Supporting Information

Substituent Modulated Adaptive Aromaticity in NHC-Pyrrolyl Cations: A Combined DFT and Machine Learning Study

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1. Aromaticity Indices of the studied systems:

Table S1. Overview of aromaticity indices (HOMA, $NICS(1)_{zz}$, $EDDB_{\pi}$ and MCI for the studied systems, based on structures optimized at the M06-2X/def2-TZVPP level of theory

Compound (Substitution)	Charge	$NICS(1)_{zz}$		HOMA		$EDDB_{\pi}$		MCI	
		S_0	T_1	S_0	T_1	S_0	T_1	S_0	T_1
A(NO)	-1	-18.52	-22.91	0.731	0.892	2.30	3.71	0.541	0.558
B(NO_2)	-1	-22.03	10.77	0.852	0.381	3.01	2.28	0.560	0.466
C(CHO)	-1	-19.95	14.88	0.810	0.261	3.09	2.18	0.562	0.434
D($COCH_3$)	-1	-17.82	17.32	0.514	0.186	3.33	2.07	0.567	0.418
E (OH)	-1	-27.19	-7.30	0.947	0.465	4.619	2.276	0.587	0.511
F(NH_2)	-1	-27.87	-7.05	0.947	0.649	4.712	2.425	0.598	0.531
G(COOH)	-1	-24.46	18.91	0.832	0.108	3.052	1.573	0.569	0.378
H(CN)	-1	-27.40	17.71	0.885	-0.269	3.745	1.357	0.578	0.240
I(NO)	+1	-24.81	-24.30	0.939	0.924	3.83	3.67	0.559	0.473
J(NO_2)	+1	-26.25	-25.83	0.959	0.950	4.24	4.15	0.557	0.559
K(CHO)	+1	-27.12	-23.03	0.941	0.865	4.11	3.44	0.554	0.527
L($COCH_3$)	+1	-27.11	-23.91	0.941	0.867	4.18	3.61	0.549	0.526
M(OH)	+1	-25.52	19.72	0.918	0.277	3.573	1.102	0.557	0.434
N(NH_2)	+1	-26.22	12.11	0.916	0.399	3.669	0.935	0.559	0.426
O(COOH)	+1	-27.43	21.0	0.945	0.174	3.908	1.112	0.556	0.435
P(CN)	+1	-28.70	17.70	0.943	0.139	3.963	1.178	0.563	0.445

Table S2. Overview of aromaticity indices (HOMA, $NICS(1)_{zz}$, $EDDB_{\pi}$ and MCI for the redox systems **I-VI**, based on structures optimized at the M06-2X/def2-TZVPP level of theory.

Compound	Charge	$NICS(1)_{zz}$		HOMA		$EDDB_{\pi}$	
		S_0	T_1	S_0	T_1	S_0	T_1
I	+1	35.77	-21.63	-0.947	0.709	1.54	3.02
II	-1	-30.00	13.42	0.936	-0.203	5.13	2.10
III	+3	-16.54	4.23	0.393	-1.21	2.51	1.17
IV	+11	-29.63	17.14	0.931	0.013	4.24	1.53
V	-1	-1.29	-21.85	0.293	0.926	1.58	2.66
VI	+3	16.57	-7.03	-0.276	0.746	1.32	2.03

1. EDDB Analysis:

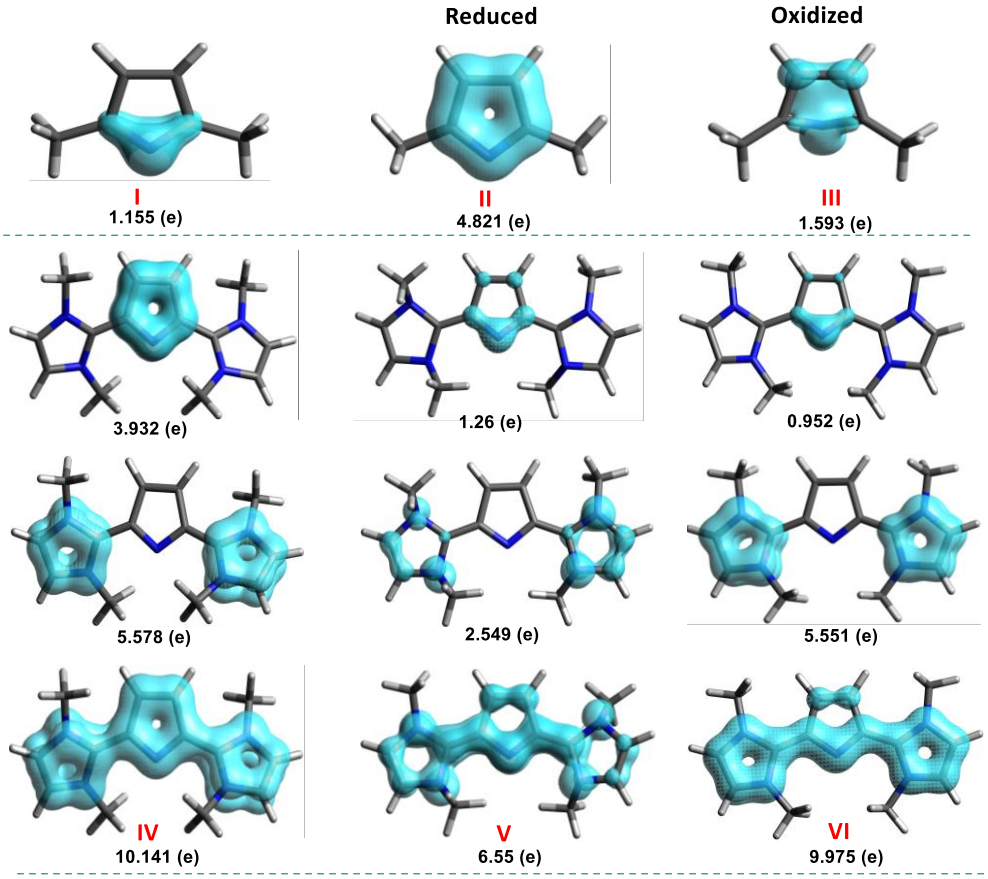

Figure S1. EDDB analysis of the compounds **I** and **IV** along with their oxidized and reduced species on π-$EDDB_{5MR}$ for their singlet states and (isovalue = 0.01 a.u.)

3. Geometrical parameters:

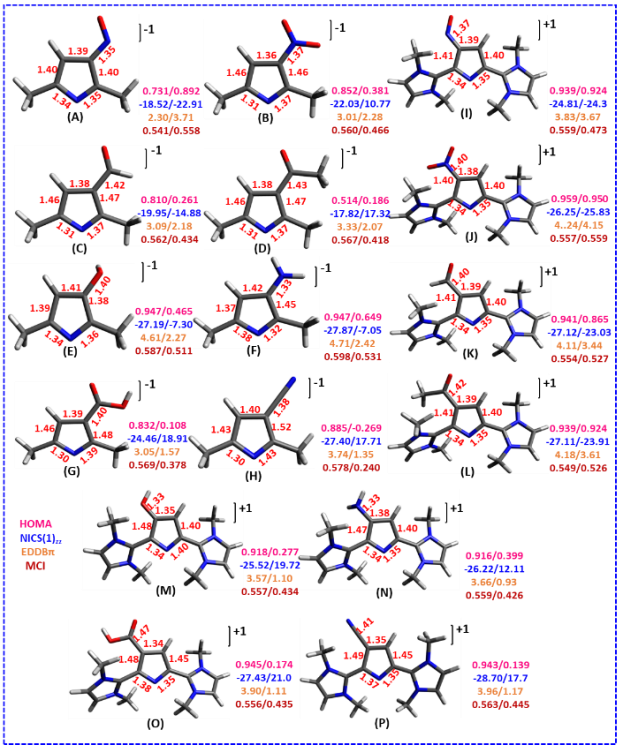

Figure S2. Geometrical parameters of interest of compounds A-P in the T_1 state.

4. Correlation Diagrams:

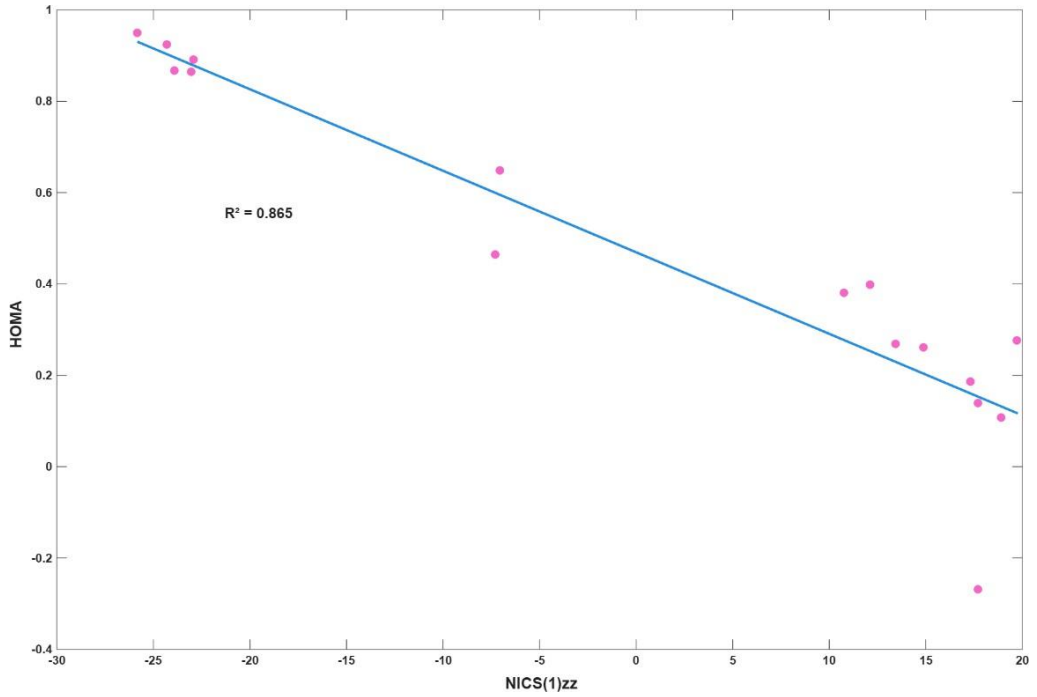

Figure S3. Correlation between HOMA and $NICS(1)_{zz}$ for compounds A-P.

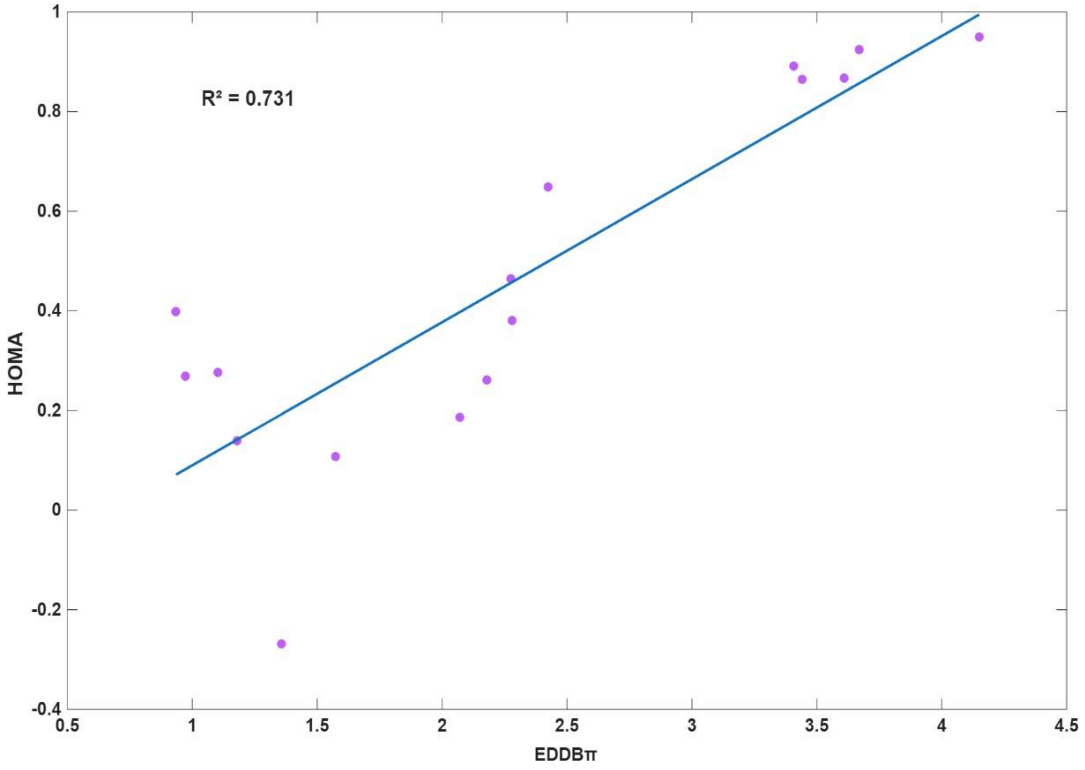

Figure S4. Correlation between HOMA and $EDDB_{\pi}$ for compounds A-P.

