*Supplementary information for:*

# Influence of Pseudo-Jahn–Teller Activity on the Singlet-Triplet Gap of Azaphenalenes

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Table S1: **Results for 1AP:** Energies of the $S_1$ and $T_1$ states with respect to the $S_0$ ground state along with the singlet-triplet gap, $S_1$-$T_1$, are given in eV. Methods used for determining the equilibrium geometries and their point groups are also stated. The barrier for automerization, $E^{\ddagger}$, determined with the method used for optimization is stated in kJ/mol. Results from other studies are included for comparison.

| Geometry | | | Excited states | | | | Source |
|---|---|---|---|---|---|---|---|
| Method | Symmetry | $E^{\ddagger}$ | Method | $S_1$ | $T_1$ | $S_1$-$T_1$ | |
| B3LYP | $D_{3h}$ , $C_{3h}$ | 0.0 | ADC(2) | 1.004 | 1.146 | −0.143 | this work |
| $\omega$B97X-D | $D_{3h}$ , $C_{3h}$ | 0.0 | " | 1.027 | 1.166 | −0.139 | " |
| MP2 | $D_{3h}$ , $C_{3h}$ | 0.0 | " | 0.997 | 1.138 | −0.141 | " |
| CCSD | $D_{3h}$ | 3.6 | " | 1.012 | 1.153 | −0.142 | " |
| " | $C_{3h}$ | | " | 1.391 | 1.334 | +0.057 | " |
| CCSD(T) | $D_{3h}$ | 0.5 | " | 0.988 | 1.134 | −0.146 | " |
| " | $C_{3h}$ | | " | 1.143 | 1.204 | −0.061 | " |
| B97-3C | | | NEVPT2(12,12) | 1.244 | 1.288 | −0.044 | Ref. 1 |
| | | | RMS-CASPT2 | 0.89 | 0.97 | −0.08 | Ref. 2 |
| MP2 | | | CC2 | 1.047 | 1.180 | −0.133 | Ref. 3 |
| MP2,ADC(2) | | | CC2(adiabatic) | 0.976 | 1.117 | −0.141 | Ref. 3 |
| MP2,ADC(2) | | | CC2 (0-0) | 0.992 | 1.068 | −0.076 | Ref. 3 |
| $\omega$B97X-D | | | EOM-CCSD | | | −0.072 | Ref. 4 |
| CCSD(T) | $D_{3h}$ | | ADC(2) | 1.001 | 1.138 | −0.137 | Ref. 5 |
| CCSD(T) | $D_{3h}$ | | ADC(3) | 0.81 | 0.87 | −0.06 | Ref. 5 |
| CCSD(T) | $D_{3h}$ | | TBE | 0.979 | 1.110 | −0.131 | Ref. 5 |
| exp. | | | exp. | 0.97 | 0.93 | +0.04 | Ref. 6[a] |

[a] Using $S_1$=0.78 $\mu m^{-1}$ and $T_1$=0.75 $\mu m^{-1}$ from Ref. 6 multiplied by 1.2398 eV/$\mu m^{-1}$.

Table S2: **Results for 5AP:** Energies of the $S_1$ and $T_1$ states with respect to the $S_0$ ground state along with the singlet-triplet gap, $S_1$-$T_1$, are given in eV. Methods used for determining the equilibrium geometries and their point groups are also stated. The barrier for automerization, $E^{\ddagger}$, determined with the method used for optimization is stated in kJ/mol. Results from other studies are included for comparison.

| Geometry | | | Excited states | | | | Source |
|---|---|---|---|---|---|---|---|
| Method | Symmetry | $E^{\ddagger}$ | Method | $S_1$ | $T_1$ | $S_1$-$T_1$ | |
| B3LYP | $C_{2v}$ , $C_s$ | 0.0 | ADC(2) | 2.129 | 2.275 | −0.146 | this work |
| $\omega$B97X-D | $C_{2v}$ , $C_s$ | 0.0 | " | 2.167 | 2.307 | −0.140 | " |
| MP2 | $C_{2v}$ | | " | 2.143 | 2.288 | −0.145 | " |
| CCSD | $C_{2v}$ | | " | 2.161 | 2.303 | −0.142 | " |
| CCSD(T) | $C_{2v}$ | | " | 2.123 | 2.273 | −0.150 | " |
| B97-3C | | | NEVPT2(8,8) | 2.26 | 2.35 | −0.089 | Ref. 1 |
| B97-3C | | | NEVPT2(10,10) | | | +0.034 | Ref. 1 |
| B97-3C | | | NEVPT2(12,12) | | | +0.036 | Ref. 1 |
| | | | RMS-CASPT2 | 2.00 | 2.08 | −0.08 | Ref. 2 |
| MP2 | | | CC2 | 2.231 | 2.365 | −0.134 | Ref. 3 |
| MP2, ADC(2) | | | CC2 (adiabatic) | 2.066 | 2.197 | −0.131 | Ref. 3 |
| MP2, ADC(2) | | | CC2 (0-0) | 1.971 | 2.056 | −0.085 | Ref. 3 |
| $\omega$B97X-D | | | EOM-CCSD | 2.359 | 2.397 | −0.08 | Ref. 7 |
| CCSD(T) | $C_{2v}$ | | ADC(2) | 2.159 | 2.298 | −0.139 | Ref. 5 |
| CCSD(T) | $C_{2v}$ | | TBE | 2.177 | 2.296 | −0.119 | Ref. 5 |
| exp. | | | exp. | 1.957 | 2.003 | −0.047 | Ref. 8 |

Table S3: **Results for 7AP:** Energies of the $S_1$ and $T_1$ states with respect to the $S_0$ ground state along with the singlet-triplet gap, $S_1$-$T_1$, are given in eV. Methods used for determining the equilibrium geometries and their point groups are also stated. The barrier for automerization, $E^{\ddagger}$, determined with the method used for optimization is stated in kJ/mol. Results from other studies are included for comparison.

| Geometry | | | Excited states | | | | Source |
|---|---|---|---|---|---|---|---|
| Method | Symmetry | $E^{\ddagger}$ | Method | $S_1$ | $T_1$ | $S_1$-$T_1$ | |
| B3LYP | $D_{3h}$ , $C_{3h}$ | 0.0 | ADC(2) | 2.643 | 2.892 | −0.249 | this work |
| $\omega$B97X-D | $D_{3h}$ , $C_{3h}$ | 0.0 | " | 2.681 | 2.925 | −0.244 | " |
| MP2 | $D_{3h}$ | | " | 2.649 | 2.900 | −0.251 | " |
| CCSD | $D_{3h}$ | | " | 2.670 | 2.918 | −0.249 | " |
| CCSD(T) | $D_{3h}$ | | " | 2.626 | 2.882 | −0.256 | " |
| B97-3C | | | NEVPT2(12,12) | 3.259 | 3.398 | −0.139 | Ref. 1 |
| | | | RMS-CASPT2 | 2.50 | 2.70 | −0.20 | Ref. 2 |
| MP2 | | | CC2 | 2.756 | 2.998 | −0.242 | Ref. 3 |
| MP2, ADC(2) | | | CC2 (adiabatic) | 2.640 | 2.894 | −0.254 | Ref. 3 |
| MP2, ADC(2) | | | CC2 (0-0) | 2.512 | 2.618 | −0.106 | Ref. 3 |
| $\omega$B97X-D | | | EOM-CCSD | | | −0.144 | Ref. 4 |
| CCSD(T) | $D_{3h}$ | | ADC(2) | 2.675 | 2.927 | −0.246 | Ref. 5 |
| CCSD(T) | $D_{3h}$ | | ADC(3) | 2.81 | 2.88 | −0.07 | Ref. 5 |
| CCSD(T) | $D_{3h}$ | | TBE | 2.717 | 2.936 | −0.219 | Ref. 5 |
| exp. | | | exp. | | | <0 | Ref. 9 |

Table S4: **Results for 2AP, 3AP, and 4AP:** Energies of the $S_1$ and $T_1$ states with respect to the $S_0$ ground state along with the singlet-triplet gap, $S_1$-$T_1$, are given in eV. Methods used for determining the equilibrium geometries and their point groups are also stated. The barrier for automerization, $E^{\ddagger}$, determined with the method used for optimization is stated in kJ/mol. Results from other studies are included for comparison.

