Carbene Derived Diradicaloids – Building Blocks for Singlet Fission?

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1.) Comparison Adiabatic *vs.* Vertical Excitation for 13

CASSCF(12,12)/NEVPT2 calculations (1 singlet root and state averaged 5 singlet roots, 5 triplet roots, def2-TZVPP basis set) were performed with the geometric parameters as obtained from:

I. The solid state structure (position of hydrogen atoms optimized using B3LYP-D3BJ/def2-SVP)
II. Geometry optimization (B3LYP-D3BJ/def2-SVP) of the restricted closed-shell singlet state
III. Geometry optimization (B3LYP-D3BJ/def2-SVP) of the broken-symmetry open-shell singlet state
IV. Geometry optimization (B3LYP-D3BJ/def2-SVP) of the triplet state

	I.	**II.**	**III.**	**IV.**
	from solid-state structure	closed-shell singlet	open-shell singlet	triplet
E(B3LYP) [Ha]	-1354.747299	-1354.759953	-1354.759757	-1354.741404
E(CASSCF/NEVPT2, state averaged) [Ha]	-1353.393725	-1353.404354	-1353.406001	-1353.399245
$E(S_0)$ [eV]	0	0.06	0.12	0.28
$E(T_1)$ [eV]	0.80	0.98	0.99	0.73
$E(S_1)$ [eV]	2.49	2.17	2.67	2.56
$E(T_2)$ [eV]	2.72	3.04	2.99	3.17

Table S1. Adiabatic and vertical excitation energies for **13**. Energies of S_1, T_1 and T_2 states are given relative to the S_0 state for the solid state structure **I**.

2.) Further Correlation Plots

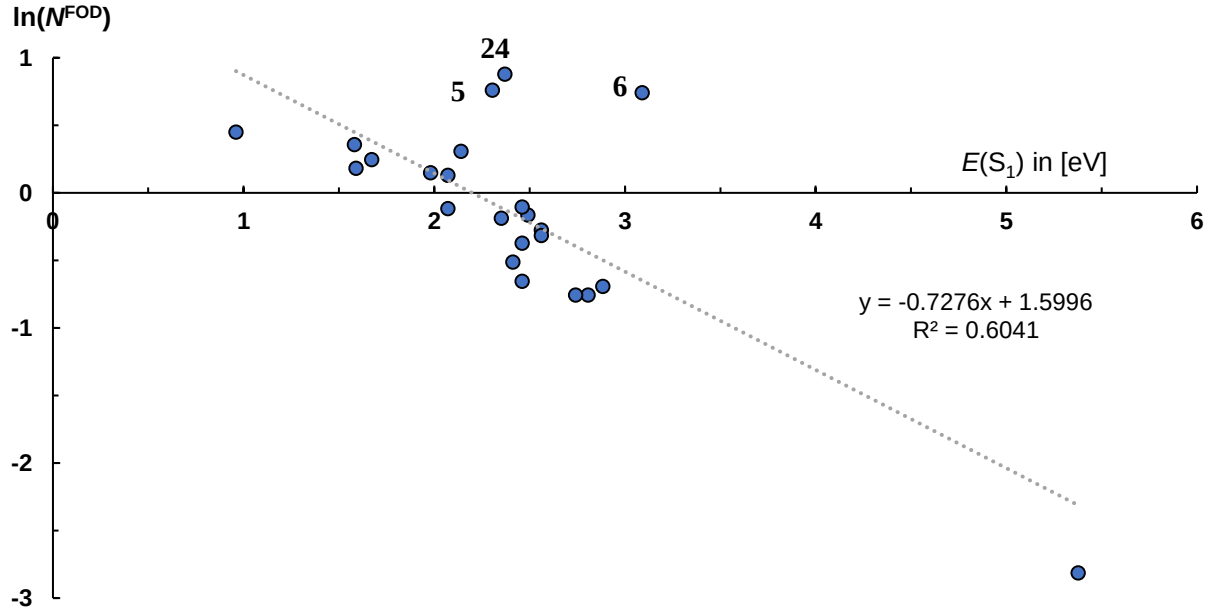


Figure S1. Correlation of N^{FOD} with $E(S_1)$. The three outliers are the compounds **5**, **6**, **24** with "perfect" diradical character. Omission of these compounds from the fit leads to an R^2 value of 0.92.

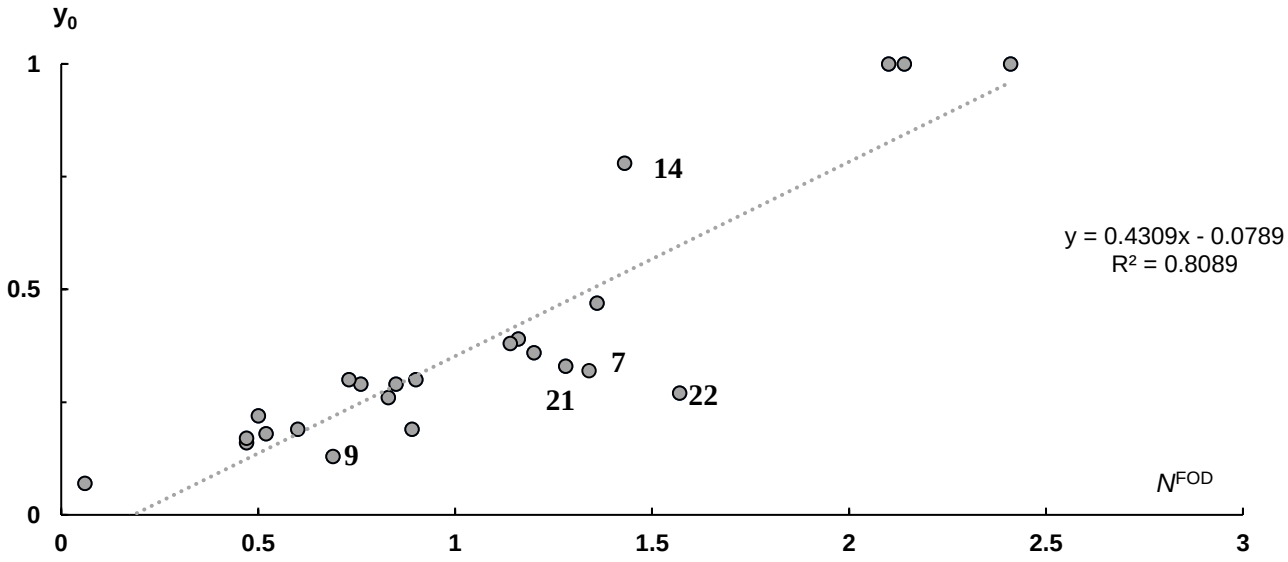


Figure S2. Correlation of y_0 with N^{FOD}. Omission of the aromatic carbenes (**7**, **9**, **21**, **22**) from the fit leads to an R^2 value of 0.90.

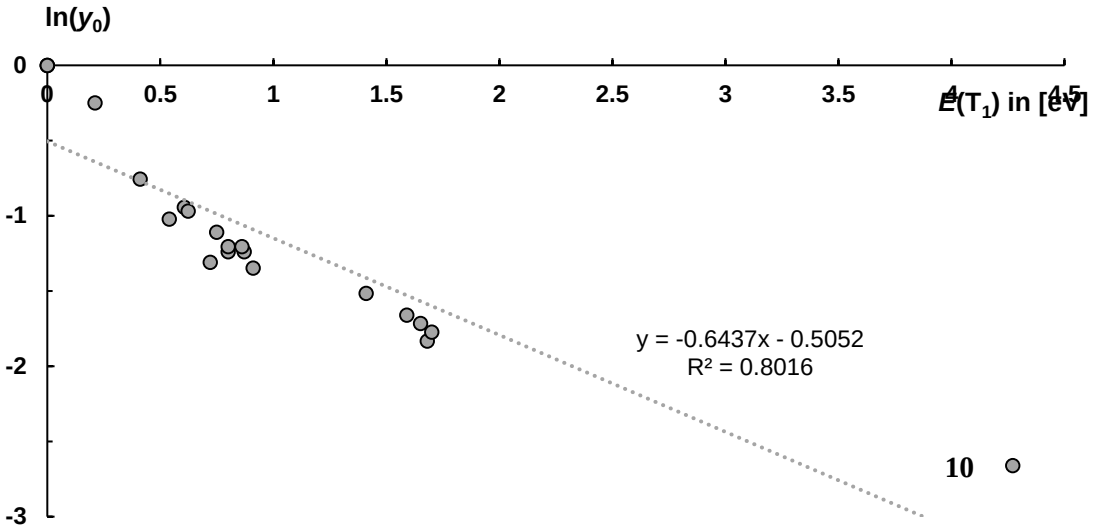


Figure S3. Correlation of ln(y_0) with $E(T_1)$. Omission of the C_1 bridged compound **10** from the fit leads to an R^2 value of 0.89.

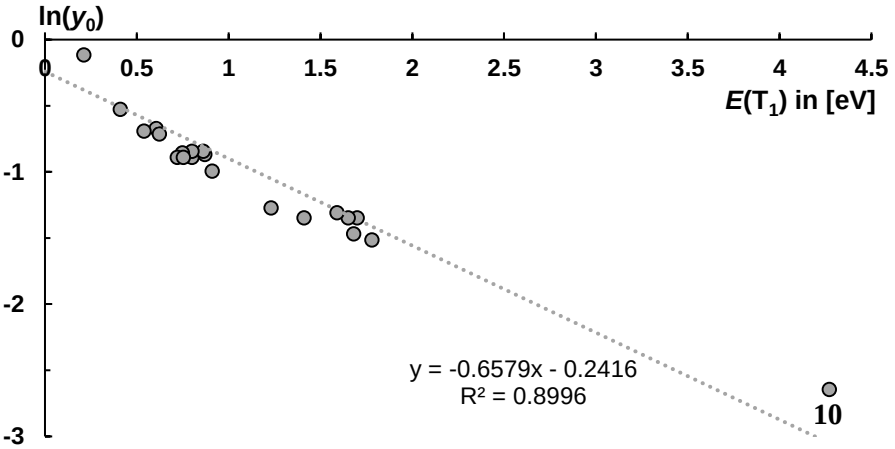


Figure S4. Correlation of ln(y_0 + y_1) with $E(T_1)$. Omission of the C_1 bridged compound **10** from the fit leads to an R^2 value of 0.92.

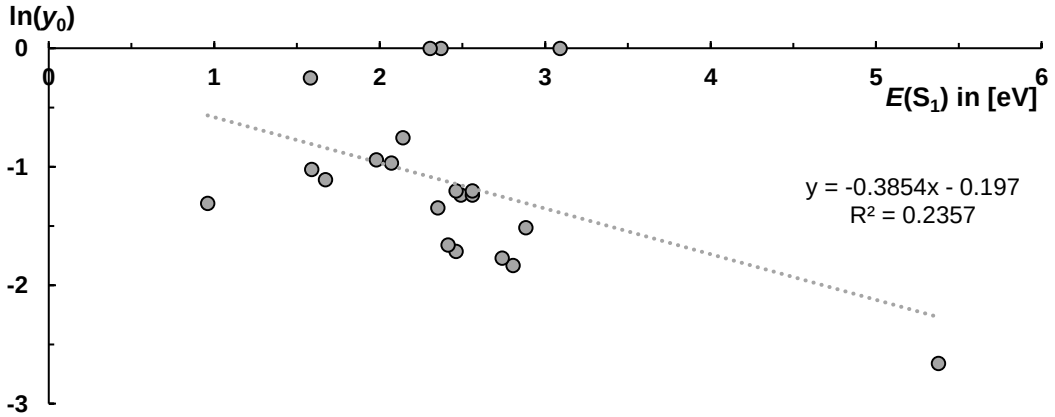


Figure S5. Correlation of ln(y_0) with $E(S_1)$.

3.) Comparison With Experimental Values and Solvation Effects

Note that the experimentally investigated compounds **7**, **8**, **9**, **11**, **17, 18** were truncated in the calculations through omitting the diisopropylphenyl *N*-substituents (*t*-butyl group, respectively, for **7**). Values for **11** (CAAC-CC-CAAC) were not include due to alleged radical impurity in the experimental UV-Vis spectrum by radical.[1] The results indicate overall that the largest error is introduced by neglecting the relaxation of the geometry upon excitation to the T_1 state (vide supra) and is in the order of magnitude of up to 0.3 eV.

Structure	**Name**	**$^{calc}\lambda$ [nm]**	**$^{exp}\lambda^{reference}$ [nm]**	**Deviation [nm]**
1	Tschitschibabin	581	576[2]	+5
2	Thiele	514	"orange"[3]	n.a.
3	Tetracene	503	475[4]	+28
4	Pentacene	599	582[5]	+16
5	Oxoverdazyl	400	417[6]	-17
6	Quinone	567	550[7]	+17
9	NHC–C_6H_4–NHC	503	444[8]	+59
13	CAAC–CC–C_6H_4–CC–CAAC	498	551[9]	-53
14	CAAC–CC–C_6H_4–C_6H_4–CC–CAAC	725	767[9]	-42
18	saNHC–CC–C_6H_4–CC–saNHC	527	595[10]	-68
Mean Absolute Deviation [nm]				**31**
Root Mean Square Deviation [nm]				**38**

Table S2. Comparison of calculated and experimentally observed absorption bands in [nm].

Structure	**$[^{exp}E(S_1) - {}^{calc}E(S_1)]$ [eV]**	**$[^{exp}E(T_1) - {}^{calc}E(T_1)]$ [eV]**
1	0.018	n.a.
1^{SMD}	0.016	
3	0.146	-0.311
3^{SMD}	0.150	-0.310
4	0.059	-0.280
4^{SMD}	0.057	-0.278
6	-0.132	
6^{SMD}	-0.142	
7	0.062	
7^{SMD}	0.067	
9	0.330	
9^{SMD}	0.320	
13	-0.242	-0.250 (from optimized triplet structure vs. closed-shell optimized singlet structure, cf. Table S1)
13^{SMD}	-0.257	
18	-0.356	
18^{SMD}	-0.258	
RMSD - Gasphase	**0.194**	**0.280**
RMSD - SMD	**0.179**	**n.a.**

Table S3. Effects of solvation on the energy levels of the S_1 and T_1 states as modeled in the gas phase or the SMD solvation model.

Solvent	***E*(S$_1$) [eV]**	***E*(T$_1$) [eV]**
gas phase	2.492	0.801
pentane	2.507	0.815
benzene	2.512	0.819
THF	2.421	0.835
methanol	2.369	0.843

Table S4. Effect of solvent polarity on **13**.

Structure	***E*(S$_1$) [eV]**	***E*(T$_1$) [eV]**
13	2.492	0.801
$^{\text{not\_truncated}}$**13**	2.481	0.789
13$^{\text{SMD}}$	2.507	0.815
$^{\text{not\_truncated}}$**13**$^{\text{SMD}}$	2.490	0.803

Table S5. Evaluation of effects of truncation on the energy levels of the S_1 and T_1 states of compound **13** in gas phase and pentane.

1. Y. Li, K. C. Mondal, P. P. Samuel, H. Zhu, C. M. Orben, S. Panneerselvam, B. Dittrich, B. Schwederski, W. Kaim, T. Mondal, D. Koley and H. W. Roesky, *Angew. Chem., Int. Ed.*, 2014, **53**, 4168-4172.
2. L. K. Montgomery, J. C. Huffman, E. A. Jurczak and M. P. Grendze, *J. Am. Chem. Soc.*, 1986, **108**, 6004-6011.
3. J. Thiele and H. Balhorn, *Ber. Dtsch. Chem. Ges.*, 1904, **37**, 1463-1470.
4. J. J. Burdett, A. M. Müller, D. Gosztola and C. J. Bardeen, *J. Chem. Phys.*, 2010, **133**, 144506.
5. M. B. Smith and J. Michl, *Chem. Rev.*, 2010, **110**, 6891-6936.
6. J. B. Gilroy, S. D. J. McKinnon, P. Kennepohl, M. S. Zsombor, M. J. Ferguson, L. K. Thompson and R. G. Hicks, *J. Org. Chem.*, 2007, **72**, 8062-8069.
7. J. Zhou and A. Rieker, *J. Chem. Soc., Perkin Trans. 2*, 1997, 931-938.
8. D. Rottschäfer, N. K. T. Ho, B. Neumann, H. G. Stammler, M. v. Gastel, D. M. Andrada and R. S. Ghadwal, *Angew. Chem., Int. Ed.*, 2018, **57**, 5838 –5842.
9. M. M. Hansmann, M. Melaimi, D. Munz and G. Bertrand, *J. Am. Chem. Soc.*, 2018, **140**, 2546–2554.
10. B. Barry, G. Soper, J. Hurmalainen, A. Mansikkamäki, K. N. Robertson, W. L. McClennan, A. J. Veinot, T. L. Roemmele, U. Werner-Zwanziger, R. T. Boeré, H. M. Tuononen, J. Clyburne and J. Masuda, *Angew. Chem., Int. Ed.*, 2018, **57**, 749-754.

4.) Effects of Enlarging Active Space for 13

The calculations were performed with the def2-TZVPP basis set. Energies are NEVPT2 corrected and were obtained from state averaged calculations with 5 singlet and 5 triplet roots. The y_0 (NOON) values were obtained from calculations with the singlet multiplicity only.

Active Space	y_0	$E(S_1)$ in [eV]	$E(T_1)$ in [eV]
(2,2)	0.14	n.a.	n.a.
(4,4)	0.19	1.93	0.76
(6,6)	0.23	2.25	0.70
(8,8)	0.25	2.28	0.84
(10,10)	0.28	2.26	0.79
(12,12)	0.29	2.49	0.80

Table S6. Effects of enlarging active space of compound **13**.

5.) Basis Set Effects

Basis set effects were evaluated for tetracene (**3**) and CAAC-CC-C_6H_4-CC-CAAC (**13**). Triple-ζ basis sets like def2-TZVPP are sufficiently large and appear reasonably close to the complete basis set limit.

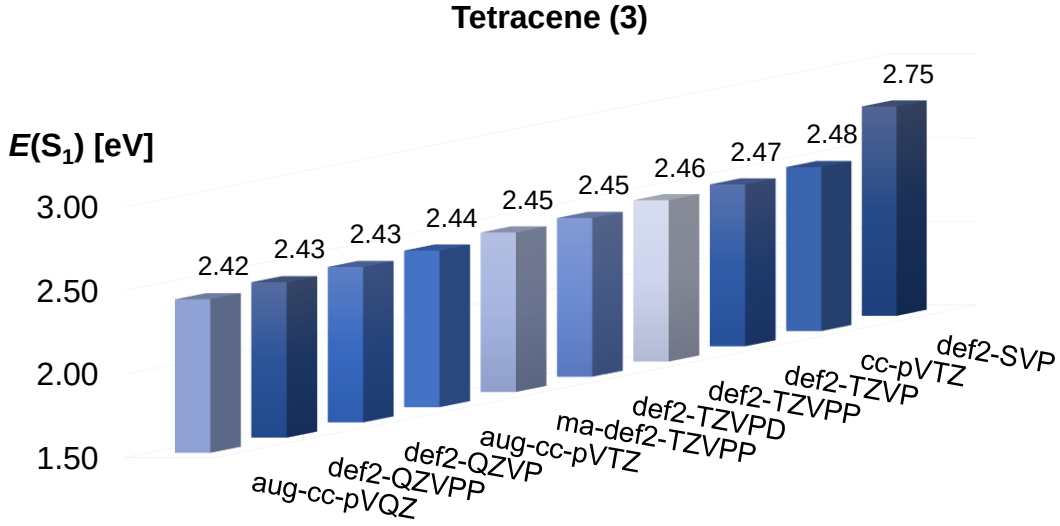


Table S7. Basis set effects on the energies of the S_1 state of tetracene (**3**).

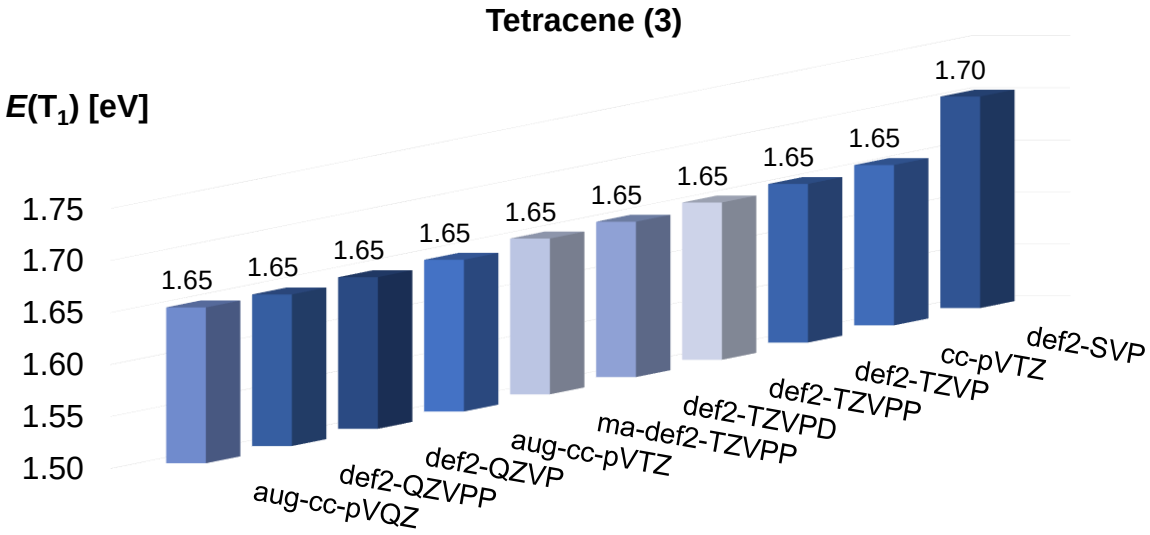


Table S8. Basis set effects on the energies of the T_1 state of tetracene (**3**).

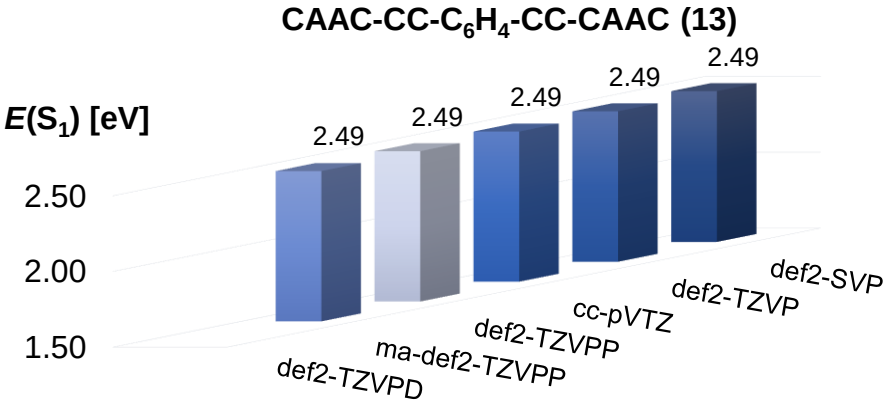


Table S9. Basis set effects on the energies of the S_1 state of CAAC-CC-C_6H_4-CC-CAAC (**13**).

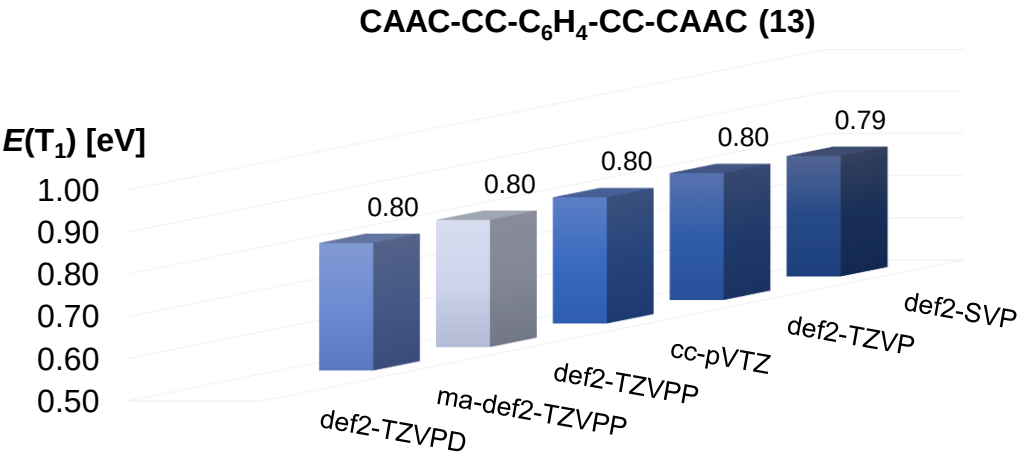


Table S10. Basis set effects on the energies of the T_1 state of CAAC-CC-C_6H_4-CC-CAAC (**13**).

6.) Choice of Active Space for all Molecules and FOD Plots

The active space of all investigated molecules comprised basically the π-system up to 14 electrons in 14 orbitals. Molecular orbitals included in the active space showed occupancy (NOON) of typically more than 0.03 electrons or less than 1.97 electrons, respectively. Out of plane orbitals of π-symmetry of the alkyne linkers were NOT included in the active space. This leads to a CASSCF(12,12) active space for e.g. saNHC-CC-C_6H_4-CC-saNHC **18**, where 6 orbitals (6 electrons) associated with the phenylene linker, 4 orbitals (4 electrons) of each CC linker, and 2 orbitals (2 electrons) from the carbene positions were allowed to mix. Inclusion of the lone pairs of the amines led to difficult to converge wave functions and did not lead to an improvement. For the aromatic carbenes, the inclusion of further molecular orbitals (4 orbitals, 4 electrons) associated with the π-system of the carbenes proved necessary. In order to keep the size of the active space manageable, the orbitals with a_{2u} (b_{2g}) symmetry associated with the *para*-phenylene linker were omitted here from the active space. Note that the numbering of the molecular orbitals shown subsequently is not necessarily in the correct order, because the out of plane π-orbitals have in many cases higher energies than the lowest energy orbital of the active space.

Tschitschibabin's Hydrocarbon (1)

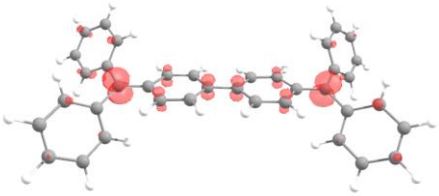
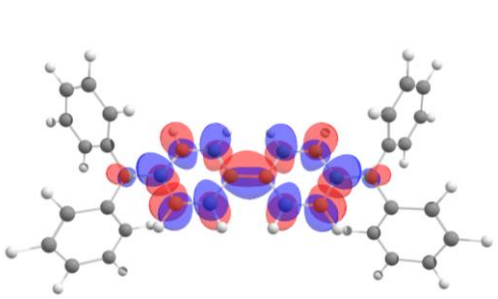
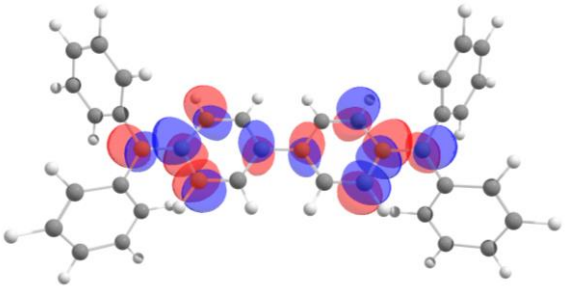


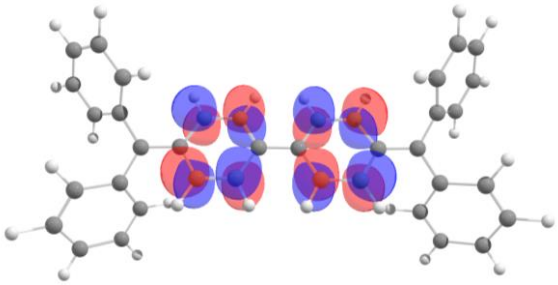
Figure S6. FOD plot of **1** with a contour value of 0.005 e Bohr^{-3}.