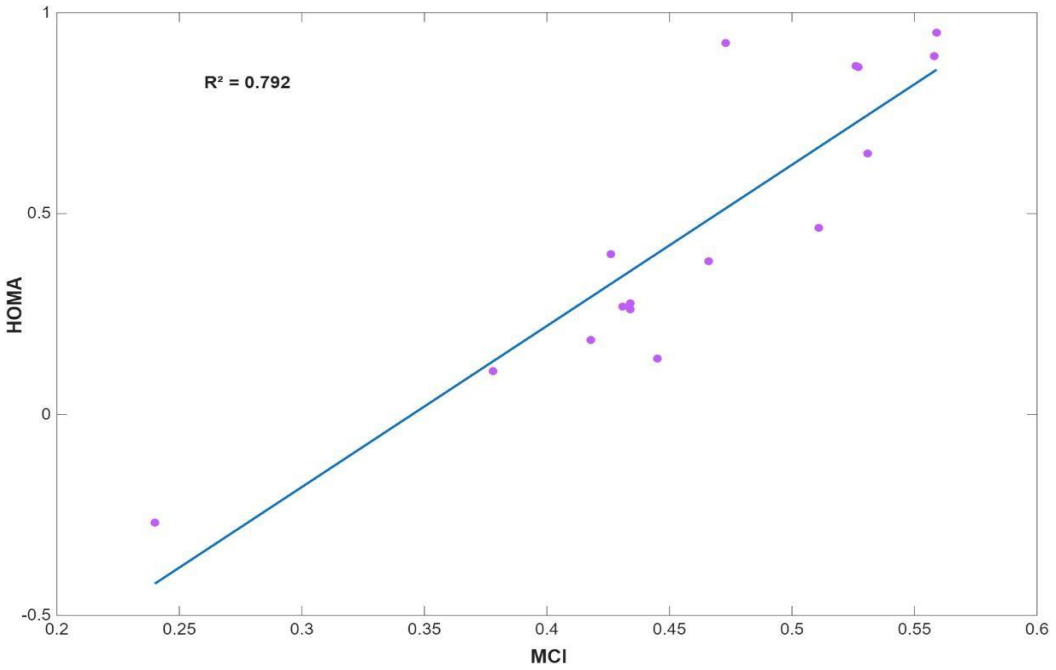

Figure S5. Correlation between HOMA and MCI for compounds A-P.

The correlation investigation between different aromatic indices is shown above. There is a strong correlation seen among different aromaticity indexes with HOMA values plotted along Y axis vs $NICS(1)_{zz}$, $EDDB_{\pi}$. And MCI along the X axis. The R^2 values for the correlations between HOMA and $NICS(1)_{zz}$ are the highest (0.865), followed by HOMA/MCI (0.792) and (0.731) with HOMA/ $EDDB_{\pi}$, respectively. These values corroborate the data well, as both the HOMA and $NICS(1)_{zz}$ prove to be the significant indicators for deciphering the (anti)aromaticity in all the studied systems.

5. Acid Plots of the model systems:

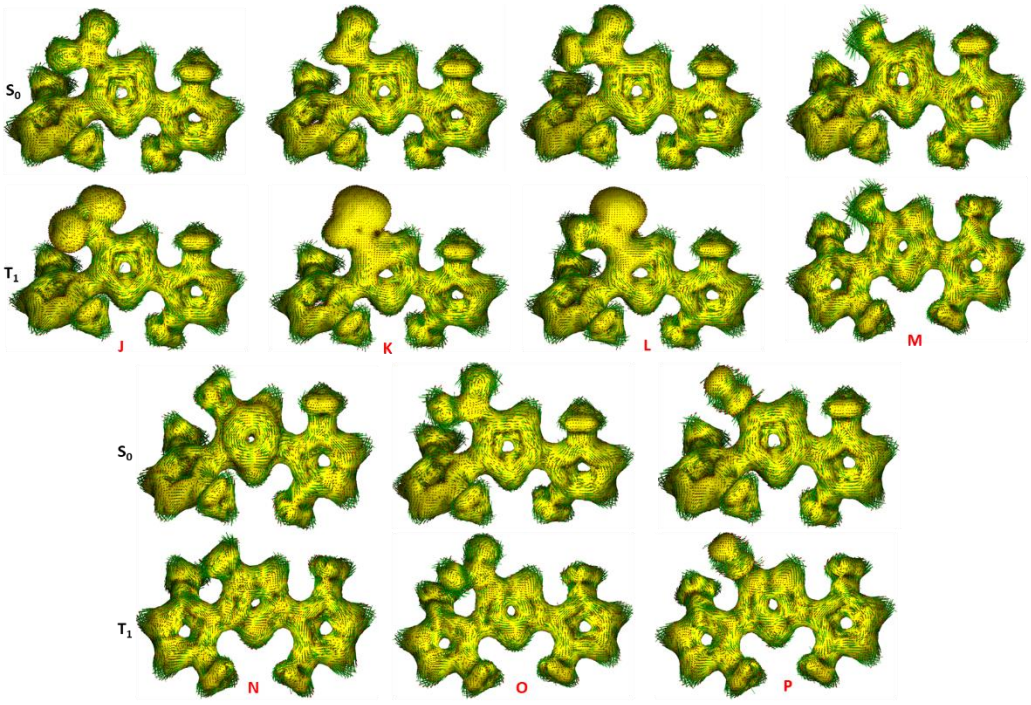

Figure S6. ACID plots showing induced current densities in the S_0 and T_1 states for the NHC substituted pyrrolyl cation bearing different substituent groups. Clockwise loops denote aromaticity and counterclockwise denote antiaromaticity.

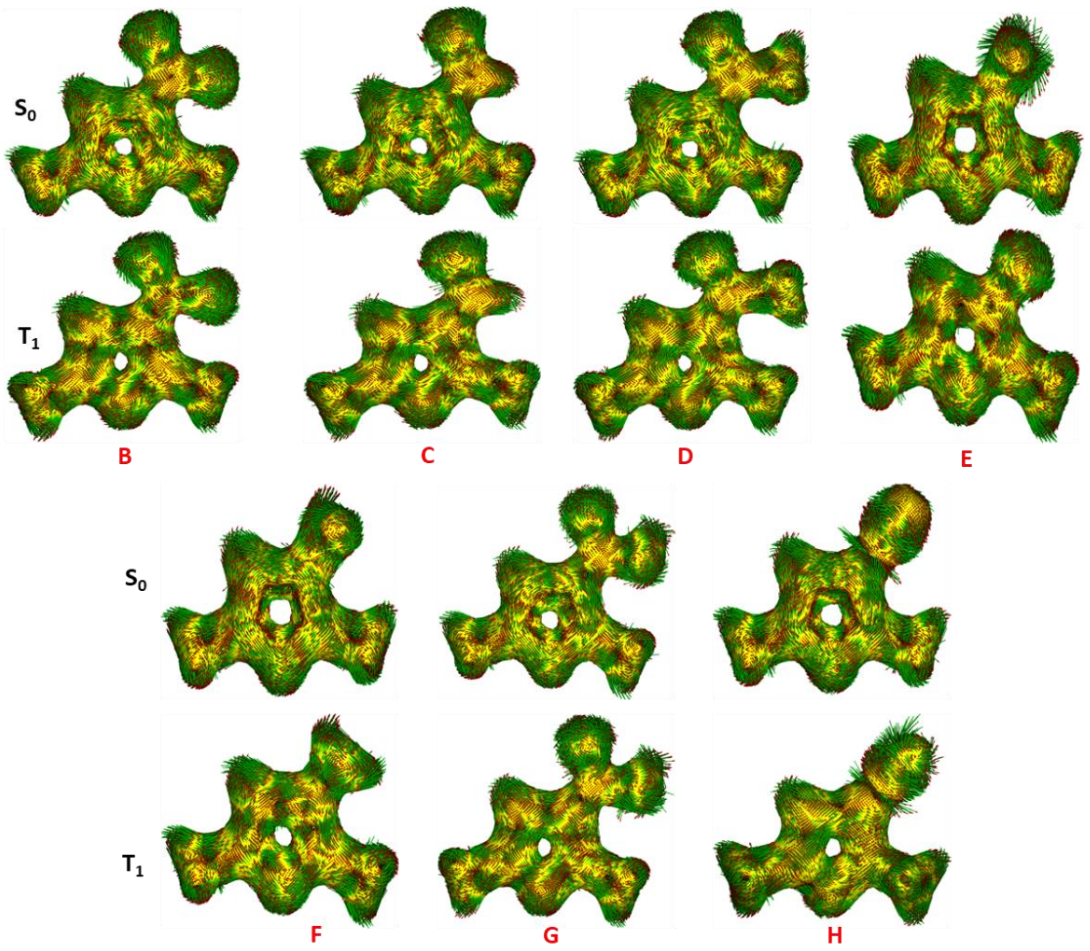

Figure S7. ACID plots showing induced current densities in the S_0 and T_1 states for the substituted pyrrolyl anion. Clockwise loops denote aromaticity and counterclockwise denote antiaromaticity.

6. Frontier MOs

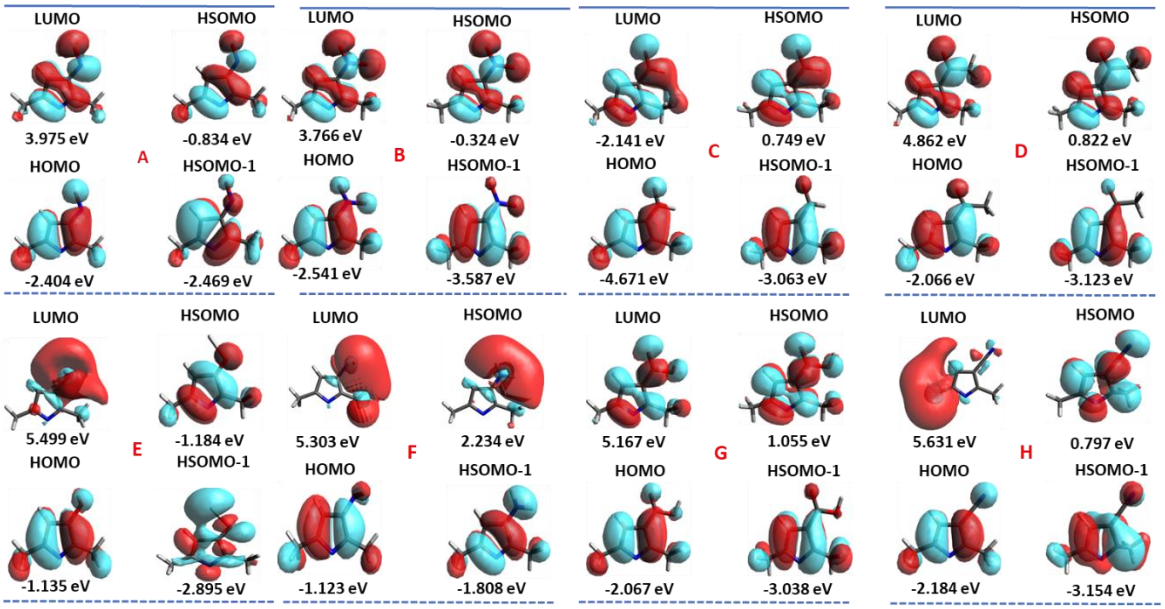

Figure S8. Frontier molecular orbitals (MOs) of the substituted pyrrolyl anion

7. Linear regression analysis

=== FULL MODEL (Linear + Quadratic Terms) === **NICS(1)$_{zz}$ as the T_1 state (dependent variable, y);**

X_1-X_4 = Dependent variables; X_5-X_8 their squared terms

X_1 = (H-L gap); X_2= (Spin density R); X_3 = (Spin 5MR); X_4 = (ΔFBO)

Linear regression model:

$y \sim 1 + X_1 + X_2 + X_3 + X_4 + X_5 + X_6 + X_7 + X_8$

Table S3: Coefficients and Significance Levels for the full Regression Model

Term	Estimate	SE	tStat	pValue
(Intercept)	-817.32	436.5	-1.8725	0.1033
X1	262.84	131.79	1.9943	0.086341
X2	-15.498	13.392	-1.1572	0.28515
X3	-13.652	62.7	-0.21774	0.83385
X4	-135.45	408.57	-0.33152	0.74996
X5	-20.285	10	-2.0285	0.082097
X6	-2.8234	12.171	-0.23198	0.82319
X7	14.627	31.126	0.46995	0.65268
X8	218.24	544	0.40117	0.70026

Performance Statistics:

RMSE	R^2	Adjusted R^2	F-statistic	p-Value
4.5	0.975	0.945	33.5	6.63e-05

=== LINEAR MODEL (Only Linear Terms) ===

Linear regression model:

