2.328579	-1.704947	2.000783
C	3.336528	0.473451	2.105169
C	3.218507	0.940456	-0.818674
C	-4.249004	-3.663169	1.728980
H	-2.244258	-3.000310	1.237923
C	-6.107993	-2.345049	0.875395
C	-4.915972	1.988572	-2.107177

H	-2.791838	1.596054	-1.935615
C	-6.433639	0.448740	-0.992972
C	2.785166	3.382540	-0.789389
C	-0.542983	3.710342	-0.585897
C	0.321017	3.261844	1.644647
C	4.378778	-4.342534	-1.907790
H	2.299877	-4.910556	-2.148701
C	4.723676	-2.122771	-0.981323
C	2.372675	-1.799867	3.392864
H	1.911917	-2.537056	1.428635
C	3.383542	0.385034	3.502459
H	3.738271	1.366876	1.624017
C	4.498978	1.243389	-1.302363
C	-5.631372	-3.433191	1.605273
H	-3.895799	-4.512988	2.316223
H	-7.180362	-2.157487	0.791848
C	-6.221135	1.584493	-1.773363
H	-4.770118	2.873635	-2.729826
H	-7.446689	0.126145	-0.744447
C	4.070233	3.626969	-1.248361
H	2.113951	4.215738	-0.591642
C	-1.288684	4.776891	-0.079109
H	-0.572513	3.451474	-1.645211
C	-0.426485	4.332109	2.141962
H	0.951078	2.651678	2.293884
C	5.243837	-3.330215	-1.460166
H	4.781104	-5.286276	-2.282096
H	5.420826	-1.376825	-0.593604
C	2.897317	-0.750015	4.153749
H	1.991837	-2.697395	3.887061
H	3.813584	1.207048	4.081465
C	4.927784	2.551960	-1.525756
H	5.183776	0.422146	-1.510446
H	-6.335154	-4.110068	2.092848
H	-7.073310	2.162854	-2.134606
H	4.401678	4.655169	-1.403476
C	-1.230861	5.087283	1.283152
H	-1.918195	5.363767	-0.750099
H	-0.383209	4.572242	3.205725
H	6.324766	-3.489534	-1.474362
H	2.931532	-0.820218	5.243374
H	5.933185	2.740279	-1.908608
H	-1.816962	5.919728	1.676770

145 **Table S15**. Coordinates for $^1P_2$

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-1.690039	-0.766109	-0.507600
C	-0.962121	-1.861869	-0.917133
C	-1.049273	0.466375	-0.200654
C	0.463283	-1.751525	-0.943722
H	-1.430947	-2.800203	-1.207066
N	-3.097660	-0.828298	-0.382253
C	0.334841	0.613039	-0.323728
H	-1.667391	1.295080	0.138614
N	1.155578	-2.844039	-1.322167
C	1.122585	-0.530993	-0.595725
C	-3.814649	-1.787258	0.347205
C	-4.003579	0.091909	-0.924177
N	0.985281	1.828847	-0.112577
C	2.507798	-2.883216	-1.340059
C	2.839166	-0.554388	1.308163
B	2.670111	-0.473909	-0.376121
C	-3.346273	-2.874917	1.090232
C	-5.198702	-1.475243	0.274021
C	-3.766046	1.194077	-1.752453
C	-5.319488	-0.277995	-0.536503
C	2.291392	2.066617	-0.636065
C	0.223225	2.929124	0.397926
C	3.065270	-4.126631	-1.781769
C	3.358275	-1.803242	-0.898504
C	2.304759	-1.630017	2.035696
C	3.500302	0.458212	2.016319
C	3.158075	0.976640	-0.886423
C	-4.290626	-3.662601	1.749980
H	-2.281714	-3.097813	1.157440
C	-6.125952	-2.283981	0.943333
C	-4.868277	1.943042	-2.167019
H	-2.758022	1.456334	-2.072961
C	-6.408330	0.489229	-0.968705
C	2.699159	3.383916	-0.900483
C	-0.617075	3.670109	-0.440582
C	0.316692	3.239139	1.757058
C	4.427639	-4.315016	-1.774357
H	2.368597	-4.904240	-2.098037
C	4.737056	-2.069349	-0.852769
C	2.421442	-1.693513	3.425698
H	1.783127	-2.436129	1.512924
C	3.620186	0.398784	3.411043

H	3.927007	1.305866	1.478344
C	4.392144	1.258161	-1.484015
C	-5.666475	-3.377355	1.675724
H	-3.950313	-4.518489	2.336289
H	-7.192544	-2.055477	0.894124
C	-6.176160	1.600840	-1.777821
H	-4.708770	2.809162	-2.812460
H	-7.424597	0.215687	-0.677866
C	3.955306	3.627857	-1.457987
H	2.035740	4.218782	-0.678814
C	-1.371675	4.720546	0.086295
H	-0.670844	3.416409	-1.500717
C	-0.434592	4.295332	2.278939
H	0.979104	2.643303	2.387168
C	5.264637	-3.277240	-1.297919
H	4.863193	-5.257488	-2.110144
H	5.409798	-1.307736	-0.455719
C	3.080003	-0.674547	4.121456
H	1.994099	-2.540800	3.968012
H	4.141699	1.200430	3.940873
C	4.801335	2.564376	-1.772033
H	5.064861	0.432510	-1.721227
H	-6.377966	-4.017302	2.200629
H	-7.015910	2.208207	-2.120155
H	4.260306	4.657149	-1.658793
C	-1.280354	5.034010	1.446112
H	-2.031863	5.295393	-0.566024
H	-0.362872	4.538613	3.340849
H	6.346342	-3.432504	-1.276716
H	3.171473	-0.719373	5.209063
H	5.777017	2.747383	-2.227111
H	-1.870864	5.855244	1.857099