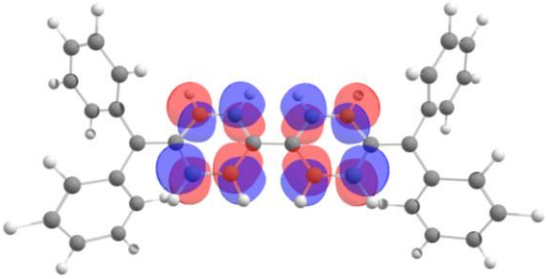
MO134 ("LUMO+5")



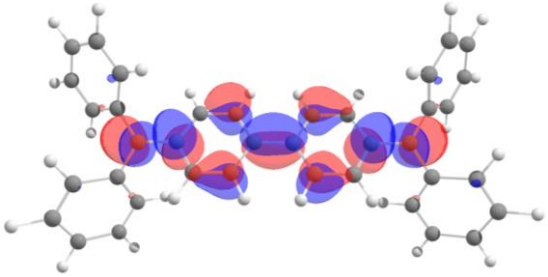
MO133 ("LUMO+4")



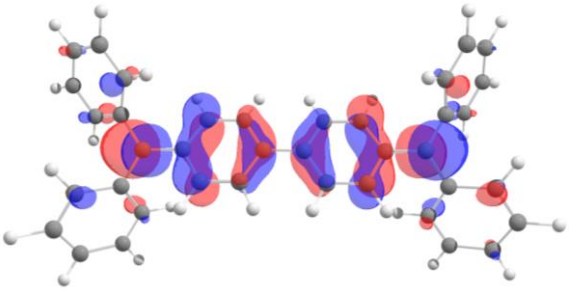
MO132 ("LUMO+3")



MO131 ("LUMO+2")



MO130 ("LUMO+1")



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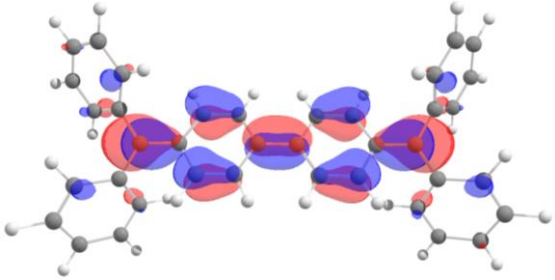

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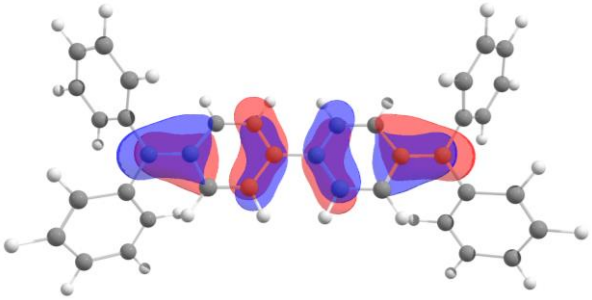


MO127 ("HOMO-1")

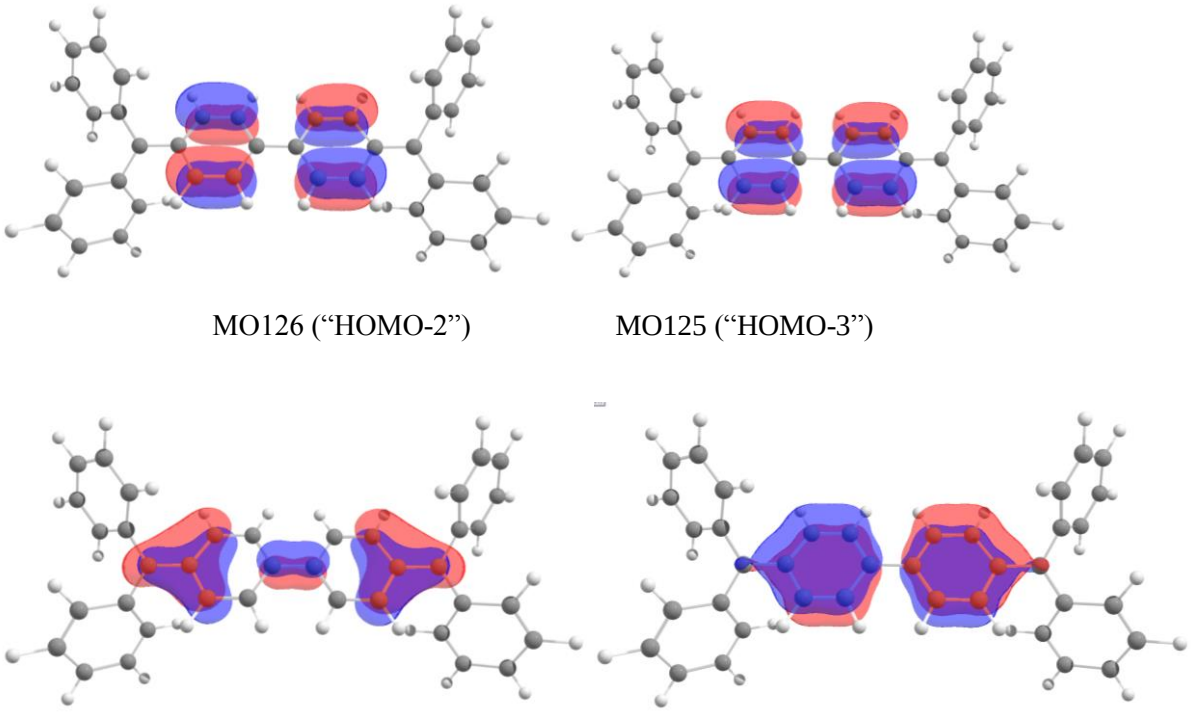


Figure S7. CASSCF optimized orbitals of **1** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.62088 [0]: 222222000000
0.15086 [7]: 222220200000
0.05012 [35]: 222211110000
0.01254 [6775]: 212221100010
0.01126 [2070]: 221122001100
0.01012 [274]: 222121101000
0.00861 [1563]: 221221100100
0.00543 [6851]: 212212010010
0.00538 [111]: 222202020000
0.00426 [24079]: 122221100001
0.00355 [781]: 222022002000
0.00347 [1639]: 221212010100
0.00333 [350]: 222112011000
0.00323 [2135]: 221120201100
0.00292 [3873]: 220222000200
0.00256 [24586]: 122122001001

Table S 11. Configurations of **1** for singlet multiplicity.

Thiele's Hydrocarbon (2)

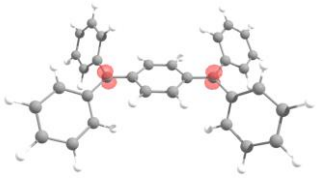
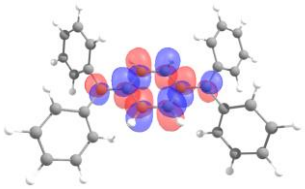
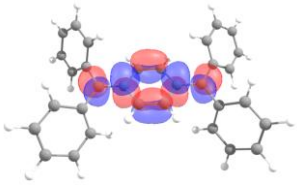


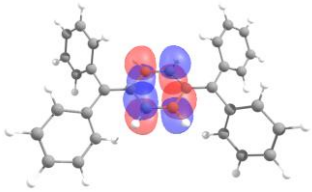
Figure S 8. FOD plot of **2** with a contour value of 0.005 e Bohr^{-3}.



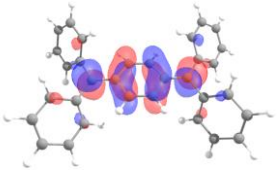
MO111 ("LUMO+3")



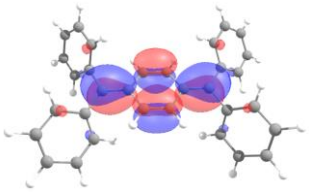
MO110 ("LUMO+2")



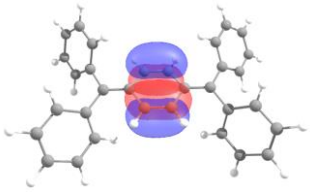
MO109 ("LUMO+1")



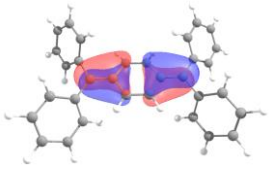
MO108 ("LUMO")



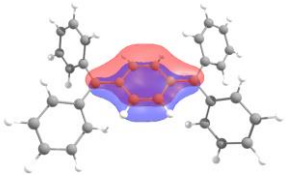
MO107 ("HOMO")



MO 106("HOMO-1")



MO 105("HOMO-2")



MO104 ("HOMO-3")

Figure S9. CASSCF optimized orbitals of **2** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.81225 [	0]:	22220000
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0.03153 [	96]:	21211010
0.01477 [	20]:	22111100
0.01244 [	49]:	22020200
0.00725 [	393]:	12120101
0.00711 [	388]:	12121100
0.00697 [	364]:	12211001
0.00593 [	223]:	20220020
0.00465 [	25]:	22110101
0.00378 [	491]:	11220011
0.00357 [	125]:	21120110
0.00325 [	48]:	22021001
0.00321 [	216]:	20222000
0.00305 [	365]:	12210200
0.00292 [	485]:	11221010

Table S12. Configurations of **2** for singlet multiplicity.

Tetracene (3)

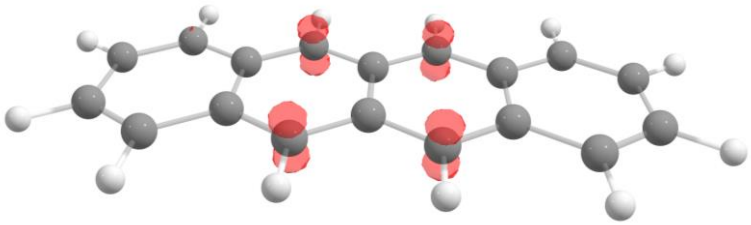
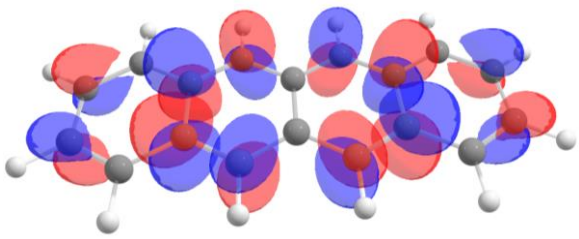
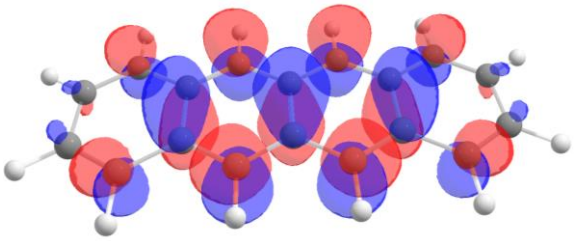


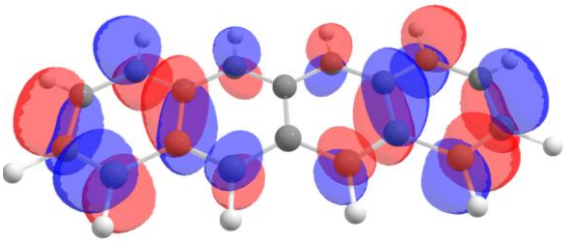
Figure S10. FOD plot of **3** with a contour value of 0.005 e Bohr^{-3}.



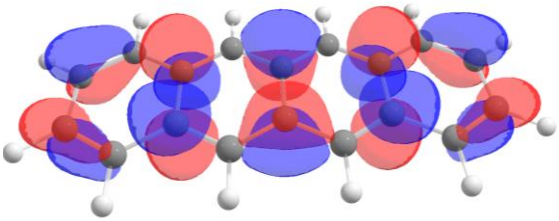
MO66 (“LUMO+5”)



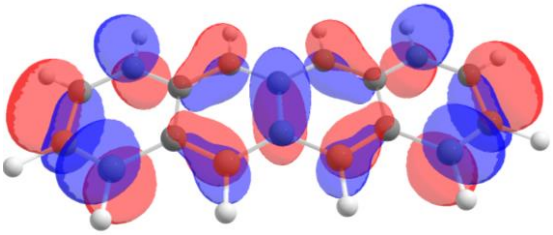
MO 65 (“LUMO+4”)



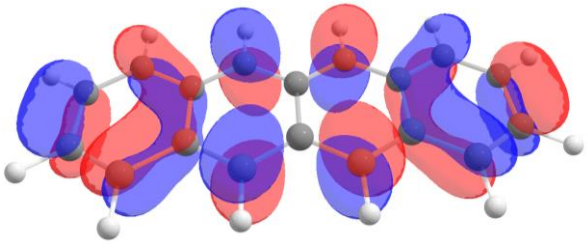
MO64 (“LUMO+3”)



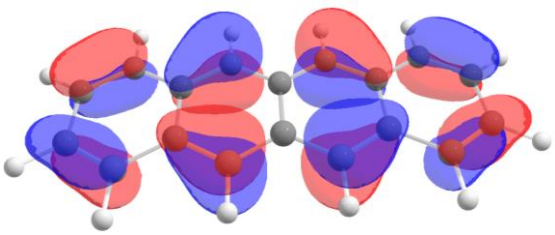
MO63 (“LUMO+2”)



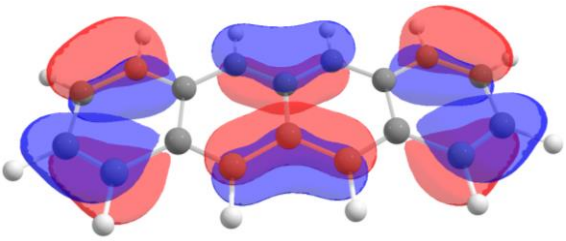
MO62 (“LUMO+1”)



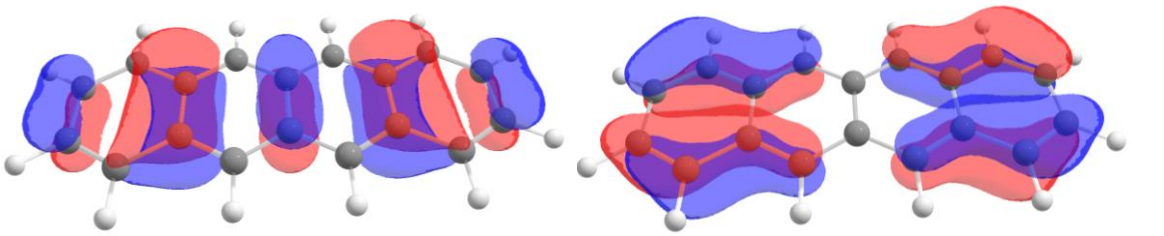
MO61 (“LUMO”)



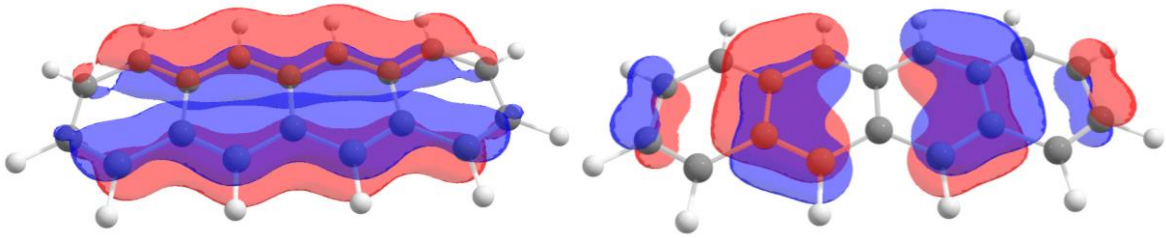
MO60 (“HOMO”)



MO59 (“HOMO-1”)



MO58 (“HOMO-2”) MO57 (“HOMO-3”)



MO56 (“HOMO-4”) MO55 (“HOMO-5”)

Figure S11. CASSCF optimized orbitals of **3** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.77191 [0]: 222222000000
0.03461 [7]: 222220200000
0.01554 [274]: 222121101000
0.01495 [35]: 222211110000
0.01102 [6775]: 212221100010
0.00846 [24079]: 122221100001
0.00773 [1563]: 221221100100
0.00640 [1639]: 221212010100
0.00622 [24586]: 122122001001
0.00523 [350]: 222112011000
0.00465 [781]: 222022002000
0.00357 [2070]: 221122001100
0.00335 [111]: 222202020000
0.00329 [7282]: 212122001010

Table S13. Configurations of **3** for singlet multiplicity.

Pentacene (4)

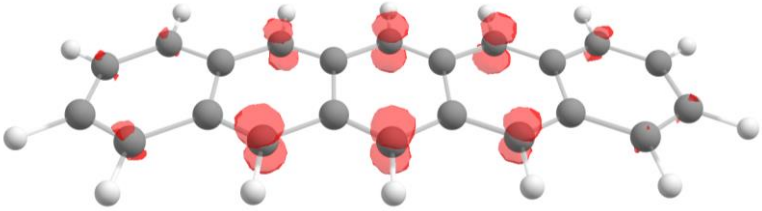
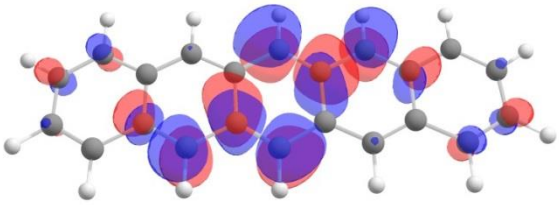
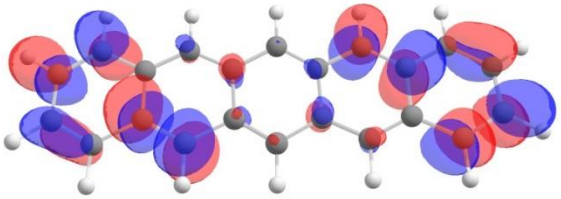


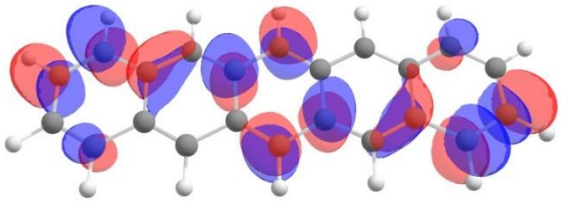
Figure S12. FOD plot of **4** with a contour value of 0.005 e Bohr^{-3}.



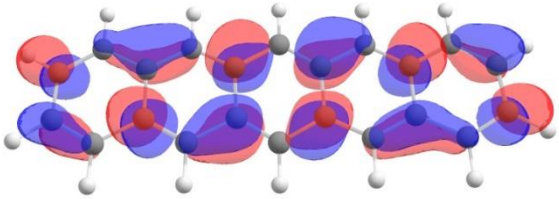
MO79 (“LUMO+5”)



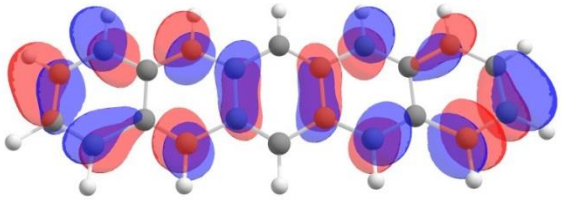
MO78 (“LUMO+4”)



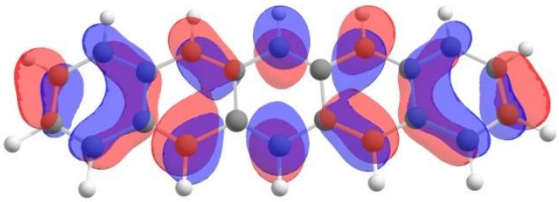
MO77 (“LUMO+3”)



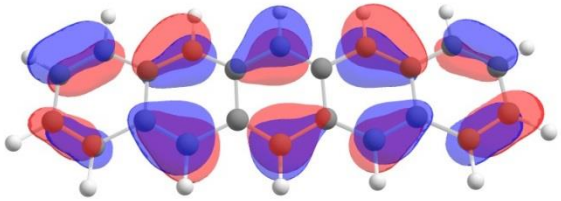
MO76 (“LUMO+2”)



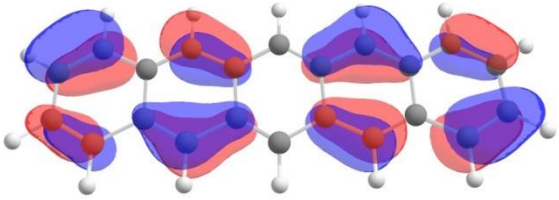
MO75 (“LUMO+1”)



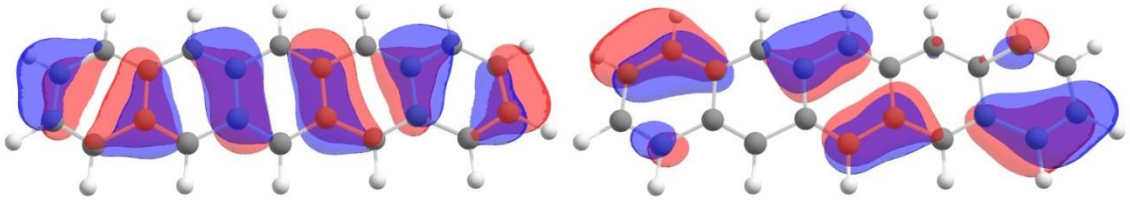
MO74 (“LUMO”)



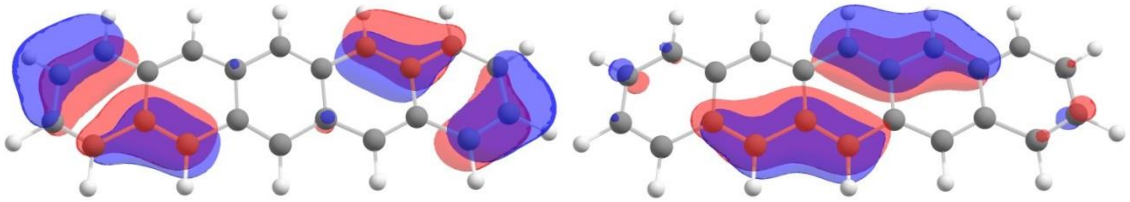
MO73 (“HOMO”)



MO72 (“HOMO-1”)



MO71 (“HOMO-2”) MO70 (“HOMO-3”)



MO69 (“HOMO-4”) MO68 (“HOMO-5”)

Figure S13. CASSCF optimized orbitals of **4** from state averaged calculation CASSCF(12,12) (5 singlet roots, 5 triplet roots).

0.75015 [0]: 22222220000000
0.03256 [8]: 22222202000000
0.01187 [44]: 22222111100000
0.01073 [423]: 22221211010000
0.01030 [2860]: 22212211001000
0.00641 [201656]: 12222211000001
0.00410 [58290]: 21222211000010
0.00407 [14477]: 22122120100100
0.00393 [2971]: 22212120101000
0.00380 [14366]: 22122211000100
0.00356 [58401]: 21222120100010
0.00354 [534]: 22221120110000
0.00347 [155]: 22222020200000
0.00342 [2859]: 22212211010000
0.00330 [3746]: 22211220011000
0.00328 [78156]: 21122220000110
0.00323 [7608]: 22202220002000
0.00300 [202542]: 12221220010001
0.00300 [424]: 22221211001000

Table S14. Configurations of **4** for singlet multiplicity and CASSCF(14,14).

<u>Bisnitroxide (5)</u>

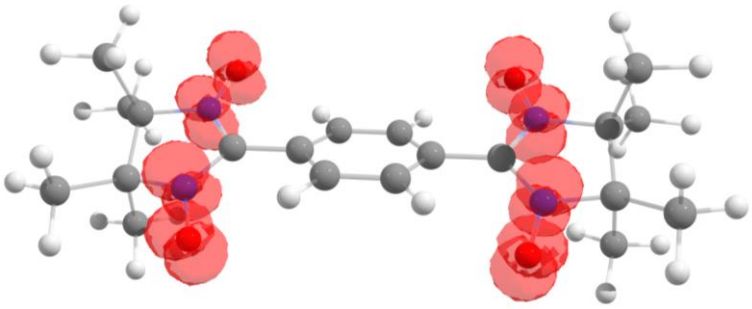
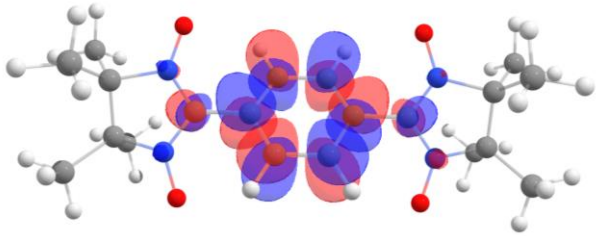
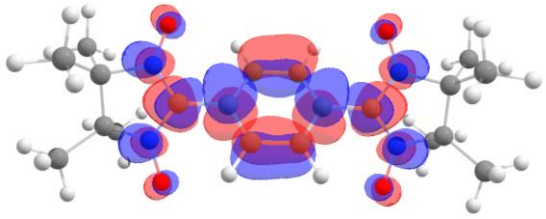


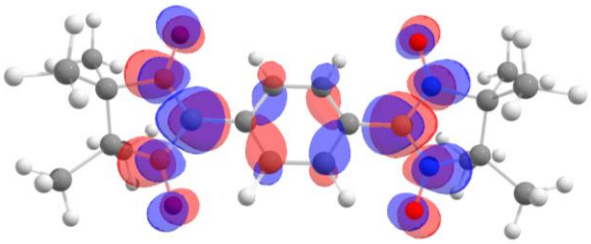
Figure S14. FOD plot of **5** with a contour value of 0.005 e Bohr^{-3}.



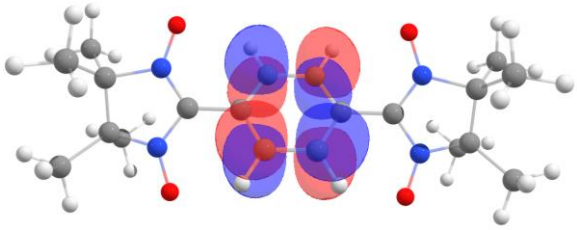
MO110 (“LUMO+5”)



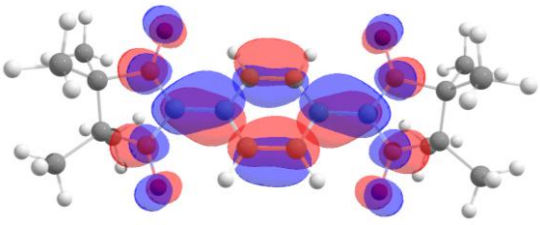
MO109 (“LUMO+4”)



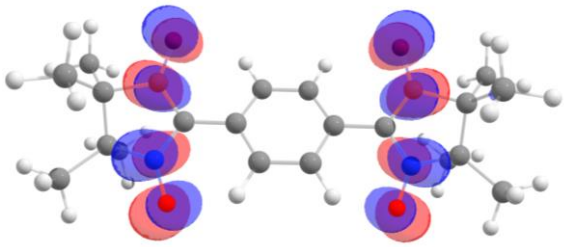
MO108 (“LUMO+3”)



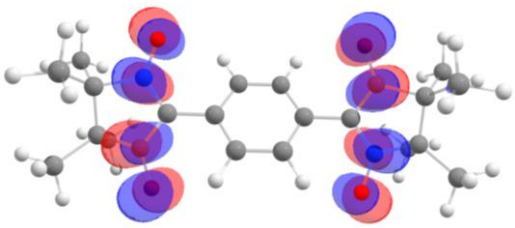
MO107 (“LUMO+2”)



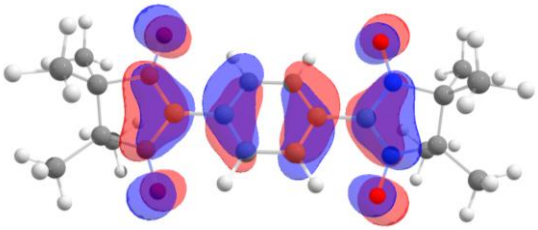
MO106 (“LUMO+1”)



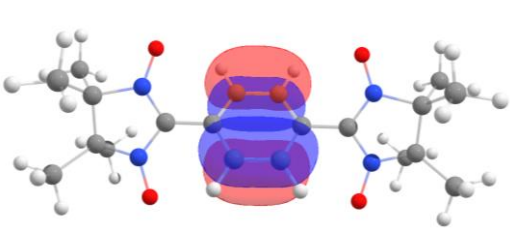
MO105 (“LUMO”)



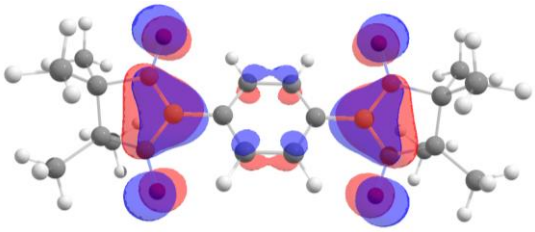
MO104 (“HOMO”)



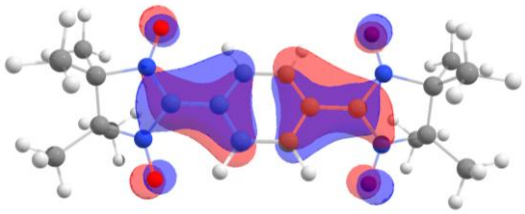
MO103 (“HOMO-1”)



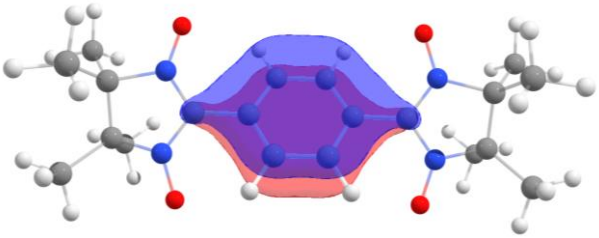
MO102 (“HOMO-2”)



MO101 (“HOMO-3”)



MO100 (“HOMO-4”)



MO99 (“HOMO-5”)

Figure S15. CASSCF optimized orbitals of **5** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.34902 [7]: 222220200000
0.34831 [0]: 222222000000
0.05322 [1563]: 221221100100
0.05248 [35]: 222211110000
0.00899 [38]: 222211100010
0.00830 [846]: 222020202000
0.00829 [781]: 222022002000
0.00711 [1639]: 221212010100
0.00711 [1704]: 221210210100
0.00586 [6772]: 212221110000
0.00524 [111]: 222202020000
0.00520 [6851]: 212212010010
0.00517 [6916]: 212210210010
0.00514 [176]: 222200220000
0.00473 [6775]: 212221100010
0.00440 [350]: 222112011000
0.00440 [415]: 222110211000
0.00383 [24651]: 122120201001
0.00382 [24586]: 122122001001
0.00364 [3938]: 220220200200
0.00357 [3873]: 220222000200
0.00357 [7341]: 212120211000
0.00356 [7276]: 212122011000

Table S15. Configurations of **5** for singlet multiplicity.