$y \sim 1 + X1 + X2 + X3 + X4$

$Y = \beta_0 + \beta_1 X_1 + \cdots \beta_4 X_4$

Table S4: Coefficients and Significance Levels for the linear Regression Model

Term	Estimate	SE	tStat	pValue
(Intercept)	21.761	26.292	0.82767	0.42545
X1(H-L)	-3.09	3.8089	-0.81127	0.43442
X2(Spin R)	-18.88	3.728	-5.0643	0.00036383
X3(Spin 5MR)	9.4895	7.3235	1.2958	0.22159
X4(ΔFBO)	19.918	28.005	0.71122	0.49175

Performance Statistics:

RMSE	R^2	Adjusted R^2	F-statistic	p-Value
4.6	0.958	0.943	63.1	1.62e-07

Non-Linear Regression Model (Symbolic regression)

$$y \sim b1 + b2*x1 + b3*x2\hat{}2 + b4*sqrt(x3) + b5*log(x4)$$

$$y = \alpha_0 + \alpha_1 x_1 + \beta x_2^2 + \alpha_2 * sqrtx_3 + \alpha 3 \log(x_4)$$

Table S5: Estimated Coefficients and Significance Levels for the Non-linear Regression Model

m	Estimate	SE (Std. Error)	tStat	pValue
b1	-0.6515	24.683	-0.026	0.979
b2	4.0187	3.9543	1.016	0.331
b3	-14.295	2.991	-4.780	0.00057
b4	-6.2251	14.308	-0.435	0.672
b5	2.8917	11.399	0.254	0.804

b3 corresponds to the spin density of the substituent and is highly significant

Performance Statistics:

RMSE	**R^2**	**Adjusted R^2**	**F-statistic**	**p-Value**
4.89	0.953	0.936	55.6	3.15e-07

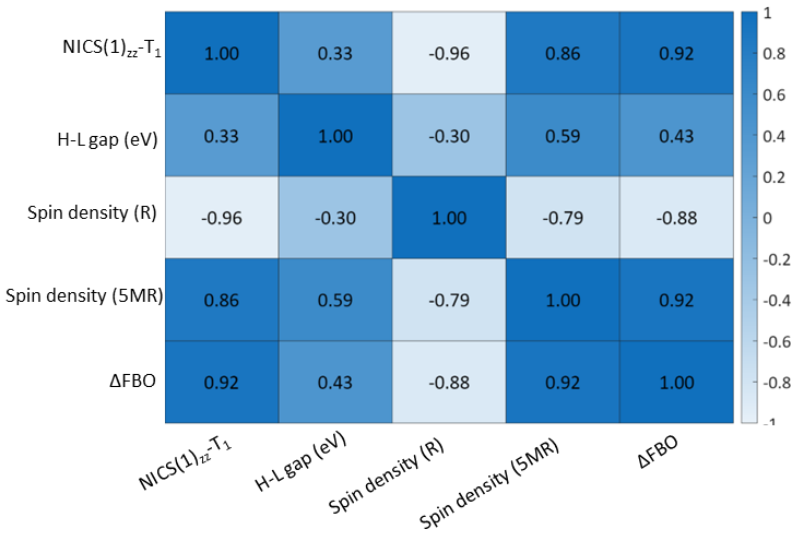

Figure S9: Heat map of excited state aromaticity predictors. Absolute value of Pearson correlation is displayed where strong colors indicate strong correlation. magnitudes. Preliminary processing of the data was performed using MATLAB (R2025a) software package.

Examination of the above heat map reveals that $NICS(1)_{zz}$ exhibits a strong negative correlation with the spin density of the substituent (-0.96), a strong positive correlation with the fuzzy bond order (ΔFBO) index (0.92), and a moderate correlation with the HOMO–LUMO gap (0.33). The correlation results highlight that the spin density on the substituent (R) emerges as the decisive factor influencing T_1 aromaticity, as evidenced by its strong inverse correlation with $NICS(1)_{zz}$, with greater spin localization corresponding to enhanced aromatic character in the ring system.

7.1 === FULL MODEL (Linear + Quadratic Terms) === **EDDB$_\pi$ as the T$_1$ state (dependent variable, y)**

Linear regression model:
y ~ 1 + X1 + X2 + X3 + X4 + X5 + X6 + X7 + X8
X_1-X_4 = Dependent variables; X_5-X_8 their squared terms
X_1 = (H-L gap); X_2= (Spin density R); X_3 = (Spin 5MR); X_4 = (ΔFBO)

Table S6: Estimated Coefficients and Significance Levels for the Linear Regression Model

Term	Estimate	SE	tStat	pValue
(Intercept)	-35.741	22.936	-1.5583	0.16313
X1	10.665	6.9253	1.5400	0.16745
X2	1.4924	0.70372	2.1207	0.07164
X3	-3.0629	3.2947	-0.9297	0.38348
X4	11.298	21.469	0.5263	0.61497
X5	-0.76646	0.52548	-1.4586	0.18804
X6	-0.3597	0.63953	-0.5624	0.59136
X7	1.965	1.6355	1.2015	0.26864
X8	-19.026	28.585	-0.6656	0.52699

Performance Statistics:

RMSE	R^2	Adjusted R^2	F-statistic	p-Value
0.236	0.977	0.951	37.2	4.68e-05

=== LINEAR MODEL (Only Linear Terms) ===

Linear regression model:
y ~ 1 + x1 + x2 + x3 + x4
$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_4 X_4$

Table S7: Estimated Coefficients and Significance Levels for the linear Regression Model

Term	Estimate(β)	SE	tStat	pValue
(Intercept)	1.3128	1.2746	1.03	0.32514
x1(H-L)	0.14112	0.18465	0.7642	0.46081
x2 (Spin R)	1.2196	0.18073	6.748	0.0000316
x3 (Spin 5MR)	0.57221	0.35504	1.6117	0.13533
x4(ΔFBO)	-3.5285	1.3577	-2.599	0.02474

Performance Statistics:

RMSE	R^2	Adjusted R^2	F-statistic	p-Value
0.223	0.968	0.956	82.9	3.87 e-08

Substituent spin density (R) is the decisive factor influencing T_1 aromaticity, with a pValue of 0.0000316

Non-Linear Regression Model (Symbolic regression)

$$y \sim b1 + b2*HL\_Gap\_eV + b3*(SpinDensity\_Subst\hat{}2) + b4*sqrt(SpinDensity\_5MR) + b5*log(\Delta FBO)$$

$$y \sim b1 + b2*X_1 + b3*X_2^2 + b4*sqrt(X_3) + b5*log(X_4)$$

Table S8: Estimated Coefficients and Significance Levels for the Nonlinear Regression Model

Term	Estimate	SE	tStat	pValue
Intercept	-0.12979	1.4028	-0.0925	0.92795
b2	-0.19425	0.22474	-0.8643	0.40586
b3	0.90651	0.16999	5.3327	0.0002401
b4	2.0515	0.81319	2.5228	0.02833
b5	-0.9312	0.64784	-1.4374	0.17844

The non-linear regression model performs poor than the linear model, as both the regression coefficients and p-values indicate a stronger, more reliable fit for the linear case.

8. PCA Analysis

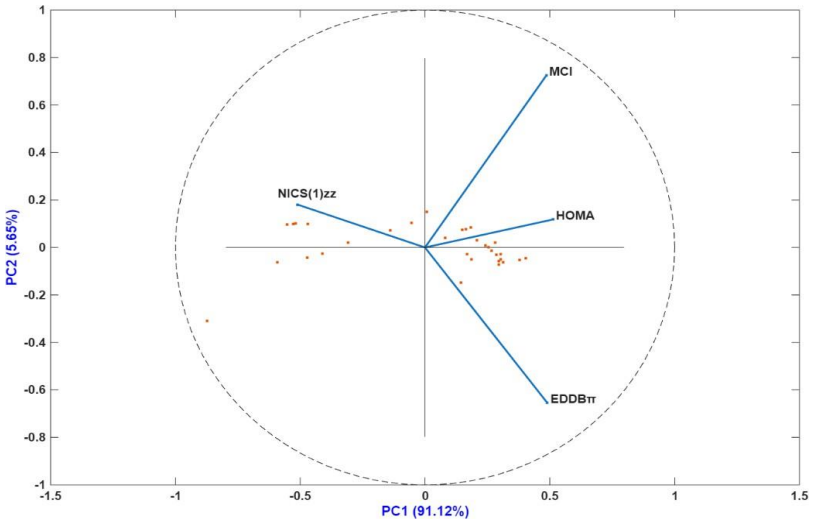

Figure S9: PCA plot of different aromatic indicators

Table S9. Variable Contributes to Each Principal Component

Variable	$NICS(1)_{zz}$ %	HOMA %	$EDDB_{\pi}$ %	MCI %
PC1	26.14	26.28	23.84	23.74
PC2	2.35	1.77	46.39	49.47

PC1 accounts for 91% of the variance, indicating that it is the primary source of variation within the dataset. (Table S9) highlights the contribution of the variables to the two principal components (PC1 and PC2). Notably, all variables contribute substantially to PC1, with $NICS(1)_{zz}$ (26.14%) and HOMA (26.28%) having the greatest impact. PC1 likely represents the shared aromatic factor, as all these variables represent aromatic indicators. Orthogonal to PC1, the less dominant secondary variation, PC2, accounts for 5.65% of the variance in the data, with the most significant impact on MCI (49.47%), followed by $EDDB_{\pi}$ (46.39%). Although HOMA makes the largest contribution to PC1 (26.28%), the total contribution of all aromatic descriptors is similar, as shown in Table S10.

Table S10. Variable Contribution of Principal Component Analysis

Total Contribution = (PC1 Variance × Contribution to PC1) + (PC2 Variance × Contribution to PC2)

Variable	$NICS(1)_{zz}$	HOMA	$EDDB_{\pi}$	MCI
Contribution	24.06	24.27	25.18	25.31

Table S11. Eigen vectors for Principal Component Analysis

Principal Component	Eigen Values	$NICS(1)_{zz}$	HOMA	$EDDB_{\pi}$	MCI
PC1	3.63044	-0.51126	0.51265	0.48822	0.48728
PC1	0.231	0.15345	0.13321	-0.68118	0.70335

Table S12: Principal components loadings

	PC1	PC2	PC3	PC4	PC5
$NICS(1)_{zz}$	0.45995	-0.1049	0.72664	-0.22443	0.44617
$EDDB_{\pi}$	-0.44466	0.48379	0.49128	-0.38573	-0.42199
HOMA	-0.45334	-0.29907	0.45264	0.70704	0.015507
Spin density(R)	0.45379	0.38798	-0.15355	-0.045788	0.78605
Spin density(5MR)	0.42341	0.71762	0.046672	0.54666	-0.068806

Table S13: Variable Contributions:

	PC1	PC2	PC3	PC4	PC5
$NICS(1)_{zz}$	21.155	1.1003	52.8	5.0371	19.907
$EDDB_{\pi}$	19.773	23.405	24.135	14.879	17.808
HOMA	20.552	8.9442	20.489	49.991	0.024047
Spin density(R)	20.592	15.053	2.3577	0.20965	61.788
Spin density(5MR)	17.928	51.497	0.21782	29.883	0.47342

Table S14: Comparative aromaticity indices for the T_1 state of compounds A-P calculated at M06-2X/def2-TZVPP and CAM-B3LYP/def2-TZVPP levels of theory.

Molecule	M06-2X/T_1				CAM-B3LYP/T_1			
	HOMA	**NICS**	**EDDB$_\pi$**	**MCI**	**HOMA**	**NICS**	**EDDB$_\pi$**	**MCI**
A	0.892	-22.91	3.71	0.558	0.894	-21.16	3.37	0.552
B	0.381	10.77	2.28	0.466	0.405	10.35	2.24	0.453
C	0.261	14.88	2.18	0.434	0.292	14.51	2.18	0.418
D	0.186	-17.32	2.07	0.418	0.232	16.71	2.04	0.394
E	0.465	-7.30	2.27	0.511	0.524	-7.18	2.62	0.504
F	0.649	-7.05	2.42	0.531	0.694	-7.62	2.74	0.517
G	0.108	18.91	1.57	0.378	0.157	18.01	1.91	0.354
H	0.269	17.71	1.35	0.240	-0.180	24.07	1.66	0.251
I	0.924	-24.3	3.67	0.473	0.928	-22.74	3.50	0.532
J	0.950	-25.83	4.15	0.559	0.956	-24.86	4.03	0.542
K	0.865	-23.03	3.44	0.527	0.873	-21.68	3.32	0.512
L	0.924	-23.91	3.61	0.526	0.876	-22.32	3.49	0.513
M	0.277	19.72	1.10	0.434	0.302	17.77	1.31	0.405
N	0.399	12.11	0.93	0.426	0.408	7.7	1.16	0.402
O	0.174	21.0	1.11	0.435	0.107	21.67	1.39	0.393
P	0.139	17.7	1.17	0.445	0.106	17.46	1.43	0.403

The table above shows comparative aromaticity indices using the M06-2X and range-separated CAM-B3LYP functionals. The qualitative classification of all A-P systems as aromatic or antiaromatic is identical for both functions. Aromatic systems consistently exhibit negative NICS and high HOMA, EDDB$_\pi$, and MCI values with both methods, while antiaromatic systems show positive NICS and low values for the aromaticity indices. Although we observed minor variations in the quantitative values of the descriptors, the overall qualitative trends remain entirely consistent. Based on these results, we are confident that our main findings regarding triplet-state aromaticity are robust and method-independent, thereby firmly supporting our original conclusions based on M06-2X.