Table S16. Coordinates for $^1P_3$

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-1.537438	-0.980450	-0.440483
C	-0.862958	-2.148135	-0.714698
C	-0.837105	0.227799	-0.149165
C	0.570831	-2.185076	-0.719084
H	-1.397789	-3.073933	-0.926777
N	-2.955886	-0.936258	-0.391963
C	0.537461	0.200242	-0.222563
H	-1.405919	1.100682	0.153457
N	1.167757	-3.363920	-0.925445

C	1.287303	-0.947160	-0.514244
C	-3.777110	-1.737872	0.409046
C	-3.750762	0.019477	-1.030053
N	1.320370	1.426191	0.280457
C	2.528484	-3.433470	-0.903470
C	1.673378	1.199014	1.748195
B	2.787264	-0.941056	-0.642034
C	-3.434071	-2.794229	1.259241
C	-5.122123	-1.296240	0.274187
C	-3.381855	1.021659	-1.934613
C	-5.105529	-0.173686	-0.644166
C	2.638954	1.626445	-0.475521
C	0.438082	2.631928	0.108814
C	3.082919	-4.742567	-1.046224
C	3.428878	-2.309036	-0.756961
C	0.951932	0.279198	2.507088
C	2.700994	1.949693	2.320843
C	3.400200	0.491788	-0.806024
C	-4.463818	-3.415586	1.966733
H	-2.400164	-3.122465	1.362767
C	-6.137000	-1.941457	0.992774
C	-4.389918	1.845639	-2.436257
H	-2.344061	1.149330	-2.240862
C	-6.098196	0.665336	-1.166472
C	3.070499	2.932316	-0.709498
C	0.053838	2.952993	-1.197077
C	-0.034142	3.354594	1.196435
C	4.443365	-4.952105	-1.016068
H	2.377188	-5.566605	-1.166635
C	4.825411	-2.583962	-0.715997
C	1.267469	0.115110	3.858679
H	0.156689	-0.310579	2.060484
C	3.002061	1.779417	3.673489
H	3.272504	2.657062	1.726077
C	4.632258	0.751685	-1.443716
C	-5.802377	-3.000654	1.834750
H	-4.222333	-4.245186	2.634440
H	-7.174263	-1.613954	0.895641
C	-5.734489	1.675164	-2.056719
H	-4.127648	2.635232	-3.143860
H	-7.142916	0.526735	-0.880308
C	4.308070	3.140896	-1.322825
H	2.465886	3.789048	-0.420425
C	-0.815847	4.018345	-1.409179

H	0.427811	2.363685	-2.033287
C	-0.909262	4.426558	0.969958
H	0.253500	3.091670	2.211164
C	5.332393	-3.862374	-0.837798
H	4.841864	-5.964721	-1.119637
H	5.520128	-1.756802	-0.550782
C	2.288501	0.861828	4.447206
H	0.707691	-0.614182	4.446248
H	3.807950	2.366970	4.116310
C	5.088238	2.044396	-1.695538
H	5.231561	-0.098048	-1.769697
H	-6.583298	-3.514245	2.398558
H	-6.498731	2.336244	-2.469614
H	4.648923	4.160526	-1.509808
C	-1.302138	4.758686	-0.324358
H	-1.123017	4.265462	-2.426448
H	-1.287096	4.992282	1.822994
H	6.409611	-4.038230	-0.792455
H	2.533076	0.724148	5.501882
H	6.049740	2.198309	-2.189754
H	-1.991183	5.587858	-0.492849

Table S17. Coordinates for ^{3}R* (BNPA-1)

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	0.000051	1.487840	0.000012
C	1.211469	0.784892	-0.051948
C	-1.211430	0.785001	0.051963
C	1.208293	-0.624922	-0.048171
H	2.140624	1.347082	-0.092554
N	0.000116	2.905688	0.000014
C	-1.208380	-0.624814	0.048165
H	-2.140535	1.347274	0.092575
N	2.422837	-1.305329	-0.100833
C	-0.000077	-1.372081	-0.000011
C	0.216089	3.716947	1.112490
C	-0.215711	3.716968	-1.112476
N	-2.422985	-1.305114	0.100821
C	2.556741	-2.700356	-0.012428
C	3.620764	-0.506908	-0.212435
B	-0.000145	-2.877089	-0.000026
C	0.465239	3.341953	2.435716
C	0.140072	5.080074	0.712721
C	-0.464909	3.341996	-2.435699
C	-0.139471	5.080087	-0.712726