Bisoxoverdazyl (6)

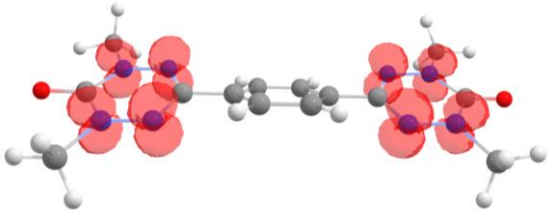
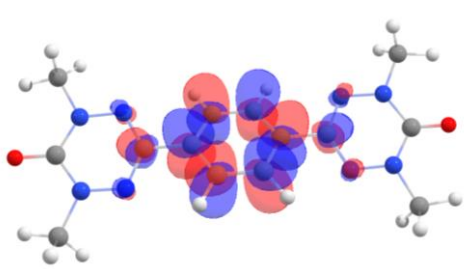
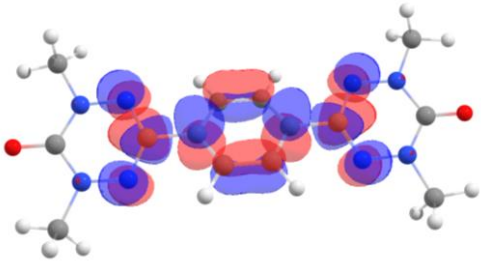


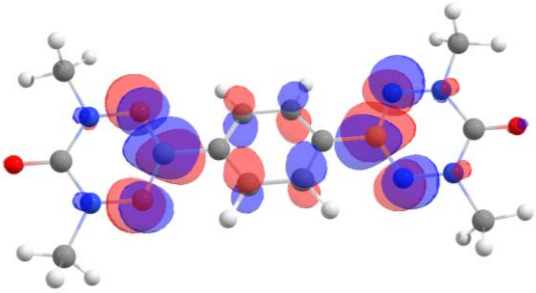
Figure S16. FOD plot of **6** with a contour value of 0.005 e Bohr^{-3}.



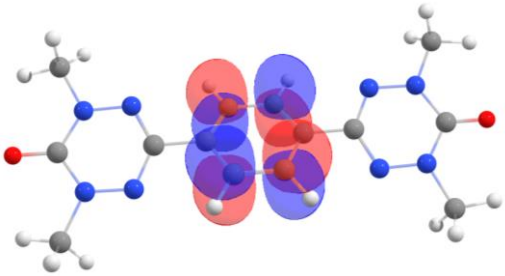
MO92 ("LUMO+5")



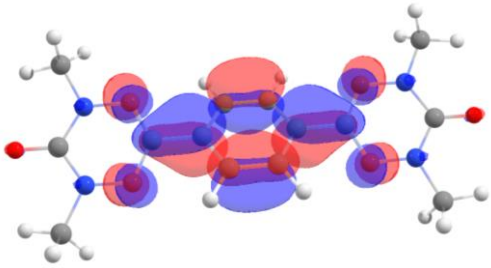
MO91 ("LUMO+4")



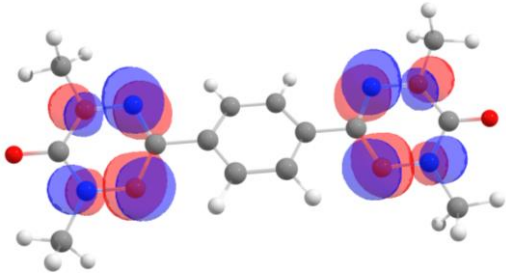
MO90 ("LUMO+3")



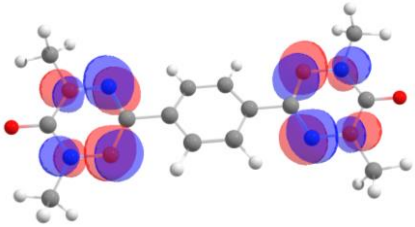
MO89 ("LUMO+2")



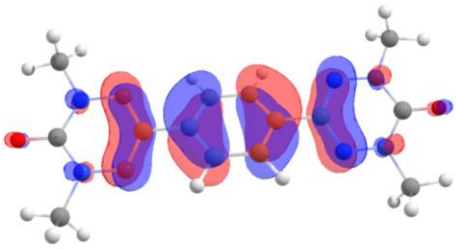
MO88 ("LUMO+1")



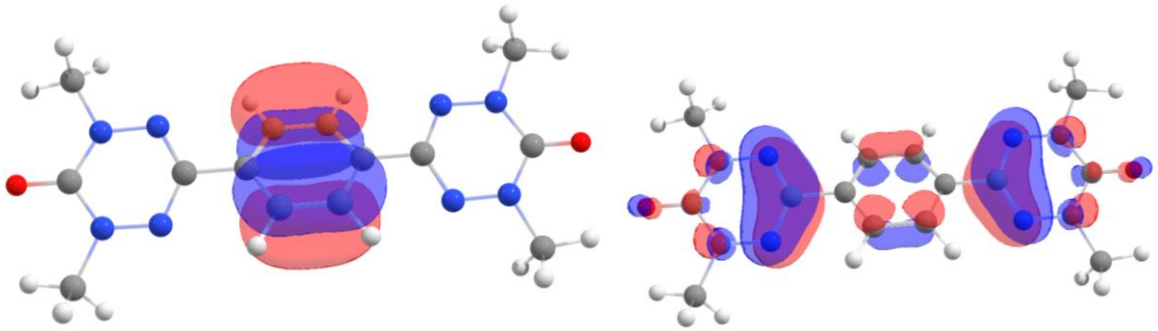
MO87 ("LUMO")



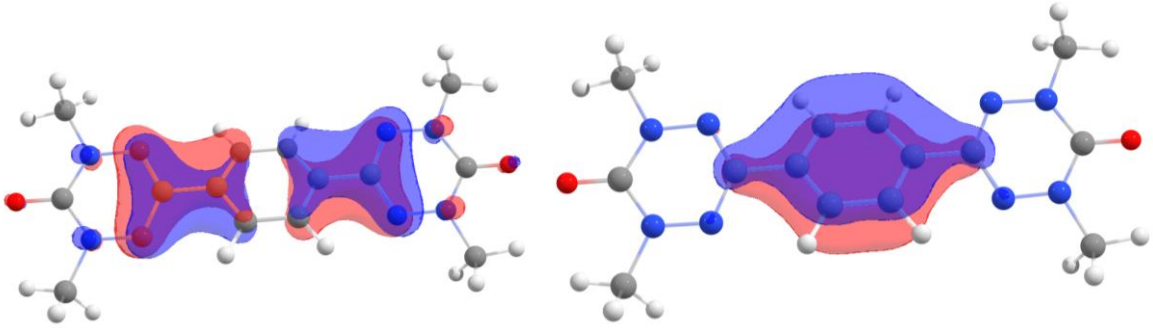
MO86 ("HOMO")



MO85 ("HOMO-1")



MO84 (“HOMO-2”) MO83 (“HOMO-3”)



MO82 (“HOMO-4”) MO81 (“HOMO-5”)

Figure S17. CASSCF optimized orbitals of **6** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.37395 [0]: 222222000000
0.37159 [7]: 222220200000
0.04400 [274]: 222121101000
0.03589 [35]: 222211110000
0.00841 [3873]: 220222000200
0.00836 [3938]: 220220200200
0.00728 [38]: 222211100010
0.00723 [6772]: 212221110000
0.00619 [6775]: 212221100010
0.00541 [6851]: 212212010010
0.00537 [6916]: 212210210010
0.00515 [1639]: 221212010100
0.00512 [1704]: 221210210100
0.00432 [26389]: 121222000101
0.00430 [26454]: 121220200101
0.00415 [350]: 222112011000
0.00414 [415]: 222110211000
0.00413 [111]: 222202020000
0.00411 [176]: 222200220000
0.00303 [9077]: 211222010100
0.00302 [9142]: 211220210100
0.00260 [846]: 222020202000
0.00260 [781]: 222022002000
0.00254 [1647]: 221212000110
0.00253 [1712]: 221210200110

Table S16. Configurations of **6** for singlet multiplicity.

Terphenoquinone (7)

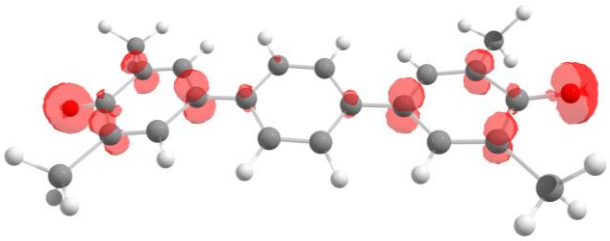
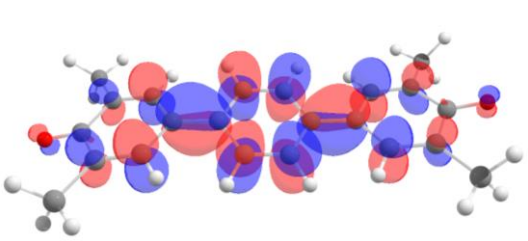
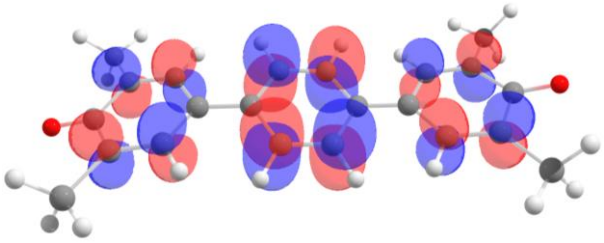


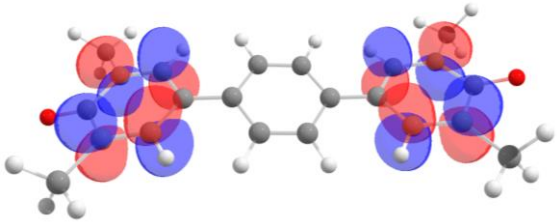
Figure S18. FOD plot of **7** with a contour value of 0.005 e Bohr^{-3}.



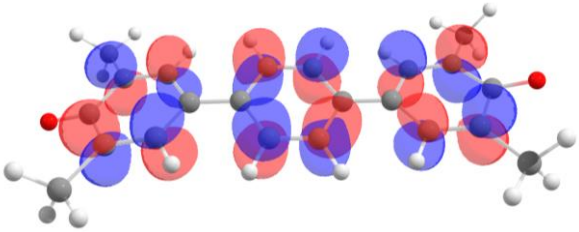
MO79 (“LUMO+5”)



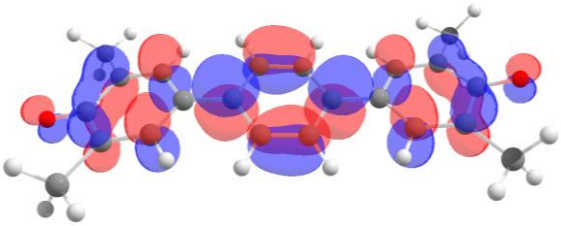
MO78 (“LUMO+4”)



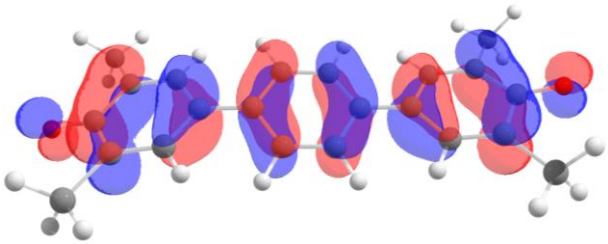
MO77 (“LUMO+3”)



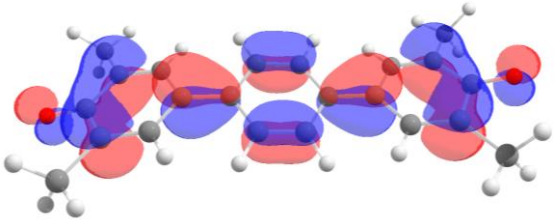
MO76 (“LUMO+2”)



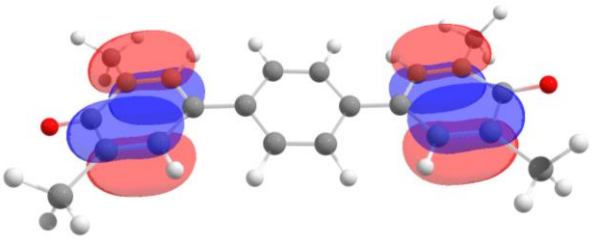
MO75 (“LUMO+1”)



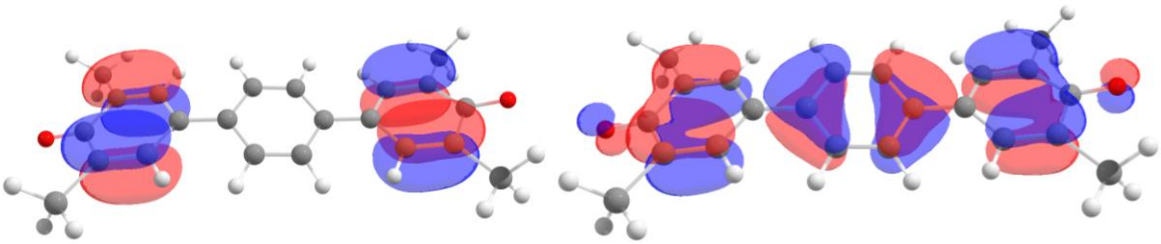
MO74 (“LUMO”)



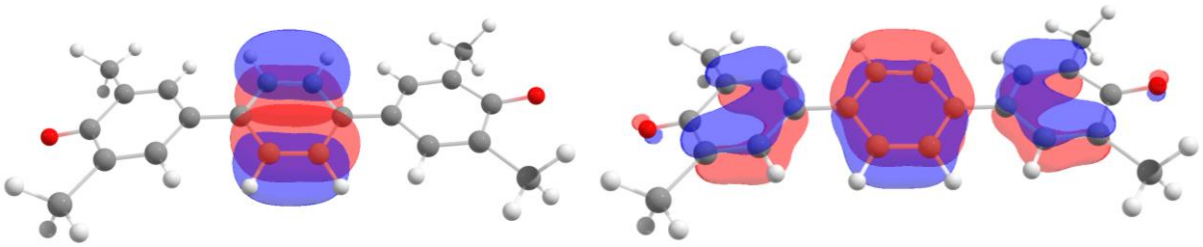
MO73 (“HOMO”)



MO72 (“HOMO-1”)



MO71 (“HOMO-2”) MO70 (“HOMO-3”)



MO69 (“HOMO-4”) MO68 (“HOMO-5”)

Figure S19. CASSCF optimized orbitals of **7** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.69987 [0]: 222222000000
0.10065 [7]: 222220200000
0.01092 [1563]: 221221100100
0.01004 [350]: 222112011000
0.00950 [6775]: 212221100010
0.00944 [35]: 222211110000
0.00927 [274]: 222121101000
0.00923 [24079]: 122221100001
0.00853 [49741]: 022222000002
0.00529 [2070]: 221122001100
0.00518 [1639]: 221212010100
0.00364 [6854]: 212212001100
0.00363 [1633]: 221212101000
0.00360 [7277]: 212122010100
0.00360 [2059]: 221122110000
0.00351 [359]: 222112000110
0.00308 [1644]: 221212001010
0.00307 [7282]: 212122001010
0.00307 [2067]: 221122010010
0.00306 [9076]: 211222011000
0.00304 [6851]: 212212010010
0.00285 [111]: 222202020000
0.00283 [781]: 222022002000
0.00260 [346]: 222112100100

Table S17. Configurations of **7** for singlet multiplicity.

CAAC–C_6H_4–CAAC (8)

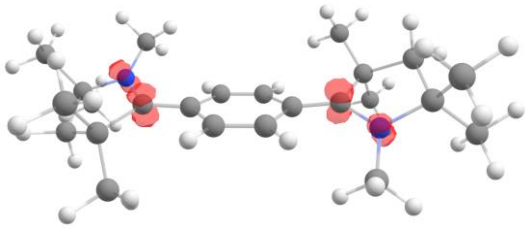
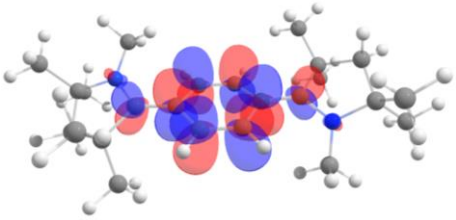
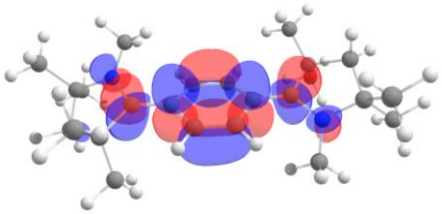


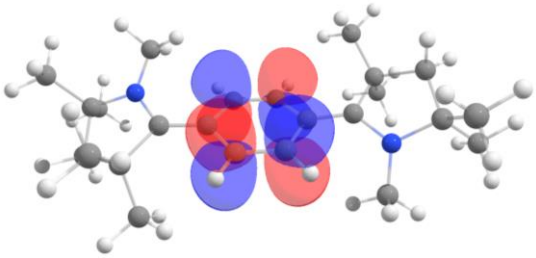
Figure S20. FOD plot of **8** with a contour value of 0.005 e $Bohr^{-3}$.



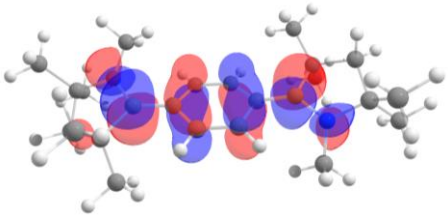
MO102 (“LUMO+3”)



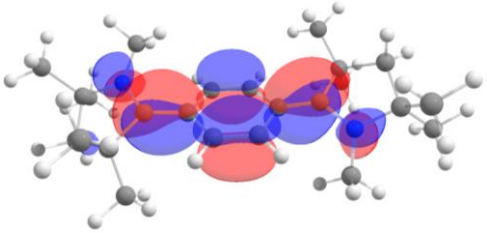
MO101 (“LUMO+2”)



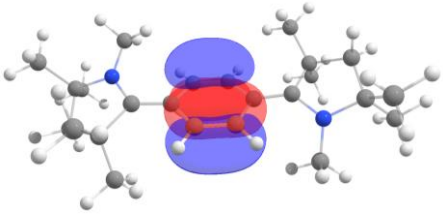
MO100 (“LUMO+1”)



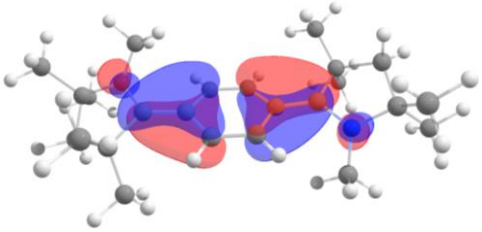
MO99 (“LUMO”)



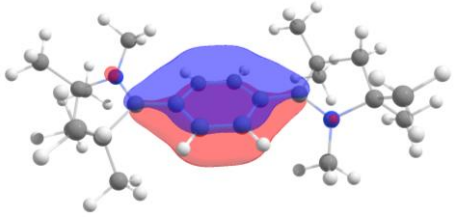
MO98 (“HOMO”)



MO97 (“HOMO-1”)



MO96 (“HOMO-2”)



MO95 (“HOMO-3”)

Figure S21. CASSCF optimized orbitals of **8** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.74596 [0]: 2222200000
0.09612 [6]: 2222020000
0.04093 [28]: 2221110100

0.01136 [432]: 2202202000
0.01135 [167]: 2212111000
0.01040 [792]: 2122110010
0.00650 [2916]: 1222110001
0.00589 [80]: 2220200200
0.00546 [1057]: 2112201010
0.00513 [217]: 2211201100
0.00393 [173]: 2212101010
0.00350 [844]: 2121200110
0.00338 [1051]: 2112211000
0.00260 [36]: 2221100110

Table S18. Configurations of **8** for singlet multiplicity.

NHC–C_6H_4–NHC (9)

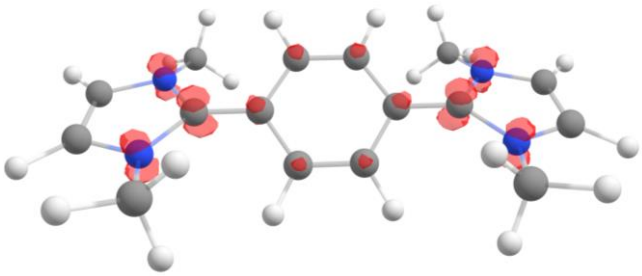
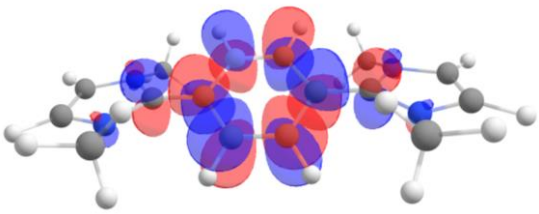
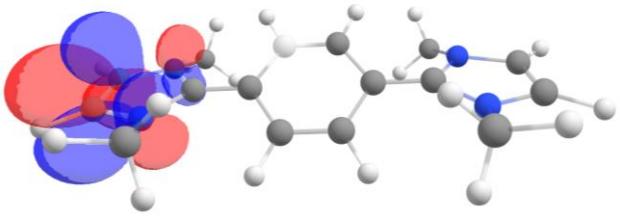


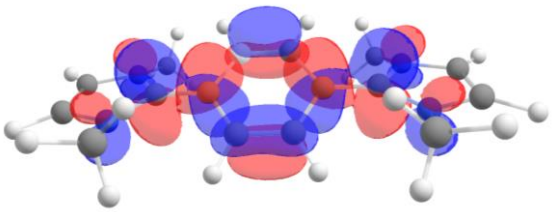
Figure S22. FOD plot of **9** with a contour value of 0.005 e $Bohr^{-3}$.



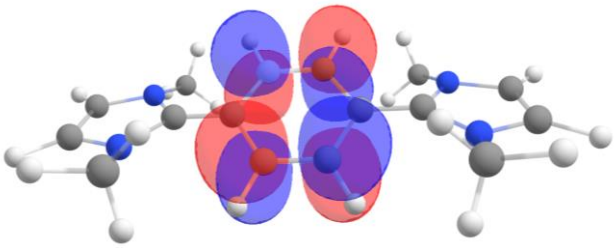
MO78 (“LUMO+4”)



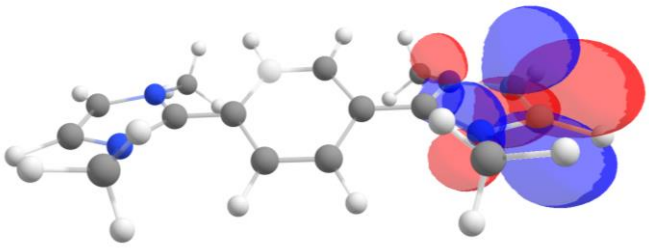
MO77 (“LUMO+3”)



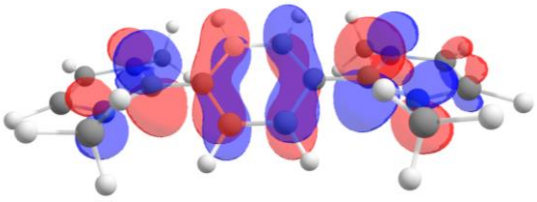
MO76 (“LUMO+2”)



MO75 (“LUMO+1”)



MO74 (“LUMO”)



MO73 (“HOMO”)

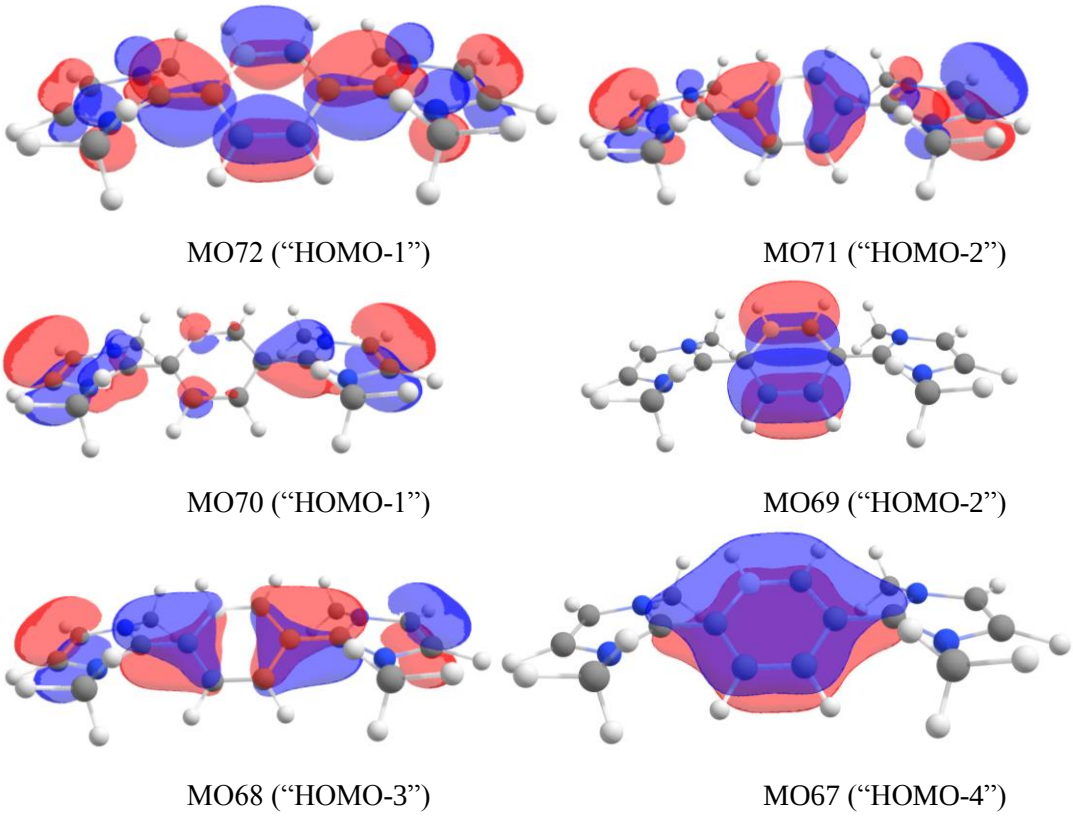


Figure S23. CASSCF optimized orbitals of **9** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.78336 [0]: 222222000000
0.02483 [7]: 222220200000
0.01609 [35]: 222211110000
0.01562 [6775]: 212221100010
0.01186 [111]: 222202020000
0.01125 [2070]: 221122001100
0.00875 [2069]: 221122002000
0.00875 [2073]: 221122000200
0.00758 [781]: 222022002000
0.00728 [785]: 222022000200
0.00709 [3873]: 220222000200
0.00681 [3869]: 220222002000
0.00568 [24079]: 122221100001
0.00512 [24146]: 122212110000
0.00494 [44]: 222211010001
0.00450 [24155]: 122212010001
0.00414 [32437]: 112222000011
0.00383 [6790]: 212221000011
0.00380 [15133]: 202222000020
0.00347 [24080]: 122221020000
0.00274 [25]: 222220000020
0.00252 [110]: 222202100001

Table S19. Configurations of **9** for singlet multiplicity.

CAAC–C–CAAC (10)

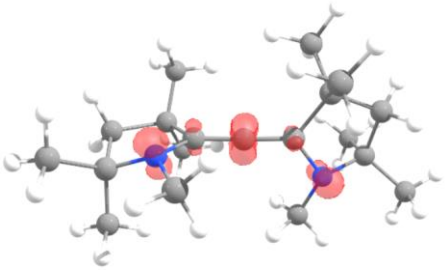
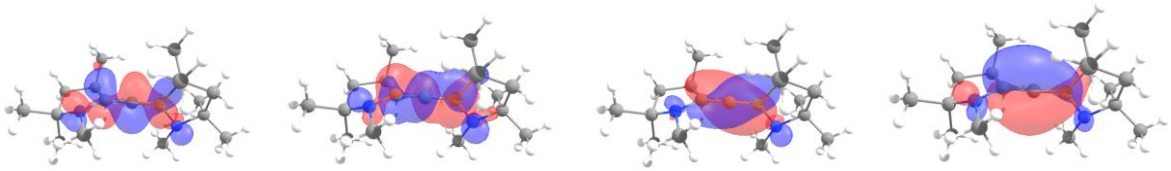


Figure S24. FOD plot of **10** with a contour value of 0.005 e Bohr^{-3}.



MO78 (“LUMO+1”) **MO79 (“LUMO”)** **MO80 (“HOMO”)** MO81 (“HOMO-1”)

Figure S25. CASSCF optimized orbitals of **10** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.88883 [	0]:	2200
0.03936 [	1]:	2110
0.02789 [	7]:	1201
0.02117 [	15]:	0202
0.01872 [	3]:	2020

Table S20. Configurations of **10** for singlet multiplicity.