| Geometry | | | Excited states | | | | Source |
|---|---|---|---|---|---|---|---|
| Method | Symmetry | $E^{\ddagger}$ | Method | $S_1$ | $T_1$ | $S_1$-$T_1$ | |
| **Results for 2AP** | | | | | | | |
| B3LYP | $C_{2v}$ , $C_s$ | 0.0 | ADC(2) | 0.872 | 0.975 | −0.103 | this work |
| $\omega$B97X-D | $C_{2v}$ ($B_2$, 340$i$ cm$^{-1}$) | 0.1 | " | 0.894 | 0.993 | −0.099 | " |
| " | $C_s$ | | " | 1.007 | 1.041 | −0.034 | " |
| MP2 | $C_{2v}$ | 0.3 | " | 0.861 | 0.960 | −0.099 | " |
| " | $C_s$ | | " | 0.851 | 0.948 | −0.097 | " |
| CCSD | $C_{2v}$ | 9.6 | " | 0.885 | 0.988 | −0.102 | " |
| " | $C_s$ | | " | 1.481 | 1.269 | +0.212 | " |
| CCSD(T) | $C_{2v}$ | 2.5 | " | 0.856 | 0.962 | −0.106 | " |
| " | $C_s$ | | " | 1.269 | 1.145 | +0.125 | " |
| B97-3C | | | NEVPT2(12,12) | | | −0.120 | Ref. 1 |
| | | | RMS-CASPT2 | 0.89 | 0.97 | −0.08 | Ref. 2 |
| CCSD(T) | $C_{2v}$ | | ADC(2) | 1.001 | 1.138 | −0.137 | Ref. 5 |
| CCSD(T) | $C_{2v}$ | | TBE | 0.833 | 0.904 | −0.071 | Ref. 5 |
| **Results for 3AP** | | | | | | | |
| B3LYP | $C_{2v}$ ,$C_s$ | 0.0 | ADC(2) | 0.743 | 0.827 | −0.084 | this work |
| $\omega$B97X-D | $C_{2v}$ ($B_2$, 773$i$ cm$^{-1}$) | 1.9 | " | 0.765 | 0.845 | −0.079 | " |
| " | $C_s$ | | " | 1.238 | 1.049 | +0.189 | " |
| MP2 | $C_{2v}$ ,$C_s$ | | " | 0.711 | 0.790 | −0.079 | " |
| CCSD | $C_{2v}$ | 16.8 | " | 0.745 | 0.826 | −0.081 | " |
| " | $C_s$ | | " | 1.555 | 1.225 | +0.330 | " |
| CCSD(T) | $C_{2v}$ | 5.9 | " | 0.714 | 0.797 | −0.083 | " |
| " | $C_s$ | | " | 1.367 | 1.093 | +0.274 | " |
| CCSD(T) | $C_{2v}$ | | ADC(2) | 2.159 | 2.298 | −0.139 | Ref. 5 |
| CCSD(T) | $C_{2v}$ | | TBE | 0.693 | 0.735 | −0.042 | Ref. 5 |
| **Results for 4AP** | | | | | | | |
| B3LYP | $D_{3h}$ ($A_2'$, 494$i$ cm$^{-1}$)) | 0.2 | ADC(2) | 0.614 | 0.689 | −0.075 | this work |
| " | $C_{3h}$ | | " | 0.916 | 0.791 | +0.125 | " |
| $\omega$B97X-D | $D_{3h}$ ($A_2'$, 1113$i$ cm$^{-1}$) | 5.5 | " | 0.636 | 0.707 | −0.071 | " |
| " | $C_{3h}$ | | " | 1.377 | 1.033 | +0.344 | " |
| MP2 | $D_{3h}$ ,$C_{3h}$ | | " | 0.573 | 0.648 | −0.074 | " |
| CCSD | $D_{3h}$ | 26.3 | " | 0.614 | 0.688 | −0.073 | " |
| " | $C_{3h}$ | | " | 1.635 | 1.203 | +0.432 | " |
| CCSD(T) | $D_{3h}$ | 11.6 | " | 0.582 | 0.660 | −0.078 | " |
| " | $C_{3h}$ | | " | 1.452 | 1.057 | +0.395 | " |
| CCSD(T) | $D_{3h}$ | | ADC(2) | 2.675 | 2.927 | −0.246 | Ref. 5 |
| CCSD(T) | $D_{3h}$ | | TBE | 0.554 | 0.583 | −0.029 | Ref. 5 |

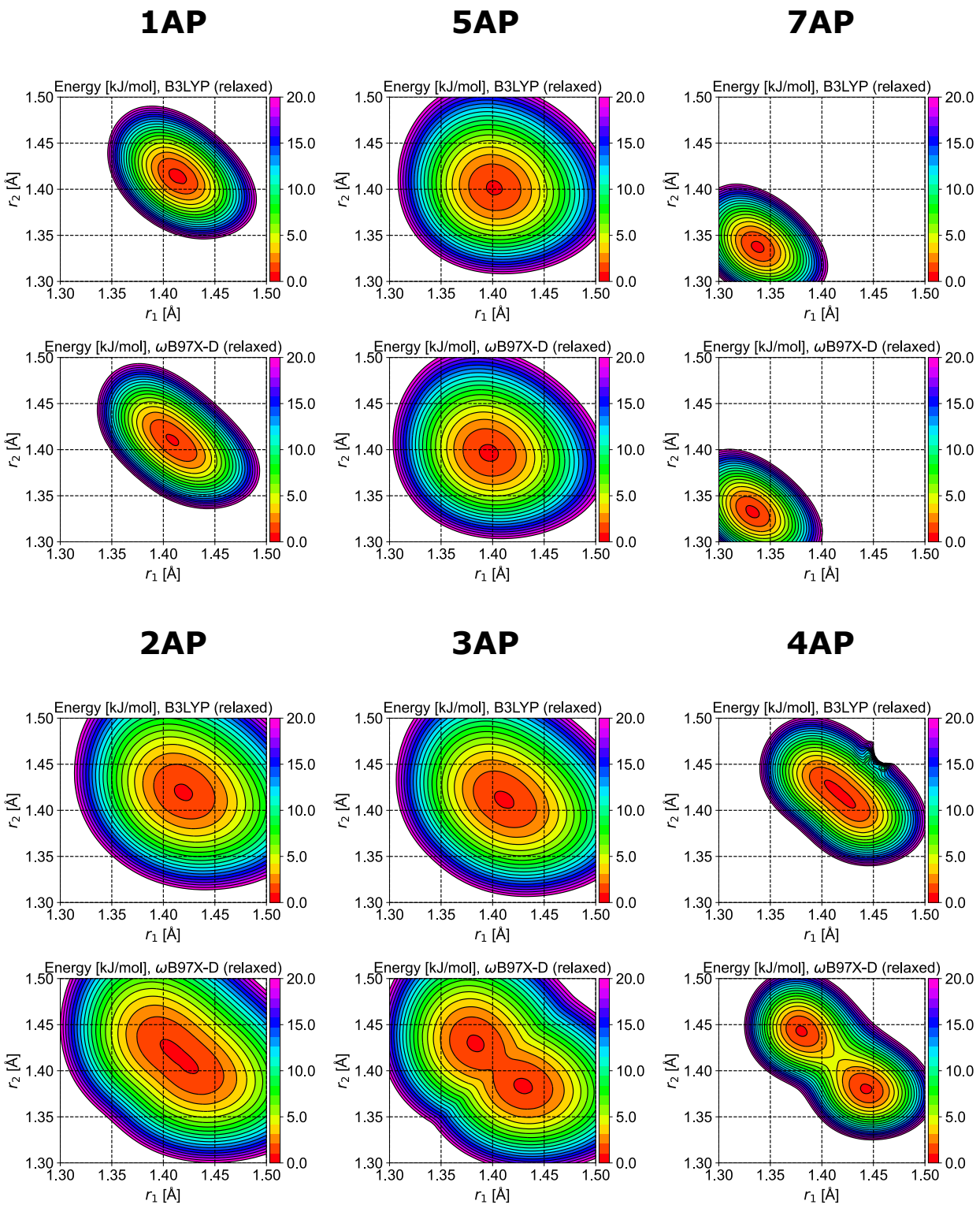


Figure S1: Contour plots of two-dimensional potential energy surfaces (of the ground state, $S_0$) of azaphenalenes calculated with the DFT methods: B3LYP and $\omega$B97X-D. See the main text for more details.