C	-2.557015	-2.700126	0.012386
C	-3.620840	-0.506588	0.212453
C	3.856484	-3.245787	-0.012008
C	1.394584	-3.536883	0.093286
C	4.070545	-0.148803	-1.509287
C	4.272428	-0.089528	0.975695
C	-1.394933	-3.536757	-0.093351
C	0.648110	4.362611	3.369960
H	0.510734	2.290108	2.720575
C	0.326663	6.083262	1.673022
C	-0.647605	4.362671	-3.369959
H	-0.510572	2.290155	-2.720545
C	-0.325892	6.083292	-1.673042
C	-3.856807	-3.245441	0.011960
C	-4.070574	-0.148470	1.509319
C	-4.272480	-0.089124	-0.975661
C	4.047377	-4.618690	0.150388
H	4.718924	-2.593899	-0.128236
C	1.651041	-4.912096	0.300261
C	5.216805	0.659645	-1.576231
C	5.429871	0.690409	0.817151
C	-1.651515	-4.911942	-0.300355
C	0.581311	5.718327	2.995332
H	0.845798	4.102248	4.411827
H	0.272763	7.136443	1.389070
C	-0.580590	5.718381	-2.995349
H	-0.845326	4.102326	-4.411824
H	-0.271822	7.136468	-1.389104
C	-4.047825	-4.618324	-0.150466
H	-4.719188	-2.593478	0.128205
C	-5.216761	0.660081	1.576292
C	-5.429852	0.690913	-0.817087
C	2.938553	-5.450637	0.330035
H	5.059408	-5.026815	0.149617
H	0.809223	-5.581442	0.464987
C	5.895447	1.066346	-0.435203
C	-2.939075	-5.450367	-0.330136
H	-0.809758	-5.581360	-0.465100
H	0.729387	6.491704	3.751294
H	-0.728533	6.491772	-3.751322
H	-5.059892	-5.026357	-0.149700
C	-5.895380	1.066866	0.435280
H	3.075795	-6.522668	0.488668
H	6.789387	1.687132	-0.522747

H	-3.076415	-6.522381	-0.488793
H	-6.789263	1.687731	0.522848
H	5.587318	0.986107	-2.546037
H	5.975983	1.023617	1.698102
H	-5.587232	0.986556	2.546109
H	-5.975944	1.024189	-1.698024
C	-3.874695	-0.379534	-2.453459
C	-3.411066	-0.484462	2.879533
C	3.874602	-0.379935	2.453483
C	3.411025	-0.484711	-2.879516
C	2.299000	-1.551029	-2.910408
H	2.636667	-2.519264	-2.520245
H	1.390590	-1.252844	-2.376503
H	2.014077	-1.703445	-3.963073
C	2.809302	0.827169	-3.434970
H	3.564304	1.622413	-3.526177
H	2.377056	0.650926	-4.433444
H	2.007112	1.199167	-2.778955
C	4.505773	-1.003608	-3.843690
H	5.300236	-0.270091	-4.036820
H	4.973685	-1.915890	-3.441285
H	4.050605	-1.254812	-4.814226
C	5.014090	-1.207424	3.092943
H	5.104023	-2.185455	2.595187
H	5.987891	-0.700382	3.028944
H	4.795523	-1.386190	4.157978
C	2.566654	-1.145821	2.731094
H	1.678668	-0.623077	2.355151
H	2.572350	-2.166550	2.334413
H	2.457032	-1.225443	3.823876
C	3.734959	0.977935	3.184697
H	3.459384	0.805432	4.237203
H	4.662386	1.567265	3.177626
H	2.945394	1.590795	2.722397
C	-5.014263	-1.206906	-3.092927
H	-5.988018	-0.699778	-3.028908
H	-4.795722	-1.385669	-4.157968
H	-5.104279	-2.184941	-2.595191
C	-2.566817	-1.145530	-2.731100
H	-1.678781	-0.622872	-2.355153
H	-2.572601	-2.166266	-2.334440
H	-2.457213	-1.225137	-3.823885
C	-3.734939	0.978340	-3.184645
H	-3.459392	0.805836	-4.237158

H	-4.662313	1.567753	-3.177549
H	-2.945313	1.591119	-2.722341
C	-2.299149	-1.550895	2.910389
H	-2.636922	-2.519087	2.520211
H	-1.390716	-1.252792	2.376477
H	-2.014227	-1.703362	3.963046
C	-4.505849	-1.003263	3.843719
H	-4.050687	-1.254531	4.814242
H	-5.300232	-0.269666	4.036878
H	-4.973864	-1.915489	3.441308
C	-2.809202	0.827349	3.434994
H	-3.564123	1.622667	3.526222
H	-2.376958	0.651050	4.433459
H	-2.006985	1.199275	2.778971

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151 **Table S18**. Coordinates for ^{1}R (BNPA-1)

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-0.000013	-1.486269	0.000007
C	1.220487	-0.815931	-0.038376
C	-1.220504	-0.815914	0.038381
C	1.220317	0.589892	-0.045938
H	2.142298	-1.388808	-0.060029
N	-0.000023	-2.906909	0.000019
C	-1.220316	0.589908	0.045923
H	-2.142323	-1.388779	0.060042
N	2.429074	1.274010	-0.075205
C	0.000005	1.318813	-0.000013
C	0.478094	-3.718018	-1.028903
C	-0.478133	-3.717994	1.028965
N	-2.429063	1.274043	0.075181
C	2.538260	2.666158	-0.169254
C	3.640153	0.490712	-0.055611
B	0.000015	2.834057	-0.000024
C	1.016334	-3.349342	-2.265192
C	0.305834	-5.080154	-0.658221
C	-1.016372	-3.349287	2.265244
C	-0.305867	-5.080138	0.658318
C	-2.538231	2.666193	0.169210
C	-3.640153	0.490761	0.055602
C	3.829251	3.240155	-0.233406
C	1.380909	3.495863	-0.214157
C	4.186867	0.126348	1.201313
C	4.230835	0.108362	-1.289806
C	-1.380869	3.495883	0.214098