CAAC–CC–CAAC (11)

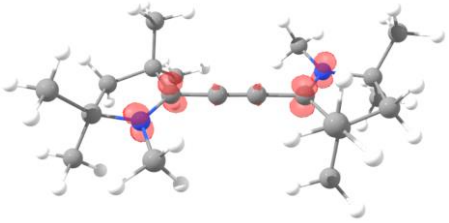
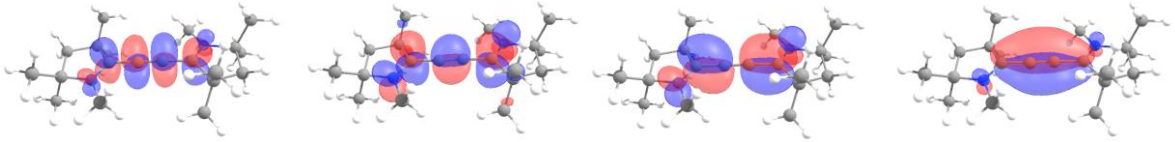


Figure S26. FOD plot of **11** with a contour value of 0.005 e Bohr^{-3}.



MO 78 (“LUMO+1”) **MO 79 (“LUMO”)** **MO 80 (“HOMO”)** MO 81 (“HOMO-1”)

Figure S27. CASSCF optimized orbitals of **11** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.87049 [	0]:	2200
0.09564 [	3]:	2020
0.02458 [	9]:	1111
0.00615 [	15]:	0202

Table S21. Configurations of **11** for singlet multiplicity.

CAAC–CCCC–CAAC (12)

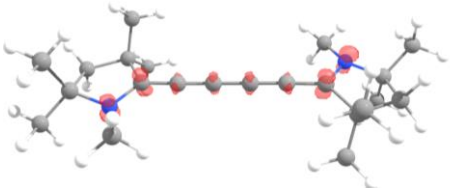
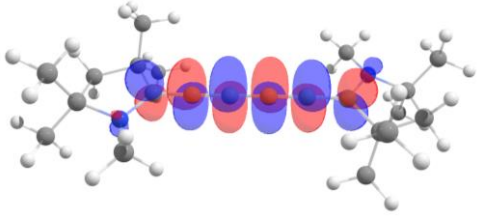
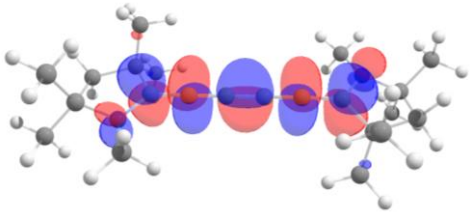


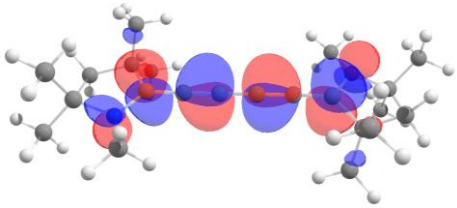
Figure S28. FOD plot of **12** with a contour value of 0.005 e Bohr^{-3}.



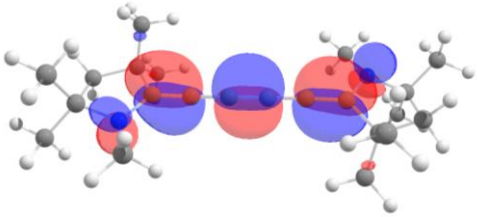
MO93 (“LUMO+2”)



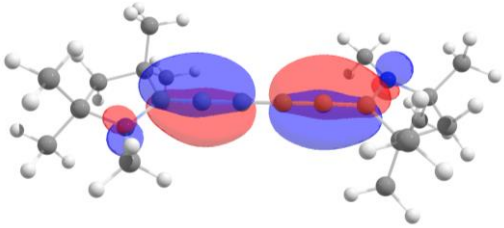
MO92 (“LUMO+1”)



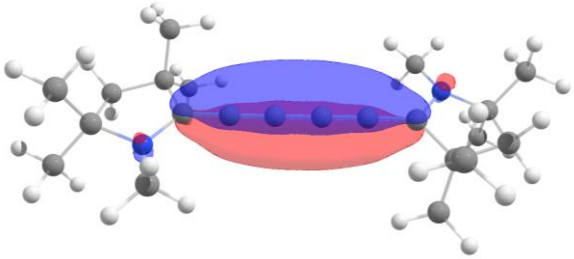
MO91 (“LUMO”)



MO90 (“HOMO”)



MO89 (“HOMO-1”)



MO88 (“HOMO-2”)

Figure S29. CASSCF optimized orbitals of **12** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.84305 [0]: 222000
0.05669 [4]: 220200
0.02856 [14]: 211110
0.02473 [10]: 212100
0.01410 [50]: 121101
0.00478 [29]: 202020
0.00433 [65]: 112011
0.00259 [7]: 220020
0.00254 [17]: 211011

Table S22. Configurations of **12** for singlet multiplicity.

CAAC–CC–C_6H_4–CC–CAAC (13)

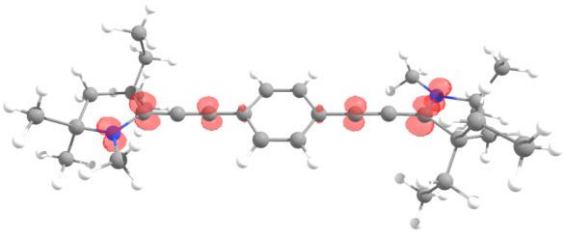
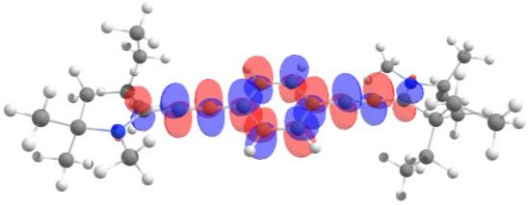
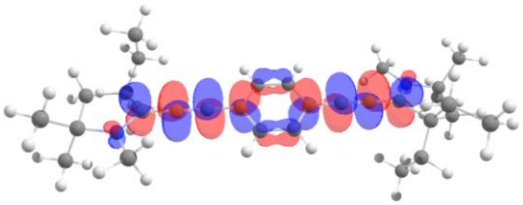


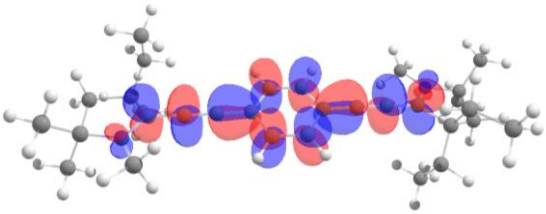
Figure S30. FOD plot of **13** with a contour value of 0.005 e $Bohr^{-3}$.



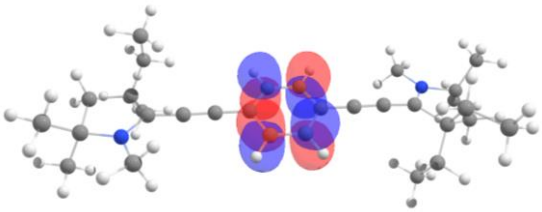
MO131 (“LUMO+5”)



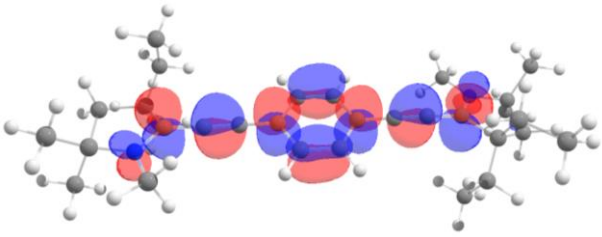
MO130 (“LUMO+4”)



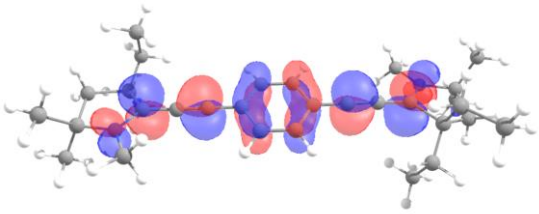
MO129 (“LUMO+3”)



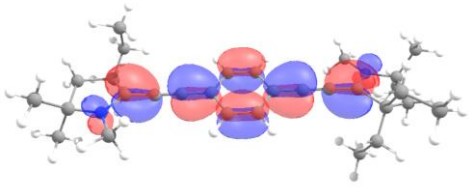
MO128 (“LUMO+2”)



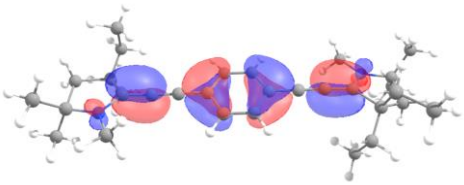
MO127 (“LUMO+1”)



MO127 (“LUMO”)



MO126 (“HOMO”)



MO125 (“HOMO-1”)

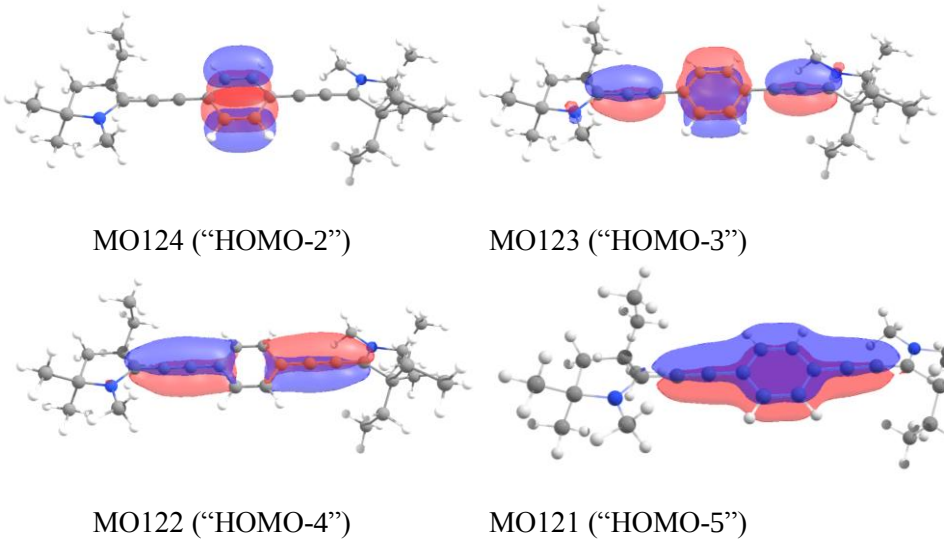


Figure S31. CASSCF optimized orbitals of **13** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.71499 [0]: 222222000000
0.07529 [7]: 222220200000
0.04106 [35]: 222211110000
0.01111 [1563]: 221221100100
0.01097 [781]: 222022002000
0.00949 [6775]: 212221100010
0.00911 [274]: 222121101000
0.00645 [111]: 222202020000
0.00535 [24079]: 122221100001
0.00443 [350]: 222112011000
0.00403 [2070]: 221122001100
0.00388 [1639]: 221212010100
0.00347 [6851]: 212212010010
0.00340 [2060]: 221122101000
0.00297 [284]: 222121001100
0.00283 [13]: 222220020000
0.00276 [42]: 222211010100
0.00254 [24155]: 122212010001

Table S23. Configurations of **13** for singlet multiplicity.

CAAC–CC–C_6H_4–C_6H_4–CC–CAAC (14)

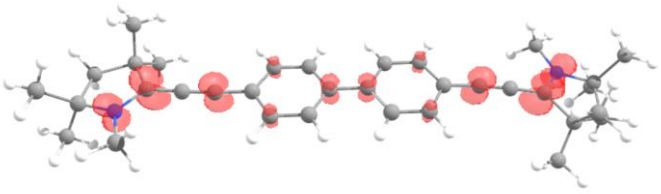
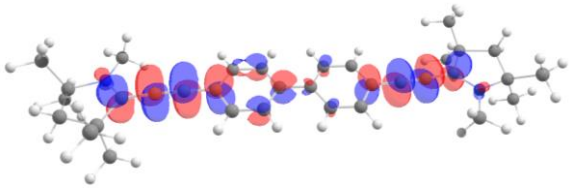
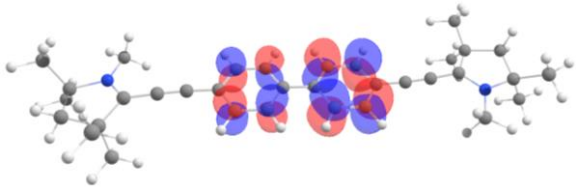


Figure S32. FOD plot of **14** with a contour value of 0.005 e $Bohr^{-3}$.

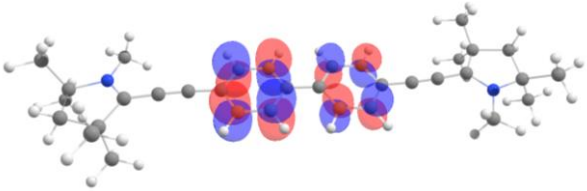


MO137 (“LUMO+6”)

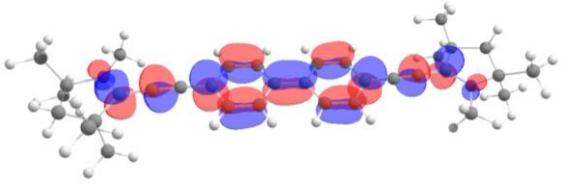
MO136 (“LUMO+5”)



MO135 (“LUMO+4”)

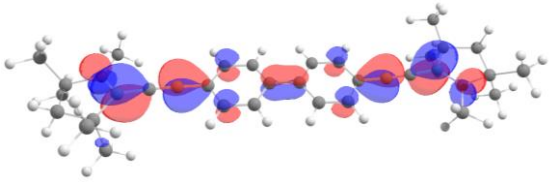


MO134 (“LUMO+3”)

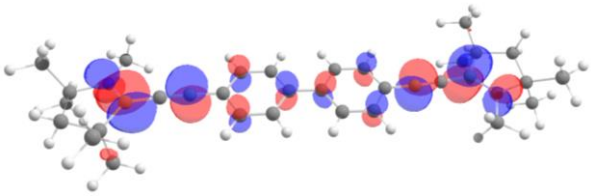


MO133 (“LUMO+2”)

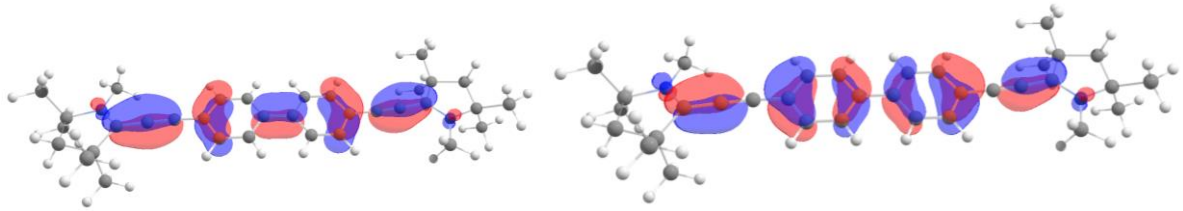
MO132 (“LUMO+1”)



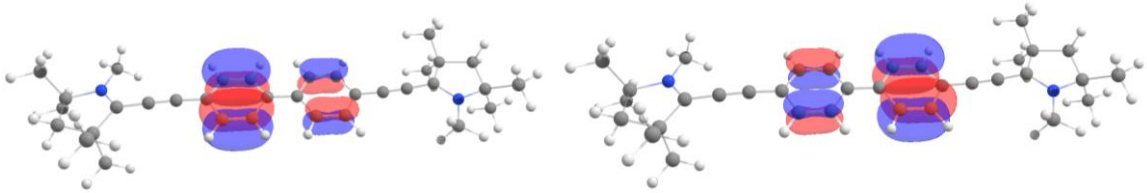
MO131 (“LUMO”)



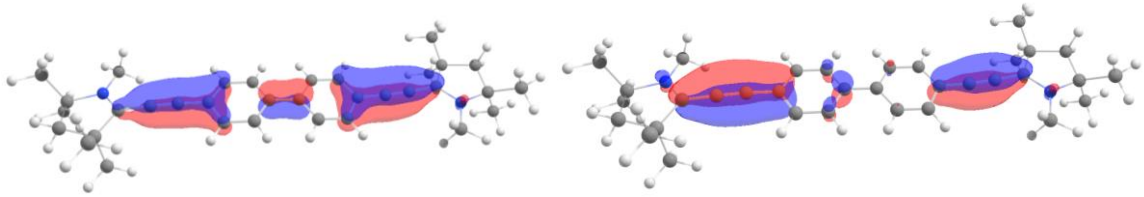
MO130 (“HOMO”)



MO129 (“HOMO-1”) MO128 (“HOMO-2”)



MO127 (“HOMO-3”) MO126 (“HOMO-4”)



MO125 (“HOMO-5”) MO124 (“HOMO-6”)

Figure S33. CASSCF optimized orbitals of **14** from state averaged calculation (4 singlet roots, 3 triplet roots).

0.47622 [0]: 22222220000000
0.30365 [8]: 22222202000000
0.03172 [44]: 22222111100000
0.01844 [423]: 22221211010000
0.01107 [58290]: 21222211000010
0.00730 [201656]: 12222211000001
0.00460 [534]: 22221120110000
0.00354 [7608]: 22202220002000
0.00327 [19114]: 22112220001100
0.00322 [155]: 22222020200000
0.00311 [632]: 22221102110000
0.00301 [34232]: 22022220000200

Table S24. Configurations of **14** for singlet multiplicity.

$Ph_2C–CC–C_6H_4–CC–CPh_2$ (15)

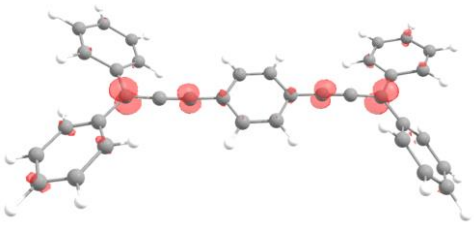
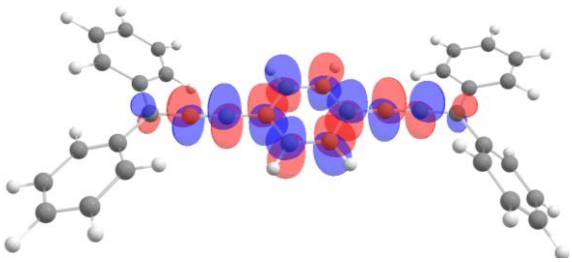
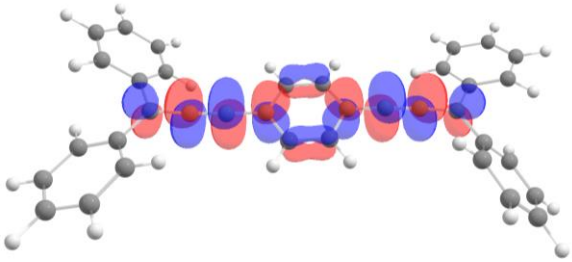


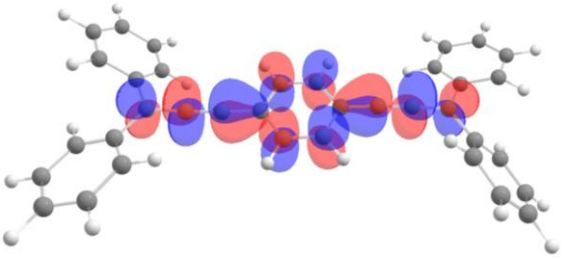
Figure S34. FOD plot of **15** with a contour value of 0.005 e $Bohr^{-3}$.



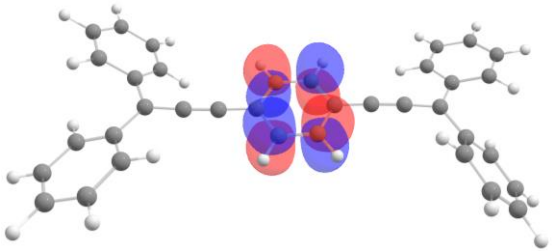
MO126 (“LUMO+5”)



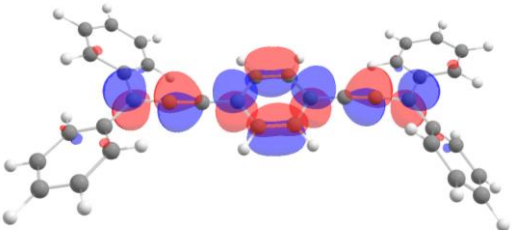
MO125 (“LUMO+4”)



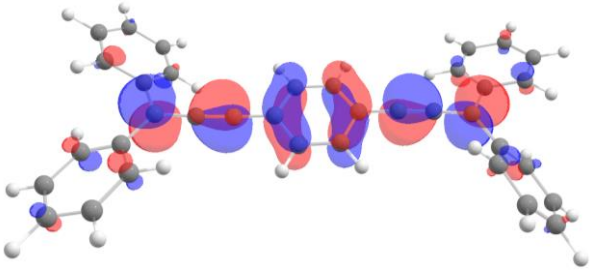
MO124 (“LUMO+3”)



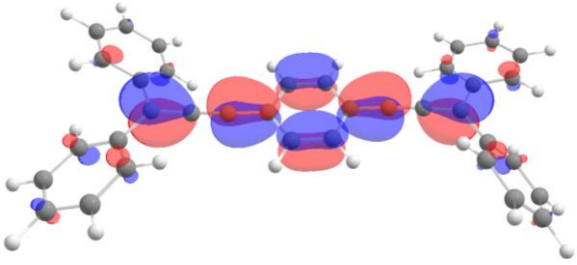
MO123 (“LUMO+2”)

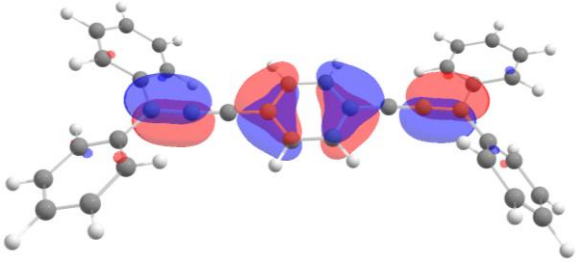


MO122 (“LUMO+1”)

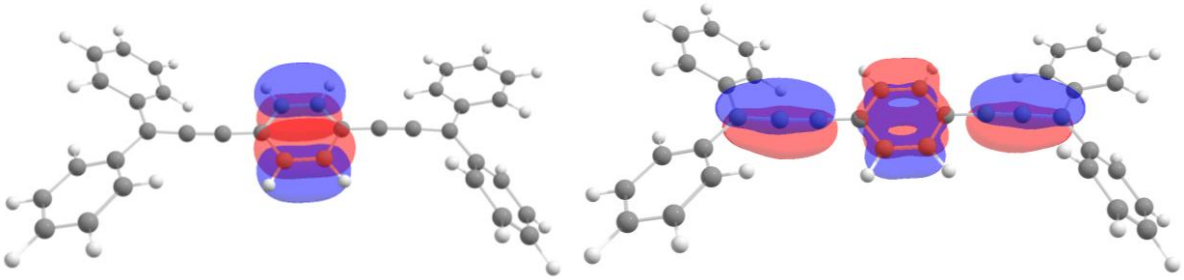


MO121 (“LUMO”)

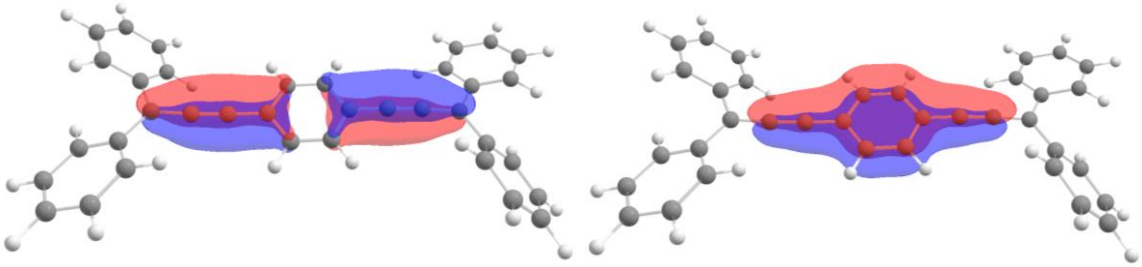




MO120 (“HOMO”) MO119 (“HOMO-1”)



MO118 (“HOMO-2”) MO117 (“HOMO-3”)



MO116 (“HOMO-4”) MO115 (“HOMO-5”)

Figure S35. CASSCF optimized orbitals of **15** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.63283 [0]: 222222000000
0.12178 [7]: 222220200000
0.05275 [35]: 222211110000
0.01515 [1563]: 221221100100
0.01141 [781]: 222022002000
0.01099 [6775]: 212221100010
0.00996 [274]: 222121101000
0.00779 [111]: 222202020000
0.00572 [350]: 222112011000
0.00505 [24079]: 122221100001
0.00489 [1639]: 221212010100
0.00392 [6851]: 212212010010
0.00328 [2070]: 221122001100
0.00304 [176]: 222200220000
0.00286 [846]: 222020202000
0.00265 [1632]: 221212110000
0.00260 [24155]: 122212010001
0.00255 [284]: 222121001100
0.00254 [24584]: 122122001100

Table S25. Configurations of **15** for singlet multiplicity.

Alkylidene–CC–C_6H_4–C_6H_4–CC–alkylidene (16)

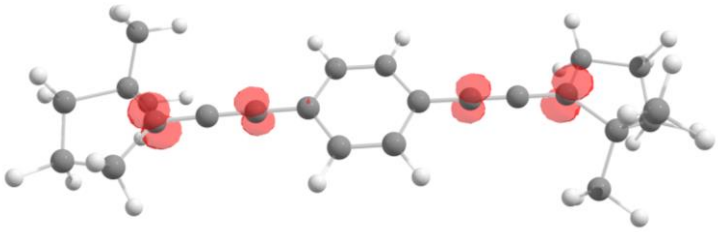
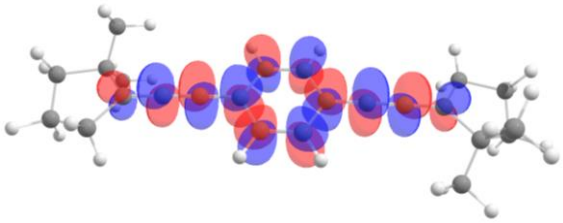
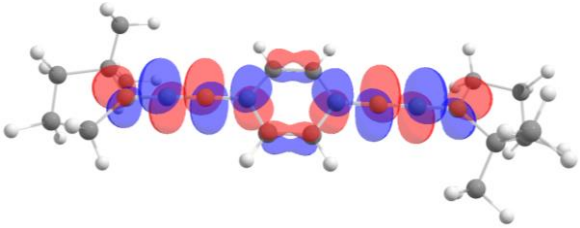


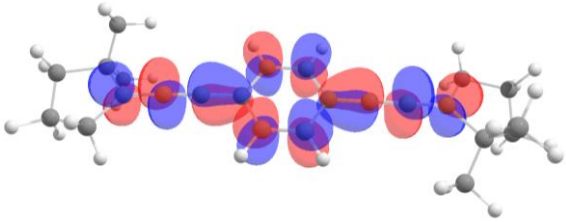
Figure S36. FOD plot of **16** with a contour value of 0.005 e Bohr^{-3}.