Table S15*:* Comparison of TD-DFT vertical and UDFT adiabatic singlet–triplet gaps for A–P.

SYSTEM	TD-DFT Vertical T_1 (eV)	Dominant Orbital Character	$\langle S^2 \rangle$	UDFT AdiabaticΔE (eV)
A	1.265	32 → 34	2.000	1.233
B	2.695	36 → 38, 37 → 38	2.000	2.328
C	3.089	32 → 34, 33 → 34	2.000	2.816
D	3.264	36 → 38, 37 → 38	2.000	2.919
E	4.180	29 → 31, 30 → 31	2.000	3.893
F	4.170	29 → 31, 30 → 31	2.000	3.083
G	3.568	36 → 38, 37 → 38	2.000	3.151
H	4.126	31 → 34, 32 → 34	2.000	3.589
I	0.699	74 → 76, 74 → 78	2.000	0.770
J	3.002	74 → 80, 74 → 82	2.000	2.831
K	3.322	73 → 76, 73 → 77, 73 → 80	2.000	3.148
L	3.488	77 → 80, 77 → 81, 77 → 83	2.000	3.148
M	3.137	72 → 73	2.000	2.811
N	3.130	72 → 73	2.000	2.596
O	3.676	79 → 80, 79 → 81	2.000	3.246
P	3.601	74 → 75, 72 → 76	2.000	3.227

Across systems A-P, UDFT triplet optimizations confirmed the same singly occupied orbitals and yielded adiabatic singlet–triplet gaps (ΔE) in close agreement with the TD-DFT vertical energies. The orbital transitions defining the T_1 state in TD-DFT match the singly occupied molecular orbitals (SOMOs) obtained from our unrestricted DFT (UDFT) optimizations, confirming consistent electronic character. TD-DFT consistently yields spin expectation value $\langle S^2 \rangle$ = 2.0 across all systems, confirming pure triplet character with negligible spin contamination.

Additionally, we compared the UDFT- and TD-DFT-optimized T_1 geometries for the adaptive aromatic systems **A**, **I**, **J**, **K**, and **L**. As anticipated, both methods give very similar geometries for the T_1 structure. Key geometric parameters (core aromatic bond lengths, ring planarity) are in close agreement, with only small quantitative differences in bond distances. This confirms that our qualitative conclusions about T_1 aromaticity are preserved regardless of whether UDFT or TD-DFT is used for geometry optimization, demonstrating the robustness of our results.

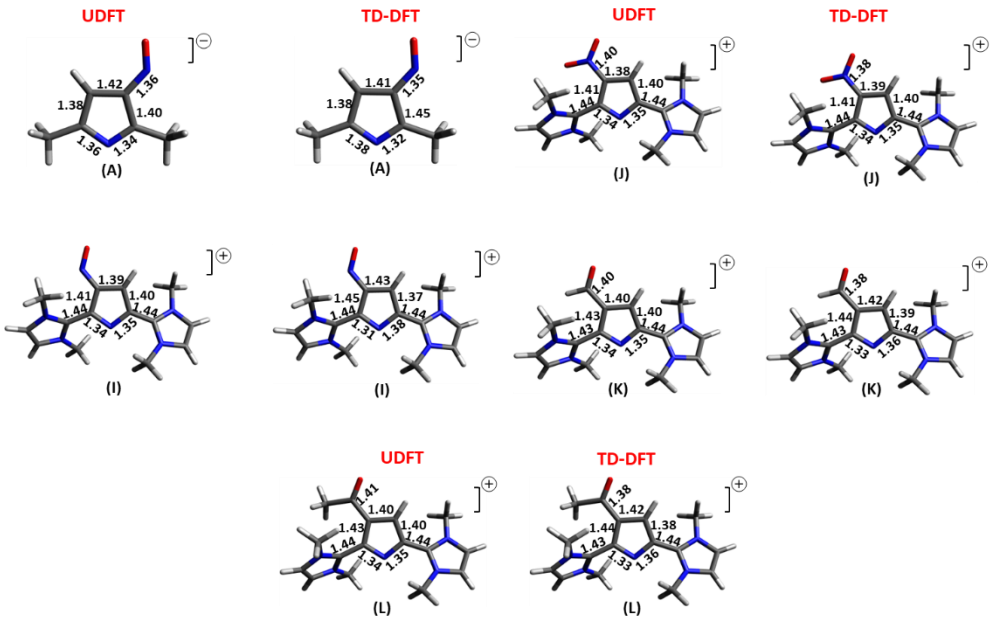

Figure S10: Comparison of the optimized T_1 triplet state geometries of adaptive aromatic systems **A**, **I**, **J**, **K**, and **L**, calculated at the M06-2X/def2-TZVPP level of theory with unrestricted DFT (UDFT) and linear-response TD-DFT. Key bond lengths are given in angstroms (Å), and all systems are classified as adaptively aromatic in the triplet state.

9. Optimized Coordinates

Computational Method: All molecules are optimized using Gaussian 16 the following method Method: M06-2X; Basis Set: def2-TZVPP

Optimized molecular coordinates for systems I-VI in the singlet (S_0) and triplet (T_1) electronic states.

I (S_0)

Total Energy: -287.842907 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.057797	-0.149787	-0.000071
6	-0.660907	1.314583	0.000056
6	0.660922	1.314577	0.000031
6	1.057800	-0.149773	-0.000064
7	-0.000005	-0.955984	-0.000113
1	-1.356710	2.138629	0.000127
1	1.356728	2.138621	0.000082
6	-2.426517	-0.620110	-0.000015
1	-2.941357	-0.180122	0.865838
1	-2.942062	-0.179065	-0.864868
1	-2.498415	-1.701570	-0.000539
6	2.426508	-0.620123	-0.000020
1	2.498385	-1.701584	-0.000812
1	2.942232	-0.178810	-0.864618
1	2.941188	-0.180415	0.866082

I (T_1)

Total Energy: -287.806901 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.103421	-0.079228	0.000038
6	-0.721769	1.289238	-0.000014
6	0.721777	1.289228	0.000018
6	1.103411	-0.079238	0.000033
7	-0.000005	-0.871344	-0.000052
1	-1.374186	2.148980	-0.000130
1	1.374206	2.148961	0.000007
6	-2.458458	-0.647930	0.000023
1	-2.575275	-1.295240	0.873330
1	-3.227059	0.118548	0.000101
1	-2.575268	-1.294995	-0.873483
6	2.458463	-0.647930	0.000004
1	2.575315	-1.294831	-0.873607
1	3.227070	0.118535	0.000324
1	2.575215	-1.295398	0.873208

II (S_0)

Total Energy: -288.199257 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.080393	-0.074109	-0.000003
6	-0.708651	1.268730	0.000003
6	0.708665	1.268729	-0.000003

6	1.080401	-0.074124	-0.000017
7	-0.000006	-0.892011	-0.000015
1	-1.372452	2.123612	0.000020
1	1.372468	2.123609	0.000001
6	-2.470694	-0.635524	0.000010
1	-3.211130	0.168078	0.000062
1	-2.655073	-1.262029	-0.878865
1	-2.655049	-1.262134	0.878816
6	2.470681	-0.635532	0.000013
1	2.655030	-1.262192	-0.878763
1	3.211113	0.168078	-0.000106
1	2.655080	-1.261972	0.878929

II (T_1)
Total Energy: -288.053509 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.151344	0.131323	0.487696
6	0.802051	-1.327100	0.226269
6	-0.516076	-1.263655	-0.212536
6	-0.989170	0.053057	0.047883
7	-0.082443	0.865087	0.599715
1	1.497744	-2.149837	0.156352
1	-1.117146	-2.058743	-0.638279
6	2.143493	0.764073	-0.463599
1	3.102243	0.238306	-0.448739
1	1.754447	0.720942	-1.496098
1	2.301638	1.814413	-0.207363
6	-2.381034	0.535492	-0.210569
1	-2.405169	1.279385	-1.014741
1	-3.044309	-0.287855	-0.484142
1	-2.776003	1.028639	0.684141

III (S_0)
Total Energy: -286.517231 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	3.071880	-0.359717	0.431128
6	-1.153245	-0.095746	-0.001557
6	-0.710616	1.303918	-0.141442
6	0.706984	1.303550	-0.137209
7	1.152841	-0.096281	-0.004574
1	0.001932	-0.293321	0.754740
1	-1.339558	2.170648	0.120543
6	1.334947	2.168462	0.133482
1	-2.276606	-0.899166	-0.201830
1	-3.101367	-0.338848	0.370654
1	-2.719726	-0.737143	-1.216099
6	-2.216819	-1.932747	0.147887
1	2.278956	-0.896077	-0.210513
1	2.210330	-1.939068	0.110489
1	2.756900	-0.699519	-1.198515

III (T_1)
Total energy: -286.518080 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.712566	1.301345	0.000001
6	-1.184301	-0.152864	-0.000012
6	0.712575	1.301344	-0.000002
6	1.184305	-0.152866	0.000000
7	-0.000004	-0.795991	-0.000016
1	-1.378516	2.172986	0.000012
1	1.378525	2.172984	-0.000010
6	-2.485456	-0.686248	0.000003
1	-3.081303	-0.193252	0.827473
1	-3.081390	-0.193184	-0.827358
1	-2.568112	-1.773937	-0.000029
6	2.485444	-0.686260	0.000012
1	2.568110	-1.773947	0.000041
1	3.081349	-0.193244	-0.827410
1	3.081367	-0.193173	0.827377

IV (S_0)
Total Energy: -817.849857 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.068719	-0.586634	-0.032312
6	0.691199	-1.947086	-0.017473
6	-0.691199	-1.947086	0.017473
6	-1.068719	-0.586634	0.032313
6	-2.396412	-0.033652	0.094763
6	-4.592600	0.239389	-0.117927
6	-4.098116	1.339449	0.485453
1	-5.596165	-0.020304	-0.400093
1	-4.586599	2.229293	0.837289
7	-2.739798	1.157453	0.616907
7	-3.528975	-0.601226	-0.360786
6	-1.844162	2.108126	1.264270
1	-1.147259	1.569485	1.898009
1	-1.281183	2.660899	0.517821
1	-2.452866	2.783996	1.857767
6	-3.633882	-1.878936	-1.050312
1	-3.679503	-2.697129	-0.334737
1	-4.541868	-1.868107	-1.645751
1	-2.771228	-2.007263	-1.698465
6	2.396412	-0.033652	-0.094763
6	4.098116	1.339449	-0.485454
6	4.592601	0.239389	0.117926
1	4.586599	2.229293	-0.837289
1	5.596165	-0.020304	0.400093
7	3.528976	-0.601226	0.360786
7	2.739798	1.157453	-0.616907
6	3.633882	-1.878936	1.050312
1	2.771229	-2.007263	1.698465
1	3.679503	-2.697129	0.334737
1	4.541869	-1.868107	1.645750
6	1.844162	2.108126	-1.264269
1	1.281183	2.660899	-0.517821
1	2.452865	2.783996	-1.857766
1	1.147259	1.569485	-1.898009
7	0.000000	0.235787	0.000000
1	1.328637	-2.813646	-0.057961

1	-1.328637	-2.813646	0.057961

IV (T_1)
Total Energy: -817.741716 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.089778	-0.551732	0.002761
6	0.668237	-1.967253	0.002968
6	-0.668237	-1.967253	-0.002969
6	-1.089778	-0.551732	-0.002761
6	-2.388222	-0.048411	0.010777
6	-4.621398	0.144976	-0.004719
6	-4.101104	1.394967	0.055153
1	-5.645777	-0.179215	-0.031882
1	-4.596125	2.348144	0.093790
7	-2.739875	1.289502	0.062793
7	-3.584458	-0.743496	-0.032475
6	-1.847854	2.434218	0.147574
1	-1.231151	2.364177	1.039486
1	-1.199570	2.472197	-0.722934
1	-2.467881	3.325293	0.192278
6	-3.756159	-2.178796	-0.122476
1	-3.358088	-2.669835	0.764073
1	-4.819968	-2.385109	-0.189833
1	-3.265120	-2.565338	-1.014019
6	2.388222	-0.048411	-0.010777
6	4.101104	1.394967	-0.055153
6	4.621398	0.144976	0.004719
1	4.596125	2.348144	-0.093790
1	5.645777	-0.179216	0.031882
7	3.584458	-0.743496	0.032475
7	2.739875	1.289502	-0.062793
6	3.756159	-2.178796	0.122476
1	3.265119	-2.565338	1.014019
1	3.358088	-2.669835	-0.764073
1	4.819968	-2.385109	0.189834
6	1.847854	2.434218	-0.147575
1	1.199570	2.472197	0.722933
1	2.467881	3.325293	-0.192278
1	1.231152	2.364176	-1.039486
7	0.000000	0.268989	0.000000
1	1.292674	-2.841640	0.002472
1	-1.292674	-2.841640	-0.002473