C	1.406452	-4.372393	-3.129940
H	1.121215	-2.300275	-2.540412
C	0.705827	-6.086846	-1.547198
C	-1.406484	-4.372317	3.130021
H	-1.121256	-2.300214	2.540437
C	-0.705855	-6.086809	1.547322
C	-3.829215	3.240208	0.233354
C	-4.186876	0.126388	-1.201315
C	-4.230838	0.108438	1.289804
C	3.982654	4.605739	-0.423056
H	4.709468	2.607386	-0.148138
C	1.595669	4.873630	-0.456912
C	5.360122	-0.646111	1.183601
C	5.423329	-0.629406	-1.217659
C	-1.595612	4.873658	0.456832
C	1.258264	-5.727222	-2.776202
H	1.833407	-4.112925	-4.100912
H	0.582700	-7.138623	-1.280396
C	-1.258291	-5.727154	2.776317
H	-1.833438	-4.112825	4.100986
H	-0.582724	-7.138592	1.280547
C	-3.982599	4.605797	0.422983
H	-4.709440	2.607449	0.148097
C	-5.360144	-0.646051	-1.183589
C	-5.423343	-0.629313	1.217671
C	2.860502	5.433499	-0.568006
H	4.989453	5.025769	-0.477307
H	0.729764	5.520214	-0.586347
C	5.979354	-1.010006	-0.003578
C	-2.860437	5.433545	0.567919
H	-0.729697	5.520233	0.586257
H	1.575239	-6.502925	-3.475677
H	-1.575262	-6.502840	3.475813
H	-4.989393	5.025841	0.477228
C	-5.979379	-1.009919	0.003597
H	2.979589	6.501346	-0.759508
H	6.899346	-1.597835	0.016244
H	-2.979510	6.501396	0.759404
H	-6.899381	-1.597733	-0.016214
H	5.804397	-0.969336	2.123551
H	5.931011	-0.920660	-2.134920
H	-5.804428	-0.969280	-2.123533
H	-5.931028	-0.920545	2.134937
C	-3.747738	0.444645	2.732403

C	-3.635392	0.447718	-2.621343
C	3.747744	0.444555	-2.732411
C	3.635382	0.447705	2.621335
C	2.434587	1.404641	2.743624
H	2.633789	2.392630	2.310817
H	1.516109	1.001902	2.303795
H	2.237196	1.552908	3.816958
C	3.211404	-0.890305	3.271320
H	4.040235	-1.611851	3.320240
H	2.855136	-0.713195	4.299088
H	2.390977	-1.354064	2.701729
C	4.771910	1.097215	3.448061
H	5.657564	0.454475	3.545592
H	5.089521	2.045465	2.985917
H	4.410349	1.318884	4.464514
C	4.712829	1.499870	-3.319548
H	4.642058	2.446730	-2.764025
H	5.758699	1.158498	-3.285074
H	4.454306	1.701902	-4.371914
C	2.313290	0.980617	-2.907265
H	1.558428	0.286350	-2.516168
H	2.156940	1.964334	-2.452843
H	2.127495	1.093015	-3.986784
C	3.819554	-0.842336	-3.593343
H	3.397425	-0.640491	-4.590007
H	4.845650	-1.204087	-3.745566
H	3.240990	-1.657186	-3.132759
C	-4.712805	1.499984	3.319525
H	-5.758680	1.158628	3.285059
H	-4.454276	1.702028	4.371888
H	-4.642020	2.446834	2.763988
C	-2.313275	0.980686	2.907246
H	-1.558425	0.286402	2.516158
H	-2.156910	1.964394	2.452809
H	-2.127477	1.093097	3.986763
C	-3.819567	-0.842232	3.593355
H	-3.397433	-0.640379	4.590014
H	-4.845669	-1.203964	3.745585
H	-3.241019	-1.657098	3.132782
C	-2.434571	1.404618	-2.743650
H	-2.633741	2.392618	-2.310854
H	-1.516102	1.001857	-2.303821
H	-2.237181	1.552867	-3.816986
C	-4.771909	1.097253	-3.448065

H	-4.410352	1.318902	-4.464524
H	-5.657583	0.454538	-3.545579
H	-5.089488	2.045517	-2.985927
C	-3.211456	-0.890309	-3.271321
H	-4.040307	-1.611832	-3.320232
H	-2.855190	-0.713216	-4.299093
H	-2.391038	-1.354086	-2.701732

Table S19. Coordinates for $^{3}TS_{3}$* (BNPA-1)

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-0.059918	1.415567	-0.211613
C	-1.251669	0.697025	-0.314835
C	1.170991	0.770787	-0.086873
C	-1.206518	-0.724631	-0.300644
H	-2.188882	1.231694	-0.431418
N	-0.078459	2.830604	-0.239610
C	1.223932	-0.645427	-0.075426
H	2.073118	1.368374	0.003419
N	-2.382621	-1.418751	-0.348238
C	0.046583	-1.411059	-0.211632
C	0.640874	3.627449	-1.135070
C	-0.685017	3.657800	0.712383
N	2.447619	-1.266967	0.086701
C	-2.427042	-2.789731	-0.490425
C	-3.885692	-0.520454	0.035870
B	0.109992	-2.917430	-0.275193
C	1.394146	3.247313	-2.249695
C	0.474776	4.991120	-0.770283
C	-1.452723	3.304106	1.823355
C	-0.371574	5.009874	0.409541
C	2.608253	-2.654711	0.168520
C	3.614340	-0.425973	0.241674
C	-3.709996	-3.387148	-0.594635
C	-1.246661	-3.603197	-0.571443
C	-3.840973	-0.018096	1.382499
C	-4.322359	0.306347	-1.056874
C	1.493403	-3.533303	0.008531
C	2.000741	4.258633	-2.996055
H	1.497863	2.199250	-2.530782
C	1.092243	5.986063	-1.539371
C	-1.931273	4.338041	2.628266
H	-1.684415	2.263047	2.040478
C	-0.866644	6.028639	1.234250
C	3.897944	-3.167625	0.441179