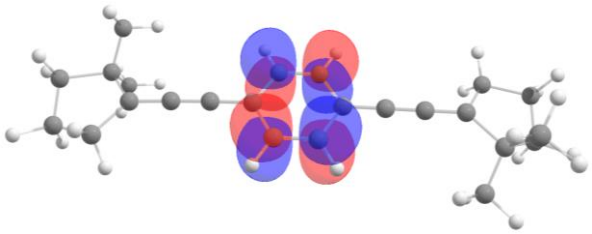
MO92 (“LUMO+5”)



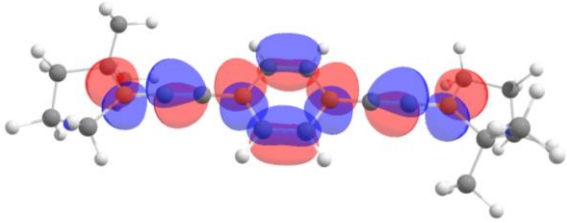
MO91 (“LUMO+4”)



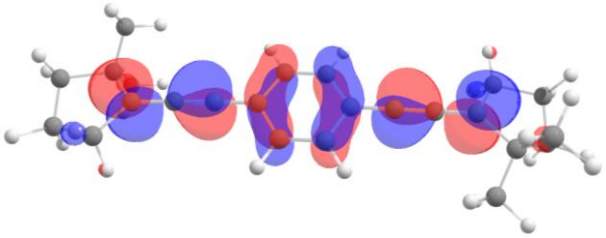
MO90 (“LUMO+3”)



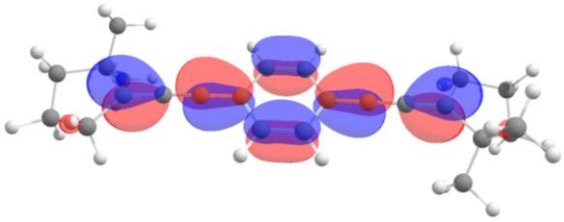
MO89 (“LUMO+2”)



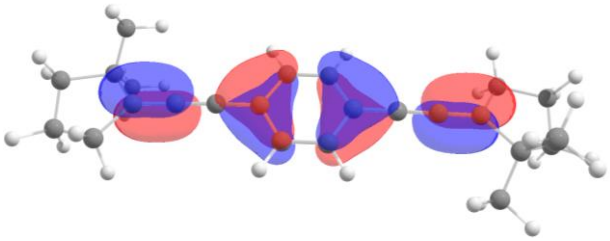
MO88 (“LUMO+1”)



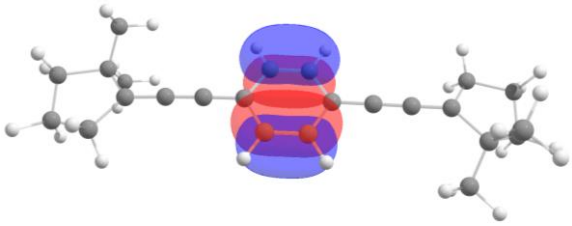
MO87 (“LUMO”)



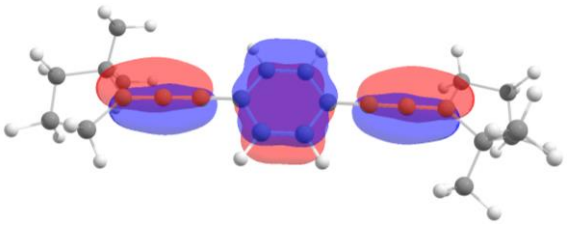
MO86 (“HOMO”)



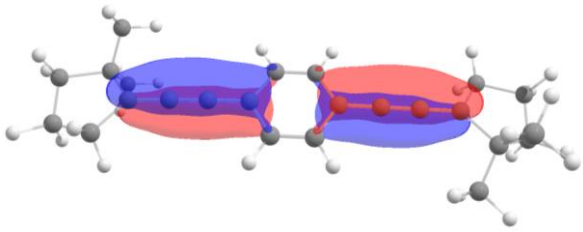
MO85 (“HOMO-1”)



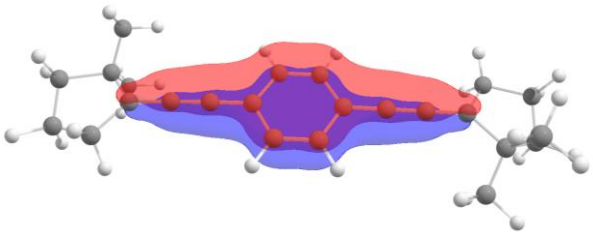
MO84 (“HOMO-2”)



MO83 (“HOMO-3”)



MO82 (“HOMO-4”)



MO81 (“HOMO-5”)

Figure S37. CASSCF optimized orbitals of **16** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.65992 [0]: 222222000000
0.08465 [7]: 222220200000
0.04914 [35]: 222211110000
0.01390 [1563]: 221221100100
0.01148 [781]: 222022002000
0.01127 [6775]: 212221100010
0.01066 [274]: 222121101000
0.00725 [111]: 222202020000
0.00621 [28]: 222212100000
0.00602 [24079]: 122221100001
0.00487 [1639]: 221212010100
0.00468 [350]: 222112011000
0.00406 [6851]: 212212010010
0.00404 [2070]: 221122001100
0.00351 [284]: 222121001100
0.00322 [2060]: 221122101000
0.00310 [1632]: 221212110000
0.00274 [24155]: 122212010001

Table S26. Configurations of **16** for singlet multiplicity.

Fischer–CC–C_6H_4–C_6H_4–CC–Fischer (17)

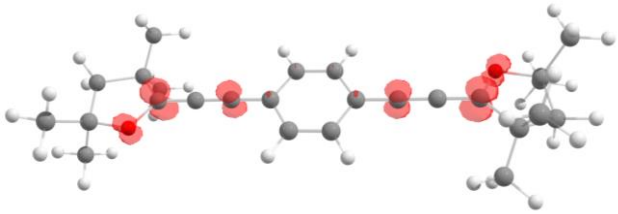
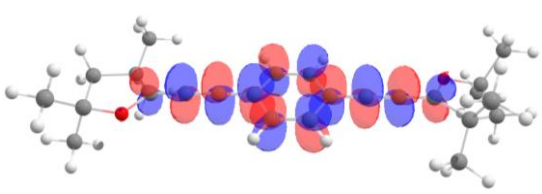
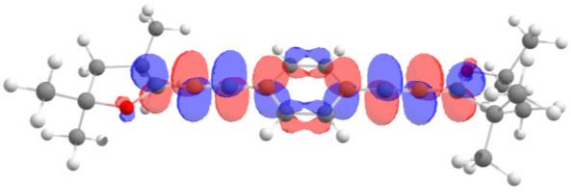


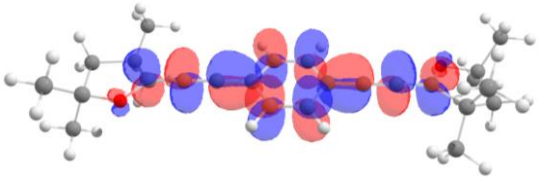
Figure S38. FOD plot of **17** with a contour value of 0.005 e Bohr^{-3}.



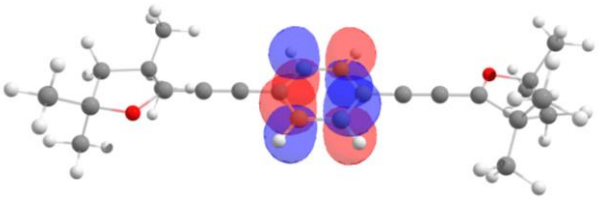
MO106 (“LUMO+5”)



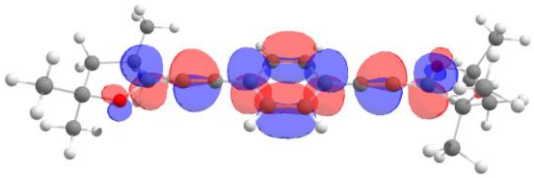
MO105 (“LUMO+4”)



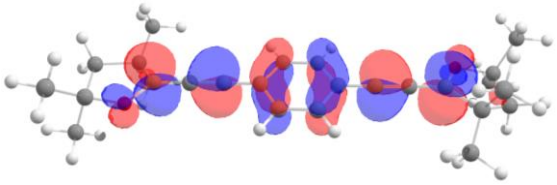
MO106 (“LUMO+3”)



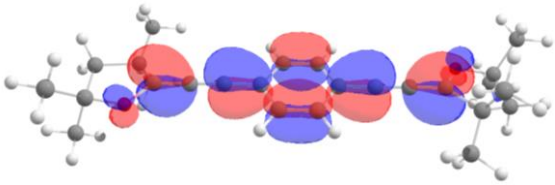
MO105 (“LUMO+2”)



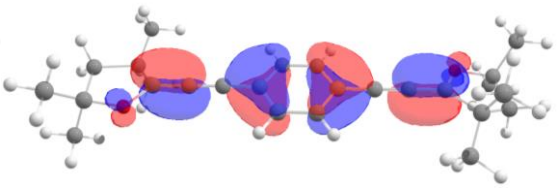
MO104 (“LUMO+1”)



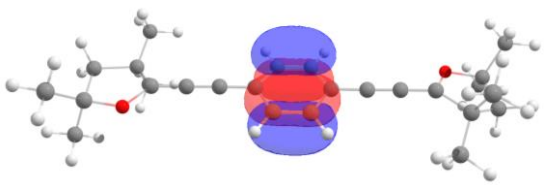
MO103 (“LUMO”)



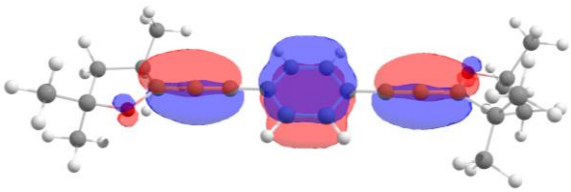
MO102 (“HOMO”)



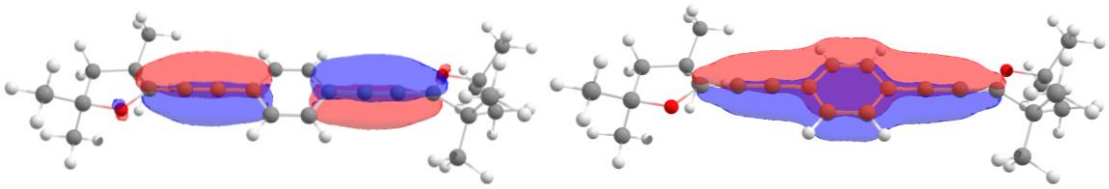
MO101 (“HOMO-1”)



MO100 (“HOMO-2”)



MO99 (“HOMO-3”)



MO98 (“HOMO-4”) MO97 (“HOMO-5”)

Figure S39. CASSCF optimized orbitals of **17** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.67047 [0]: 222222000000
0.08302 [7]: 222220200000
0.04947 [35]: 222211110000
0.01422 [1563]: 221221100100
0.01114 [781]: 222022002000
0.01102 [6775]: 212221100010
0.00922 [274]: 222121101000
0.00694 [111]: 222202020000
0.00613 [28]: 222212100000
0.00521 [2]: 222221010000
0.00508 [24079]: 122221100001
0.00471 [1639]: 221212010100
0.00447 [350]: 222112011000
0.00390 [6851]: 212212010010
0.00284 [24586]: 122122001001
0.00282 [2070]: 221122001100
0.00275 [2060]: 221122101000
0.00258 [42]: 222211010100
0.00258 [1632]: 221212110000

Table S27. Configurations of **17** for singlet multiplicity.

saNHC–CC–C_6H_4–C_6H_4–CC–saNHC (18)

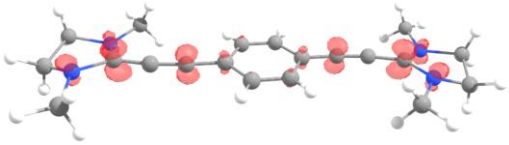
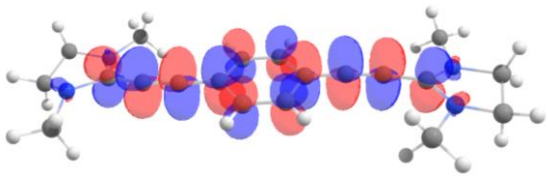
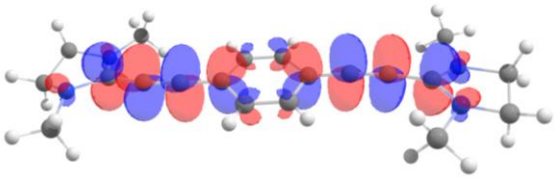


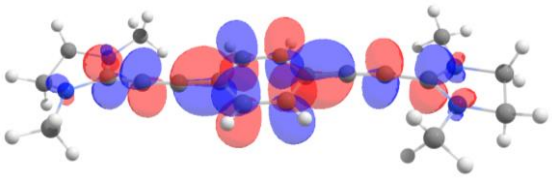
Figure S40. FOD plot of **18** with a contour value of 0.005 e Bohr^{-3}.



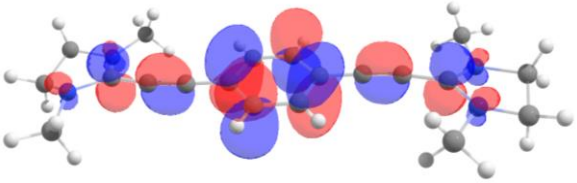
MO92 (“LUMO+5”)



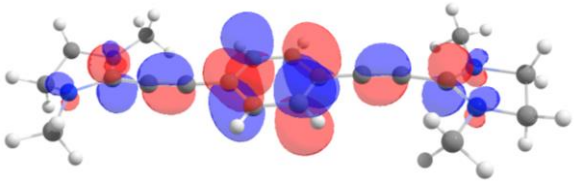
MO91 (“LUMO+4”)



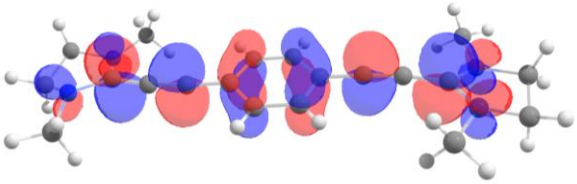
MO90 (“LUMO+3”)



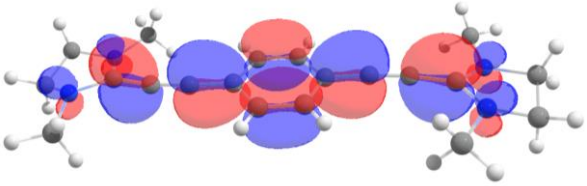
MO89 (“LUMO+2”)



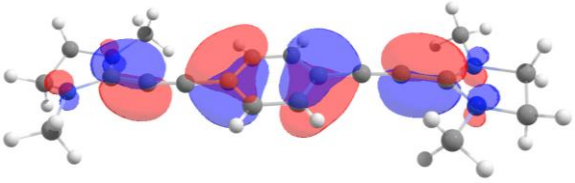
MO88 (“LUMO+1”)



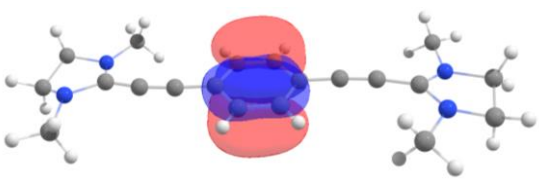
MO87 (“LUMO”)



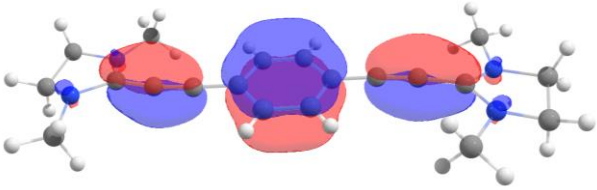
MO86 (“HOMO”)



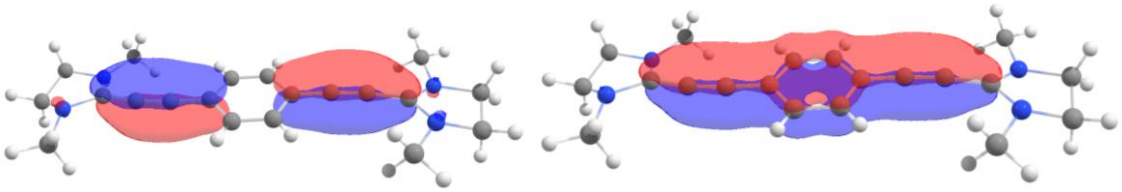
MO85 (“HOMO-1”)



MO84 (“HOMO-2”)



MO83 (“HOMO-3”)



MO82 (“HOMO-4”) MO81 (“HOMO-5”)

Figure S41. CASSCF optimized orbitals of **18** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.71362 [0]: 222222000000
0.06994 [7]: 222220200000
0.03865 [35]: 222211110000
0.01210 [781]: 222022002000
0.01071 [1563]: 221221100100
0.01054 [274]: 222121101000
0.00872 [6775]: 212221100010
0.00587 [111]: 222202020000
0.00536 [24079]: 122221100001
0.00476 [2070]: 221122001100
0.00464 [350]: 222112011000
0.00400 [284]: 222121001100
0.00385 [2060]: 221122101000
0.00377 [1639]: 221212010100
0.00324 [6851]: 212212010010
0.00312 [13]: 222220020000
0.00298 [42]: 222211010100

Table S28. Configurations of **18** for singlet multiplicity.

<u>Pyrazolidin-derivative (19)</u>

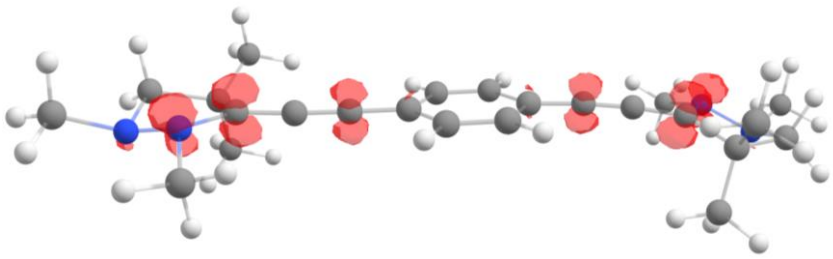
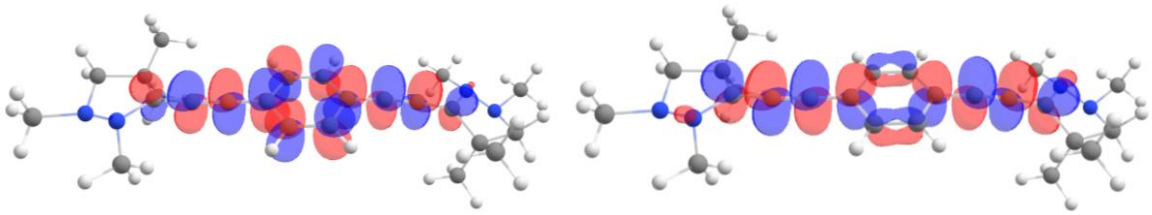
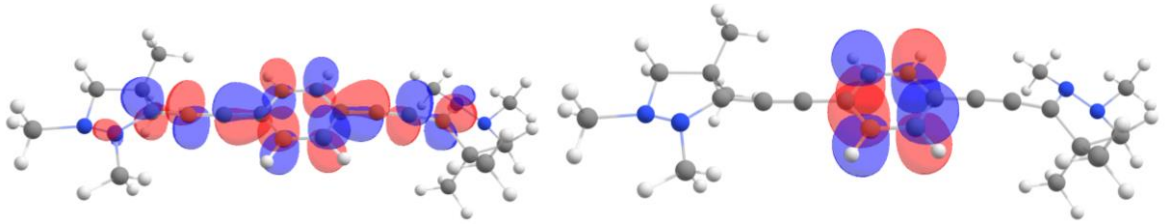


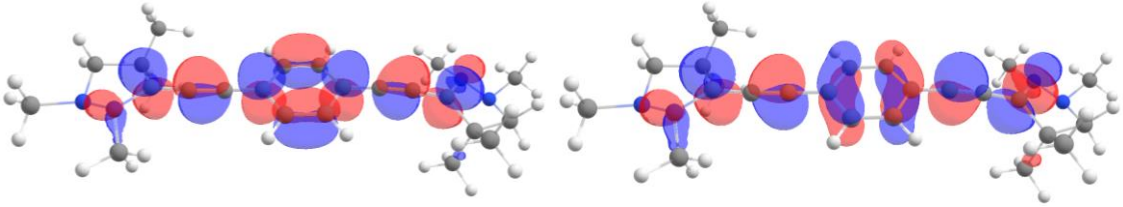
Figure S42. FOD plot of **19** with a contour value of 0.005 e Bohr^{-3}.



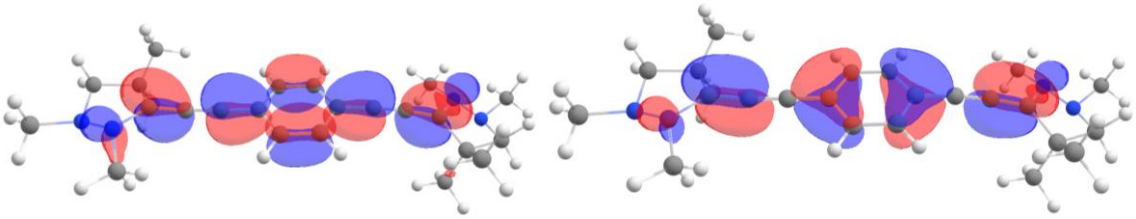
MO108 (“LUMO+5”) MO107 (“LUMO+4”)



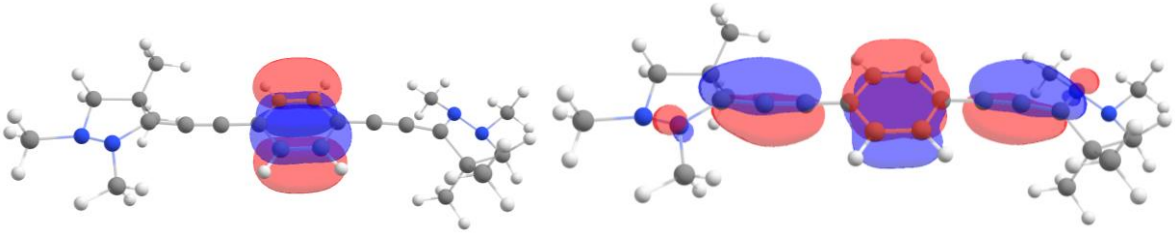
MO106 (“LUMO+3”) MO105 (“LUMO+2”)



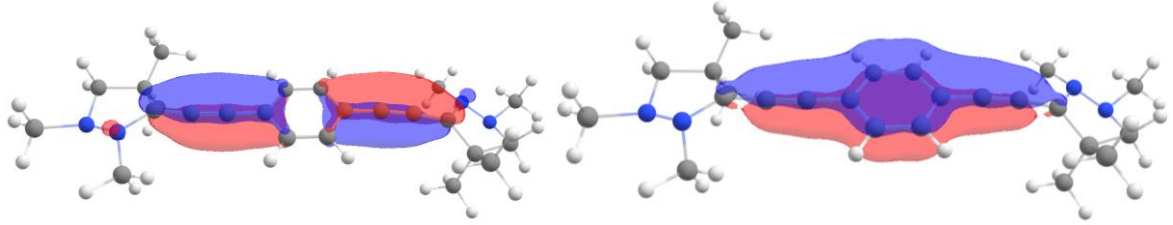
MO104 (“LUMO+1”) **MO103 (“LUMO”)**



MO102 (“HOMO”) MO101 (“HOMO-1”)



MO100 (“HOMO-2”) MO99 (“HOMO-3”)



MO98 (“HOMO-4”) MO97 (“HOMO-5”)

Figure S43. CASSCF optimized orbitals of **19** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.70742 [0]: 222222000000
0.07080 [7]: 222220200000

0.04111 [35]: 222211110000
0.01197 [1563]: 221221100100
0.01149 [781]: 222022002000
0.01012 [6775]: 212221100010
0.00993 [274]: 222121101000
0.00654 [111]: 222202020000
0.00561 [24079]: 122221100001
0.00438 [1639]: 221212010100
0.00413 [350]: 222112011000
0.00395 [2070]: 221122001100
0.00388 [6851]: 212212010010
0.00361 [2060]: 221122101000
0.00306 [284]: 222121001100
0.00280 [42]: 222211010100
0.00279 [13]: 222220020000
0.00261 [24155]: 122212010001
0.00254 [1632]: 221212110000

Table S29. Configurations of **19** for singlet multiplicity.

TTF-derivative (20)

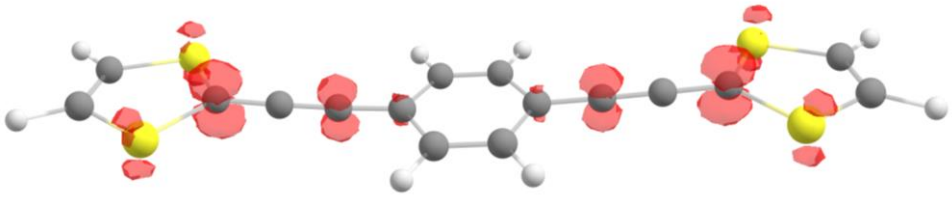
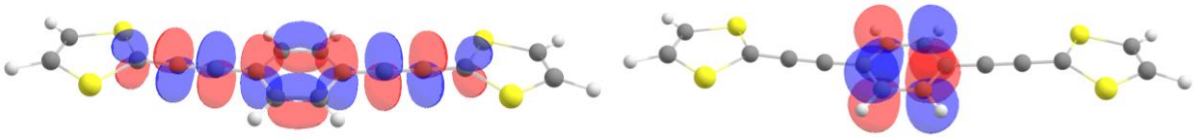
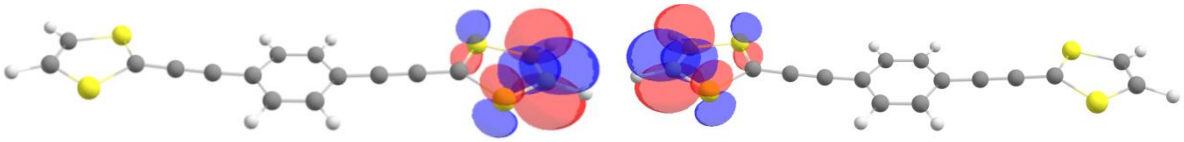


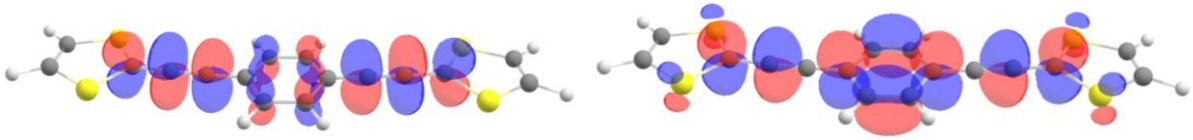
Figure S44. FOD plot of **20** with a contour value of 0.005 e Bohr^{-3}.



MO91 (“LUMO+6”) MO90 (“LUMO+5”)



MO89 (“LUMO+4”) MO88 (“LUMO+3”)



MO87 (“LUMO+2”) MO86 (“LUMO+1”)

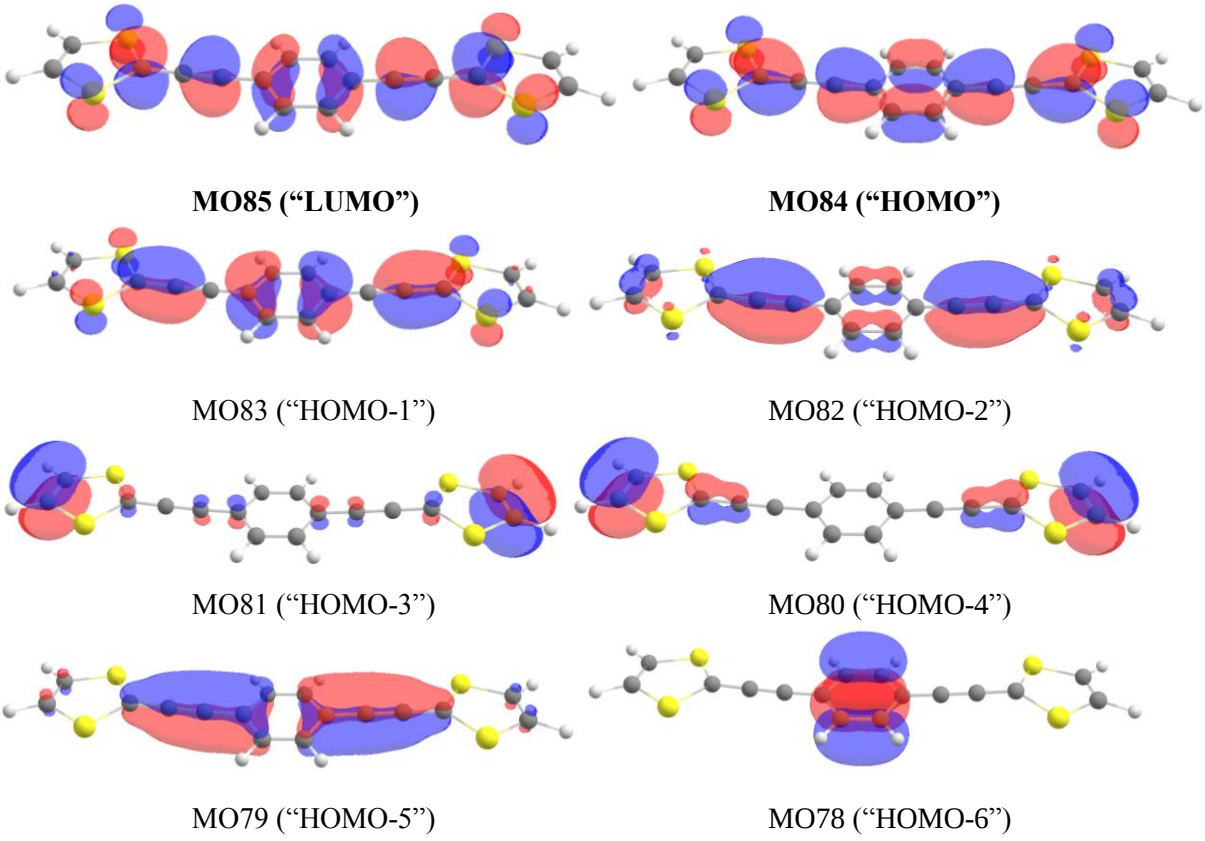


Figure S45. CASSCF optimized orbitals of **20** from state averaged calculation (4 singlet roots, 3 triplet roots).