V (S_0)
Total Energy: -817.941061 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.068031	-0.493629	-0.115756
6	0.640457	-1.885223	-0.240243
6	-0.707133	-1.893690	-0.176146
6	-1.135652	-0.505797	-0.004802
6	-2.418935	-0.036818	0.097335
6	-4.677527	0.160798	0.247603
6	-4.174212	1.397904	0.214679
1	-5.698636	-0.165139	0.353346
1	-4.685067	2.344637	0.265337

7	-2.777431	1.340187	0.190953
7	-3.633857	-0.761197	0.262301
6	-2.088289	2.308999	-0.645626
1	-1.017285	2.202221	-0.495469
1	-2.314375	2.139679	-1.708457
1	-2.426225	3.308602	-0.366153
6	-3.812573	-2.096528	-0.230171
1	-3.299066	-2.821583	0.402656
1	-4.877163	-2.330991	-0.226141
1	-3.423985	-2.199960	-1.252908
6	2.368546	-0.079684	-0.115060
6	4.143616	1.258041	-0.464409
6	4.579378	-0.000538	-0.563296
1	4.694792	2.173574	-0.620922
1	5.564097	-0.353315	-0.828173
7	3.534668	-0.922269	-0.292900
7	2.778782	1.296902	-0.180137
6	3.858443	-1.797495	0.832560
1	4.023279	-1.221247	1.755650
1	3.039573	-2.492929	1.002318
1	4.763702	-2.366255	0.600303
6	2.338946	2.188175	0.879920
1	2.783554	1.913579	1.849654
1	2.626389	3.213638	0.634032
1	1.255358	2.112872	0.954546
7	-0.025522	0.317294	0.029548
1	1.286500	-2.733639	-0.413640
1	-1.330487	-2.767257	-0.273867

V (T_1)
Total energy: -817.923835 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.067191	-0.560168	-0.167801
6	0.744559	-1.819787	-0.707818
6	-0.656571	-1.836497	-0.819367
6	-1.098223	-0.599532	-0.324697
6	-2.466966	-0.105994	-0.237582
6	-4.492854	0.210993	0.727364
6	-4.036990	1.414065	0.340860
1	-5.420565	-0.049020	1.208799
1	-4.503683	2.381442	0.420918
7	-2.738633	1.276968	-0.121919
7	-3.488920	-0.729892	0.533554
6	-2.184397	2.189772	-1.090232
1	-1.108092	2.039046	-1.128941
1	-2.611508	2.010380	-2.087837
1	-2.399686	3.214325	-0.783931
6	-3.792149	-2.119996	0.330930
1	-2.891628	-2.709715	0.491529
1	-4.557097	-2.429781	1.044175
1	-4.150640	-2.304556	-0.694069
6	2.380111	-0.045121	0.135136
6	4.123681	1.372058	-0.072376
6	4.617112	0.129751	-0.151123
1	4.641546	2.316359	-0.117308
1	5.635545	-0.195019	-0.286349
7	3.564292	-0.793614	-0.124885

7	2.738811	1.322910	0.001591
6	3.774095	-1.999200	0.655460
1	3.941675	-1.753551	1.714489
1	2.894034	-2.632067	0.583739
1	4.639883	-2.538527	0.266698
6	2.026608	2.327730	0.764778
1	2.245251	2.225929	1.838108
1	2.333899	3.318602	0.424932
1	0.959908	2.184210	0.614371
7	-0.053452	0.175484	0.067442
1	1.435318	-2.577803	-1.045532
1	-1.270079	-2.611690	-1.255477

VI (S_0)
Total Energy: -816.954609 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.071488	-0.525621	-0.003156
6	0.664664	-1.960173	-0.005440
6	-0.664727	-1.960150	0.005777
6	-1.071508	-0.525630	0.003227
6	-2.386127	-0.028146	-0.009132
6	-4.590498	0.085345	0.011880
6	-4.078599	1.389154	-0.065760
1	-5.618313	-0.244376	0.046158
1	-4.607053	2.329642	-0.114487
7	-2.757026	1.299243	-0.074068
7	-3.561904	-0.750450	0.042606
6	-1.873900	2.475202	-0.160971
1	-1.246016	2.507573	0.723574
1	-1.269914	2.392971	-1.059570
1	-2.509549	3.353794	-0.209911
6	-3.744460	-2.215296	0.133772
1	-3.257722	-2.585008	1.032114
1	-4.811503	-2.403070	0.203081
1	-3.357087	-2.683971	-0.767100
6	2.386135	-0.028154	0.009120
6	4.078616	1.389144	0.065686
6	4.590506	0.085346	-0.012030
1	4.607067	2.329632	0.114422
1	5.618317	-0.244377	-0.046390
7	3.561901	-0.750458	-0.042712
7	2.757032	1.299230	0.074078
6	3.744476	-2.215299	-0.133917
1	3.357475	-2.683964	0.767121
1	3.257426	-2.585059	-1.032066
1	4.811500	-2.403031	-0.203642
6	1.873914	2.475189	0.161079
1	1.269886	2.392854	1.059638
1	2.509566	3.353770	0.210171
1	1.246074	2.507680	-0.723494
7	0.000003	0.284585	-0.000034
1	1.298815	-2.827806	-0.007033
1	-1.298898	-2.827767	0.007519

VI (T_1)
Total energy: -816.916134 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.093776	-0.587025	0.026569
6	0.684254	-1.956098	0.010469
6	-0.684250	-1.956098	-0.010379
6	-1.093776	-0.587027	-0.026527
6	-2.395662	-0.032720	-0.047111
6	-4.597808	0.132799	0.057421
6	-4.067801	1.397773	-0.241806
1	-5.627467	-0.164238	0.193935
1	-4.582633	2.331108	-0.415949
7	-2.740678	1.276331	-0.294495
7	-3.574018	-0.713630	0.165856
6	-1.843906	2.401141	-0.618632
1	-1.239616	2.631928	0.252575
1	-1.220979	2.126824	-1.464402
1	-2.470712	3.249170	-0.876891
6	-3.735413	-2.140375	0.507610
1	-3.090012	-2.382038	1.348348
1	-4.771801	-2.293071	0.793431
1	-3.507640	-2.748733	-0.364733
6	2.395665	-0.032722	0.047117
6	4.067811	1.397766	0.241764
6	4.597806	0.132792	-0.057484
1	4.582651	2.331099	0.415896
1	5.627460	-0.164246	-0.194033
7	3.574011	-0.713635	-0.165889
7	2.740689	1.276327	0.294493
6	3.735385	-2.140380	-0.507656
1	3.507666	-2.748740	0.364699
1	3.089928	-2.382042	-1.348353
1	4.771754	-2.293076	-0.793545
6	1.843920	2.401126	0.618675
1	1.221032	2.126796	1.464469
1	2.470727	3.249161	0.876914
1	1.239591	2.631912	-0.252504
7	0.000002	0.244380	0.000012
1	1.299876	-2.837967	0.030612
1	-1.299868	-2.837971	-0.030486

Optimized molecular coordinates for systems A–P in the singlet (S_0) and triplet (T_1) electronic states.

A. NO (S_0)

Total energy = -417.541281 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	-1.510877	0.311275	-0.000028
6	-0.420329	1.135975	-0.000037
6	0.710623	0.252979	0.000010
6	0.162784	-1.063313	0.000029
7	-1.158324	-1.032683	0.000011
1	-0.396784	2.213523	-0.000053
6	-2.957746	0.686780	0.000012
1	-3.078354	1.770797	0.000043
1	-3.468346	0.282613	-0.878247
1	-3.468298	0.282589	0.878291
6	0.937699	-2.342313	-0.000023
1	0.692059	-2.942239	0.879139
1	0.693358	-2.941453	-0.880090
1	2.006015	-2.132063	0.000813
7	2.041991	0.488609	0.000067
8	2.412720	1.673307	-0.000028

A. NO (T_1)

Total energy = -417.495960 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.530948	0.327063	-0.005147
6	-0.404067	1.134908	-0.013242
6	0.688675	0.220735	-0.001986
6	0.125141	-1.069881	0.009362
7	-1.217442	-0.998491	0.008138
1	-0.346073	2.212125	-0.017785
6	-2.961621	0.768468	0.002791
1	-3.031275	1.857218	-0.030854
1	-3.506648	0.365754	-0.855652
1	-3.481461	0.422827	0.901152
6	0.864287	-2.368411	-0.003494
1	0.370431	-3.093085	0.646920
1	0.908285	-2.808086	-1.005767
1	1.891338	-2.231784	0.340472
7	2.029139	0.496360	-0.008775
8	2.603089	1.589082	0.012034

B. NO_2 (S_0)

Total energy = -492.760104 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.825016	0.275705	-0.000059
6	-0.745648	1.122664	-0.000054
6	0.383577	0.259696	-0.000034
6	-0.112193	-1.066283	-0.000012
7	-1.441088	-1.048753	-0.000038
1	-0.730779	2.199859	-0.000063
6	-3.277351	0.630363	0.000059
1	-3.783764	0.222159	0.878785
1	-3.412028	1.712844	-0.000095
1	-3.783874	0.221844	-0.878420
6	0.654276	-2.347574	0.000031
1	-0.054473	-3.175135	-0.000203

1	1.306831	-2.421360	-0.871740
1	1.306415	-2.421531	0.872062
7	1.717772	0.653193	0.000006
8	1.989024	1.857071	0.000039
8	2.604604	-0.209218	0.000000

B. NO_2 (T1)

Total energy = -492.674539 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.842952	0.241809	0.000015
6	-0.675272	1.119303	-0.000024
6	0.406715	0.281703	-0.000021
6	-0.143962	-1.074111	0.000026
7	-1.517961	-1.035513	0.000036
1	-0.650307	2.195570	-0.000055
6	-3.257966	0.698814	-0.000003
1	-3.464612	1.317948	0.877490
1	-3.464648	1.317822	-0.877586
1	-3.926274	-0.159756	0.000064
6	0.586781	-2.362399	-0.000026
1	-0.130564	-3.182090	0.000385
1	1.246288	-2.430602	-0.866360
1	1.246999	-2.430266	0.865795
7	1.735028	0.639559	0.000002
8	2.028529	1.887324	0.000001
8	2.619420	-0.298281	0.000025

C. CHO (S_0)

Total energy = -401.561461 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.546484	0.354523	-0.000028
6	-0.423984	1.144900	-0.000026
6	0.685388	0.243332	-0.000019
6	0.100847	-1.050099	-0.000017
7	-1.227782	-0.987450	-0.000030
1	-0.373650	2.223315	-0.000033

6	-2.980680	0.779958	0.000037
1	-3.061115	1.868183	0.000058
1	-3.508730	0.398461	-0.878513
1	-3.508657	0.398441	0.878620
6	0.802499	-2.377185	0.000017
1	0.050793	-3.166115	-0.000467
1	1.439247	-2.507331	-0.878880
1	1.438459	-2.507690	0.879454
8	2.638447	1.613343	0.000018
6	2.078366	0.519997	0.000004
1	2.714843	-0.394417	0.000009

C. CHO (T_1)

Total energy = - -401.457945 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.563481	0.324088	-0.000007
6	-0.337242	1.123036	-0.000037
6	0.718639	0.223203	-0.000000
6	0.039497	-1.087359	0.000046
7	-1.335479	-0.971611	0.000036
1	-0.272969	2.199689	-0.000082
6	-2.943243	0.881215	-0.000024
1	-3.103002	1.514695	0.877936
1	-3.102454	1.516016	-0.877096
1	-3.674455	0.075061	-0.000820
6	0.735881	-2.387110	0.000069
1	0.024360	-3.211547	0.000074
1	1.397004	-2.470058	-0.873327
1	1.396994	-2.470043	0.873453
8	2.661088	1.610568	-0.000069
6	2.122594	0.457908	-0.000020
1	2.758298	-0.446959	0.000011

D. $COCH_3$ (S_0)

Total energy = -440.874442 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	1.897536	0.280763	0.000004
6	0.816419	1.126697	0.000128
6	-0.342435	0.291723	0.000203
6	0.172454	-1.035028	0.000076
7	1.506631	-1.036391	-0.000062
1	0.814508	2.206142	0.000139
6	3.352271	0.631210	-0.000081
1	3.488463	1.713947	-0.000230
1	3.860578	0.223736	0.878594
1	3.860516	0.223490	-0.878675
6	-0.545163	-2.353943	-0.000023
1	0.207615	-3.141583	-0.001233
1	-1.181249	-2.490169	0.878851
1	-1.183075	-2.489093	-0.877711
8	-2.002526	1.963066	-0.000114
6	-1.694873	0.771043	0.000056
6	-2.832738	-0.247041	-0.000031
1	-2.779703	-0.890924	-0.878597
1	-2.778509	-0.892721	0.877118
1	-3.776174	0.294852	0.001088