C	4.366081	-0.091981	-0.915535
C	3.940533	0.042319	1.540010
C	-3.843422	-4.729546	-0.899656
H	-4.570303	-2.742496	-0.433113
C	-1.435234	-4.958517	-0.908489
C	-4.168825	1.325689	1.583218
C	-4.632423	1.639861	-0.762270
C	1.746867	-4.915176	0.195093
C	1.855993	5.613969	-2.645536
H	2.594958	3.988917	-3.871577
H	0.974110	7.038933	-1.275060
C	-1.647453	5.685782	2.337903
H	-2.542567	4.091946	3.498922
H	-0.639005	7.074296	1.017193
C	4.092546	-4.532496	0.582489
H	4.738586	-2.488137	0.558859
C	5.499076	0.712801	-0.716900
C	5.068799	0.873315	1.642365
C	-2.697567	-5.518591	-1.092285
H	-4.838800	-5.168869	-0.988330
H	-0.562530	-5.594693	-1.048664
C	-4.521688	2.167923	0.526828
C	3.008222	-5.418371	0.472520
H	0.909887	-5.609114	0.146407
H	2.343230	6.380623	-3.250673
H	-2.041109	6.469824	2.987378
H	5.094170	-4.910317	0.797081
C	5.844906	1.195699	0.538398
H	-2.794401	-6.573043	-1.359117
H	-4.735936	3.221207	0.711485
H	3.156578	-6.490685	0.612156
H	6.723276	1.833567	0.654929
H	-4.167687	1.745202	2.588145
H	-4.979775	2.304339	-1.550843
H	6.126737	0.976237	-1.564917
H	5.349051	1.279338	2.612638
C	3.191035	-0.212771	2.882634
C	4.121362	-0.563767	-2.379157
C	-4.565322	-0.204319	-2.501865
C	-3.552404	-0.915758	2.612355
C	-2.059924	-1.308125	2.729087
H	-1.748026	-2.030336	1.966162
H	-1.409488	-0.422661	2.648657
H	-1.872522	-1.776119	3.709766

C	-3.915891	-0.200419	3.929927
H	-4.964382	0.133454	3.939264
H	-3.774609	-0.897190	4.770961
H	-3.274335	0.673860	4.120826
C	-4.407582	-2.196099	2.548726
H	-5.476149	-1.946021	2.455612
H	-4.132948	-2.831030	1.699127
H	-4.270147	-2.792164	3.466572
C	-5.789612	-1.145864	-2.509663
H	-5.632875	-2.030435	-1.880586
H	-6.681592	-0.619629	-2.135138
H	-6.000081	-1.496945	-3.534501
C	-3.349529	-0.934287	-3.114066
H	-2.434734	-0.327445	-3.027271
H	-3.161163	-1.909756	-2.656665
H	-3.533169	-1.112871	-4.186220
C	-4.890968	0.953073	-3.469600
H	-5.030312	0.546181	-4.483133
H	-5.818605	1.478252	-3.199336
H	-4.075461	1.691805	-3.513303
C	4.216393	-0.748121	3.912104
H	5.049279	-0.055305	4.093878
H	3.714582	-0.922455	4.876597
H	4.639025	-1.706486	3.570926
C	2.024491	-1.219162	2.901132
H	1.165884	-0.903985	2.299417
H	2.328143	-2.226146	2.591088
H	1.668736	-1.293865	3.940228
C	2.621387	1.142237	3.365189
H	5.048577	-2.002238	-3.736257
H	6.166021	-1.369039	-2.498482
H	4.932813	-2.576847	-2.053451
C	4.384256	0.618909	-3.345670
H	5.437815	0.928268	-3.375992
H	4.109707	0.320912	-4.368875
H	3.780607	1.497121	-3.069054
H	2.131577	1.015574	4.343896
H	3.401542	1.909724	3.473925
H	1.867789	1.523747	2.658616
C	2.712826	-1.079582	-2.734867
H	2.448367	-2.015345	-2.232049
H	1.932050	-0.335419	-2.527871
H	2.691419	-1.282227	-3.816506
C	5.130368	-1.694940	-2.680857

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155 **Table S20**. Coordinates for $^{3}IM_{3}$* (BNPA-1)