0.64624 [0]: 22222220000000
0.11334 [8]: 22222202000000
0.04062 [44]: 22222111100000
0.01719 [14366]: 22122211000100
0.01272 [3750]: 22211220002000
0.01269 [3745]: 22211220020000
0.01147 [201656]: 12222211000001
0.00944 [127879]: 20222220000020
0.00692 [1309]: 22220220020000
0.00638 [7608]: 22202220002000
0.00636 [1314]: 22220220002000
0.00584 [7603]: 22202220020000
0.00562 [58290]: 21222211000010
0.00526 [155]: 22222020200000
0.00472 [14477]: 22122120100100
0.00335 [201767]: 12222120100001
0.00324 [58401]: 21222120100010

Table S30. Configurations of **20** for singlet multiplicity.

NHC–CC–C_6H_4–CC–NHC (21)

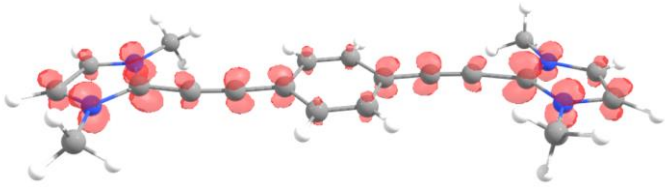
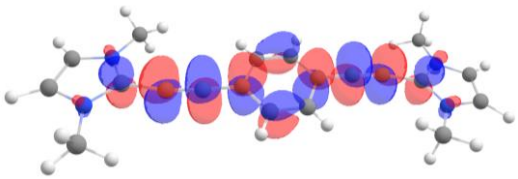
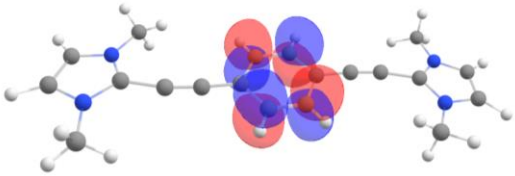


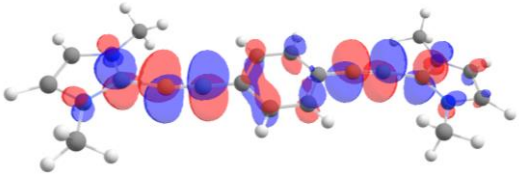
Figure S46. FOD plot of **21** with a contour value of 0.005 e Bohr^{-3}.



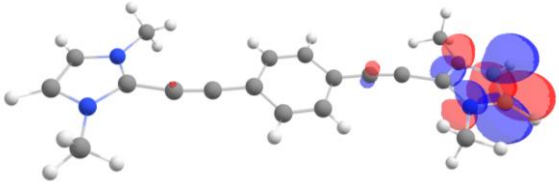
MO87 (“LUMO+6”)



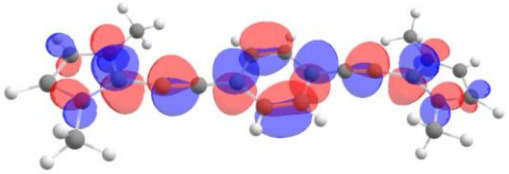
MO86 (“LUMO+5”)



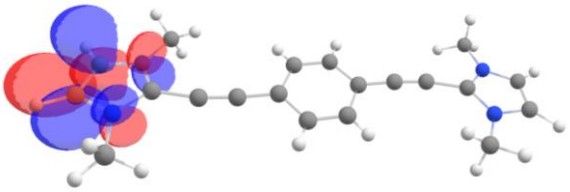
MO85 (“LUMO+4”)



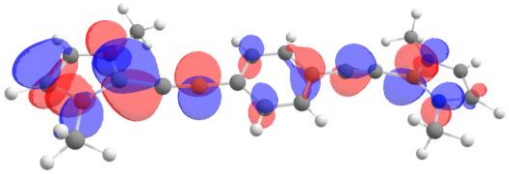
MO84 (“LUMO+3”)



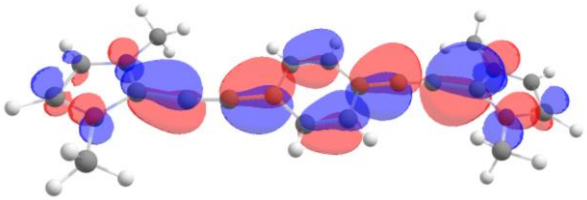
MO83 (“LUMO+2”)



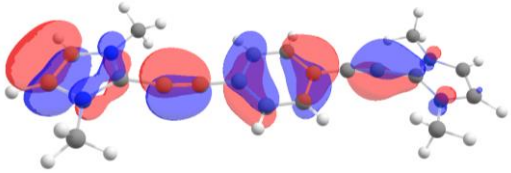
MO82 (“LUMO+1”)



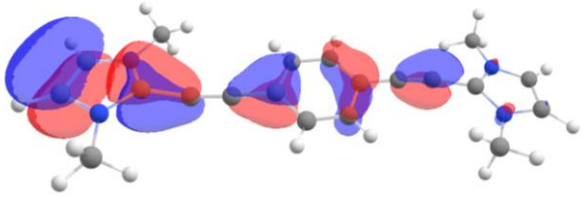
MO81 (“LUMO”)



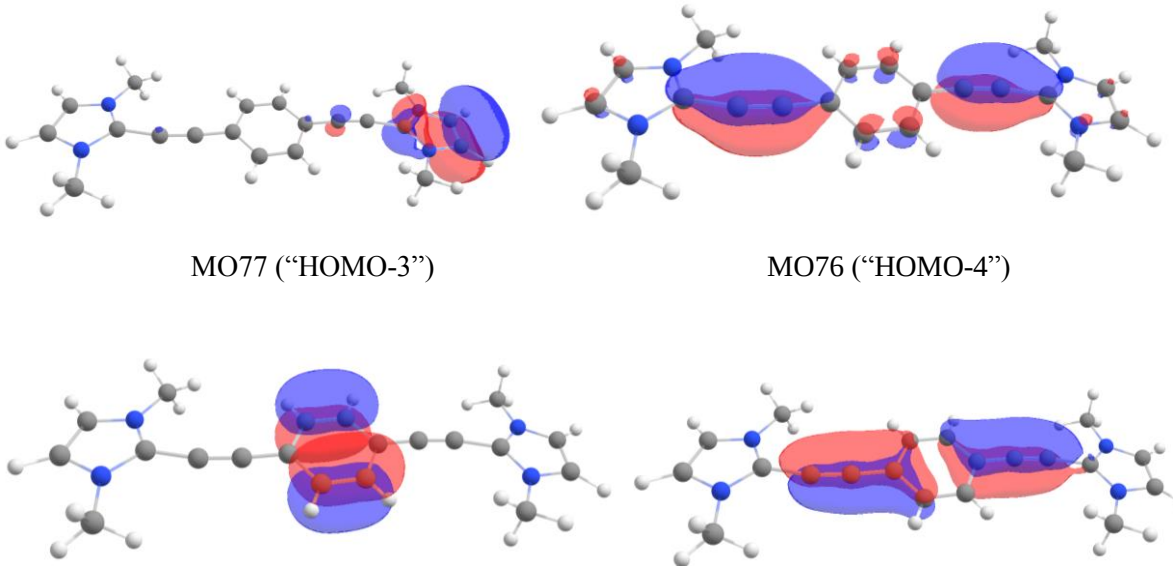
MO80 (“HOMO”)



MO79 (“HOMO-1”)



MO78 (“HOMO-2”)



MO77 (“HOMO-3”) MO76 (“HOMO-4”)

MO75 (“HOMO-5”) MO74 (“HOMO-6”)

Figure S47. CASSCF optimized orbitals of **21** from state averaged calculation (4 singlet roots, 3 triplet roots).

0.68085 [0]: 22222220000000
0.10619 [8]: 22222202000000
0.02170 [44]: 22222111100000
0.01450 [3746]: 22211220011000
0.01076 [58290]: 21222211000010
0.00920 [34232]: 22022220000200
0.00857 [2858]: 22212211100000
0.00842 [540]: 22221120011000
0.00706 [201656]: 12222211000001
0.00650 [1309]: 22220220020000
0.00494 [1314]: 22220220002000
0.00457 [14366]: 22122211000100
0.00317 [2975]: 22212120020000
0.00282 [14477]: 22122120100100
0.00279 [271245]: 11222220000011
0.00266 [7603]: 22202220020000

Table S31. Configurations of **21** for singlet multiplicity.

MIC–CC–C_6H_4–C_6H_4–CC–MIC (22)

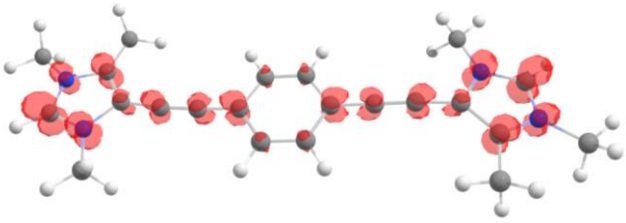
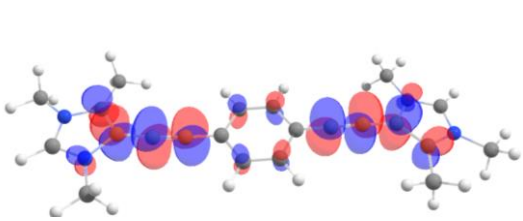
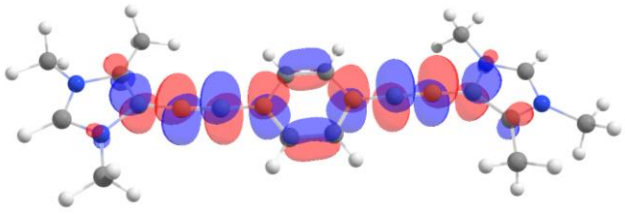


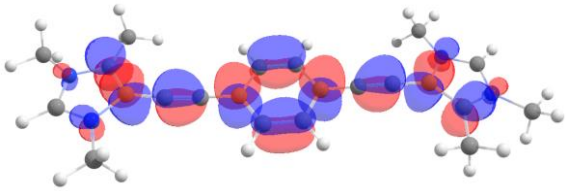
Figure S48. FOD plot of **22** with a contour value of 0.3 e $Bohr^{-3}$.



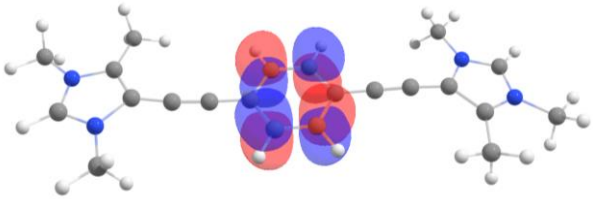
MO99 (“LUMO+6”)



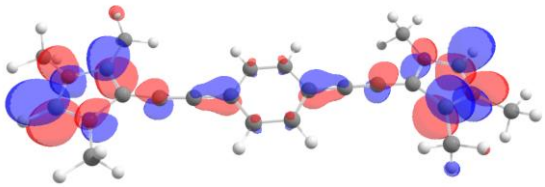
MO98 (“LUMO+5”)



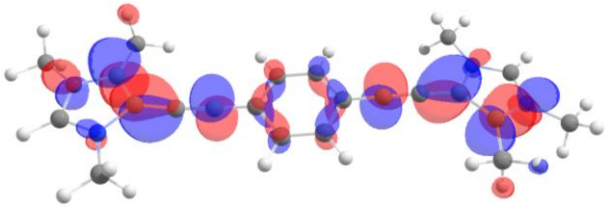
MO97 (“LUMO+4”)



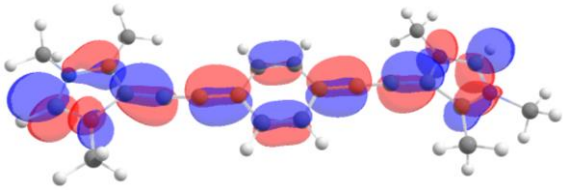
MO96 (“LUMO+3”)



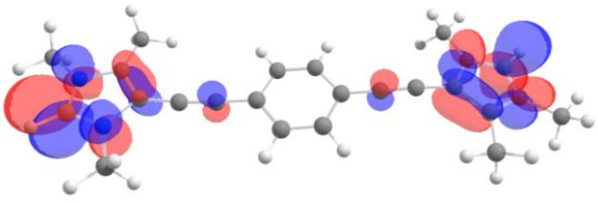
MO95 (“LUMO+2”)



MO94 (“LUMO+1”)



MO93 (“LUMO”)



MO92 (“HOMO”)

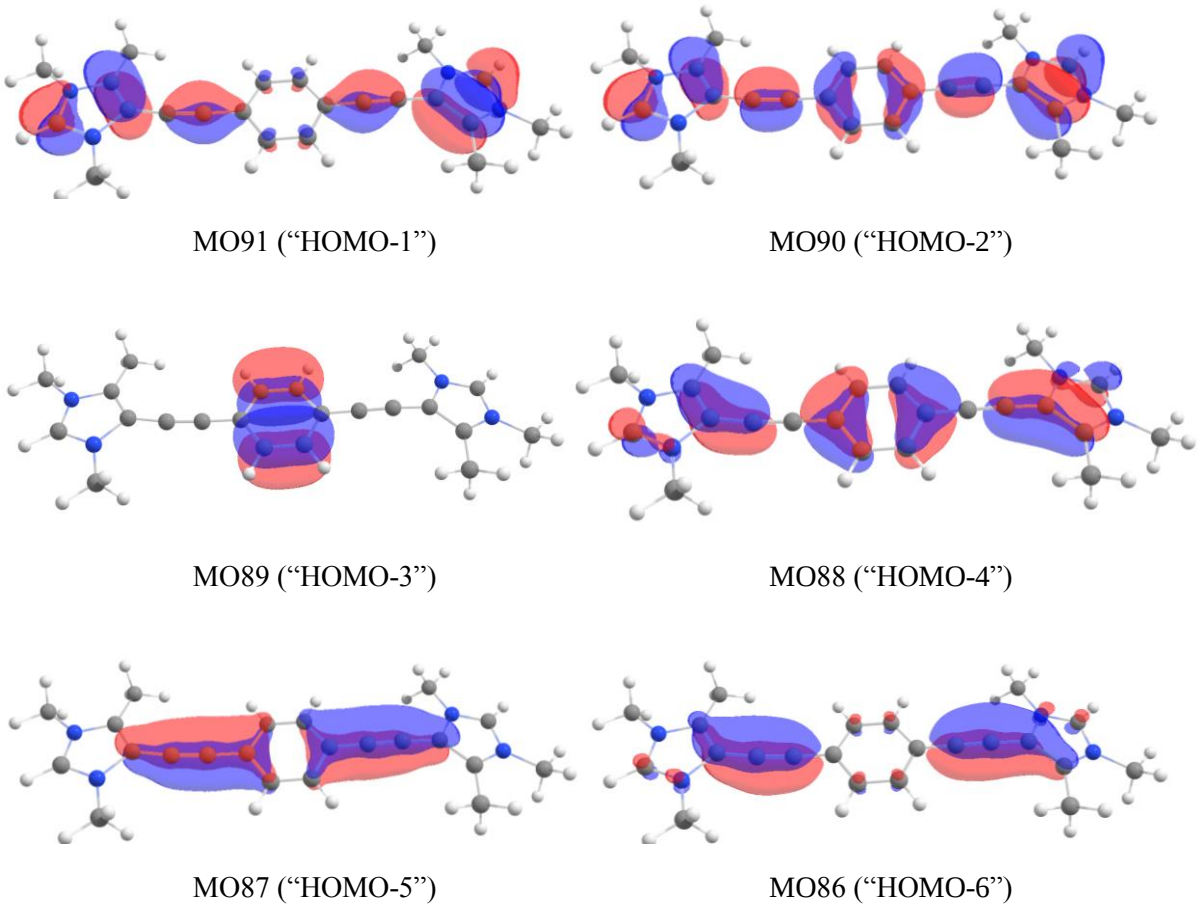


Figure S49. CASSCF optimized orbitals of **22** from state averaged calculation (4 singlet roots, 3 triplet roots).

0.68218 [0]: 22222220000000
0.06406 [8]: 22222202000000
0.02301 [44]: 22222111100000
0.01663 [423]: 22221211010000
0.01490 [534]: 22221120110000
0.01187 [2860]: 22212211001000
0.01069 [51]: 22222110110000
0.00957 [34232]: 22022220000200
0.00705 [155]: 22222020200000
0.00544 [428]: 22221210200000
0.00471 [58290]: 21222211000010
0.00450 [161]: 22222020020000
0.00412 [201656]: 12222211000001
0.00368 [14366]: 22122211000100
0.00350 [1309]: 22220220020000
0.00319 [15]: 22222200200000
0.00286 [527]: 22221121100000
0.00264 [540]: 22221120011000

Table S32. Configurations of **22** for singlet multiplicity.

Pyrazolin-derivative (23)

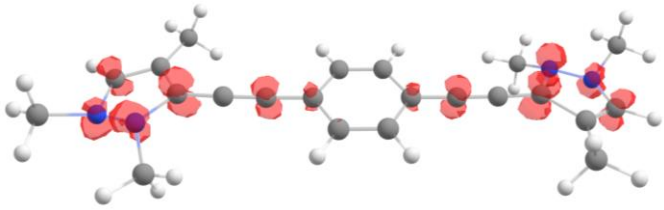
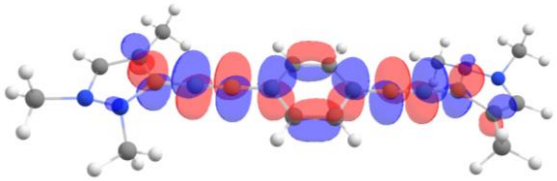
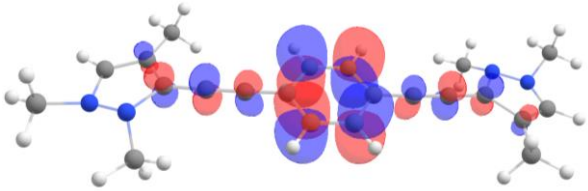


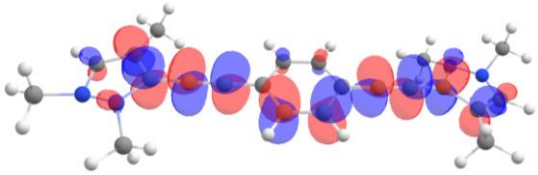
Figure S50. FOD plot of **23** with a contour value of 0.005 e Bohr^{-3}.



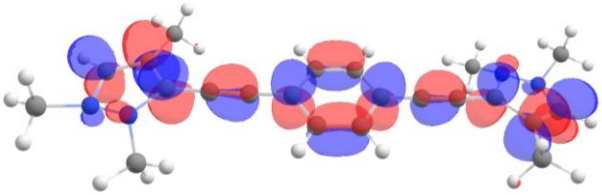
MO99 (“LUMO+6”)



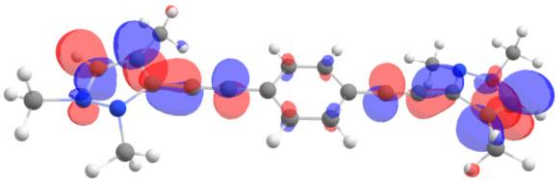
MO98 (“LUMO+5”)



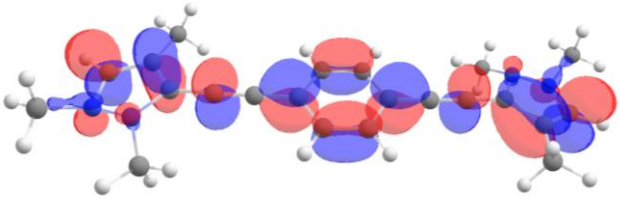
MO97 (“LUMO+4”)



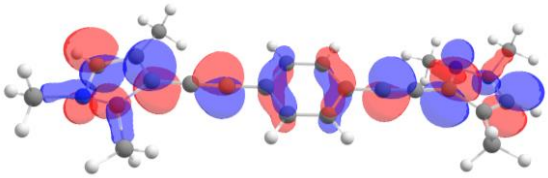
MO96 (“LUMO+3”)



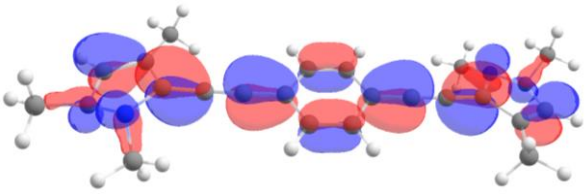
MO95 (“LUMO+2”)



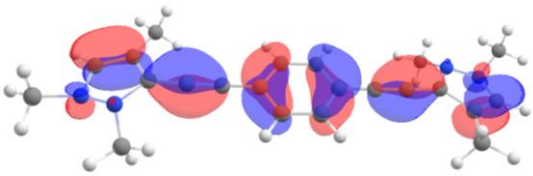
MO94 (“LUMO+1”)



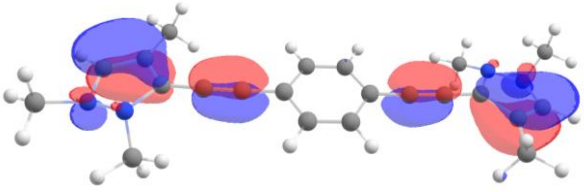
MO93 (“LUMO”)



MO92 (“HOMO”)



MO95 (“HOMO-1”)



MO94 (“HOMO-2”)

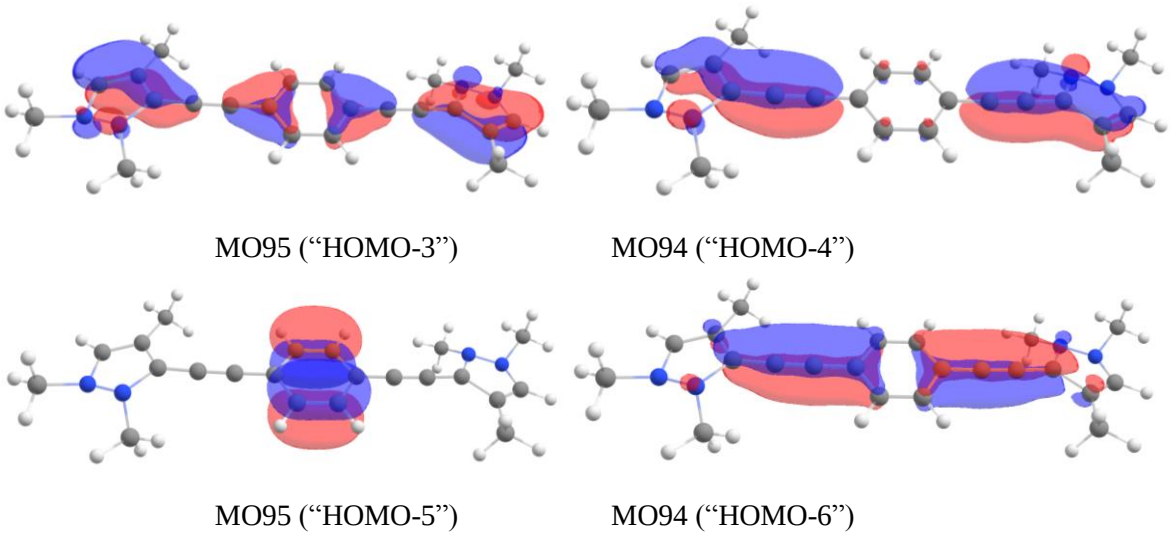


Figure S51. CASSCF optimized orbitals of **23** from state averaged calculation (4 singlet roots, 3 triplet roots).

0.64813 [0]: 22222220000000
0.11552 [8]: 22222202000000
0.03472 [44]: 22222111100000
0.01031 [14367]: 22122211000010
0.00950 [423]: 22221211010000
0.00938 [127876]: 20222220000200
0.00872 [201656]: 12222211000001
0.00836 [2860]: 22212211001000
0.00636 [3746]: 22211220011000
0.00513 [58289]: 21222211000100
0.00420 [534]: 22221120110000
0.00413 [155]: 22222020200000
0.00358 [2971]: 22212120101000
0.00300 [1309]: 22220220020000
0.00268 [3740]: 22211220110000
0.00267 [14478]: 22122120100010
0.00259 [58400]: 21222120100100

Table S33. Configurations of **23** for singlet multiplicity.

<u>Bentallene–CC–C_6H_4–C_6H_4–CC–bentallene (24)</u>

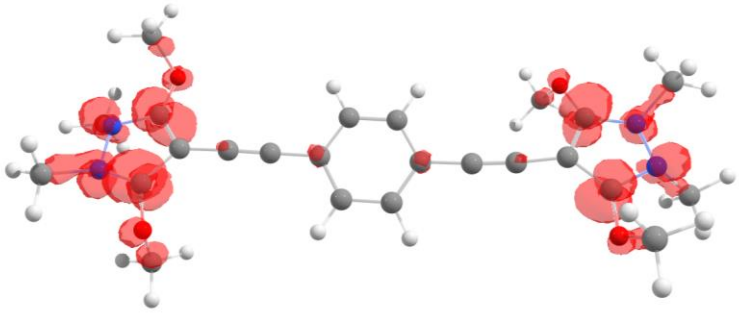
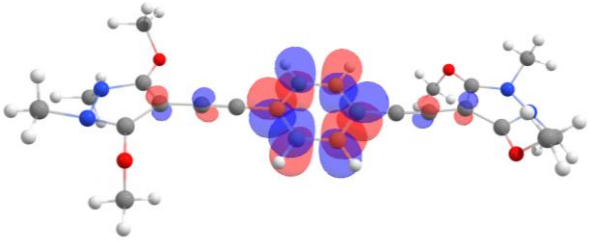
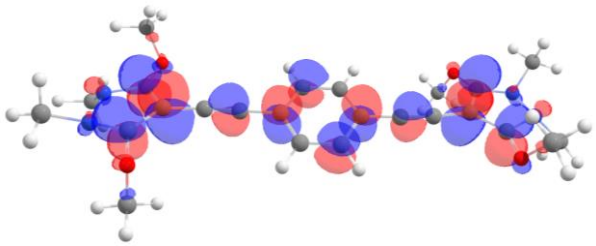


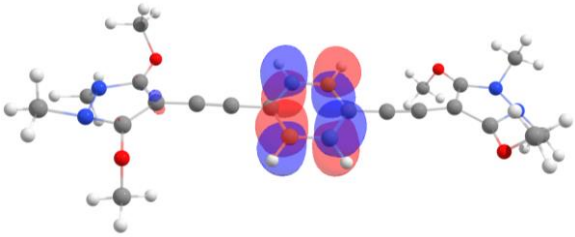
Figure S52. FOD plot of **24** with a contour value of 0.005 e $Bohr^{-3}$.



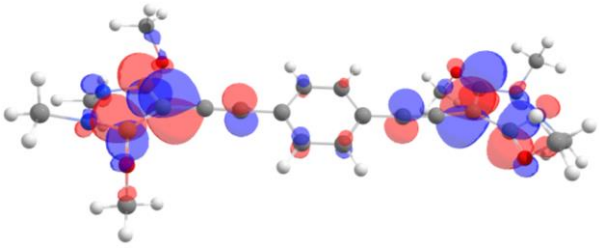
MO122 (“LUMO+5”)



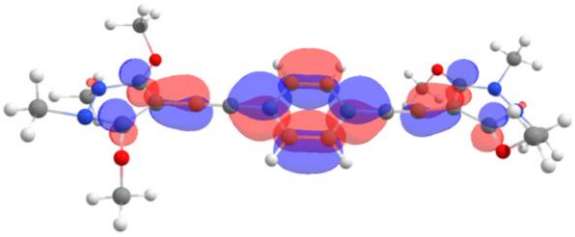
MO121 (“LUMO+4”)



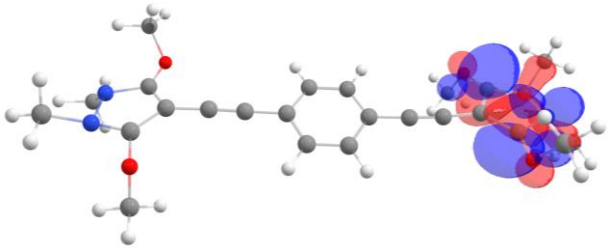
MO120 (“LUMO+3”)



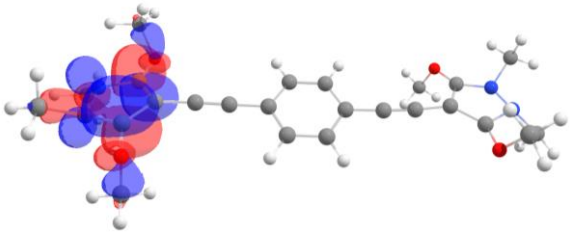
MO119 (“LUMO+2”)



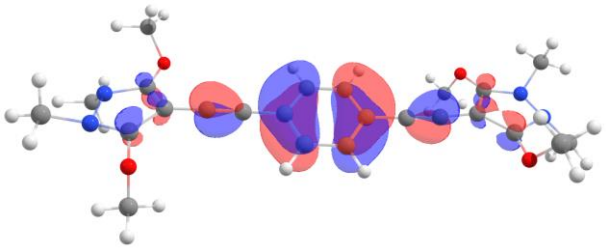
MO118 (“LUMO+1”)



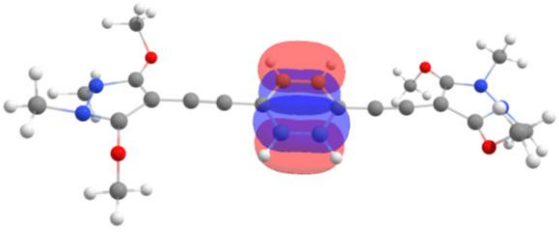
MO117 (“LUMO”)



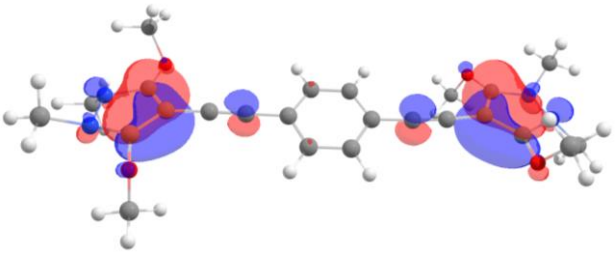
MO116 (“HOMO”)



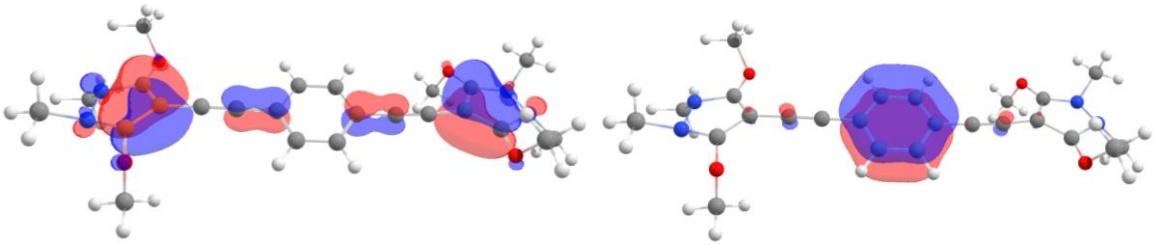
MO115 (“HOMO-1”)



MO114 (“HOMO-2”)



MO113 (“HOMO-3”)



MO112 (“HOMO-4”) MO111 (“HOMO-5”)

Figure S53. CASSCF optimized orbitals of **24** from state averaged calculation (5 singlet roots, 5 triplet roots).