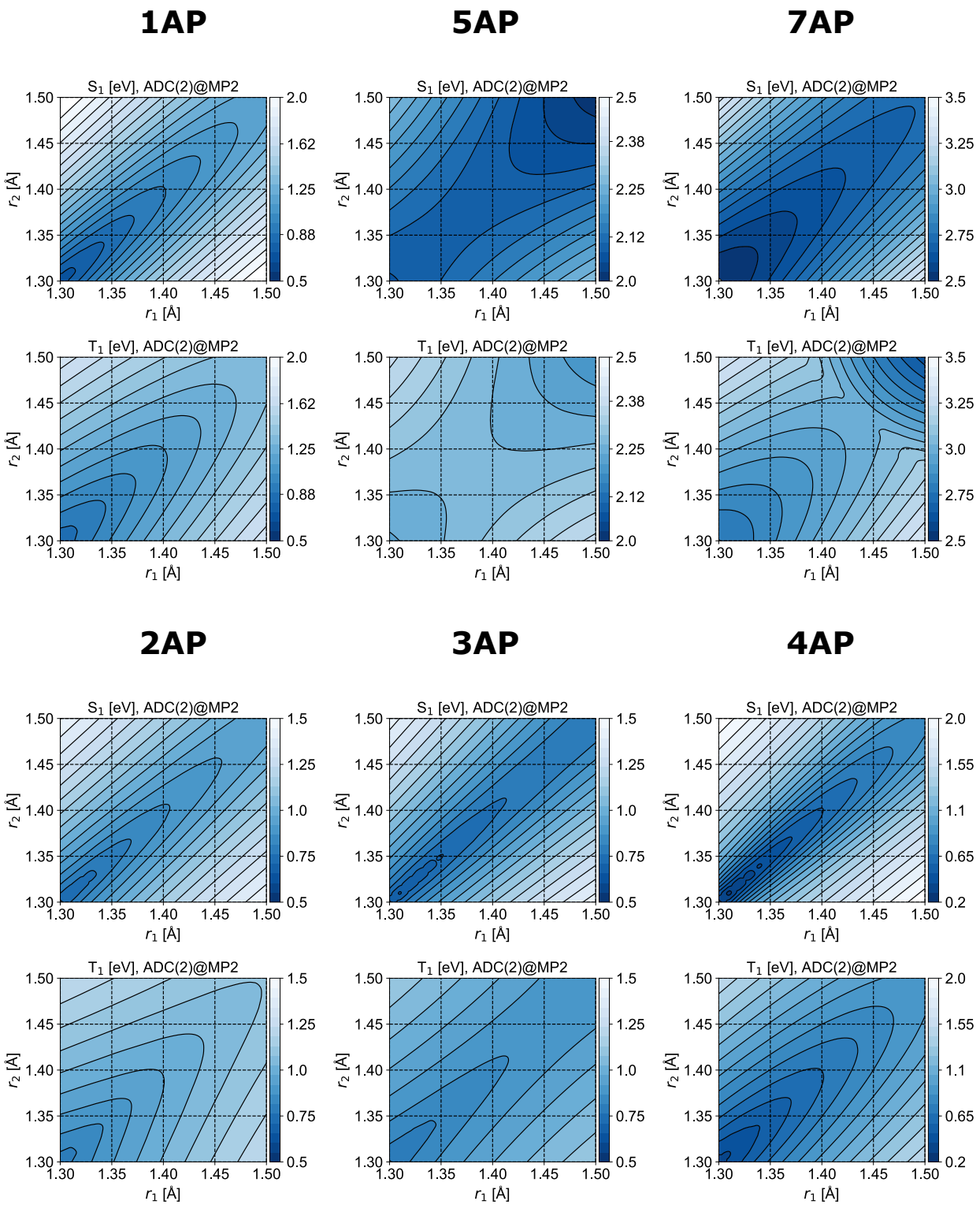


Figure S2: Contour plots of $S_1$ and $T_1$ energies of azaphenalenes. See the main text for more details.

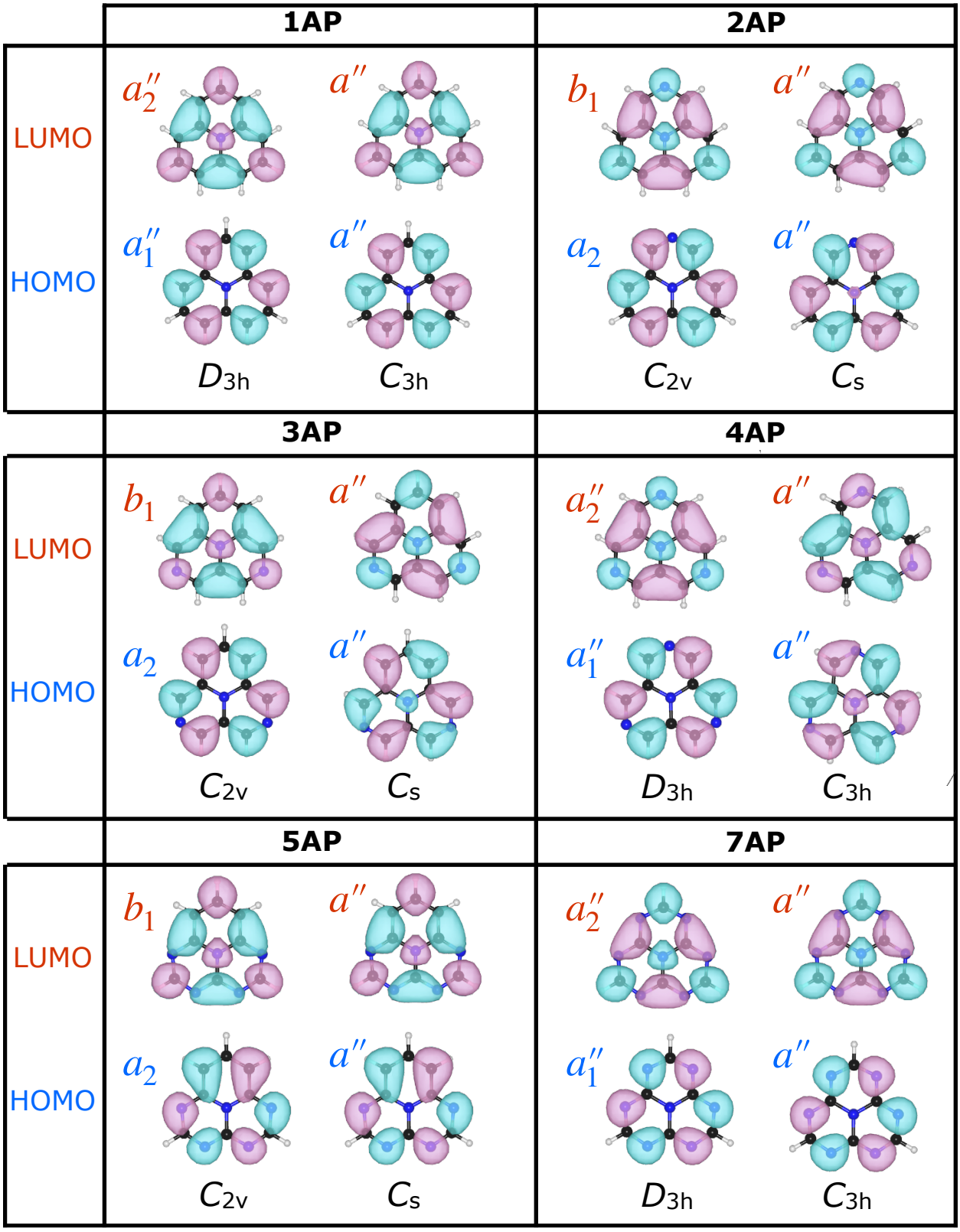


Figure S3: Frontier MOs of azaphenalenes calculated with the ωB97X-D/cc-pVTZ method in the respective equilibrium geometries.