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	2.351523	0.800354	0.722981
C	1.736790	-0.388406	0.328314
C	1.729415	1.669766	1.621053
C	0.443786	-0.712051	0.813208
H	2.259829	-1.051271	-0.354876
N	3.614198	1.127127	0.171462
C	0.434454	1.362939	2.104778
H	2.198794	2.603099	1.928564
N	-0.144274	-1.905934	0.428381
C	-0.233974	0.166656	1.683334
C	4.781838	1.401890	0.889875
C	3.895639	1.212480	-1.196338
N	-0.117353	2.272619	2.945195
C	-1.406197	-2.316208	0.870758
C	0.615272	-2.793576	-0.427205
B	-1.635865	-0.129673	2.176608
C	4.992938	1.405467	2.271939
C	5.833117	1.664951	-0.030323
C	3.037489	1.058313	-2.289475
C	5.266766	1.546198	-1.361419
C	-1.398583	2.108984	3.380893
C	-3.386852	1.979375	-1.361191
C	-1.881089	-3.583214	0.453254
C	-2.193523	-1.501730	1.742658
C	0.440393	-2.709012	-1.835025
C	1.518402	-3.703778	0.181459
C	-2.259626	0.999108	3.047952
C	6.279842	1.695610	2.727116
H	4.182685	1.187894	2.968159
C	7.115267	1.953122	0.454638
C	3.578744	1.223307	-3.564770
H	1.982764	0.825990	-2.151654
C	5.784479	1.705253	-2.653792
C	-1.884401	3.173460	4.192436
C	-2.416277	2.768667	-1.949444
C	-4.256999	1.088684	-1.960743
C	-3.105352	-4.055776	0.894156
H	-1.274138	-4.197667	-0.206972
C	-3.424762	-2.050760	2.180359
C	1.191445	-3.598242	-2.619475
C	2.261114	-4.528133	-0.680686

C	-3.584543	1.072782	3.517057
C	7.330736	1.970078	1.832059
H	6.472579	1.707899	3.801743
H	7.933569	2.157758	-0.238806
C	4.938197	1.538186	-3.749274
H	2.928870	1.107696	-4.434609
H	6.836108	1.961408	-2.798084
C	-3.191386	3.187550	4.644177
H	-1.185920	3.980091	4.419928
C	-2.327592	2.638522	-3.350314
C	-4.125467	0.994497	-3.361078
C	-3.887250	-3.291365	1.775247
H	-3.451128	-5.035633	0.558353
H	-4.028385	-1.478731	2.880934
C	2.095969	-4.489063	-2.057473
C	-4.052664	2.133725	4.293592
H	-4.294530	0.291567	3.252703
H	8.324721	2.194929	2.222933
H	5.330057	1.658570	-4.760849
H	-3.555102	4.015221	5.256646
C	-3.174199	1.763860	-4.038371
H	-4.843267	-3.672055	2.138640
H	2.679299	-5.153796	-2.697839
H	-5.092953	2.143734	4.625840
H	-3.089214	1.678063	-5.123963
H	1.072753	-3.589759	-3.700455
H	2.988586	-5.222037	-0.263676
H	-1.587528	3.220795	-3.904525
H	-4.768930	0.313739	-3.923905
C	-5.263095	0.252148	-1.165350
C	-1.489242	3.678899	-1.139120
C	1.834582	-3.893127	1.695734
C	-0.531837	-1.780086	-2.614660
C	-1.028458	-0.521903	-1.885695
H	-1.678408	-0.731837	-1.032213
H	-0.197940	0.107939	-1.545567
H	-1.618145	0.071638	-2.593399
C	0.166151	-1.260833	-3.897845
H	0.342431	-2.047253	-4.645007
H	-0.474562	-0.502403	-4.372379
H	1.134760	-0.794267	-3.661842
C	-1.764459	-2.614341	-3.029450
H	-1.471952	-3.498550	-3.617257
H	-2.327212	-2.956450	-2.149566

H	-2.440948	-1.997775	-3.642895
C	0.947015	-3.174814	2.729536
H	1.021699	-2.083437	2.686983
H	-0.108139	-3.463307	2.651352
H	1.292887	-3.477885	3.729950
C	3.286498	-3.415614	1.932313
H	4.007781	-3.945026	1.292376
H	3.380294	-2.337655	1.728211
H	3.573155	-3.587942	2.982311
C	1.718140	-5.400270	2.033245
H	1.936946	-5.556451	3.101061
H	0.695069	-5.759957	1.839873
H	2.412944	-6.029344	1.460626
C	-6.681123	0.465144	-1.726958
H	-6.758731	0.139326	-2.775823
H	-7.413037	-0.115428	-1.141657
H	-6.967130	1.527684	-1.679765
C	-5.233032	0.671445	0.311501
H	-4.225916	0.549120	0.732038
H	-5.519219	1.727235	0.434231
H	-5.928734	0.051964	0.900065
C	-4.881201	-1.237642	-1.270553
H	-5.605311	-1.858709	-0.718768
H	-4.866551	-1.578052	-2.317514
H	-3.887258	-1.420604	-0.838371
C	-1.957134	3.725538	0.322539
H	-2.958270	4.176126	0.405559
H	-2.011999	2.714543	0.748593
H	-1.256758	4.310576	0.937622
C	-1.498130	5.102941	-1.724199
H	-0.858530	5.764196	-1.117311
H	-1.115326	5.125853	-2.756329
H	-2.517461	5.520129	-1.729678
C	-0.057948	3.108107	-1.190747
H	0.309030	3.022296	-2.225484
H	0.637037	3.758296	-0.635414
H	-0.022327	2.111195	-0.730259

Table S21. Coordinates for $^{1}IM_{3}$ (BNPA-1)

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	-2.279375	-0.778996	0.759385
C	-1.682432	0.420988	0.349752
C	-1.621367	-1.653824	1.615208
C	-0.377339	0.740782	0.779747