0.35445 [0]: 222222000000
0.35438 [7]: 222220200000
0.05420 [1]: 222221100000
0.04005 [1563]: 221221100100
0.01883 [6775]: 212221100010
0.00892 [38]: 222211100010
0.00882 [6772]: 212221110000
0.00826 [781]: 222022002000
0.00826 [846]: 222020202000
0.00766 [350]: 222112011000
0.00766 [415]: 222110211000
0.00733 [35]: 222211110000
0.00530 [24586]: 122122001001
0.00530 [24651]: 122120201001
0.00405 [111]: 222202020000
0.00405 [176]: 222200220000
0.00309 [6916]: 212210210010
0.00309 [6851]: 212212010010
0.00299 [24155]: 122212010001
0.00298 [24220]: 122210210001
0.00297 [9085]: 211222000110
0.00297 [9150]: 211220200110
0.00257 [3873]: 220222000200
0.00256 [3938]: 220220200200

Table S34. Configurations of **24** for singlet multiplicity.

1.) XYZ Coordinates and Energies

Tschitschibabin's Hydrocarbon (1)
Energy: -1461.6876457
NImag: from solid state structure

C	1.39855	0.25728	9.28925
C	0.91349	1.41271	9.95362
C	-0.33761	1.92981	9.71582
C	-1.21882	1.33809	8.77434
C	-0.72427	0.18268	8.09957
C	0.50633	-0.33998	8.37216
C	-2.53305	1.83352	8.50359
C	-3.26040	2.67083	9.48523
C	-4.18379	3.62584	9.03671
C	-4.95337	4.32691	9.96166
C	-4.81953	4.11007	11.28892
C	-3.91252	3.18644	11.74971
C	-3.14025	2.47021	10.85772
C	-3.20981	1.51230	7.21846
C	-2.52029	1.57139	6.01115
C	-3.16488	1.31804	4.82306
C	-4.50109	1.00166	4.81116
C	-5.18054	0.91121	5.99390
C	-4.55615	1.16316	7.19059
H	1.55364	1.93946	10.66155
H	-0.63993	2.84111	10.23268
H	-1.37454	-0.33447	7.39401
H	0.79799	-1.25256	7.85155
H	-4.30450	3.81551	7.96950
H	-5.67030	5.06779	9.59505
H	-5.43539	4.66766	11.99993
H	-3.81190	2.99414	12.82138
H	-2.46335	1.69928	11.22934
H	-1.46656	1.85656	6.01318
H	-2.60970	1.39179	3.88374
H	-5.01450	0.80752	3.86571
H	-6.23820	0.63050	5.99311
H	-5.11063	1.08403	8.12748
C	2.73685	-0.25728	9.51755
C	3.22191	-1.41271	8.85318
C	3.62917	0.33998	10.43465
C	4.47301	-1.92981	9.09098
H	2.58176	-1.93949	8.14527
C	4.85967	-0.18268	10.70714
H	3.33754	1.25258	10.95525
C	5.35432	-1.33809	10.03246
H	4.77530	-2.84112	8.57412
H	5.50996	0.33449	11.41269
C	6.66855	-1.83352	10.30321
C	7.39580	-2.67083	9.32158
C	7.34521	-1.51230	11.58835
C	8.31919	-3.62584	9.77010
C	7.27565	-2.47021	7.94909
C	6.65569	-1.57139	12.79565
C	8.69155	-1.16316	11.61621
C	9.08877	-4.32691	8.84514
H	8.43991	-3.81551	10.83731
C	8.04792	-3.18644	7.05710
H	6.59876	-1.69927	7.57747
C	7.30028	-1.31804	13.98375
H	5.60196	-1.85656	12.79362
C	9.31594	-0.91121	12.81281
H	9.24600	-1.08403	10.67930
C	8.95494	-4.11007	7.51788
H	9.80570	-5.06779	9.21175
H	7.94731	-2.99414	5.98543
C	8.63649	-1.00166	13.99565
H	6.74510	-1.39179	14.92307
H	10.37360	-0.63049	12.81359
H	9.57079	-4.66766	6.80687
H	9.14994	-0.80751	14.94108

Thiele's Hydrocarbon (2)
Energy: -1232.3021272
NImag: from solid state structure

C	-1.36236	-1.38786	5.91946
C	-2.69075	-1.60222	5.95350
C	-0.77925	-0.12970	5.49711
C	0.57805	0.12618	5.50779
C	1.55549	-0.74517	6.19464
C	2.81784	-0.97479	5.62741
C	3.73610	-1.80898	6.23155
C	3.43366	-2.42620	7.43100
C	2.21307	-2.18670	8.03296
C	1.29043	-1.35255	7.42938
C	1.15378	1.29787	4.80097
C	2.07834	2.11927	5.44849
C	2.66965	3.18662	4.78739
C	2.35427	3.45554	3.46827
C	1.44921	2.64566	2.80968
C	0.84987	1.56848	3.46747
H	-0.69232	-2.21389	6.15826
H	-3.05778	-2.59138	6.23097
H	3.06343	-0.50123	4.67463
H	4.70207	-1.98917	5.75209
H	4.16133	-3.08838	7.90764
H	1.97395	-2.64799	8.99524
H	0.34744	-1.13583	7.93442
H	2.34269	1.90894	6.48738
H	3.38475	3.82009	5.31961
H	2.82483	4.29314	2.94687
H	1.19268	2.84515	1.76524
H	0.15339	0.91877	2.93264
C	-3.65934	-0.60324	5.54785

C	-1.74785	0.86927	5.09146
C	-3.07624	0.65492	5.12550
C	-5.01664	-0.85913	5.53716
H	-1.38081	1.85843	4.81399
H	-3.74627	1.48094	4.88669
C	-5.99408	0.01222	4.85032
C	-5.59237	-2.03082	6.24399
C	-7.25644	0.24184	5.41755
C	-5.72902	0.61960	3.61558
C	-6.51694	-2.85222	5.59647
C	-5.28846	-2.30143	7.57749
C	-8.17469	1.07603	4.81341
H	-7.50202	-0.23171	6.37033
C	-6.65167	1.45375	3.01200
H	-4.78603	0.40288	3.11054
C	-7.10824	-3.91956	6.25757
H	-6.78129	-2.64188	4.55758
C	-5.88780	-3.37861	8.23528
H	-4.59198	-1.65171	8.11232
C	-7.87226	1.69326	3.61396
H	-9.14067	1.25622	5.29286
H	-6.41254	1.91504	2.04972
C	-6.79286	-4.18849	7.57669
H	-7.82334	-4.55303	5.72535
H	-5.63127	-3.57810	9.27972
H	-8.59993	2.35543	3.13732
H	-7.26343	-5.02609	8.09809

Tetracene (3)
Energy: -688.1354248
NImag: from solid state structure

C	0.64174	-0.74082	-6.21821
C	-0.49851	-1.26174	-5.66657
C	-0.64956	-1.37084	-4.24345
C	-1.80054	-1.89455	-3.65425
C	-1.94191	-1.99516	-2.25280
C	0.30869	-1.01208	-2.00961
C	0.43934	-0.91624	-3.39518
C	1.61589	-0.37979	-4.01953
C	1.71546	-0.29476	-5.38298
C	-0.85304	-1.53977	-1.40413
C	-0.99436	-1.64025	-0.00278
C	-2.14526	-2.16437	0.58647
C	-3.23394	-2.61930	-0.26178
C	-3.10343	-2.52311	-1.64744
C	-4.41031	-3.15613	0.36251
C	-4.50960	-3.24177	1.72599
C	-3.43630	-2.79487	2.56120
C	-2.29614	-2.27367	2.00955
H	-1.31954	-1.60269	-6.30317
H	2.43436	-0.03860	-3.37997
H	1.12854	-0.66937	-1.37171
H	-2.62024	-2.23713	-4.29249
H	-0.17508	-1.29754	0.63595
H	-3.92361	-2.86595	-2.28485
H	-1.47538	-1.93233	2.64628
H	-3.53588	-2.87609	3.64683
H	-5.40979	-3.65489	2.18853
H	-5.22870	-3.49776	-0.27692
H	0.74156	-0.65966	-7.30382
H	2.61584	0.11772	-5.84573

Pentacene (4)
Energy: -845.6984220
NImag: from solid state structure

C	-1.31277	-1.05271	5.90621
C	-1.93947	-2.39039	4.04448
C	-1.93690	-2.14855	5.37848
C	-0.73075	-0.17413	5.06373
C	-0.69617	-0.35138	3.63826
C	-0.08242	0.45719	2.74647
C	-0.08898	0.30378	1.37762
C	0.61572	1.17207	0.48419
C	-0.57933	-0.90449	0.82364
C	-1.27678	-1.75721	1.77940
C	-1.26271	-1.53161	3.11920
H	-1.30730	-0.86487	6.98288
H	-2.44178	-3.27782	3.64838
H	-2.44994	-2.85459	6.03875
H	-0.24474	0.72316	5.46164
H	0.40205	1.36401	3.13137
H	1.08589	2.08198	0.86589
H	-1.75998	-2.66032	1.39334
C	0.57933	0.90449	-0.82364
C	-0.61572	-1.17207	-0.48419
C	0.08898	-0.30378	-1.37762
C	1.27677	1.75721	-1.77940
H	-1.08589	-2.08198	-0.86589
C	0.08242	-0.45719	-2.74647
C	1.26271	1.53161	-3.11920
H	1.75997	2.66032	-1.39334
C	0.69617	0.35138	-3.63826
H	-0.40205	-1.36401	-3.13137
C	1.93947	2.39039	-4.04448
C	0.73075	0.17413	-5.06373
C	1.93689	2.14855	-5.37848
H	2.44178	3.27782	-3.64838
C	1.31277	1.05271	-5.90621
H	0.24474	-0.72316	-5.46164
H	2.44995	2.85459	-6.03875
H	1.30731	0.86487	-6.98288

Bisnitroxide (5)
Energy: -1297.035468914125
NImag: from solid state structure

C	4.63485	2.24888	12.22291
C	5.09901	1.09559	13.00394
C	6.38224	1.04346	13.51012
C	4.22768	0.04859	13.25825

C	3.54724	3.53186	10.56698
C	4.35050	3.35191	9.25939
C	4.22907	4.48086	11.57986
C	2.10501	3.79079	10.27857
C	5.06091	5.59788	10.99129
C	3.26701	5.06296	12.60191
N	3.68590	2.21523	11.29136
N	5.09902	3.51718	12.33502
O	3.01849	1.20510	10.90999
O	6.00572	3.91763	13.13094
H	7.06664	1.87102	13.33316
H	3.22016	0.07289	12.85069
H	4.28260	4.24786	8.62651
H	3.92746	2.49656	8.71413
H	5.40946	3.14223	9.46720
H	1.48877	3.79876	11.18641
H	1.71556	3.00260	9.62158
H	1.98575	4.75806	9.76676
H	5.85278	5.22897	10.32801
H	5.54240	6.15727	11.80423
H	4.41565	6.28471	10.42334
H	2.61680	5.81960	12.13936
H	3.85188	5.53994	13.40094
H	2.63277	4.28933	13.05900
C	6.79459	-0.04859	14.26237
C	4.64002	-1.04346	14.01050
C	5.92326	-1.09559	14.51668
H	7.80210	-0.07288	14.66993
H	3.95562	-1.87102	14.18746
C	6.38741	-2.24888	15.29771
N	7.33637	-2.21523	16.22926
N	5.92325	-3.51718	15.18560
C	7.47502	-3.53186	16.95364
O	8.00378	-1.20510	16.61063
C	6.79319	-4.48086	15.94076
O	5.01654	-3.91763	14.38968
C	6.67177	-3.35191	18.26123
C	8.91726	-3.79079	17.24205
C	5.96135	-5.59788	16.52933
C	7.75525	-5.06296	14.91871
H	6.73967	-4.24786	18.89411
H	7.09480	-2.49656	18.80649
H	5.61281	-3.14223	18.05342
H	9.53349	-3.79877	16.33421
H	9.30671	-3.00259	17.89903
H	9.03652	-4.75805	17.75387
H	5.16949	-5.22897	17.19263
H	5.47986	-6.15726	15.71639
H	6.60662	-6.28472	17.09727
H	8.40548	-5.81959	15.38126
H	7.17039	-5.53994	14.11968
H	8.38950	-4.28933	14.46162

Bisoxoverdazyl (6)

Energy: -1129.994476663918

NImag: from solid state structure

O	7.28676	2.65017	1.43727
N	9.04969	1.33177	2.02385
N	10.28373	0.79771	1.77042
N	9.02545	2.40320	-0.02378
N	10.27401	1.93752	-0.31833
C	12.13207	0.55595	0.29343
C	13.01596	1.20558	-0.56494
H	12.71781	2.15752	-1.00715
C	12.50881	-0.66031	0.85227
H	11.82024	-1.17151	1.52649
C	10.81496	1.14506	0.60244
C	8.37598	2.16512	1.16848
O	19.47315	-2.65035	-1.43724
N	17.71023	-1.33195	-2.02382
N	16.47619	-0.79789	-1.77039
N	17.73446	-2.40338	0.02380
N	16.48590	-1.93771	0.31836
C	14.62784	-0.55613	-0.29340
C	13.74395	-1.20576	0.56496
H	14.04202	-2.15773	1.00718
C	14.25110	0.66012	-0.85224
H	14.93958	1.17141	-1.52650
C	15.94495	-1.14524	-0.60242
C	18.38393	-2.16530	-1.16846
C	18.24037	-1.01763	-3.35838
H	18.19130	0.07072	-3.50450
H	19.27301	-1.37718	-3.41466
H	17.62260	-1.51147	-4.12537
C	18.33914	-3.29466	1.02424
H	17.76367	-4.23270	1.08004
H	19.37038	-3.50013	0.72099
H	18.30479	-2.79565	2.00328
C	8.51526	1.01725	3.35665
H	8.57410	-0.07010	3.50632
H	9.12371	1.51917	4.12594
H	7.47910	1.36755	3.40574
C	8.41446	3.25992	-1.05024
H	7.39729	3.50652	-0.72979
H	9.01333	4.17700	-1.16665
H	8.40744	2.71443	-2.00523

Terphenoquinone (7)

Energy: -999.557381772516

NImag: from solid state structure

O	0.79502	16.97931	4.71349
C	0.58965	17.96151	4.00101
C	-0.69752	18.11372	3.29340
C	-0.82273	19.12183	2.40873
C	0.20316	20.09106	2.15170
C	1.38404	19.99815	2.95055
C	1.62783	19.00366	3.83037
C	0.07706	21.04357	1.11084
C	-0.93937	20.97596	0.12625
C	1.01208	22.10279	0.92009

H	-1.76754	19.21558	1.86973
H	2.17151	20.73805	2.79410
H	-1.67867	20.17663	0.18158
H	1.80954	22.25414	1.64718
C	-1.01232	21.82322	-0.92001
C	0.93914	22.95005	-0.12617
C	-0.07729	22.88245	-1.11076
H	-1.80987	21.67204	-1.64702
H	1.67836	23.74946	-0.18145
C	-0.20340	23.83495	-2.15162
C	0.82249	24.80418	-2.40865
C	-1.38427	23.92786	-2.95046
C	0.69728	25.81229	-3.29332
H	1.76728	24.70999	-1.86981
C	-1.62807	24.92235	-3.83029
H	-2.17157	23.18721	-2.79559
C	-0.58988	25.96449	-4.00093
O	-0.79525	26.94670	-4.71341
C	-2.96471	25.04817	-4.58472
H	-2.78954	25.09721	-5.67117
H	-3.62162	24.19843	-4.35363
H	-3.46580	25.98901	-4.30609
C	1.83439	26.81856	-3.55024
H	2.69842	26.59795	-2.90888
H	2.14331	26.78337	-4.60744
H	1.48314	27.84495	-3.36083
C	2.97639	18.89475	4.56598
H	2.81980	18.84204	5.65522
H	3.48777	17.96190	4.27852
H	3.61688	19.75412	4.32559
C	-1.82562	17.09920	3.55747
H	-2.69819	17.31629	2.92641
H	-1.46890	16.07630	3.35984
H	-2.12263	17.12777	4.61815

CAAC-C_6H_4-CAAC (8)
Energy: -1045.5753899
NImag: 0

N	0.03263	1.21788	3.67755
N	-0.17569	-1.18470	-3.57475
C	-0.24123	1.47367	6.15653
C	-0.64316	-2.38084	3.20859
C	0.10636	-0.74551	4.95125
C	-2.31928	-0.75271	4.14511
C	1.99782	0.94771	5.14195
C	0.47785	0.75563	5.00345
C	-0.84348	-0.95496	3.74308
C	-0.98461	-0.76145	-0.71893
C	-0.37718	0.18972	2.83704
C	-1.11646	-0.68876	0.63046
C	-0.32644	0.21443	1.45593
C	0.62539	-1.79725	-5.86210
C	0.31967	2.44841	-3.50487
C	0.00066	0.56203	-5.13135
C	2.22535	0.85261	-3.92115
C	-1.78760	-1.22441	-5.43864
C	-0.33570	-0.94270	-5.01844
C	0.69327	0.98991	-3.81015
C	0.53506	1.11356	0.69540
C	0.12736	-0.04956	-2.83737
C	0.66210	1.04404	-0.65683
C	-0.05905	0.07643	-1.47154
H	-0.00555	2.54895	6.18628
H	0.08527	1.04210	7.11543
H	-1.33282	1.35883	6.08358
H	-0.73612	-3.09762	4.04165
H	-1.38892	-2.66445	2.45574
H	1.01740	-1.33858	4.78197
H	-0.34367	-1.09484	5.89277
H	-2.49892	0.27087	4.50623
H	-2.98415	-0.92751	3.28478
H	2.51991	0.45795	4.30562
H	2.36872	0.51124	6.08400
H	2.26986	2.01585	5.13664
H	-1.66488	-1.41260	-1.26712
H	-1.89716	-1.28225	1.10409
H	0.38391	-2.87003	-5.80701

NHC-C_6H_4-NHC (9)
Energy: -839.6016334
NImag: 0

N	1.09535	0.21515	-3.75248
C	-0.00003	-0.00043	-2.87801
N	-1.09538	-0.21654	-3.75237
C	0.66009	0.13024	-5.08162
H	1.34969	0.28798	-5.90508
C	-0.66006	-0.13263	-5.08155
C	0.00000	-0.00019	-1.48497
C	-1.21641	-0.01110	-0.68199
C	1.21641	0.01111	-0.68200
C	-1.21646	0.00018	0.68200
C	1.21645	0.00000	0.68199
C	0.00000	0.00000	1.48497
H	-2.18614	-0.01709	-1.17392
H	2.18615	0.01727	-1.17393
H	-2.18621	-0.00234	1.17392
H	2.18620	0.00286	1.17392
H	-1.34966	-0.29080	-5.90492
C	2.38923	0.75501	-3.45065
C	-2.38945	-0.75583	-3.45027
C	0.00000	-0.00013	2.87801
N	1.09724	-0.20616	3.75242
C	0.66119	-0.12591	5.08158
C	-0.66130	0.12493	5.08159
N	-1.09729	0.20560	3.75243
H	-1.35236	0.27639	5.90500
H	1.35219	-0.27771	5.90497
C	-2.39610	0.73347	3.45051
C	2.39626	-0.73343	3.45038
H	-2.98119	-0.78353	-4.34132

H	-2.87156	-0.13890	-2.72098
H	-2.28110	-1.74743	-3.06311
H	2.98110	0.78208	-4.34163
H	2.87139	0.13882	-2.72075
H	2.28058	1.74691	-3.06435
H	2.55108	-0.71569	2.39179
H	2.46316	-1.74116	3.80379
H	3.14375	-0.13683	3.93021
H	-2.55095	0.71601	2.39192
H	-2.46258	1.74116	3.80412
H	-3.14383	0.13709	3.93023

CAAC-C-CAAC (10)
Energy: -852.8736485
NImag = 0

N	5.69132	4.99033	1.68240
C	5.28824	5.86884	0.67152
C	4.25447	5.15834	-0.22110
C	4.17721	3.74849	0.41638
C	5.42950	3.58833	1.30957
C	2.89989	5.87776	-0.16533
C	4.74158	5.10811	-1.67823
C	6.62410	2.98198	0.54659
C	5.10950	2.73386	2.53959
C	6.84348	5.35293	2.46804
C	5.73509	7.09988	0.48956
H	3.28120	3.67639	1.05199
H	4.10496	2.94865	-0.33629
H	2.54688	5.97357	0.87318
H	2.14030	5.32071	-0.73932
H	2.98084	6.88916	-0.59204
H	5.69731	4.57231	-1.77223
H	4.89147	6.12722	-2.06592
H	4.00155	4.59647	-2.31583
H	6.37202	1.99056	0.13671
H	7.49239	2.85991	1.21374
H	6.93228	3.62879	-0.28784
H	4.31999	3.21127	3.13906
H	5.99297	2.58620	3.18105
H	4.75687	1.73794	2.22540
N	7.23237	8.74343	-0.47642
C	6.14604	8.34300	0.31456
C	5.53089	9.60275	0.94963
C	6.25582	10.75127	0.19522
C	6.99439	10.10307	-0.99877
C	5.85604	9.63049	2.45204
C	4.01055	9.63937	0.75248
C	6.10794	10.06321	-2.25851
C	8.31154	10.81870	-1.30366
C	7.88912	7.74956	-1.28647
H	6.99394	11.22953	0.85682
H	5.55836	11.53470	-0.13718
H	6.94218	9.55766	2.61849
H	5.49765	10.56528	2.91532
H	5.37326	8.78518	2.96651
H	3.74012	9.68248	-0.31326
H	3.54818	8.73683	1.17961
H	3.57402	10.52027	1.25093
H	5.82789	11.07951	-2.57844
H	6.63432	9.57851	-3.09600
H	5.18426	9.49500	-2.06861
H	8.97734	10.78112	-0.42800
H	8.83549	10.36121	-2.15737
H	8.12188	11.87288	-1.56221
H	7.75472	5.48805	1.84938
H	6.65812	6.31351	2.97470
H	7.21984	7.29119	-2.04282
H	8.75396	8.18998	-1.80257
H	8.24719	6.93372	-0.63983
H	7.04357	4.59007	3.23330

CAAC-CC-CAAC (11)
Energy: -890.9041553
NImag: from solid state structure

N	6.26283	4.98037	1.20737
C	5.58552	5.64958	0.34213
C	4.50381	4.88262	-0.36009
C	4.52434	3.55241	0.42766
C	5.79855	3.51526	1.29357
C	3.15948	5.61248	-0.22090
C	4.87006	4.72021	-1.84213
C	6.87782	2.60332	0.72357
C	5.51309	3.14571	2.74225
C	7.31914	5.59635	2.00957
C	5.88057	7.03488	0.10123
H	3.64039	3.49709	1.08104
H	4.47309	2.67917	-0.24052
H	2.90563	5.76673	0.83874
H	2.34517	5.03856	-0.69702
H	3.20885	6.60143	-0.70186
H	5.81446	4.16627	-1.95782
H	5.00435	5.70723	-2.30935
H	4.08402	4.17294	-2.39237
H	6.55004	1.55043	0.74711
H	7.80886	2.68037	1.30752
H	7.11031	2.86957	-0.31895
H	4.78944	3.84305	3.19083
H	6.43198	3.16380	3.34905
H	5.09334	2.12806	2.80721
N	5.69743	10.23674	-1.22664
C	6.37473	9.56753	-0.36141
C	7.45644	10.33449	0.34082
C	7.43591	11.66470	-0.44694
C	6.16170	11.70186	-1.31284
C	8.80077	9.60464	0.20163
C	7.09019	10.49691	1.82286
C	5.08244	12.61379	-0.74284
C	6.44716	12.07141	-2.76152
C	4.64111	9.62076	-2.02885
C	6.07969	8.18223	-0.12050

H	8.31987	11.72003	-1.10032
H	7.48717	12.53793	0.22126
H	9.05465	9.45042	-0.85802
H	9.61507	10.17855	0.67778
H	8.75140	8.61568	0.68257
H	6.14577	11.05080	1.93854
H	6.95597	9.50989	2.29009
H	7.87622	11.04422	2.37307
H	5.41025	13.66668	-0.76631
H	4.15143	12.53683	-1.32686
H	4.84988	12.34751	0.29965
H	7.17087	11.37411	-3.21008
H	5.52829	12.05321	-3.36835
H	6.86685	13.08907	-2.82647
H	8.07789	6.05586	1.34987
H	6.90186	6.39971	2.64549
H	3.88231	9.16133	-1.36916
H	4.15829	10.37662	-2.66244
H	5.05846	8.81740	-2.66475
H	7.80195	4.84049	2.64317

CAAC-CCCC-CAAC (12)
Energy: -966.9705539
NImag: 0

N	4.13621	0.89960	0.33044
C	3.25634	-0.15784	0.16401
C	4.03678	-1.47405	0.07585
C	5.50249	-0.99117	0.23787
C	5.51686	0.53107	-0.03482
C	3.62962	-2.42775	1.20966
C	3.79047	-2.16109	-1.27867
C	5.80615	0.85462	-1.51320
C	6.53220	1.24609	0.86290
C	3.65613	2.25509	0.22785
C	1.92248	-0.05911	0.09220
H	5.83496	-1.16999	1.27178
H	6.19464	-1.52938	-0.42671
H	3.75812	-1.94775	2.19210
H	4.24572	-3.34239	1.18661
H	2.57273	-2.71948	1.11027
H	4.08098	-1.51781	-2.12193
H	2.72309	-2.40315	-1.39568
H	4.36982	-3.09700	-1.34503
H	6.81287	0.50929	-1.79775
H	5.76054	1.94013	-1.69507
H	5.07538	0.36994	-2.17683
H	6.28340	1.09142	1.92388
H	6.56276	2.32963	0.66699
H	7.54383	0.85132	0.67857
N	-4.13613	-0.89898	-0.33220
C	-3.25638	0.15832	-0.16413
C	-4.03700	1.47428	-0.07394
C	-5.50268	0.99142	-0.23634
C	-5.51674	-0.53125	0.03400
C	-3.63023	2.42963	-1.20651
C	-3.79053	2.15946	1.28149
C	-5.80559	-0.85711	1.51195
C	-6.53218	-1.24504	-0.86457
C	-3.65582	-2.25456	-0.23182
C	-1.92250	0.05963	-0.09256
H	-5.83545	1.17178	-1.26989
H	-6.19474	1.52849	0.42924
H	-3.75881	1.95094	-2.18959
H	-4.24651	3.34411	-1.18209
H	-2.57338	2.72144	-1.10689
H	-4.08082	1.51496	2.12389
H	-2.72316	2.40148	1.39865
H	-4.36996	3.09522	1.34927
H	-6.81227	-0.51233	1.79730
H	-5.75981	-1.94290	1.69216
H	-5.07470	-0.37336	2.17613
H	-6.28365	-1.08871	-1.92538
H	-6.56251	-2.32889	-0.67031
H	-7.54383	-0.85073	-0.67941
H	3.33950	2.52146	-0.80077
H	2.78083	2.38292	0.88336
H	-3.33923	-2.52259	0.79638
H	-4.43512	-2.95828	-0.55547
H	-2.78046	-2.38115	-0.88747
H	4.43557	2.95921	0.55026
C	-0.65097	0.02250	-0.03254
C	0.65097	-0.02189	0.03192