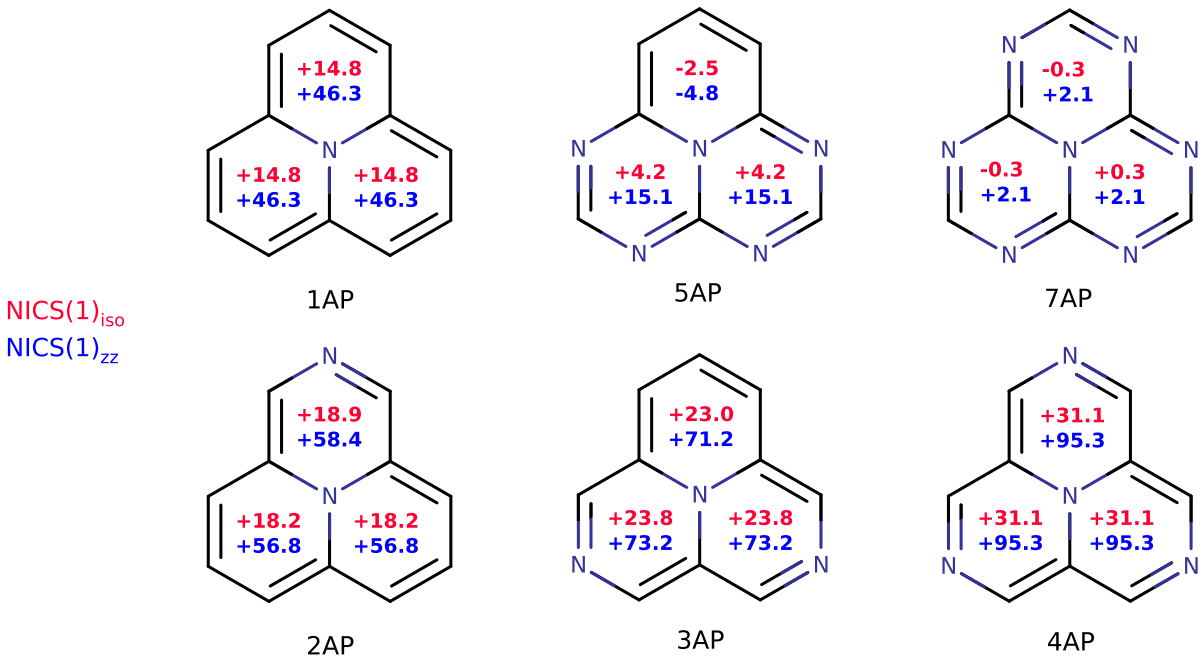


Figure S4: Nucleus-independent chemical shifts (NICS) calculated with the $\omega$B97X-D3/cc-pVTZ method.

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-----------------------------------------------------------------
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MOLECULE: 1AP, POINT GROUP: D3H
-----------------------------------------------------------------
CARTESIAN COORDINATES
---------------------
   22
 CCSD(T)/CC-PVTZ  ENERGY=-516.45718151
 N         -0.0000000000        0.0000000000        0.0000000000
 C          1.4090613106        0.0000000000        0.0000000000
 C         -0.7045306553       -1.2202828904        0.0000000000
 C         -0.7045306553        1.2202828904        0.0000000000
 C          2.0972867575       -1.2322296003        0.0000000000
 C         -2.1157855159       -1.2001888109        0.0000000000
 C          0.0184987584        2.4324184112        0.0000000000
 C          1.4038057208       -2.4314628324        0.0000000000
 C         -2.8076114416        0.0000000000        0.0000000000
 C          1.4038057208        2.4314628324        0.0000000000
 C          0.0184987584       -2.4324184112        0.0000000000
 C         -2.1157855159        1.2001888109        0.0000000000
 C          2.0972867575        1.2322296003        0.0000000000
 H          3.1771396445       -1.1950402229        0.0000000000
 H         -2.6235050138       -2.1539635320        0.0000000000
 H         -0.5536346307        3.3490037549        0.0000000000
 H          1.9455458220       -3.3697842121        0.0000000000
 H         -3.8910916439        0.0000000000        0.0000000000
 H          1.9455458220        3.3697842121        0.0000000000
 H         -0.5536346307       -3.3490037549        0.0000000000
 H         -2.6235050138        2.1539635320        0.0000000000
 H          3.1771396445        1.1950402229        0.0000000000
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C5   ,  C2   ,  R2  ,  N1  ,  A1     ,  C1  ,  180.0
C6   ,  C3   ,  R2  ,  N1  ,  A1     ,  C2  ,  180.0
C7   ,  N1   ,  R3  ,  C1  ,  60.0   ,  C4  ,  0.0
C8   ,  N1   ,  R3  ,  C2  ,  60.0   ,  C5  ,  0.0
C9   ,  N1   ,  R3  ,  C3  ,  60.0   ,  C6  ,  0.0
C10  ,  C2   ,  R2  ,  N1  ,  A1     ,  C3  ,  180.0
C11  ,  C3   ,  R2  ,  N1  ,  A1     ,  C1  ,  180.0
C12  ,  C1   ,  R2  ,  N1  ,  A1     ,  C2  ,  180.0
```

```
H13  ,  C4   ,  R4  ,  C1  ,  A2     ,  N1  ,  180.0
H14  ,  C5   ,  R4  ,  C2  ,  A2     ,  N1  ,  180.0
H15  ,  C6   ,  R4  ,  C3  ,  A2     ,  N1  ,  180.0
H16  ,  N1   ,  R5  ,  C1  ,  60.0   ,  C4  ,  0.0
H17  ,  N1   ,  R5  ,  C2  ,  60.0   ,  C5  ,  0.0
H18  ,  N1   ,  R5  ,  C3  ,  60.0   ,  C6  ,  0.0
H19  ,  C10  ,  R4  ,  C2  ,  A2     ,  N1  ,  180.0
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H21  ,  C12  ,  R4  ,  C1  ,  A2     ,  N1  ,  180.0}