D. COCH3 (T1)

Total energy = -440.767161 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.912263	0.270531	0.000105
6	0.717179	1.108632	0.000053
6	-0.384255	0.257666	0.000050
6	0.247753	-1.084868	-0.000101
7	1.637552	-1.008973	0.000079
1	0.680005	2.186277	0.000035
6	3.310941	0.779593	0.000238
1	3.491047	1.407800	-0.877181
1	3.490858	1.407851	0.877655
1	4.013882	-0.051350	0.000329
6	-0.399035	-2.416195	-0.000542
1	0.368738	-3.188769	-0.001677
1	-1.043042	-2.555868	0.876121
1	-1.044447	-2.554501	-0.876392

8	-2.018806	1.949761	-0.000801
6	-1.741110	0.705837	-0.000104
6	-2.917923	-0.249708	0.000891
1	-3.547949	-0.056752	-0.875829
1	-2.648395	-1.304282	0.002160
1	-3.547986	-0.054616	0.877097

E. OH (S_0)
Total energy = -363.425514a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.357565	-0.004796	-0.000033
6	0.604696	1.172880	-0.028481
6	-0.736022	0.731881	-0.030096
6	-0.710392	-0.653484	-0.001779
7	0.574793	-1.104134	0.011808
1	0.964825	2.192100	-0.064630
6	2.852539	-0.123980	0.014298
1	3.319583	0.863430	-0.011348
1	3.209014	-0.640737	0.911355
1	3.220397	-0.692249	-0.845867
6	-1.882847	-1.581466	0.002571
1	-1.864700	-2.251071	0.868548
1	-2.812919	-1.010057	0.030623
1	-1.904659	-2.216597	-0.889294
8	-1.889247	1.532815	-0.074260
1	-1.954344	1.975388	0.773148

E. OH (T_1)
Total energy = -363.327103a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.338237	0.009460	-0.000564
6	0.622334	-1.160327	-0.001539
6	-0.771199	-0.772565	0.000090
6	-0.716760	0.688221	0.001423
7	0.525539	1.138172	0.001320
1	1.000283	-2.171276	-0.001921
6	2.820776	0.186854	-0.000008
1	3.146961	0.749356	0.879441
1	3.329991	-0.777543	-0.002146
1	3.147177	0.753395	-0.876769
6	-1.915321	1.574930	-0.000874
1	-1.602546	2.616943	0.062920
1	-2.509632	1.437507	-0.908680
1	-2.576826	1.344864	0.838291
8	-1.826436	-1.467980	0.001318
1	-1.271096	-3.336045	-0.002090

F. NH_2 (S_0)
Total energy = -343.550644a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.377288	0.023098	0.000019
6	-0.601162	1.181224	0.000039
6	0.739129	0.733929	0.000004
6	0.674486	-0.659539	-0.000023
7	-0.611159	-1.092931	0.000003
1	-0.939273	2.208538	0.000096
6	-2.873740	-0.072689	-0.000019
1	-3.323892	0.922830	0.000427
1	-3.245584	-0.609047	-0.879193
1	-3.245539	-0.609830	0.878692
6	1.822090	-1.621926	-0.000010
1	1.807080	-2.274480	0.879209
1	1.806279	-2.275328	-0.878576
1	2.776485	-1.087673	-0.000701
7	1.909358	1.584108	0.000071
1	2.488271	1.390578	0.809080
1	2.487692	1.391592	-0.809603

F. NH_2 (T_1)
Total energy = -343.437341a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.364069	-0.025905	0.000008
6	0.624816	-1.183315	0.000128
6	-0.740230	-0.764353	0.000019
6	-0.684181	0.685099	-0.000067
7	0.566629	1.109511	-0.000093
1	0.973531	-2.203293	0.000192
6	2.848115	0.120898	-0.000013
1	3.337475	-0.853211	-0.000013
1	3.183012	0.679079	-0.878155
1	3.183003	0.679121	0.878095
6	-1.849945	1.615066	0.000086
1	-1.489885	2.645648	-0.000043
1	-2.491504	1.440505	-0.868959
1	-2.491134	1.440597	0.869431
7	-1.848548	-1.516853	-0.000168
1	-1.791764	-2.562451	0.000346
1	-2.815167	-1.099544	-0.000038

G. COOH (S_0)
Total energy = -476.824988a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.883124	-0.298669	0.000129
6	0.792319	-1.133108	0.000034

6	-0.349167	-0.276444	-0.000030
6	0.175702	1.040544	0.000040
7	1.508191	1.024565	0.000134
1	0.778781	-2.212558	0.000004
6	3.332985	-0.668021	0.000213
1	3.455519	-1.752482	0.000209
1	3.846533	-0.267070	-0.878371
1	3.846426	-0.267089	0.878870
6	-0.566520	2.342269	0.000042
1	0.160985	3.153690	-0.000002
1	-1.213166	2.441264	-0.874443
1	-1.213095	2.441303	0.874575
8	-2.132260	-1.856026	-0.000173
6	-1.706124	-0.710663	-0.000141
8	-2.632200	0.313929	-0.000228
1	-3.477564	-0.147690	-0.000293

G. COOH (T_1)
Total energy = -476.709170a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.911549	-0.262387	-0.000002
6	0.732910	-1.135452	0.000004
6	-0.384974	-0.294975	-0.000022
6	0.214631	1.062190	-0.000058
7	1.611644	1.005950	-0.000032
1	0.731549	-2.213967	0.000055
6	3.318560	-0.747653	0.000016
1	3.509146	-1.373039	0.877734
1	3.509156	-1.373072	-0.877676
1	4.006841	0.095399	0.000004
6	-0.492839	2.360372	0.000043
1	0.232950	3.173196	-0.000084
1	-1.151547	2.456083	-0.869888
1	-1.151248	2.456113	0.870204
8	-2.193957	-1.858201	0.000023
6	-1.731359	-0.691616	-0.000013
8	-2.665772	0.370669	-0.000013
1	-3.501397	-0.104985	-0.000019

H. CN (S_0)
Total energy = -380.488770a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.573125	-0.254321	0.000012
6	0.557773	-1.189984	0.000026
6	-0.648561	-0.430689	0.000007
6	-0.246055	0.918656	-0.000010
7	1.087026	1.021933	-0.000010
1	0.648121	-2.265694	0.000022
6	3.048656	-0.506232	-0.000010
1	3.258210	-1.577301	0.000017
1	3.527683	-0.065976	-0.878872
1	3.527718	-0.065924	0.878806

6	-1.138576	2.119557	0.000006
1	-0.958213	2.742973	-0.879141
1	-2.187782	1.821406	-0.000586
1	-0.959093	2.742378	0.879764
6	-1.976094	-0.905857	-0.000004
7	-3.069633	-1.284597	-0.000014

H. CN (T_1)

Total energy = -380.488770a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.532508	-0.282483	0.046607
6	0.427452	-1.167492	-0.184015
6	-0.740186	-0.428099	0.077305
6	-0.220462	0.974474	0.365340
7	1.211621	0.932586	0.408071
1	0.499828	-2.188272	-0.528006
6	2.966471	-0.679647	-0.122188
1	3.126122	-1.713497	0.189459
1	3.262776	-0.600442	-1.171236
1	3.602363	-0.016989	0.463085
6	-0.834859	2.143990	-0.320500
1	-0.394709	3.074904	0.040218
1	-0.656406	2.088167	-1.408431
1	-1.915337	2.164599	-0.170186
6	-2.066156	-0.812846	0.049844
7	-3.199228	-1.117706	0.036321

I. NO (S_0)

Total energy = -947.149283 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.181314	0.329395	-0.058448
6	-0.745274	1.653254	-0.024893
6	0.648379	1.561623	0.019743
6	0.954561	0.182122	0.006568
6	2.267176	-0.433257	0.078667
6	4.399619	-0.925421	-0.241837
6	3.906411	-1.801895	0.661621
1	5.383168	-0.825052	-0.662781
1	4.376413	-2.613488	1.186021
7	2.584353	-1.482775	0.851763
7	3.370743	-0.088360	-0.599666
6	1.683407	-2.169851	1.770785
1	1.028829	-1.440774	2.237537
1	1.080213	-2.894028	1.230689
1	2.287868	-2.666669	2.523670
6	3.489716	0.965473	-1.604526
1	3.844428	1.881154	-1.141751
1	4.181895	0.622925	-2.368533
1	2.513137	1.143205	-2.044346
6	-2.539938	-0.154159	-0.122461
6	-4.310832	-1.425222	-0.530169
6	-4.742829	-0.312100	0.098932

1	-4.848276	-2.280056	-0.897305
1	-5.729654	-0.004801	0.392423
7	-3.635399	0.464907	0.351600
7	-2.946275	-1.313825	-0.665481
6	-3.670379	1.739069	1.058013
1	-2.805552	1.811134	1.711844
1	-3.666635	2.566500	0.351896
1	-4.580373	1.771543	1.649256
6	-2.104858	-2.299148	-1.337725
1	-1.556647	-2.885213	-0.606556
1	-2.754302	-2.937863	-1.928807
1	-1.394932	-1.787138	-1.979025
7	-0.148054	-0.565967	-0.034240
1	-1.314063	2.566265	-0.048597
8	1.208687	3.688054	0.186439
7	1.626334	2.558679	0.132777

I. NO (T1)

Total energy = -947.120960 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.960639	0.176281	0.007023
6	0.659328	1.562166	0.024623
6	-0.732907	1.664160	-0.017969
6	-1.179416	0.331803	-0.054275
6	-2.539454	-0.141137	-0.119723
6	-4.746528	-0.280984	0.089323
6	-4.318007	-1.407697	-0.516344
1	-5.733094	0.037841	0.370997
1	-4.858729	-2.265626	-0.871130
7	-2.951474	-1.308005	-0.645451
7	-3.635282	0.493564	0.335346
6	-2.114820	-2.311978	-1.293767
1	-1.398069	-1.817983	-1.941596
1	-1.573079	-2.886787	-0.548699
1	-2.766568	-2.958750	-1.873602
6	-3.666600	1.776493	1.024666
1	-3.645140	2.595282	0.308700
1	-4.584359	1.826080	1.602636
1	-2.810590	1.847917	1.690004
6	2.255389	-0.452993	0.079420
6	3.873665	-1.869551	0.620406
6	4.398569	-0.943568	-0.210835
1	4.323287	-2.716755	1.104785
1	5.394051	-0.826676	-0.598003
7	3.383903	-0.077071	-0.546242
7	2.547749	-1.551663	0.796017
6	3.520095	1.008644	-1.511564
1	2.556555	1.183319	-1.981374
1	3.850533	1.917946	-1.017073
1	4.244289	0.703948	-2.261714
6	1.622803	-2.278099	1.657496
1	1.007555	-2.949603	1.065327
1	2.208229	-2.838715	2.380130
1	0.979121	-1.567002	2.165764

7	-0.162988	-0.560472	-0.033950
1	-1.294758	2.580814	-0.044773
7	1.575702	2.575560	0.128935
8	1.355120	3.766265	0.192020

J. NO_2 (S_0)

Total energy = -1022.363328 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.848026	0.055537	0.003782
6	0.565996	1.434854	-0.022695
6	-0.813468	1.576797	-0.073324
6	-1.290845	0.263691	-0.071537
6	-2.662483	-0.181550	-0.124150
6	-4.869512	-0.268902	0.094460
6	-4.467410	-1.415976	-0.491633
1	-5.848036	0.076807	0.372610
1	-5.027613	-2.268569	-0.828731
7	-3.099733	-1.348127	-0.626224
7	-3.740954	0.485312	0.322933
6	-2.284982	-2.381763	-1.258041
1	-1.563389	-1.914815	-1.920453
1	-1.750579	-2.951419	-0.504195
1	-2.951887	-3.026825	-1.822084
6	-3.741291	1.785238	0.981501
1	-3.702943	2.585630	0.245790
1	-4.656012	1.869556	1.560128
1	-2.882356	1.853136	1.643608
6	2.126173	-0.637114	0.080686
6	3.694241	-2.043764	0.753338
6	4.158144	-1.394880	-0.339167
1	4.148823	-2.793098	1.374953
1	5.097003	-1.467159	-0.857034
7	3.170332	-0.534033	-0.748110
7	2.432676	-1.560998	1.000580
6	3.270585	0.346217	-1.906023
1	2.274022	0.684238	-2.174343
1	3.887498	1.205116	-1.658502
1	3.701580	-0.216279	-2.729813
6	1.568537	-1.985555	2.096213
1	0.885308	-2.757915	1.754020
1	2.197900	-2.364064	2.895974