H	-2.239259	1.090913	-0.298699
N	-3.566747	-1.097576	0.258595
C	-0.308676	-1.343611	2.058630
H	-2.071757	-2.594613	1.928089
N	0.199348	1.939002	0.375848
C	0.338278	-0.139926	1.622830
C	-4.695567	-1.405716	1.023786
C	-3.913903	-1.147114	-1.095389
N	0.276059	-2.253783	2.870817
C	1.468403	2.359298	0.787378
C	-0.585364	2.818211	-0.462305
B	1.745715	0.172246	2.090260
C	-4.840602	-1.450123	2.413913
C	-5.787648	-1.656167	0.148525
C	-3.114598	-0.947288	-2.225656
C	-5.288031	-1.493392	-1.204006
C	1.549571	-2.067841	3.297683
C	3.167183	-2.056877	-1.367383
C	1.923609	3.628917	0.357135
C	2.281615	1.553940	1.644500
C	-0.450976	2.724966	-1.874570
C	-1.471669	3.732705	0.163695
C	2.388274	-0.936517	2.968761
C	-6.100997	-1.767466	2.921530
H	-3.999917	-1.242368	3.076012
C	-7.042020	-1.973124	0.685684
C	-3.716490	-1.082127	-3.476973
H	-2.058608	-0.699965	-2.133713
C	-5.867469	-1.621401	-2.473380
C	2.058640	-3.122816	4.116255
C	2.208057	-2.848238	-1.950329
C	4.118745	-1.232719	-1.917751
C	3.152620	4.115943	0.771827
H	1.297513	4.236452	-0.291651
C	3.515391	2.116103	2.053426
C	-1.222124	3.609911	-2.643935
C	-2.234514	4.555637	-0.682412
C	3.704999	-0.969573	3.472703
C	-7.191058	-2.030274	2.070616
H	-6.241655	-1.811074	4.003438
H	-7.890312	-2.168509	0.026383
C	-5.079164	-1.411149	-3.604045
H	-3.112498	-0.930243	-4.374016
H	-6.922091	-1.886582	-2.572837

C	3.354036	-3.098847	4.588545
H	1.378103	-3.947128	4.334816
C	2.199643	-2.753992	-3.363120
C	4.052310	-1.181478	-3.330793
C	3.958802	3.361660	1.637509
H	3.480695	5.098837	0.426977
H	4.141996	1.550995	2.738814
C	-2.107771	4.507759	-2.062697
C	4.189413	-2.013587	4.256761
H	4.394591	-0.163283	3.232854
H	-8.162627	-2.277682	2.502194
H	-5.519456	-1.506896	-4.598217
H	3.732757	-3.915101	5.207359
C	3.105129	-1.929212	-4.031609
H	4.918699	3.751114	1.981090
H	-2.706078	5.170701	-2.691032
H	5.221065	-1.989118	4.614386
H	3.076258	-1.872892	-5.121789
H	-1.134271	3.595204	-3.727678
H	-2.946556	5.255827	-0.249143
H	1.466694	-3.333709	-3.929817
H	4.760358	-0.549396	-3.873121
C	5.160104	-0.426856	-1.132233
C	1.207622	-3.729410	-1.193291
C	-1.743510	3.936307	1.684414
C	0.504015	1.792929	-2.672614
C	0.993262	0.522928	-1.958605
H	1.658221	0.720476	-1.114326
H	0.159441	-0.095790	-1.606028
H	1.562915	-0.075158	-2.679870
C	-0.209348	1.293066	-3.954899
H	-0.379876	2.087234	-4.695079
H	0.417692	0.530180	-4.440609
H	-1.182416	0.837184	-3.715995
C	1.743054	2.616571	-3.089767
H	1.455104	3.513473	-3.660383
H	2.320382	2.937931	-2.211438
H	2.403993	2.001451	-3.722048
C	-0.859436	3.188893	2.700061
H	-0.969142	2.100540	2.654065
H	0.202405	3.445102	2.604923
H	-1.178806	3.499300	3.707141
C	-3.204438	3.508723	1.959441
H	-3.925938	4.062353	1.340802

H	-3.338788	2.434587	1.757534
H	-3.455941	3.689013	3.017022
C	-1.565907	5.439863	2.009994
H	-1.762884	5.611991	3.079755
H	-0.532745	5.758706	1.799183
H	-2.244457	6.089855	1.440851
C	6.566881	-0.706770	-1.692166
H	6.669803	-0.379972	-2.738262
H	7.318994	-0.161722	-1.099070
H	6.804171	-1.781077	-1.644585
C	5.114538	-0.831346	0.345744
H	4.110405	-0.675905	0.757538
H	5.366422	-1.895156	0.476734
H	5.828748	-0.229312	0.929002
C	4.836859	1.074548	-1.264366
H	5.590186	1.673254	-0.728218
H	4.831444	1.394955	-2.317820
H	3.854950	1.307193	-0.830453
C	1.609092	-3.806100	0.284272
H	2.572702	-4.324208	0.406579
H	1.718056	-2.797533	0.704607
H	0.845421	-4.338405	0.869269
C	1.190185	-5.146521	-1.793276
H	0.512163	-5.787770	-1.207558
H	0.832850	-5.153487	-2.834616
H	2.194411	-5.598030	-1.771872
C	-0.192050	-3.097251	-1.316058
H	-0.495623	-2.983776	-2.368349
H	-0.942554	-3.725116	-0.811077
H	-0.213472	-2.106610	-0.842684

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159 **Table S22**. Coordinates for MECP (BNPA-1)