R1=  1.40906131    ANG
R2=  1.41139791    ANG
R3=  2.80761144    ANG
R4=  1.08049309    ANG
R5=  3.89109164    ANG
A1=  119.18425212  DEGREE
A2=  117.21180516  DEGREE
-----------------------------------------------------------------
```

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-----------------------------------------------------------------
EQUILIBRIUM COORDINATES (ANGSTROEM), FROZEN-CORE CCSD(T)/cc-pVTZ
MOLECULE: 1AP, POINT GROUP: C3H
-----------------------------------------------------------------
CARTESIAN COORDINATES
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 C          1.4102958789        0.0000000000        0.0000000000
 C         -0.7051479395       -1.2213520580        0.0000000000
 C         -0.7051479395        1.2213520580        0.0000000000
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 C         -2.1353040760       -1.1775980685        0.0000000000
 C          0.0478221953        2.4380266088        0.0000000000
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 C          1.4172360202        2.4262566999        0.0000000000
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 H         -0.5174110747        3.3596006228        0.0000000000
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C8   ,  N1   ,  R3   ,  C2  ,  A3     ,  C5  ,  0.0
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C12  ,  C1   ,  R22  ,  N1  ,  A12    ,  C2  ,  180.0
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H14  ,  C5   ,  R41  ,  C2  ,  A21    ,  N1  ,  180.0
H15  ,  C6   ,  R41  ,  C3  ,  A21    ,  N1  ,  180.0
H16  ,  N1   ,  R5   ,  C1  ,  A4     ,  C4  ,  0.0
H17  ,  N1   ,  R5   ,  C2  ,  A4     ,  C5  ,  0.0
H18  ,  N1   ,  R5   ,  C3  ,  A4     ,  C6  ,  0.0
H19  ,  C10  ,  R42  ,  C2  ,  A22    ,  N1  ,  180.0
H20  ,  C11  ,  R42  ,  C3  ,  A22    ,  N1  ,  180.0
H21  ,  C12  ,  R42  ,  C1  ,  A22    ,  N1  ,  180.0}

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R21=  1.43082528    ANG
R22=  1.39145026    ANG
R3=   2.80985400    ANG
R41=  1.08110467    ANG
R42=  1.08016779    ANG
R5=   3.89318035    ANG
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A12=  120.11375054  DEGREE
A21=  116.72541599  DEGREE
A22=  117.71594276  DEGREE
A3=   60.29024792   DEGREE
A4=   60.35855774   DEGREE
-----------------------------------------------------------------
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MOLECULE: 5AP, POINT GROUP: C2V
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 C          0.0000000000        0.0000000000        1.3959162652
 C          0.0000000000        1.2239982977       -0.6919457558
 C          0.0000000000       -1.2239982977       -0.6919457558
 C          0.0000000000        1.2095528292       -2.0899593840
 C          0.0000000000       -1.2095528292       -2.0899593840
 C          0.0000000000        0.0000000000       -2.7748568006
 N          0.0000000000        2.3932182796       -0.0052415583
 N          0.0000000000       -2.3932182796       -0.0052415583
 C          0.0000000000        2.2752712648        1.3127808253
 C          0.0000000000       -2.2752712648        1.3127808253
 N          0.0000000000       -1.1592137265        2.0571477735
 N          0.0000000000        1.1592137265        2.0571477735
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 H          0.0000000000       -2.1667462052       -2.5888851619
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C3   ,  N2   ,  R1   ,Q1   ,  90.0
C4   ,  N2   ,  R2   ,C3   ,  A1    ,  Q1  ,  90.0
C5   ,  N2   ,  R2   ,C3   ,  A1    ,  Q1  ,  -90.0
C6   ,  C4   ,  R3   ,N2   ,  A2    ,  C3  ,  180.0
C7   ,  C5   ,  R3   ,N2   ,  A2    ,  C3  ,  180.0
C8   ,  N2   ,  R4   ,Q1   ,  90.0  ,  C3  ,  180.0
N9   ,  C4   ,  R5   ,C6   ,  A3    ,  C8  ,  180.0
N10  ,  C5   ,  R5   ,C7   ,  A3    ,  C8  ,  180.0
C11  ,  N9   ,  R6   ,C4   ,  A4    ,  C6  ,  180.0
C12  ,  N10  ,  R6   ,C5   ,  A4    ,  C7  ,  180.0
N13  ,  C3   ,  R7   ,N2   ,  A5    ,  Q1  ,  90.0
N14  ,  C3   ,  R7   ,N2   ,  A5    ,  Q1  ,  -90.0
H15  ,  C6   ,  R8   ,C4   ,  A6    ,  N2  ,  180.0
H16  ,  C7   ,  R8   ,C5   ,  A6    ,  N2  ,  180.0
H17  ,  N2   ,  R9   ,Q1   ,  90.0  ,  C3  ,  180.0
```

```
H18  ,  C11  ,  R10  ,N9   ,  A7    ,  C4  ,  180.0
H19  ,  C12  ,  R10  ,N10  ,  A7    ,  C5  ,  180.0}

R1=   1.41684998    ANG
R2=   1.39586138    ANG
R3=   1.39808826    ANG
R4=   2.75392309    ANG
R5=   1.35596387    ANG
R6=   1.32328927    ANG
R7=   1.33454246    ANG
R8=   1.07941933    ANG
R9=   3.83689884    ANG
R10=  1.08479019    ANG
A1=   118.73213541  DEGREE
A2=   118.14012765  DEGREE
A3=   121.01850011  DEGREE
A4=   115.31283627  DEGREE
A5=   119.70103198  DEGREE
A6=   116.93824030  DEGREE
A7=   115.90926862  DEGREE
 ---------------------------------------------------------------
```

```
------------------------------------------------------------------
EQUILIBRIUM COORDINATES (ANGSTROEM), FROZEN-CORE CCSD(T)/cc-pVTZ
MOLECULE: 7AP, POINT GROUP: D3H
------------------------------------------------------------------
CARTESIAN COORDINATES
---------------------
   16
 CCSD(T)/CC-PVTZ  ENERGY=-612.67978274
 N         -0.0000000000        0.0000000000        0.0000000000
 C          1.4025590960        0.0000000000        0.0000000000
 C         -0.7012795480       -1.2146518075        0.0000000000
 C         -0.7012795480        1.2146518075        0.0000000000
 N          2.0624112763       -1.1624036292        0.0000000000
 N         -2.0378767105       -1.2048987437        0.0000000000
 N         -0.0245345658        2.3673023730        0.0000000000
 C          1.3055871332       -2.2613432484        0.0000000000
 C         -2.6111742664        0.0000000000        0.0000000000
 C          1.3055871332        2.2613432484        0.0000000000
 N         -0.0245345658       -2.3673023730        0.0000000000
 N         -2.0378767105        1.2048987437        0.0000000000
 N          2.0624112763        1.1624036292        0.0000000000
 H          1.8477262446       -3.2003557341        0.0000000000
 H         -3.6954524892        0.0000000000        0.0000000000
 H          1.8477262446        3.2003557341        0.0000000000
------------------------------------------------------------------
Z-MATRIX
--------
geometry={
N1
C1   ,  N1  ,  R1
C2   ,  N1  ,  R1  ,  C1  ,  120.0
C3   ,  N1  ,  R1  ,  C1  ,  120.0  ,  C2  ,  180.0
N4   ,  C1  ,  R2  ,  N1  ,  A1     ,  C3  ,  180.0
N5   ,  C2  ,  R2  ,  N1  ,  A1     ,  C1  ,  180.0
N6   ,  C3  ,  R2  ,  N1  ,  A1     ,  C2  ,  180.0
C7   ,  N1  ,  R3  ,  C1  ,  60.0   ,  N4  ,  0.0
C8   ,  N1  ,  R3  ,  C2  ,  60.0   ,  N5  ,  0.0
C9   ,  N1  ,  R3  ,  C3  ,  60.0   ,  N6  ,  0.0
N10  ,  C2  ,  R2  ,  N1  ,  A1     ,  C3  ,  180.0
N11  ,  C3  ,  R2  ,  N1  ,  A1     ,  C1  ,  180.0
N12  ,  C1  ,  R2  ,  N1  ,  A1     ,  C2  ,  180.0
H16  ,  N1  ,  R4  ,  C1  ,  60.0   ,  N4  ,  0.0
H17  ,  N1  ,  R4  ,  C2  ,  60.0   ,  N5  ,  0.0
H18  ,  N1  ,  R4  ,  C3  ,  60.0   ,  N6  ,  0.0}

R1=  1.40255910    ANG
R2=  1.33663275    ANG
```

```
R3=  2.61117427    ANG
R4=  3.69545249    ANG
A1=  119.58192379  DEGREE
-----------------------------------------------------------------
```

```
-------------------------------------------------------------
EQUILIBRIUM COORDINATES (ANGSTROEM), FROZEN-CORE CCSD(T)/cc-pVTZ
MOLECULE: 2AP, POINT GROUP: C2V
-------------------------------------------------------------
CARTESIAN COORDINATES
---------------------
   21
 CCSD(T)/CC-PVTZ  ENERGY=-532.47959209
 N          0.0000000000        0.0000000000        0.0248325005
 C          0.0000000000        0.0000000000        1.4290623782
 C          0.0000000000        1.2078318281       -0.6816722169
 C          0.0000000000       -1.2078318281       -0.6816722169
 C          0.0000000000        1.1361626851       -2.0998624488
 C          0.0000000000       -1.1361626851       -2.0998624488
 N          0.0000000000        0.0000000000       -2.7913610218
 C          0.0000000000        2.4312143725        0.0133915849
 C          0.0000000000       -2.4312143725        0.0133915849
 C          0.0000000000        2.4361423616        1.4014105437
 C          0.0000000000       -2.4361423616        1.4014105437
 C          0.0000000000       -1.2409740228        2.1053260238
 C          0.0000000000        1.2409740228        2.1053260238
 H          0.0000000000        2.0691835901       -2.6488864922
 H          0.0000000000       -2.0691835901       -2.6488864922
 H          0.0000000000        3.3405675958       -0.5697082153
 H          0.0000000000       -3.3405675958       -0.5697082153
 H          0.0000000000        3.3764935994        1.9393551417
 H          0.0000000000       -3.3764935994        1.9393551417
 H          0.0000000000       -1.2161284987        3.1855901804
 H          0.0000000000        1.2161284987        3.1855901804
-------------------------------------------------------------
Z-MATRIX
--------
geometry={
Q1
N2   ,  Q1   ,  1.0
C3   ,  N2   ,  R1    ,  Q1   ,  90.0
C4   ,  N2   ,  R21   ,  C3   ,  A11   ,  Q1  ,  90.0
C5   ,  N2   ,  R21   ,  C3   ,  A11   ,  Q1  ,  -90.0
C6   ,  C4   ,  1.42  ,  N2   ,  A21   ,  C3  ,  180.0
C7   ,  C5   ,  1.42  ,  N2   ,  A21   ,  C3  ,  180.0
N8   ,  N2   ,  R4    ,  Q1   ,  90.0  ,  C3  ,  180.0
C9   ,  C4   ,  R51   ,  C6   ,  A31   ,  N8  ,  180.0
C10  ,  C5   ,  R51   ,  C7   ,  A31   ,  N8  ,  180.0
C11  ,  C9   ,  R61   ,  C4   ,  A41   ,  C6  ,  180.0
C12  ,  C10  ,  R61   ,  C5   ,  A41   ,  C7  ,  180.0
C13  ,  C3   ,  R71   ,  N2   ,  A51   ,  Q1  ,  90.0
C14  ,  C3   ,  R71   ,  N2   ,  A51   ,  Q1  ,  -90.0
```

```
H15  ,  C6   ,  R81   ,  C4   ,  A61   ,  N2  ,  180.0
H16  ,  C7   ,  R81   ,  C5   ,  A61   ,  N2  ,  180.0
H17  ,  C9   ,  R91   ,  C4   ,  A71   ,  N2  ,  180.0
H18  ,  C10  ,  R91   ,  C5   ,  A71   ,  N2  ,  180.0
H19  ,  C11  ,  R101  ,  C9   ,  A81   ,  C4  ,  180.0
H20  ,  C12  ,  R101  ,  C10  ,  A81   ,  C5  ,  180.0
H21  ,  C13  ,  R111  ,  C3   ,  A91   ,  N2  ,  180.0
H22  ,  C14  ,  R111  ,  C3   ,  A91   ,  N2  ,  180.0}

R1=    1.40422988    ANG
R21=   1.39928790    ANG
R4=    2.81619352    ANG
R51=   1.40704603    ANG
R61=   1.38802771    ANG
R71=   1.41327600    ANG
R81=   1.08256889    ANG
R91=   1.08024472    ANG
R101=  1.08334890    ANG
R111=  1.08054984    ANG
A11=   120.32491617  DEGREE
A21=   117.43189871  DEGREE
A31=   122.49605497  DEGREE
A41=   119.80645820  DEGREE
A51=   118.58799201  DEGREE
A61=   117.58111363  DEGREE
A71=   117.72796459  DEGREE
A81=   119.97590106  DEGREE
A91=   117.27045062  DEGREE
-----------------------------------------------------------------
```

```
-------------------------------------------------------------
EQUILIBRIUM COORDINATES (ANGSTROEM), FROZEN-CORE CCSD(T)/cc-pVTZ
MOLECULE: 2AP, POINT GROUP: CS
-------------------------------------------------------------
CARTESIAN COORDINATES
---------------------
   21
 CCSD(T)/CC-PVTZ  ENERGY=-532.48054565
 N          0.0000000000       -0.0045831784        0.0256744030
 C          0.0000000000       -0.0653222374        1.4328110801
 C          0.0000000000        1.2349703896       -0.6238470103
 C          0.0000000000       -1.1796125221       -0.7439882171
 C          0.0000000000        1.2001927918       -2.0721810380
 C          0.0000000000       -1.0755525634       -2.1230678573
 N          0.0000000000        0.1172406921       -2.7966089725
 C          0.0000000000        2.4209431626        0.0784696912
 C          0.0000000000       -2.4422851071       -0.0575750796
 C          0.0000000000        2.3859073808        1.4986888985
 C          0.0000000000       -2.4928065436        1.3058067208
 C          0.0000000000       -1.2937083640        2.0669099437
 C          0.0000000000        1.1868583471        2.1491593335
 H          0.0000000000        2.1601623484       -2.5787913104
 H          0.0000000000       -1.9796425986       -2.7154936531
 H          0.0000000000        3.3481710306       -0.4755702300
 H          0.0000000000       -3.3337207740       -0.6698562121
 H          0.0000000000        3.3094589364        2.0645423722
 H          0.0000000000       -3.4495452735        1.8138331151
 H          0.0000000000       -1.3101702046        3.1471666469
 H          0.0000000000        1.1246713808        3.2292659990
-------------------------------------------------------------
Z-MATRIX
--------
geometry={
Q1
N2   ,  Q1   ,  1.0
C3   ,  N2   ,  R1    ,  Q1   ,  90.0
C4   ,  N2   ,  R21   ,  C3   ,  A11   ,  Q1  ,  90.0
C5   ,  N2   ,  R22   ,  C3   ,  A12   ,  Q1  ,  -90.0
C6   ,  C4   ,  R31   ,  N2   ,  A21   ,  C3  ,  180.0
C7   ,  C5   ,  R32   ,  N2   ,  A22   ,  C3  ,  180.0
N8   ,  N2   ,  R4    ,  Q1   ,  90.0  ,  C3  ,  180.0
C9   ,  C4   ,  R51   ,  C6   ,  A31   ,  N8  ,  180.0
C10  ,  C5   ,  R52   ,  C7   ,  A32   ,  N8  ,  180.0
C11  ,  C9   ,  R61   ,  C4   ,  A41   ,  C6  ,  180.0
C12  ,  C10  ,  R62   ,  C5   ,  A42   ,  C7  ,  180.0
C13  ,  C3   ,  R71   ,  N2   ,  A51   ,  Q1  ,  90.0
C14  ,  C3   ,  R72   ,  N2   ,  A52   ,  Q1  ,  -90.0
```

```
H15  ,  C6   ,  R81   ,  C4   ,  A61   ,  N2  ,  180.0
H16  ,  C7   ,  R82   ,  C5   ,  A62   ,  N2  ,  180.0
H17  ,  C9   ,  R91   ,  C4   ,  A71   ,  N2  ,  180.0
H18  ,  C10  ,  R92   ,  C5   ,  A72   ,  N2  ,  180.0
H19  ,  C11  ,  R101  ,  C9   ,  A81   ,  C4  ,  80.0
H20  ,  C12  ,  R102  ,  C10  ,  A82   ,  C5  ,  180.0
H21  ,  C13  ,  R111  ,  C3   ,  A91   ,  N2  ,  180.0
H22  ,  C14  ,  R112  ,  C3   ,  A92   ,  N2  ,  180.0}

R1=    1.40844697    ANG
R21=   1.39941813    ANG
R22=   1.40466171    ANG
R31=   1.44875151    ANG
R32=   1.38300005    ANG
R4=    2.82491142    ANG
R51=   1.37832513    ANG
R52=   1.43718651    ANG
R61=   1.42065130    ANG
R62=   1.36431754    ANG
R71=   1.38239424    ANG
R72=   1.44260564    ANG
R81=   1.08544715    ANG
R82=   1.08090107    ANG
R91=   1.08014432    ANG
R92=   1.08145538    ANG
R101=  1.08311478    ANG
R102=  1.08325427    ANG
R111=  1.08038213    ANG
R112=  1.08189539    ANG
A11=   120.12600781  DEGREE
A12=   120.75378845  DEGREE
A21=   116.27883973  DEGREE
A22=   118.91028829  DEGREE
A31=   122.00896152  DEGREE
A32=   122.84449320  DEGREE
A41=   119.22027278  DEGREE
A42=   120.65153460  DEGREE
A51=   119.77464009  DEGREE
A52=   117.30139889  DEGREE
A61=   116.44668394  DEGREE
A62=   118.92060510  DEGREE
A71=   118.50728259  DEGREE
A72=   116.98748256  DEGREE
A81=   120.08234665  DEGREE
A82=   120.09039442  DEGREE
A91=   118.17605456  DEGREE
A92=   116.47787965  DEGREE
```