1	0.997268	-1.131598	2.446561
7	-0.283507	-0.652555	-0.022365
1	-1.344973	2.510533	-0.121562
7	1.503039	2.512770	0.077826
8	1.075964	3.641349	0.032760
8	2.680929	2.217795	0.211004

J. NO_2 (T_1)

Total energy = -1022.259284 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.842064	0.019005	-0.032608
6	0.592566	1.405752	-0.073506
6	-0.781947	1.575168	-0.126236
6	-1.290546	0.264121	-0.096751
6	-2.671490	-0.149431	-0.126970
6	-4.879269	-0.183209	0.111097
6	-4.506993	-1.354219	-0.445832
1	-5.847669	0.191007	0.387645
1	-5.088207	-2.203418	-0.754650
7	-3.139128	-1.319918	-0.593304
7	-3.732594	0.552580	0.309747
6	-2.352960	-2.388323	-1.201295
1	-1.624657	-1.956279	-1.879856
1	-1.826246	-2.949152	-0.435235
1	-3.038161	-3.033690	-1.742754
6	-3.699502	1.866177	0.938859
1	-3.652673	2.649435	0.185344
1	-4.606379	1.982291	1.524391
1	-2.832590	1.930764	1.590761
6	2.106637	-0.680855	0.048729
6	3.658106	-2.134978	0.666284
6	4.182847	-1.361331	-0.309763
1	4.084021	-2.945513	1.228550
1	5.155295	-1.364713	-0.766921
7	3.205883	-0.472656	-0.690052
7	2.372398	-1.699260	0.879788
6	3.354013	0.510504	-1.756225
1	2.366586	0.792267	-2.111203
1	3.873903	1.389658	-1.383237

1	3.915808	0.056083	-2.567467
6	1.457359	-2.242135	1.876932
1	0.779838	-2.954506	1.414679
1	2.049062	-2.726792	2.647680
1	0.879625	-1.428917	2.305060
7	-0.312763	-0.668275	-0.034433
1	-1.302418	2.514415	-0.183870
7	1.556939	2.426299	-0.069912
8	1.180213	3.668739	0.121599
8	2.694086	2.262284	0.514896

K. CHO (S0)
Total energy = -931.175254 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.951184	0.194460	0.050565
6	0.647563	1.576085	0.049116
6	-0.743465	1.644414	-0.018886
6	-1.181813	0.316431	-0.046505
6	-2.537543	-0.170269	-0.121015
6	-4.744858	-0.325572	0.066607
6	-4.301877	-1.452902	-0.527735
1	-5.736605	-0.012054	0.335769
1	-4.832401	-2.317043	-0.882820
7	-2.934875	-1.343388	-0.642731
7	-3.641998	0.458542	0.319305
6	-2.082126	-2.343477	-1.276313
1	-1.366698	-1.846899	-1.923654
1	-1.539194	-2.905619	-0.522680
1	-2.722053	-3.002213	-1.855776
6	-3.690188	1.748629	0.994796
1	-3.666420	2.559729	0.270395
1	-4.614219	1.796925	1.562765
1	-2.841147	1.833866	1.667437
6	2.256679	-0.435891	0.095794
6	3.900681	-1.815877	0.645561
6	4.366207	-0.982689	-0.311004
1	4.381103	-2.617635	1.175827
1	5.329565	-0.918167	-0.782957
7	3.334595	-0.136981	-0.648019
7	2.595196	-1.462407	0.889081
6	3.405022	0.848268	-1.723257
1	2.396186	1.140338	-1.998532
1	3.963171	1.722846	-1.398097
1	3.900769	0.391932	-2.575873
6	1.722036	-2.098519	1.869676
1	1.105730	-2.851102	1.385975
1	2.346602	-2.552402	2.633280
1	1.078288	-1.343660	2.309994
7	-0.147013	-0.567687	-0.003626
1	-1.315778	2.555698	-0.049993

8	1.236116	3.858048	0.139279
1	2.618405	2.435055	0.419303
6	1.563236	2.701820	0.205490

K. CHO (T_1)
Total energy = -931.059555 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.966662	0.201650	0.038006
6	0.661307	1.599212	0.040852
6	-0.742655	1.655950	-0.033858
6	-1.172841	0.318874	-0.051498
6	-2.522886	-0.178573	-0.124262
6	-4.732033	-0.348772	0.051475
6	-4.274793	-1.487855	-0.507660
1	-5.728398	-0.037253	0.305272
1	-4.795204	-2.366324	-0.841829
7	-2.907851	-1.369909	-0.616664
7	-3.637880	0.452429	0.289645
6	-2.045023	-2.381913	-1.215199
1	-1.331872	-1.900413	-1.876298
1	-1.497798	-2.913369	-0.442461
1	-2.678201	-3.065681	-1.772870
6	-3.703284	1.755526	0.936548
1	-3.678610	2.551657	0.195590
1	-4.633918	1.808688	1.493336
1	-2.862334	1.861657	1.616227
6	2.259004	-0.426559	0.091984
6	3.896394	-1.827819	0.629614
6	4.384448	-0.959637	-0.281594
1	4.365003	-2.649207	1.139932
1	5.358322	-0.880318	-0.728838
7	3.359390	-0.101481	-0.614896
7	2.583854	-1.484192	0.856690
6	3.428149	0.876412	-1.693859
1	2.418373	1.112333	-2.015719
1	3.922265	1.786027	-1.360199
1	3.986483	0.439428	-2.517406
6	1.695400	-2.143313	1.804767
1	1.064485	-2.862854	1.290124
1	2.307068	-2.641374	2.551269
1	1.063623	-1.394947	2.273479
7	-0.144716	-0.556914	-0.002300
1	-1.332272	2.554988	-0.081055
8	1.100676	3.923581	0.222661
6	1.548672	2.685296	0.175370
1	2.598866	2.597909	0.438712

L. COCH3 (S_0)
Total energy = -970.491678 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.817440	0.045813	0.023772
6	0.580842	1.438829	-0.050107
6	-0.807313	1.560480	-0.115544

6	-1.309492	0.256072	-0.066355
6	-2.684790	-0.172590	-0.100121
6	-4.897206	-0.212612	0.101533
6	-4.508341	-1.402701	-0.400019
1	-5.872481	0.166437	0.345159
1	-5.078719	-2.267895	-0.683363
7	-3.137991	-1.365094	-0.524985
7	-3.758643	0.538776	0.289040
6	-2.336135	-2.450837	-1.078359
1	-1.619988	-2.044271	-1.785121
1	-1.793675	-2.958788	-0.287203
1	-3.013085	-3.136737	-1.578960
6	-3.745976	1.879664	0.857520
1	-3.670345	2.627240	0.071000
1	-4.672811	2.021661	1.404883
1	-2.901396	1.975264	1.534442
6	2.081616	-0.671811	0.064970
6	3.687467	-2.049700	0.720833
6	4.077246	-1.487763	-0.445716
1	4.179845	-2.759276	1.360362
1	4.973629	-1.614458	-1.025120
7	3.068416	-0.641496	-0.842341
7	2.451354	-1.530963	1.023414
6	3.050965	0.083000	-2.108295
1	2.157720	0.698893	-2.147432
1	3.935195	0.711435	-2.179656
1	3.042514	-0.631385	-2.928187
6	1.657551	-1.863535	2.201171
1	0.992943	-2.693692	1.977454
1	2.335344	-2.127897	3.007458
1	1.064332	-0.997265	2.477606
7	-0.313735	-0.669075	0.015198
1	-1.331748	2.497437	-0.191713
8	1.095346	3.708830	-0.208721
6	1.494061	2.595899	0.040465
6	2.923830	2.375509	0.489414
1	2.997243	1.613266	1.265310
1	3.537375	2.063672	-0.357332
1	3.318950	3.318395	0.856920

L.COCH3 (T_1)
Total energy = -970.374484 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.834692	0.023318	0.046263
6	0.622310	1.435576	-0.025529
6	-0.774345	1.575844	-0.119449
6	-1.293618	0.271665	-0.059683
6	-2.673277	-0.140345	-0.107217
6	-4.889877	-0.153688	0.061932
6	-4.506214	-1.357284	-0.410151
1	-5.864583	0.239665	0.284137
1	-5.081689	-2.221900	-0.684810

7	-3.134059	-1.336595	-0.515986
7	-3.746340	0.589717	0.251179
6	-2.338149	-2.443318	-1.033647
1	-1.598156	-2.059745	-1.728427
1	-1.822781	-2.946988	-0.221452
1	-3.014806	-3.126773	-1.538153
6	-3.728981	1.937268	0.802647
1	-3.639773	2.674447	0.007662
1	-4.660556	2.093687	1.338019
1	-2.891197	2.034180	1.487619
6	2.071542	-0.711820	0.053231
6	3.606000	-2.246497	0.526028
6	4.103238	-1.457806	-0.450974
1	4.032333	-3.093342	1.031723
1	5.044745	-1.485585	-0.968124
7	3.139647	-0.518545	-0.744162
7	2.351589	-1.771448	0.832375
6	3.220465	0.443626	-1.834929
1	2.214025	0.665141	-2.178703
1	3.696138	1.363359	-1.502762
1	3.798635	-0.001124	-2.639949
6	1.471049	-2.317264	1.856042
1	0.759714	-3.007066	1.409758
1	2.083120	-2.828328	2.593488
1	0.923936	-1.501572	2.319072
7	-0.325620	-0.663418	0.047076
1	-1.302732	2.509161	-0.206941
8	1.093524	3.719730	-0.189634
6	1.559218	2.500529	0.048380
6	2.875340	2.517926	0.769015
1	3.219361	1.500309	0.939200
1	3.635493	3.064127	0.208948
1	2.767697	3.006143	1.741632

M. OH (S_0)
Total energy = -893.078811 a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.000091	0.383088	0.029540
6	0.655199	1.749428	0.082927
6	-0.725711	1.810634	0.045404
6	-1.140236	0.456788	-0.029123
6	-2.480624	-0.058036	-0.113053
6	-4.686378	-0.278927	0.072642
6	-4.212233	-1.383721	-0.537478
1	-5.686221	0.002289	0.347171
1	-4.718568	-2.257325	-0.904377
7	-2.848246	-1.234785	-0.652958
7	-3.604836	0.532718	0.336201
6	-1.973366	-2.203660	-1.302603
1	-1.270390	-1.680031	-1.942170

1	-1.413945	-2.762925	-0.558688
1	-2.599146	-2.869861	-1.889296
6	-3.686553	1.802657	1.041508
1	-3.680733	2.632665	0.337942
1	-4.613589	1.816293	1.606713
1	-2.842633	1.890652	1.720350
6	2.313474	-0.200383	0.086402
6	3.983911	-1.576926	0.577162
6	4.476190	-0.598491	-0.211983
1	4.463021	-2.426446	1.027908
1	5.467807	-0.428247	-0.588884
7	3.429598	0.241843	-0.517341
7	2.645605	-1.316240	0.759271
6	3.520244	1.369662	-1.436507
1	2.547756	1.522872	-1.895227
1	3.806532	2.271229	-0.903903
1	4.255103	1.125828	-2.198540
6	1.745410	-2.109613	1.585498
1	1.164623	-2.787132	0.965729
1	2.346865	-2.668527	2.296443
1	1.065678	-1.443450	2.107568
7	-0.103130	-0.397989	-0.034808
1	-1.328797	2.702768	0.038212
8	1.568021	2.752579	0.186855
1	1.123030	3.584899	0.363630

M.OH (T_1)
Total energy = -892.975500a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.019290	0.359635	0.034097
6	0.610289	1.743410	0.364814
6	-0.745537	1.791733	0.379357
6	-1.174412	0.452660	0.075988
6	-2.468117	-0.038164	-0.037696
6	-4.698968	-0.188376	-0.212695
6	-4.192940	-1.443609	-0.296558
1	-5.717153	0.152685	-0.261105
1	-4.699450	-2.384096	-0.415479
7	-2.833796	-1.366416	-0.198677
7	-3.656064	0.677626	-0.053002
6	-1.969784	-2.536435	-0.154025
1	-1.253822	-2.509931	-0.968977
1	-1.429194	-2.566896	0.788864
1	-2.607437	-3.411985	-0.239344
6	-3.796542	2.116611	0.008487
1	-3.172201	2.587448	-0.749096
1	-4.835992	2.362811	-0.186565
1	-3.526155	2.489998	0.995455
6	2.324793	-0.171040	-0.010534
6	3.992133	-1.657637	0.073539
6	4.523309	-0.469202	-0.280142
1	4.460405	-2.611689	0.232103
1	5.537569	-0.197592	-0.508238
7	3.499474	0.447639	-0.345471
7	2.639194	-1.481862	0.231101
6	3.657945	1.772934	-0.920236
1	2.760528	2.030359	-1.477663
1	3.826883	2.519508	-0.150062
1	4.503993	1.745205	-1.601815