Atoms	X/Angstrom	Y/Angstrom	Z/Angstrom
C	0.140181	1.578326	-0.398460
C	-1.073050	0.908896	-0.499637
C	1.349692	0.873964	-0.407288
C	-1.104239	-0.487212	-0.662332
H	-2.007904	1.453067	-0.408821
N	0.149848	2.987890	-0.254612
C	1.333125	-0.534595	-0.492754
H	2.281973	1.420070	-0.337823
N	-2.342684	-1.071218	-0.778681
C	0.117041	-1.238836	-0.678771
C	-0.666452	3.889671	-0.953661

C	0.891276	3.707281	0.694570
N	2.531215	-1.238978	-0.390549
C	-2.452323	-2.426117	-1.050019
C	-3.962663	-0.491483	0.739622
B	0.090413	-2.746729	-0.851569
C	-1.557713	3.655931	-2.008200
C	-0.441801	5.197816	-0.451602
C	1.803757	3.250582	1.649573
C	0.552007	5.084419	0.597326
C	2.623626	-2.634526	-0.497721
C	3.722421	-0.477127	-0.080239
C	-3.764114	-2.917707	-1.291726
C	-1.323836	-3.318873	-1.168268
C	-3.855933	-1.364248	1.811893
C	-5.129329	-0.079715	0.092544
C	1.464746	-3.451526	-0.686319
C	-2.244024	4.751300	-2.537186
H	-1.722201	2.655743	-2.406443
C	-1.140871	6.282926	-1.003844
C	2.399910	4.188530	2.491369
H	2.050839	2.193419	1.739610
C	1.164758	6.007945	1.455209
C	3.905797	-3.229025	-0.409471
C	4.475179	0.068161	-1.153911
C	4.062271	-0.266269	1.291318
C	-3.981077	-4.236505	-1.658454
H	-4.603913	-2.237939	-1.183303
C	-1.598416	-4.636613	-1.596801
C	-4.994802	-2.183282	1.994500
C	-6.243969	-0.904377	0.364130
C	1.674814	-4.854733	-0.691759
C	-2.043683	6.051413	-2.039959
H	-2.949400	4.586241	-3.354784
H	-0.973830	7.293184	-0.625755
C	2.089687	5.559433	2.393351
H	3.123284	3.847836	3.234282
H	0.914588	7.070680	1.385829
C	4.053424	-4.606131	-0.453876
H	4.786203	-2.601243	-0.293382
C	5.600510	0.840319	-0.811686
C	5.209617	0.505182	1.537486
C	-2.890936	-5.099113	-1.832871
H	-5.000875	-4.582665	-1.840882
H	-0.764899	-5.312084	-1.787560

C	-6.146644	-2.001560	1.227652
C	2.929469	-5.435625	-0.576582
H	0.809522	-5.511461	-0.767777
H	-2.597256	6.886117	-2.475805
H	2.580060	6.269442	3.062333
H	5.055014	-5.035387	-0.378118
C	5.966131	1.055072	0.508871
H	-3.049200	-6.127351	-2.166354
H	-6.991373	-2.685993	1.337103
H	3.041057	-6.520636	-0.580952
H	6.846007	1.658324	0.742771
H	-4.972153	-2.971656	2.750871
H	-7.195072	-0.698966	-0.132788
H	6.206070	1.287576	-1.599001
H	5.527815	0.684994	2.561606
C	3.360179	-0.867983	2.557825
C	4.213225	-0.069283	-2.690203
C	-5.243165	1.181492	-0.797461
C	-2.664514	-1.431335	2.796155
C	-1.722036	-2.590709	2.421512
H	-2.278647	-3.536192	2.330882
H	-1.224132	-2.402229	1.463427
H	-0.938056	-2.724419	3.185765
C	-1.888902	-0.096035	2.806427
H	-2.535359	0.744373	3.105734
H	-1.057179	-0.151878	3.528347
H	-1.458842	0.144644	1.826056
C	-3.187680	-1.657977	4.232840
H	-3.911401	-0.880813	4.525935
H	-3.666593	-2.639714	4.361422
H	-2.340787	-1.616161	4.937742
C	-6.712195	1.545743	-1.091790
H	-7.220940	0.786046	-1.705158
H	-7.292858	1.692767	-0.167185
H	-6.741189	2.492421	-1.655527
C	-4.522135	0.950739	-2.141236
H	-3.479804	0.645169	-1.994332
H	-5.017717	0.143690	-2.704730
H	-4.546816	1.862589	-2.760929
C	-4.628881	2.387653	-0.042024
H	-4.604291	3.275404	-0.693831
H	-5.222125	2.640285	0.851603
H	-3.602413	2.196306	0.299908
C	4.136968	-2.143371	2.965869

H	5.206334	-1.929230	3.119749
H	3.728910	-2.549147	3.906527
H	4.051595	-2.925066	2.197867
C	1.866895	-1.237869	2.429541
H	1.252500	-0.385190	2.111130
H	1.677119	-2.077570	1.753780
H	1.502823	-1.545479	3.422256
C	3.424918	0.137913	3.737863
H	2.849626	-0.266280	4.584854
H	4.443757	0.318770	4.107056
H	2.978684	1.108126	3.469585
C	3.020696	-0.927466	-3.165440
H	3.096045	-1.975954	-2.852455
H	2.049570	-0.530598	-2.846865
H	3.021260	-0.920729	-4.267080
C	5.474423	-0.703791	-3.330159
H	5.338216	-0.789565	-4.420108
H	6.387340	-0.117604	-3.152307
H	5.640847	-1.717609	-2.931492
C	3.984275	1.351413	-3.266395
H	4.827641	2.030820	-3.075386
H	3.837669	1.295465	-4.357178
H	3.080311	1.806401	-2.831234

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