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```
------------------------------------------------------------------
EQUILIBRIUM COORDINATES (ANGSTROEM), FROZEN-CORE CCSD(T)/cc-pVTZ
MOLECULE: 3AP, POINT GROUP: C2V
------------------------------------------------------------------
CARTESIAN COORDINATES
---------------------
   20
 CCSD(T)/CC-PVTZ  ENERGY=-548.50029036
 N          0.0000000000        0.0000000000       -0.0290948978
 C          0.0000000000        0.0000000000        1.3669984084
 C         -1.2168465284        0.0000000000       -0.7084797812
 C          1.2168465284        0.0000000000       -0.7084797812
 C         -1.2064367713        0.0000000000       -2.1185246596
 C          1.2064367713        0.0000000000       -2.1185246596
 C          0.0000000000        0.0000000000       -2.8062433640
 C         -2.4039234215        0.0000000000        0.0664921221
 C          2.4039234215        0.0000000000        0.0664921221
 N         -2.4222905439        0.0000000000        1.3968479847
 N          2.4222905439        0.0000000000        1.3968479847
 C          1.2485138341        0.0000000000        2.0294160803
 C         -1.2485138341        0.0000000000        2.0294160803
 H         -2.1584950794        0.0000000000       -2.6293185356
 H          2.1584950794        0.0000000000       -2.6293185356
 H          0.0000000000        0.0000000000       -3.8894859148
 H         -3.3500423056        0.0000000000       -0.4592347960
 H          3.3500423056        0.0000000000       -0.4592347960
 H          1.2501853399        0.0000000000        3.1116676060
 H         -1.2501853399        0.0000000000        3.1116676060
------------------------------------------------------------------
Z-MATRIX
--------
geometry={
Q1
N2   ,  Q1   ,  1.
C3   ,  N2   ,  R1    ,  Q1  ,  90.
C4   ,  N2   ,  R21   ,  C3  ,  A11  ,  Q1  ,  90.
C5   ,  N2   ,  R21   ,  C3  ,  A11  ,  Q1  ,  -90.
C6   ,  C4   ,  R31   ,  N2  ,  A21  ,  C3  ,  180.
C7   ,  C5   ,  R31   ,  N2  ,  A21  ,  C3  ,  180.
C8   ,  N2   ,  R4    ,  Q1  ,  90.  ,  C3  ,  180.
C9   ,  C4   ,  R51   ,  C6  ,  A31  ,  C8  ,  180.
C10  ,  C5   ,  R51   ,  C7  ,  A31  ,  C8  ,  180.
N11  ,  C9   ,  R61   ,  C4  ,  A41  ,  C6  ,  180.
N12  ,  C10  ,  R61   ,  C5  ,  A41  ,  C7  ,  180.
C13  ,  C3   ,  R71   ,  N2  ,  A51  ,  Q1  ,  90.
C14  ,  C3   ,  R71   ,  N2  ,  A51  ,  Q1  ,  -90.
H15  ,  C6   ,  R81   ,  C4  ,  A61  ,  N2  ,  180.
```