6	1.732775	-2.508646	0.713927
1	1.040279	-2.802998	-0.069662
1	2.332215	-3.358967	1.026294
1	1.163199	-2.130071	1.559884
7	-0.073679	-0.402699	-0.118132
1	-1.340490	2.647604	0.640097
8	1.498558	2.685020	0.674135
1	1.057041	3.495190	0.951548

N. NH_2 (S_0)
Total energy = -873.206453a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.992097	0.402861	0.084165
6	0.646854	1.773169	0.132690
6	-0.737559	1.806355	0.067057
6	-1.143657	0.451637	-0.005768
6	-2.477109	-0.076447	-0.112244
6	-4.686211	-0.309780	0.017998
6	-4.187337	-1.427689	-0.546451
1	-5.695344	-0.028653	0.256099
1	-4.676922	-2.315399	-0.901983
7	-2.821715	-1.271376	-0.627898
7	-3.618257	0.517541	0.288236
6	-1.922920	-2.251655	-1.225266
1	-1.213899	-1.742782	-1.870049
1	-1.370911	-2.776216	-0.451238
1	-2.529416	-2.946359	-1.799031
6	-3.729693	1.806448	0.953476
1	-3.697019	2.616318	0.227667
1	-4.678400	1.833165	1.481010
1	-2.913163	1.916115	1.662126
6	2.309083	-0.181649	0.101428
6	3.997508	-1.552520	0.547761
6	4.442124	-0.623002	-0.325198
1	4.499290	-2.383614	1.008255
1	5.406104	-0.486916	-0.779887
7	3.384689	0.213791	-0.601833
7	2.677980	-1.264362	0.808019
6	3.410437	1.274432	-1.602522
1	2.400483	1.424058	-1.972205
1	3.759388	2.204515	-1.164484
1	4.064981	0.959605	-2.410561
6	1.820584	-2.009331	1.720001
1	1.234257	-2.740747	1.170266
1	2.452870	-2.503853	2.451749
1	1.143462	-1.317226	2.210877
7	-0.097620	-0.394808	0.022227
1	-1.349148	2.692662	0.058583
7	1.554384	2.847275	0.217853
1	1.089510	3.742605	0.172694
1	2.112441	2.819312	1.061125

N. NH_2 (T_1)
Total energy = -873.111020a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	1.005485	0.317156	0.084063
6	0.620016	1.681691	0.507512
6	-0.764327	1.737817	0.474793
6	-1.191706	0.450173	0.107719
6	-2.497257	-0.040823	-0.036136
6	-4.719938	-0.170356	-0.275732
6	-4.229965	-1.428065	-0.303903
1	-5.728809	0.188629	-0.364755
1	-4.737465	-2.369260	-0.409214
7	-2.866437	-1.356573	-0.162823
7	-3.659632	0.686192	-0.113071
6	-2.011936	-2.530263	-0.052091
1	-1.298668	-2.559199	-0.869448
1	-1.467852	-2.508357	0.888830
1	-2.657157	-3.403746	-0.081354
6	-3.769429	2.129422	-0.113882
1	-3.047634	2.554395	-0.809487
1	-4.772573	2.393232	-0.435259
1	-3.600391	2.533906	0.883506
6	2.319051	-0.174861	-0.021890
6	4.073469	-1.561041	0.029396
6	4.537660	-0.346431	-0.312942
1	4.597307	-2.487448	0.180840
1	5.535060	-0.023328	-0.549056
7	3.459494	0.529517	-0.362560
7	2.708226	-1.471163	0.193781
6	3.485472	1.717870	-1.208154
1	2.470711	1.968518	-1.503853
1	3.926512	2.567874	-0.689184
1	4.070154	1.509098	-2.102693
6	1.854345	-2.524938	0.703166
1	1.112793	-2.805910	-0.040473
1	2.479882	-3.378156	0.949187
1	1.336547	-2.181729	1.598704
7	-0.086181	-0.416035	-0.125521
1	-1.356505	2.577517	0.790417
7	1.484244	2.607938	0.941827
1	1.153586	3.468034	1.345829
1	2.440855	2.352707	1.124519

O. COOH (S_0)

Total energy = -1006.446431a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.827336	0.045530	0.007712
6	0.585427	1.437331	-0.036376
6	-0.800220	1.570624	-0.091114
6	-1.302505	0.265730	-0.071865
6	-2.677896	-0.161532	-0.119316
6	-4.889563	-0.209988	0.083793
6	-4.500073	-1.382855	-0.456752
1	-5.864915	0.159854	0.340960
1	-5.070017	-2.238932	-0.767424
7	-3.130034	-1.339779	-0.582339
7	-3.751461	0.535915	0.294330
6	-2.327072	-2.406276	-1.171256
1	-1.602671	-1.974848	-1.854407
1	-1.794402	-2.947810	-0.395750

1	-3.001753	-3.068962	-1.705021
6	-3.737892	1.857167	0.907064
1	-3.671290	2.630854	0.145286
1	-4.660321	1.978321	1.466738
1	-2.887995	1.932442	1.580005
6	2.090986	-0.671911	0.075029
6	3.646990	-2.102137	0.733623
6	4.104793	-1.471778	-0.371568
1	4.097509	-2.855524	1.353351
1	5.031910	-1.569059	-0.906222
7	3.124939	-0.595541	-0.771540
7	2.398622	-1.593156	0.997694
6	3.206812	0.246191	-1.958043
1	2.225524	0.667265	-2.154182
1	3.916131	1.050499	-1.787773
1	3.521415	-0.366661	-2.798772
6	1.542522	-1.991373	2.108979
1	0.846771	-2.760714	1.785582
1	2.175753	-2.364587	2.908343
1	0.983005	-1.125531	2.449084
7	-0.306909	-0.661268	-0.009332
1	-1.324705	2.508942	-0.147226
8	1.182727	3.725092	0.020818
6	1.502518	2.570881	0.073500
8	2.791897	2.192606	0.270283
1	3.303988	3.006031	0.376479

O. COOH (T_1)
Total energy = -1006.327123a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.867624	-0.040721	-0.003797
6	-0.609894	1.410883	-0.172900
6	0.730292	1.560019	-0.115653
6	1.293155	0.226993	0.020334
6	2.668485	-0.102779	0.064239
6	4.884988	0.005873	0.278406
6	4.557232	-1.283744	0.032972
1	5.842333	0.465069	0.444072
1	5.178865	-2.154829	-0.064455
7	3.195407	-1.350751	-0.093772
7	3.722968	0.730830	0.302319
6	2.471394	-2.576906	-0.404650
1	1.835896	-2.854970	0.430772
1	1.851603	-2.427276	-1.283805
1	3.209675	-3.350345	-0.594941
6	3.661667	2.150795	0.604451
1	2.891745	2.335831	1.350533
1	4.625487	2.450306	1.004363
1	3.454266	2.729179	-0.293973
6	-2.075463	-0.691289	0.158347
6	-3.616655	-2.314088	0.126053
6	-4.225087	-1.175415	0.552364
1	-4.029800	-3.291618	-0.046974
1	-5.240891	-1.013671	0.866300
7	-3.295985	-0.177511	0.585171
7	-2.299311	-2.043918	-0.084857
6	-3.492804	1.039327	1.360843
1	-2.539476	1.533139	1.515085
1	-4.168887	1.713309	0.842204

1	-3.904020	0.777932	2.334540
6	-1.370458	-2.957496	-0.725186
1	-0.516261	-3.136981	-0.080176
1	-1.899145	-3.885987	-0.920914
1	-1.019313	-2.532264	-1.664422
7	0.334974	-0.726481	0.051757
1	1.242145	2.493615	-0.272763
8	-1.204591	3.667836	-0.555688
6	-1.480126	2.502573	-0.633373
8	-2.609703	2.053737	-1.217730
1	-3.080865	2.827641	-1.557128

P. CN (S_0)
Total energy = -910.100291a.u

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.924529	0.217275	0.008028
6	0.652457	1.605084	0.024017
6	-0.735701	1.718863	-0.016665
6	-1.207587	0.399674	-0.052303
6	-2.576447	-0.051068	-0.118512
6	-4.782569	-0.164191	0.103814
6	-4.374519	-1.282026	-0.532258
1	-5.762468	0.161982	0.400122
1	-4.929982	-2.123366	-0.903723
7	-3.007811	-1.198282	-0.668681
7	-3.658416	0.587798	0.360610
6	-2.187296	-2.196981	-1.346543
1	-1.465807	-1.695874	-1.983624
1	-1.652512	-2.799633	-0.618835
1	-2.849540	-2.817864	-1.942388
6	-3.665120	1.855793	1.078070
1	-3.650643	2.689616	0.379473
1	-4.570569	1.900822	1.675478
1	-2.795534	1.904887	1.727813
6	2.221115	-0.428100	0.076602
6	3.834299	-1.826716	0.663005
6	4.344715	-0.963513	-0.243103
1	4.288626	-2.645411	1.190224
1	5.329920	-0.883508	-0.664646
7	3.331711	-0.107626	-0.604455
7	2.518902	-1.480356	0.853903
6	3.466050	0.924699	-1.630380
1	2.480796	1.161505	-2.020814
1	3.908892	1.821343	-1.205600
1	4.090284	0.528793	-2.426481
6	1.605500	-2.141164	1.779618
1	0.978261	-2.848417	1.244495
1	2.200662	-2.654014	2.529089
1	0.975051	-1.393218	2.250034
7	-0.198165	-0.507076	-0.033097
1	-1.293045	2.639076	-0.038913
6	1.612049	2.644581	0.132303
7	2.432173	3.445543	0.213742

P. CN (T_1)
Total energy = -909.981673a.u

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
6	0.978062	0.189027	-0.000335
6	0.648947	1.622939	0.240517
6	-0.699610	1.708637	0.243735
6	-1.199353	0.365188	0.018882
6	-2.554796	-0.031732	-0.040317
6	-4.779326	-0.025826	-0.203313
6	-4.376734	-1.313775	-0.104699
1	-5.763874	0.393492	-0.301951
1	-4.948510	-2.223531	-0.091842
7	-3.010968	-1.318004	-0.009325
7	-3.659732	0.762044	-0.167841
6	-2.219038	-2.530091	0.155061
1	-1.580024	-2.677634	-0.710277
1	-1.598718	-2.448669	1.042958
1	-2.912985	-3.358870	0.259997
6	-3.685381	2.207045	-0.312766
1	-2.969363	2.515307	-1.071905
1	-4.683415	2.494691	-0.628349
1	-3.459596	2.694251	0.634215
6	2.215020	-0.416465	-0.078025
6	3.783168	-2.016018	0.006741
6	4.406041	-0.839254	-0.276615
1	4.200686	-2.996408	0.150867
1	5.445494	-0.640851	-0.467877
7	3.467141	0.143455	-0.340930
7	2.448167	-1.783506	0.100410
6	3.740831	1.443521	-0.942599
1	2.858057	1.787126	-1.475186
1	4.014618	2.175743	-0.188987
1	4.551864	1.322282	-1.656325
6	1.487633	-2.770644	0.559966
1	0.715712	-2.919792	-0.187951
1	2.027111	-3.696924	0.736211
1	1.022666	-2.436885	1.486200
7	-0.191532	-0.529970	-0.109628
1	-1.257194	2.602867	0.457328
6	1.512011	2.684580	0.608486
7	2.203013	3.547553	0.92225

10. References:

1. G. W. T. M. J. Frisch, H. B. Schlegel, G. E. Scuseria,, J. R. C. M. A. Robb, G. Scalmani, V. Barone,, H. N. G. A. Petersson, X. Li, M. Caricato,, J. B. A. V. Marenich, B. G. Janesko, R. Gomperts,, H. P. H. B. Mennucci, J. V. Ortiz, A. F. Izmaylov,, D. W.-Y. J. L. Sonnenberg, F. Ding, F. Lipparini,, J. G. F. Egidi, B. Peng, A. Petrone, T. Henderson,, V. G. Z. D. Ranasinghe, J. Gao, N. Rega, G. Zheng,, M. H. W. Liang, M. Ehara, K. Toyota, R. Fukuda,, M. I. J. Hasegawa, T. Nakajima, Y. Honda, O. Kitao,, T. V. H. Nakai, K. Throssell, J. A. Montgomery Jr.,, F. O. J. E. Peralta, M. J. Bearpark, J. J. Heyd,, K. N. K. E. N. Brothers, V. N. Staroverov, T. A. Keith,, J. N. R. Kobayashi, K. Raghavachari, A. P. Rendell,, S. S. I. J. C. Burant, J. Tomasi, M. Cossi,, M. K. J. M. Millam, C. Adamo, R. Cammi,, R. L. M. J. W. Ochterski, K. Morokuma, O. Farkas, and J. B. F. a. D. J. Fox, Gaussian 16, Revision Revision A.03, *Gaussian Inc. Wallingford CT*, 2016, **1**, 572.