```
H16  ,  C7   ,  R81   ,  C5  ,  A61  ,  N2  ,  180.
H17  ,  N2   ,  R9    ,  Q1  ,  90.  ,  C3  ,  180.
H18  ,  C9   ,  R101  ,  C4  ,  A71  ,  N2  ,  180.
H19  ,  C10  ,  R101  ,  C5  ,  A71  ,  N2  ,  180.
H20  ,  C13  ,  R111  ,  C3  ,  A81  ,  N2  ,  180.
H21  ,  C14  ,  R111  ,  C3  ,  A81  ,  N2  ,  180.}

R1=    1.39609331    ANG
R21=   1.39365681    ANG
R31=   1.41008330    ANG
R4=    2.77714847    ANG
R51=   1.41765052    ANG
R61=   1.33048265    ANG
R71=   1.41335911    ANG
R81=   1.08042834    ANG
R9=    3.86039102    ANG
R101=  1.08237227    ANG
R111=  1.08225282    ANG
A11=   119.17532185  DEGREE
A21=   118.75233935  DEGREE
A31=   123.56111295  DEGREE
A41=   123.92911561  DEGREE
A51=   117.94885423  DEGREE
A61=   117.79125752  DEGREE
A71=   117.80239208  DEGREE
A81=   118.03734581  DEGREE
-----------------------------------------------------------------
```

```
-----------------------------------------------------------------
EQUILIBRIUM COORDINATES (ANGSTROEM), FROZEN-CORE CCSD(T)/cc-pVTZ
MOLECULE: 3AP, POINT GROUP: CS
-----------------------------------------------------------------
CARTESIAN COORDINATES
---------------------
   20
 CCSD(T)/CC-PVTZ  ENERGY=-548.50254805
 N         -0.0301087996        0.0000000000       -0.0071919123
 C          1.3672653196        0.0000000000        0.0434018915
 C         -0.7451386686        0.0000000000        1.1985859497
 C         -0.6743830266        0.0000000000       -1.2451826933
 C         -2.1854701157        0.0000000000        1.1008388321
 C         -2.0478183588        0.0000000000       -1.3162538802
 C         -2.8111683861        0.0000000000       -0.1078839037
 C         -0.0667671869        0.0000000000        2.3955584988
 C          0.1946360907        0.0000000000       -2.4104311060
 N          1.3092378138        0.0000000000        2.4841624359
 N          1.4945797827        0.0000000000       -2.3753924311
 C          2.0868659377        0.0000000000       -1.1279470207
 C          1.9703973364        0.0000000000        1.3638484277
 H         -2.7395722113        0.0000000000        2.0300723981
 H         -2.5188281841        0.0000000000       -2.2885833186
 H         -3.8933635152        0.0000000000       -0.1470662294
 H         -0.6238735158        0.0000000000        3.3211015155
 H         -0.2953113948        0.0000000000       -3.3792420842
 H          3.1668701502        0.0000000000       -1.0931161855
 H          3.0551323907        0.0000000000        1.4020293484
-----------------------------------------------------------------
Z-MATRIX
--------
geometry={
Q1
N2   ,  Q1   ,  1.
C3   ,  N2   ,  R1    ,  Q1  ,  90.
C4   ,  N2   ,  R21   ,  C3  ,  A11  ,  Q1  ,  90.
C5   ,  N2   ,  R22   ,  C3  ,  A12  ,  Q1  ,  -90.
C6   ,  C4   ,  R31   ,  N2  ,  A21  ,  C3  ,  180.
C7   ,  C5   ,  R32   ,  N2  ,  A22  ,  C3  ,  180.
C8   ,  N2   ,  R4    ,  Q1  ,  90.  ,  C3  ,  180.
C9   ,  C4   ,  R51   ,  C6  ,  A31  ,  C8  ,  180.
C10  ,  C5   ,  R52   ,  C7  ,  A32  ,  C8  ,  180.
N11  ,  C9   ,  R61   ,  C4  ,  A41  ,  C6  ,  180.
N12  ,  C10  ,  R62   ,  C5  ,  A42  ,  C7  ,  180.
C13  ,  C3   ,  R71   ,  N2  ,  A51  ,  Q1  ,  90.
C14  ,  C3   ,  R72   ,  N2  ,  A52  ,  Q1  ,  -90.
H15  ,  C6   ,  R81   ,  C4  ,  A61  ,  N2  ,  180.
```

```
H16  ,  C7   ,  R82   ,  C5  ,  A62  ,  N2  ,  180.
H17  ,  N2   ,  R9    ,  Q1  ,  90.  ,  C3  ,  180.
H18  ,  C9   ,  R101  ,  C4  ,  A71  ,  N2  ,  180.
H19  ,  C10  ,  R102  ,  C5  ,  A72  ,  N2  ,  180.
H20  ,  C13  ,  R111  ,  C3  ,  A81  ,  N2  ,  180.
H21  ,  C14  ,  R112  ,  C3  ,  A82  ,  N2  ,  180.}

R1=    1.39828973    ANG
R21=   1.40184449    ANG
R22=   1.39560397    ANG
R31=   1.44364441    ANG
R32=   1.37527296    ANG
R4=    2.78288183    ANG
R51=   1.37583834    ANG
R52=   1.45361552    ANG
R61=   1.37885475    ANG
R62=   1.30041582    ANG
R71=   1.37473027    ANG
R72=   1.45167052    ANG
R81=   1.08189840    ANG
R82=   1.08040492    ANG
R9=    3.86578605    ANG
R101=  1.08027651    ANG
R102=  1.08565337    ANG
R111=  1.08056573    ANG
R112=  1.08540680    ANG
A11=   118.59450254  DEGREE
A12=   119.56690131  DEGREE
A21=   116.78568095  DEGREE
A22=   120.45558028  DEGREE
A31=   123.42432210  DEGREE
A32=   123.75260069  DEGREE
A41=   123.22624833  DEGREE
A42=   125.17086814  DEGREE
A51=   119.49029669  DEGREE
A52=   116.62276352  DEGREE
A61=   116.92524294  DEGREE
A62=   118.80843317  DEGREE
A71=   119.41333011  DEGREE
A72=   116.45850051  DEGREE
A81=   119.71667571  DEGREE
A82=   116.56508535  DEGREE
-----------------------------------------------------------------
```

```
-------------------------------------------------------------
EQUILIBRIUM COORDINATES (ANGSTROEM), FROZEN-CORE CCSD(T)/cc-pVTZ
MOLECULE: 4AP, POINT GROUP: D3H
-------------------------------------------------------------
CARTESIAN COORDINATES
---------------------
   19
 CCSD(T)/CC-PVTZ  ENERGY=-564.51919933
 N         -0.0000000000        0.0000000000        0.0000000000
 C          1.3895222367        0.0000000000        0.0000000000
 C         -0.6947611183       -1.2033615561        0.0000000000
 C         -0.6947611183        1.2033615561        0.0000000000
 C          2.0427788439       -1.2553814140        0.0000000000
 C         -2.1085816179       -1.1414076661        0.0000000000
 C          0.0658027740        2.3967890801        0.0000000000
 N          1.3980302792       -2.4214594740        0.0000000000
 N         -2.7960605583        0.0000000000        0.0000000000
 N          1.3980302792        2.4214594740        0.0000000000
 C          0.0658027740       -2.3967890801        0.0000000000
 C         -2.1085816179        1.1414076661        0.0000000000
 C          2.0427788439        1.2553814140        0.0000000000
 H          3.1249114130       -1.2687198584        0.0000000000
 H         -2.6611993341       -2.0718927391        0.0000000000
 H         -0.4637120789        3.3406125974        0.0000000000
 H         -0.4637120789       -3.3406125974        0.0000000000
 H         -2.6611993341        2.0718927391        0.0000000000
 H          3.1249114130        1.2687198584        0.0000000000
-------------------------------------------------------------
Z-MATRIX
--------
geometry={
N1
C1  ,  N1  ,  R1
C2  ,  N1  ,  R1   ,  C1  ,  120.0
C3  ,  N1  ,  R1   ,  C1  ,  120.0  ,  C2  ,  180.0
C4  ,  C1  ,  R2   ,  N1  ,  A11    ,  C3  ,  180.0
C5  ,  C2  ,  R2   ,  N1  ,  A11    ,  C1  ,  180.0
C6  ,  C3  ,  R2   ,  N1  ,  A11    ,  C2  ,  180.0
N2  ,  N1  ,  R3   ,  C1  ,  60.0   ,  C4  ,  0.0
N3  ,  N1  ,  R3   ,  C2  ,  60.0   ,  C5  ,  0.0
N4  ,  N1  ,  R3   ,  C3  ,  60.0   ,  C6  ,  0.0
C7  ,  C2  ,  R2   ,  N1  ,  A11    ,  C3  ,  180.0
C8  ,  C3  ,  R2   ,  N1  ,  A11    ,  C1  ,  180.0
C9  ,  C1  ,  R2   ,  N1  ,  A11    ,  C2  ,  180.0
H1  ,  C4  ,  R41  ,  C1  ,  A21    ,  N1  ,  180.0
H2  ,  C5  ,  R41  ,  C2  ,  A21    ,  N1  ,  180.0
H3  ,  C6  ,  R41  ,  C3  ,  A21    ,  N1  ,  180.0
```

```
H4  ,  C7  ,  R41  ,  C2  ,  A21    ,  N1  ,  180.0
H5  ,  C8  ,  R41  ,  C3  ,  A21    ,  N1  ,  180.0
H6  ,  C9  ,  R41  ,  C1  ,  A21    ,  N1  ,  180.0}

R1=   1.38952224    ANG
R2=   1.41517726    ANG
R3=   2.79606056    ANG
R41=  1.08221477    ANG
A11=  117.49089295  DEGREE
A21=  118.19708911  DEGREE
-----------------------------------------------------------------
```

```
-----------------------------------------------------------------
EQUILIBRIUM COORDINATES (ANGSTROEM), FROZEN-CORE CCSD(T)/cc-pVTZ
MOLECULE: 4AP, POINT GROUP: C3H
-----------------------------------------------------------------
CARTESIAN COORDINATES
---------------------
   19
 CCSD(T)/CC-PVTZ  ENERGY=-564.52363202
 N         -0.0000000000        0.0000000000        0.0000000000
 C          1.3943168701        0.0000000000        0.0000000000
 C         -0.6971584351       -1.2075138304        0.0000000000
 C         -0.6971584351        1.2075138304        0.0000000000
 C          2.0196953303       -1.3136437071        0.0000000000
 C         -2.1474964870       -1.0922856104        0.0000000000
 C          0.1278011567        2.4059293175        0.0000000000
 N          1.3797047458       -2.4440919420        0.0000000000
 N         -2.8064980839        0.0271866114        0.0000000000
 N          1.4267933381        2.4169053306        0.0000000000
 C         -0.0029504215       -2.3888647060        0.0000000000
 C         -2.0673423109        1.1969874930        0.0000000000
 C          2.0702927324        1.1918772130        0.0000000000
 H          3.1047933775       -1.3373701978        0.0000000000
 H         -2.7105932543       -2.0201448396        0.0000000000
 H         -0.3942001232        3.3575150373        0.0000000000
 H         -0.5363847240       -3.3282397792        0.0000000000
 H         -2.6141478367        2.1286426868        0.0000000000
 H          3.1505325607        1.1995970924        0.0000000000
-----------------------------------------------------------------
Z-MATRIX
--------
geometry={
N1
C1  ,  N1  ,  R1
C2  ,  N1  ,  R1   ,  C1  ,  120.0
C3  ,  N1  ,  R1   ,  C1  ,  120.0  ,  C2  ,  180.0
C4  ,  C1  ,  R21  ,  N1  ,  A11    ,  C3  ,  180.0
C5  ,  C2  ,  R21  ,  N1  ,  A11    ,  C1  ,  180.0
C6  ,  C3  ,  R21  ,  N1  ,  A11    ,  C2  ,  180.0
N2  ,  N1  ,  R3   ,  C1  ,  A3     ,  C4  ,  0.0
N3  ,  N1  ,  R3   ,  C2  ,  A3     ,  C5  ,  0.0
N4  ,  N1  ,  R3   ,  C3  ,  A3     ,  C6  ,  0.0
C7  ,  C2  ,  R22  ,  N1  ,  A12    ,  C3  ,  180.0
C8  ,  C3  ,  R22  ,  N1  ,  A12    ,  C1  ,  180.0
C9  ,  C1  ,  R22  ,  N1  ,  A12    ,  C2  ,  180.0
H1  ,  C4  ,  R41  ,  C1  ,  A21    ,  N1  ,  180.0
H2  ,  C5  ,  R41  ,  C2  ,  A21    ,  N1  ,  180.0
H3  ,  C6  ,  R41  ,  C3  ,  A21    ,  N1  ,  180.0
```

```
H4  ,  C7  ,  R42  ,  C2  ,  A22    ,  N1  ,  180.0
H5  ,  C8  ,  R42  ,  C3  ,  A22    ,  N1  ,  180.0
H6  ,  C9  ,  R42  ,  C1  ,  A22    ,  N1  ,  180.0}

R1=   1.39431687    ANG
R21=  1.45490825    ANG
R22=  1.37022431    ANG
R3=   2.80662976    ANG
R41=  1.08535742    ANG
R42=  1.08026741    ANG
A11=  115.45743707  DEGREE
A12=  119.55983802  DEGREE
A21=  116.71005308  DEGREE
A22=  119.96929245  DEGREE
A3=   60.55500817   DEGREE
-----------------------------------------------------------------
```

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