CAAC-CC-C_6H_4-CC-CAAC_oss (13^{oss})
Energy: -1354.7597565
NImag: 0

N	-1.36351	0.72433	6.26117
N	1.36805	-0.70736	-6.28622
C	2.64529	-1.94885	6.32078
C	1.73819	2.40739	5.56173
C	-1.67979	-1.01823	8.00026
C	2.07312	0.91902	5.64459
C	0.51507	0.23757	7.58526
C	1.27442	-1.48714	5.82254
C	-1.47888	1.41165	8.63608
C	-1.03122	0.33358	7.64532
C	-0.34422	0.37293	2.77372
C	0.91283	-0.00293	6.10436
C	-0.97583	0.34962	-0.90995
C	-0.46078	0.38117	4.00522
C	-0.37523	0.34818	5.37620
C	-1.20757	0.41336	0.45473
C	-0.13475	0.35018	1.37757
C	-2.76719	1.76752	-6.40730
C	-1.58049	-2.42659	-5.19552
C	1.51484	0.77054	-8.27250
C	-2.00915	-0.98001	-5.44199
C	-0.60812	-0.46127	-7.54347
C	-1.35182	1.42435	-5.94061
C	1.35216	-1.73503	-8.53561

C	0.93458	-0.53078	-7.68680
C	0.52796	0.09767	-2.82220
C	-0.92964	-0.06330	-6.07680
C	1.18146	0.24323	0.85864
C	0.58589	-0.07967	-4.04552
C	0.41605	-0.25780	-5.39670
C	1.41367	0.17795	-0.50685
C	0.33869	0.21503	-1.42835
H	2.77845	-3.02745	6.13624
H	2.77502	-1.77660	7.40311
H	3.46301	-1.42833	5.80140
H	2.62331	2.98705	5.25370
H	1.39594	2.81328	6.52798
H	0.94402	2.59554	4.82440
H	-2.77880	-0.94185	8.01429
H	-1.35230	-1.35484	8.99675
H	-1.40316	-1.79004	7.26776
H	2.92892	0.76595	6.32387
H	2.40491	0.57438	4.64996
H	0.94675	1.18136	7.94665
H	0.88606	-0.55601	8.24916
H	0.49115	-2.12482	6.26265
H	1.20998	-1.64527	4.73290
H	-1.08430	2.39437	8.33454
H	-1.10112	1.17650	9.64370
H	-2.57625	1.48147	8.70177
H	-1.81418	0.39004	-1.60851
H	-2.22804	0.50454	0.83318
H	-2.95075	2.85041	-6.31339
H	-2.93565	1.49009	-7.46203
H	-3.53038	1.25625	-5.80277
H	-2.41870	-3.01630	-4.79058
H	-1.24096	-2.92279	-6.11936
H	-0.75276	-2.47676	-4.47215
H	2.61133	0.71645	-8.36322
H	1.10389	0.96151	-9.27644
H	1.26943	1.62914	-7.62963
H	-2.90462	-0.95852	-6.08635
H	-2.31162	-0.53207	-4.48002
H	-1.03843	-1.44581	-7.77569
H	-1.03630	0.24864	-8.26470
H	-0.62414	2.04308	-6.49040
H	-1.24084	1.70501	-4.87971
H	1.00669	-2.66815	-8.06493
H	0.90437	-1.66429	-9.53909
H	2.44478	-1.79237	-8.66294
H	2.01984	0.20570	1.55732
H	2.43438	0.08651	-0.88481
C	-2.72160	0.93020	5.82200
H	-3.29894	1.44500	6.60289
H	-2.72149	1.55934	4.91906
H	-3.23937	-0.01597	5.56626
C	2.76075	-0.75815	-5.91551
H	3.33226	-1.32938	-6.65961
H	3.21512	0.24812	-5.81996
H	2.86028	-1.26046	-4.94153

CAAC-CC-C_6H_4-CC-CAAC_singlet ($13^{singlet}$)

Energy: -1354.7599535

NImag: 0

N	-1.24465	0.28606	6.07540
N	1.24460	-0.28769	-6.07587
C	2.74518	-1.88286	7.13493
C	2.06020	2.23779	5.44953
C	-1.65657	-0.83845	8.26420
C	2.32937	0.77675	5.74404
C	0.54941	0.42562	7.59978
C	1.56310	-1.53971	6.25386
C	-1.56761	1.62419	8.15039
C	-1.02235	0.34308	7.55175
C	-0.01029	-0.01396	2.78825
C	1.13861	-0.07115	6.25717
C	-1.21814	-0.01628	-0.67360
C	-0.05683	0.00171	4.02320
C	-0.09353	0.09776	5.36213
C	-1.22841	-0.01025	0.67233
C	-0.00160	-0.00243	1.42581
C	-2.74516	1.88117	-7.13535
C	-2.06016	-2.23938	-5.45005
C	1.65659	0.83676	-8.26462
C	-2.32933	-0.77835	-5.74456
C	-0.54940	-0.42731	-7.60020
C	-1.56308	1.53802	-6.25428
C	1.56763	-1.62588	-8.15081
C	1.02237	-0.34477	-7.55217
C	0.01030	0.01227	-2.78867
C	-1.13852	0.06950	-6.25763
C	1.21815	0.01459	0.67318
C	0.05685	-0.00340	-4.02361
C	0.09355	-0.09945	-5.36254
C	1.22836	0.00861	-0.67280
C	0.00161	0.00074	-1.42623
H	2.92672	-2.96964	7.13279
H	2.58068	-1.57993	8.18274
H	3.67284	-1.40083	6.79051
H	2.97136	2.73652	5.08186
H	1.72220	2.79258	6.34068
H	1.28541	2.35423	4.67622
H	-2.74803	-0.83896	8.11285
H	-1.46333	-0.79349	9.34784
H	-1.26457	-1.79525	7.88451
H	3.14599	0.69421	6.48103
H	2.69947	0.28986	4.82579
H	0.83083	1.47356	7.76446
H	0.93566	-0.14450	8.45867
H	0.69914	-2.15601	6.55969
H	1.77711	-1.82591	5.21110
H	-1.19931	2.50346	7.59972
H	-1.24458	1.71613	9.19973
H	-2.66984	1.65479	8.14568

H	-2.15956	-0.02920	-1.22932
H	-2.17307	-0.02688	1.22115
H	-2.92672	2.96794	-7.13311
H	-2.58074	1.57822	-8.18315
H	-3.67277	1.39910	-6.79083
H	-2.97137	-2.73810	-5.08243
H	-1.72206	-2.79425	-6.34110
H	-1.28552	-2.35586	-4.67660
H	2.74814	0.83686	-8.11401
H	1.46264	0.79220	-9.34814
H	1.26510	1.79358	-7.88441
H	-3.14603	-0.69585	-6.48145
H	-2.69939	-0.29151	-4.82625
H	-0.83088	-1.47523	-7.76485
H	-0.93549	0.14289	-8.45909
H	-0.69915	2.15446	-6.55991
H	-1.77721	1.82408	-5.21150
H	1.19875	-2.50512	-7.60049
H	1.24518	-1.71749	-9.20036
H	2.66987	-1.65679	-8.14529
H	2.15957	0.02747	1.22890
H	2.17302	0.02540	-1.22164
C	-2.52468	0.47591	5.37799
H	-3.28340	0.83003	6.08873
H	-2.40395	1.22194	4.57589
H	-2.87461	-0.46268	4.91302
C	2.52466	-0.46336	-5.37481
H	3.28317	-0.83357	-6.07786
H	2.87713	0.48412	-4.92983
H	2.40135	-1.19247	-4.55807

CAAC-CC-C_6H_4-CC-CAAC_triplet ($13^{triplet}$)

Energy: -1354.7414040

NImag: 0

N	-1.24465	0.28606	6.07540
N	1.24460	-0.28769	-6.07587
C	2.74518	-1.88286	7.13493
C	2.06020	2.23779	5.44953
C	-1.65657	-0.83845	8.26420
C	2.32937	0.77675	5.74404
C	0.54941	0.42562	7.59978
C	1.56310	-1.53971	6.25386
C	-1.56761	1.62419	8.15039
C	-1.02235	0.34308	7.55175
C	-0.01029	-0.01396	2.78825
C	1.13861	-0.07115	6.25717
C	-1.21814	-0.01628	-0.67360
C	-0.05683	0.00171	4.02320
C	-0.09353	0.09776	5.36213
C	-1.22841	-0.01025	0.67233
C	-0.00160	-0.00243	1.42581
C	-2.74516	1.88117	-7.13535
C	-2.06016	-2.23938	-5.45005
C	1.65659	0.83676	-8.26462
C	-2.32933	-0.77835	-5.74456
C	-0.54940	-0.42731	-7.60020
C	-1.56308	1.53802	-6.25428
C	1.56763	-1.62588	-8.15081
C	1.02237	-0.34477	-7.55217
C	0.01030	0.01227	-2.78867
C	-1.13852	0.06950	-6.25763
C	1.21815	0.01459	0.67318
C	0.05685	-0.00340	-4.02361
C	0.09355	-0.09945	-5.36254
C	1.22836	0.00861	-0.67280
C	0.00161	0.00074	-1.42623
H	2.92672	-2.96964	7.13279
H	2.58068	-1.57993	8.18274
H	3.67284	-1.40083	6.79051
H	2.97136	2.73652	5.08186
H	1.72220	2.79258	6.34068
H	1.28541	2.35423	4.67622
H	-2.74803	-0.83896	8.11285
H	-1.46333	-0.79349	9.34784
H	-1.26457	-1.79525	7.88451
H	3.14599	0.69421	6.48103
H	2.69947	0.28986	4.82579
H	0.83083	1.47356	7.76446
H	0.93566	-0.14450	8.45867
H	0.69914	-2.15601	6.55969
H	1.77711	-1.82591	5.21110
H	-1.19931	2.50346	7.59972
H	-1.24458	1.71613	9.19973
H	-2.66984	1.65479	8.14568
H	-2.15956	-0.02920	-1.22932
H	-2.17307	-0.02688	1.22115
H	-2.92672	2.96794	-7.13311
H	-2.58074	1.57822	-8.18315
H	-3.67277	1.39910	-6.79083
H	-2.97137	-2.73810	-5.08243
H	-1.72206	-2.79425	-6.34110
H	-1.28552	-2.35586	-4.67660
H	2.74814	0.83686	-8.11401
H	1.46264	0.79220	-9.34814
H	1.26510	1.79358	-7.88441
H	-3.14603	-0.69585	-6.48145
H	-2.69939	-0.29151	-4.82625
H	-0.83088	-1.47523	-7.76485
H	-0.93549	0.14289	-8.45909
H	-0.69915	2.15446	-6.55991
H	-1.77721	1.82408	-5.21150
H	1.19875	-2.50512	-7.60049
H	1.24518	-1.71749	-9.20036
H	2.66987	-1.65679	-8.14529
H	2.15957	0.02747	1.22890
H	2.17302	0.02540	-1.22164
C	-2.52468	0.47591	5.37799
H	-3.28340	0.83003	6.08873
H	-2.40395	1.22194	4.57589
H	-2.87461	-0.46268	4.91302
C	2.52466	-0.46336	-5.37481

H	3.28317	-0.83357	-6.07786
H	2.87713	0.48412	-4.92983
H	2.40135	-1.19247	-4.55807

CAAC-CC-C_6H_4-CC-CAAC (13)
Energy: -1354.7472986
NImag: from solid state structure

N	-1.23601	0.30398	6.07630
N	1.23594	-0.30566	-6.07676
C	2.74182	-1.88723	7.13507
C	2.07988	2.23459	5.44335
C	-1.65224	-0.81426	8.26750
C	2.34054	0.77246	5.74008
C	0.56060	0.43529	7.59842
C	1.56084	-1.53845	6.25474
C	-1.54851	1.64760	8.14935
C	-1.01169	0.36218	7.55230
C	-0.00721	-0.00914	2.78828
C	1.14525	-0.06734	6.25600
C	-1.21898	-0.01008	-0.67219
C	-0.05226	0.00893	4.02325
C	-0.08686	0.10749	5.36206
C	-1.22769	-0.00168	0.67373
C	0.00000	0.00000	1.42582
C	-2.74183	1.88550	-7.13548
C	-2.07987	-2.23623	-5.44386
C	1.65223	0.81253	-8.26790
C	-2.34052	-0.77410	-5.74058
C	-0.56061	-0.43702	-7.59882
C	-1.56085	1.53671	-6.25515
C	1.54850	-1.64934	-8.14976
C	1.01168	-0.36392	-7.55270
C	0.00720	0.00741	-2.78869
C	-1.14518	0.06564	-6.25645
C	1.21897	0.00835	0.67179
C	0.05225	-0.01066	-4.02366
C	0.08685	-0.10923	-5.36246
C	1.22762	0.00000	-0.67419
C	-0.00001	-0.00173	-1.42622
H	2.81872	-2.97543	7.25428
H	2.64639	-1.45551	8.14244
H	3.69079	-1.54325	6.70132
H	3.01969	2.76760	5.24312
H	1.59354	2.75497	6.28218
H	1.42965	2.34292	4.56171
H	-2.74189	-0.78410	8.11575
H	-1.46061	-0.74640	9.34732
H	-1.27090	-1.78136	7.91643
H	3.14312	0.69440	6.49148
H	2.71760	0.28131	4.82850
H	0.83715	1.48921	7.73123
H	0.94981	-0.11132	8.47041
H	0.68683	-2.14653	6.54523
H	1.77108	-1.81468	5.20919
H	-1.03780	2.53283	7.75043
H	-1.40560	1.63593	9.24008
H	-2.62907	1.75717	7.95671
H	-2.15887	-0.03273	-1.22795
H	-2.17166	0.01481	1.22453
H	-2.81870	2.97369	-7.25474
H	-2.64643	1.45373	-8.14283
H	-3.69081	1.54157	-6.70170
H	-3.01972	-2.76938	-5.24414
H	-1.59304	-2.75651	-6.28247
H	-1.43005	-2.34456	-4.56191
H	2.74189	0.78236	-8.11618
H	1.46057	0.74469	-9.34772
H	1.27092	1.77962	-7.91680
H	-3.14303	-0.69605	-6.49208
H	-2.71769	-0.28295	-4.82905
H	-0.83714	-1.49095	-7.73160
H	-0.94984	0.10954	-8.47084
H	-0.68687	2.14486	-6.54559
H	-1.77111	1.81289	-5.20958
H	1.03778	-2.53457	-7.75085
H	1.40561	-1.63765	-9.24049
H	2.62906	-1.75892	-7.95710
H	2.15888	0.03099	1.22752
H	2.17159	-0.01647	-1.22499
C	-2.51565	0.50039	5.38000
H	-3.26907	-0.21965	5.71913
H	-2.91610	1.50510	5.55694
H	-2.40384	0.37566	4.29693
C	2.51570	-0.48788	-5.37683
H	3.28991	0.17348	-5.78220
H	2.42048	-0.26788	-4.30742
H	2.87887	-1.51762	-5.47091

CAAC-CC-C_6H_4-C_6H_4-CC-CAAC (14)
Energy: -1428.4576602
NImag: from solid state structure

N	2.15147	-0.08821	-8.19430
C	0.82877	0.13545	3.02453
H	1.67096	0.22377	3.71480
C	-0.48449	0.08317	3.55119
N	-2.13237	0.57591	8.11841
C	0.00086	0.00006	0.72066
C	-1.29809	-0.08411	1.27342
H	-2.15989	-0.17828	0.61253
C	0.96414	-0.09938	-6.11515
C	1.06167	0.08986	1.66342
H	2.09567	0.14296	1.32227
C	-0.95217	0.58860	7.45638
C	-1.53740	-0.05053	2.62169
H	-2.56419	-0.11291	2.99065
C	0.21088	0.83215	8.39502
C	1.93511	-0.11029	-9.68020
C	0.98486	-0.10823	-7.47898

C	-0.70337	0.20413	4.91618
C	-0.83629	-1.65897	-8.24517
H	-1.65145	-1.79638	-8.97350
H	-0.07662	-2.43560	-8.42377
C	-0.84081	0.36398	6.10754
C	1.54010	0.00824	-1.25264
H	2.40654	0.05261	-0.59264
C	0.88080	-0.08627	-4.88829
C	1.76619	-0.03500	-2.60579
H	2.78924	-0.01231	-2.98859
C	0.23678	-0.02052	-0.70159
C	0.42097	-0.11870	-9.79128
H	0.08050	-0.92920	-10.45081
H	0.08445	0.81508	-10.26771
C	2.54595	1.11675	-10.33285
H	2.13794	2.03915	-9.88809
H	2.31980	1.13091	-11.41109
H	3.64148	1.14043	-10.21923
C	-0.21764	-0.23925	-8.38814
C	0.69342	-0.08742	-3.51811
C	-0.61644	-0.11875	-2.97864
H	-1.46363	-0.16061	-3.66725
C	-1.99063	0.84752	9.59673
C	-1.35182	0.81715	-8.19021
H	-2.14919	0.64194	-8.92862
C	-0.83051	-0.07897	-1.63693
H	-1.86151	-0.09531	-1.28290
C	2.54852	-1.34955	-10.32625
H	3.64388	-1.37451	-10.21053
H	2.32602	-1.36058	-11.40466
H	2.13741	-2.26979	-9.88158
C	-0.52280	1.27754	9.68554
H	-0.03957	0.86981	10.58590
H	-0.47596	2.37386	9.76930
C	1.21663	1.91481	7.94501
C	-2.89811	1.98492	10.03023
H	-2.74635	2.87269	9.39737
H	-2.67825	2.26360	11.07312
H	-3.96310	1.70480	9.98133
C	0.93547	-0.48667	8.65078
C	-2.31705	-0.38381	10.42093
H	-3.35751	-0.70765	10.25712
H	-2.19530	-0.17036	11.49451
H	-1.66010	-1.22843	10.16465
H	1.96767	2.07998	8.73324
H	1.73777	1.60613	7.02531
H	0.70181	2.86618	7.74017
H	1.74218	-0.34933	9.39046
H	0.25220	-1.25709	9.03647
H	1.38592	-0.87529	7.72379
H	-1.78268	0.74044	-7.18025
H	-0.95791	1.83695	-8.32331
H	-1.24317	-1.81034	-7.23324
C	3.47391	-0.03866	-7.55430
H	4.24760	-0.27025	-8.29783
H	3.67426	0.95585	-7.11685
H	3.52462	-0.77953	-6.74078
C	-3.39081	0.27710	7.41988
H	-4.22926	0.36816	8.12277
H	-3.54280	0.98493	6.58884
H	-3.37565	-0.74172	6.99521

Thiele-derivative (15)

Energy: -1384.4275111

NImag: 0

C	1.17175	0.21392	0.74951
C	1.27426	0.03923	-0.60086
C	-0.10751	0.18058	1.41481
C	-0.22756	0.86186	5.33105
C	1.08342	1.15020	5.95415
C	1.22803	2.12291	6.96518
C	2.48800	2.44489	7.47190
C	3.63129	1.80203	6.98687
C	3.50303	0.83025	5.98700
C	2.24681	0.51046	5.47623
C	-1.49281	0.88759	6.08249
C	-1.53247	0.73976	7.48590
C	-2.74741	0.73875	8.17125
C	-3.95403	0.87040	7.47813
C	-3.93323	1.00066	6.08394
C	-2.72286	1.01036	5.39802
H	2.06288	0.38604	1.35640
H	2.24954	0.06678	-1.09107
H	0.34979	2.65713	7.33017
H	2.58009	3.21326	8.24388
H	4.61502	2.06140	7.38686
H	4.38733	0.31552	5.60197
H	2.14643	-0.24609	4.69492
H	-0.60474	0.59648	8.04054
H	-2.75186	0.61871	9.25767
H	-4.90327	0.86696	8.01927
H	-4.86892	1.10284	5.52848
H	-2.71012	1.12357	4.31219
C	0.10623	-0.19083	-1.41295
C	-1.27554	-0.04934	0.60271
C	-1.17304	-0.22403	-0.74767
C	0.22858	-0.86284	-5.33080
H	-2.25086	-0.07679	1.09287
H	-2.06419	-0.39608	-1.35457
C	-1.08276	-1.14911	-5.95411
C	1.49344	-0.88628	-6.08295
C	-1.22834	-2.12042	-6.96636
C	-2.24548	-0.50903	-5.47506
C	1.53228	-0.73675	-7.48619
C	2.72395	-1.00887	-5.39924
C	-2.48871	-2.44085	-7.47303
H	-0.35051	-2.65479	-7.33212
C	-3.50211	-0.82720	-5.98590
H	-2.14427	0.24643	-4.69281
C	2.74689	-0.73423	-8.17216
H	0.60424	-0.59348	-8.04031

C	3.93395	-0.99757	-6.08574
H	2.71176	-1.12332	-4.31353
C	-3.63136	-1.79771	-6.98684
H	-2.58176	-3.20821	-8.24591
H	-4.38592	-0.31226	-5.60003
C	3.95395	-0.86585	-7.47983
H	2.75054	-0.61306	-9.25846
H	4.87000	-1.09966	-5.53088
H	-4.61539	-2.05590	-7.38686
H	4.90295	-0.86121	-8.02138
C	0.19459	-0.38986	-2.76591
C	0.23580	-0.59528	-3.99666
C	-0.19555	0.37851	2.76796
C	-0.23425	0.58941	3.99791

Cyclopentylidene (16)

Energy: -930.0857341

NImag: 0

C	-1.15303	0.28180	6.07510
C	1.15305	-0.28388	-6.07523
H	2.43958	-1.67152	7.12496
H	2.14384	1.83772	5.78709
C	2.40308	0.77107	5.87225
C	0.59972	0.45063	7.66599
C	1.60763	-1.54493	6.41245
C	-0.93495	0.36926	7.50898
C	0.03940	0.03907	2.79741
C	1.19706	-0.05869	6.33050
C	-1.24465	0.08676	-0.66055
C	0.02149	0.06413	4.05455
C	0.00539	0.10695	5.39483
C	-1.22067	0.10175	0.70008
C	0.02543	0.01622	1.43799
H	-2.44078	1.66812	-7.12577
H	1.55045	0.87958	-8.13872
C	-2.40255	-0.77415	-5.87280
C	-0.59931	-0.45283	-7.66643
C	-1.60869	1.54230	-6.41333
H	1.63737	-1.64265	-7.97512
C	0.93529	-0.37088	-7.50917
C	-0.03979	-0.03988	-2.79782
C	-1.19708	0.05638	-6.33110
C	1.24423	-0.08699	0.66012
C	-0.02174	-0.06526	-4.05496
C	-0.00543	-0.10840	-5.39523
C	1.22026	-0.10197	-0.70050
C	-0.02586	-0.01667	-1.43841
H	3.23349	0.66832	6.58975
H	2.75650	0.42721	4.88809
H	0.89836	1.49641	7.83218
H	0.95418	-0.13423	8.52657
H	0.77681	-2.18288	6.74558
H	1.93846	-1.90664	5.42749
H	-2.19448	0.14750	-1.19655
H	-2.15027	0.17513	1.26848
H	-2.87835	-1.76490	-5.95627
H	-0.89752	-1.49876	-7.83253
H	-0.95384	0.13177	-8.52717
H	-0.77837	2.18077	-6.74667
H	-1.93969	1.90400	-5.42841
H	2.19405	-0.14791	1.19613
H	2.14984	-0.17551	-1.26891
H	-3.14916	-0.66256	-6.64515
H	-2.77774	-1.43837	-5.10831
H	-1.96651	0.99202	6.06013
H	-2.08015	-0.05037	5.63181
H	1.61611	-1.24537	-6.24104
H	2.01825	0.16474	-5.60985
H	-1.63987	1.18471	7.57630
H	-0.97498	-0.43953	8.22358

bisFischer carbene (17)

Energy: -1158.8815237

NImag: 0

O	-1.24465	0.28606	6.07540
O	1.24460	-0.28769	-6.07587
H	2.74518	-1.88286	7.13493
H	2.06020	2.23779	5.44953
C	-1.65657	-0.83845	8.26420
C	2.32937	0.77675	5.74404
C	0.54941	0.42562	7.59978
C	1.56310	-1.53971	6.25386
C	-1.56761	1.62419	8.15039
C	-1.02235	0.34308	7.55175
C	-0.01029	-0.01396	2.78825
C	1.13861	-0.07115	6.25717
C	-1.21814	-0.01628	-0.67360
C	-0.05683	0.00171	4.02320
C	-0.09353	0.09776	5.36213
C	-1.22841	-0.01025	0.67233
C	-0.00160	-0.00243	1.42581
H	-2.74516	1.88117	-7.13535
H	-2.06016	-2.23938	-5.45005
C	1.65659	0.83676	-8.26462
C	-2.32933	-0.77835	-5.74456
C	-0.54940	-0.42731	-7.60020
C	-1.56308	1.53802	-6.25428
C	1.56763	-1.62588	-8.15081
C	1.02237	-0.34477	-7.55217
C	0.01030	0.01227	-2.78867
C	-1.13852	0.06950	-6.25763
C	1.21815	0.01459	0.67318
C	0.05685	-0.00340	-4.02361
C	0.09355	-0.09945	-5.36254
C	1.22836	0.00861	-0.67280
C	0.00161	0.00074	-1.42623
H	-2.74803	-0.83896	8.11285
H	-1.46333	-0.79349	9.34784
H	-1.26457	-1.79525	7.88451
H	3.14599	0.69421	6.48103

H	2.69947	0.28986	4.82579
H	0.83083	1.47356	7.76446
H	0.93566	-0.14450	8.45867
H	0.69914	-2.15601	6.55969
H	1.77711	-1.82591	5.21110
H	-1.19931	2.50346	7.59972
H	-1.24458	1.71613	9.19973
H	-2.66984	1.65479	8.14568
H	-2.15956	-0.02920	-1.22932
H	-2.17307	-0.02688	1.22115
H	2.74814	0.83686	-8.11401
H	1.46264	0.79220	-9.34814
H	1.26510	1.79358	-7.88441
H	-3.14603	-0.69585	-6.48145
H	-2.69939	-0.29151	-4.82625
H	-0.83088	-1.47523	-7.76485
H	-0.93549	0.14289	-8.45909
H	-0.69915	2.15446	-6.55991
H	-1.77721	1.82408	-5.21150
H	1.19875	-2.50512	-7.60049
H	1.24518	-1.71749	-9.20036
H	2.66987	-1.65679	-8.14529
H	2.15957	0.02747	1.22890
H	2.17302	0.02540	-1.22164

saNHC-CC-C_6H_4-CC-saNHC (18)
Energy: -993.9871208
NImag: from solid state structure

N	0.47170	3.23090	3.21480
N	0.61530	4.98170	1.80970
C	1.06680	3.70040	2.03730
C	-0.18790	4.36530	3.91420
H	0.42030	4.79300	4.56910
H	-1.01580	4.07790	4.37430
C	-0.49050	5.29080	2.73800
H	-1.36970	5.08530	2.33320
H	-0.47310	6.24140	3.01490
C	1.94680	2.96870	1.30600
C	2.69250	2.10330	0.83060
C	3.52400	1.09090	0.40480
C	3.67060	-0.10520	1.21050
H	3.19890	-0.17040	2.03150
C	4.46280	-1.13270	0.82290
H	4.53150	-1.90110	1.37850
N	8.25130	-3.23090	-3.21480
N	8.10770	-4.98170	-1.80970
C	7.65620	-3.70040	-2.03730
C	8.91090	-4.36530	-3.91420
H	8.30270	-4.79300	-4.56910
H	9.73880	-4.07790	-4.37430
C	9.21350	-5.29080	-2.73800
H	10.09270	-5.08530	-2.33320
H	9.19610	-6.24140	-3.01490
C	6.77620	-2.96870	-1.30600
C	6.03050	-2.10330	-0.83060
C	5.19900	-1.09090	-0.40480
C	5.05240	0.10520	-1.21050
H	5.52410	0.17040	-2.03150
C	4.26020	1.13270	-0.82290
H	4.19150	1.90110	-1.37850
C	1.01399	2.03821	3.88137
H	0.80772	1.17268	3.28706
H	2.07197	2.14578	3.99967
H	0.55699	1.92803	4.84258
C	0.70845	5.64142	0.49936
H	1.73695	5.81037	0.25741
H	0.26448	5.01637	-0.24703
H	0.19172	6.57774	0.53392
C	8.01455	-5.64142	-0.49936
H	6.98544	-5.79342	-0.24892
H	8.51520	-6.58623	-0.53933
H	8.47522	-5.02484	0.24395
C	7.70901	-2.03821	-3.88137
H	6.65164	-2.14761	-4.00345
H	7.91159	-1.17321	-3.28501
H	8.16907	-1.92567	-4.84084

Pyrazolidin-CC-C_6H_4-CC-pyrazolidin (19)
Energy: -1151.1443073
NImag: 0

N	6.64862	-3.12465	-4.23415
N	-0.65663	5.15416	2.16192
N	7.48987	-3.36346	-5.38422
N	-0.76491	5.83309	3.43040
C	6.76891	-2.71351	-6.47973
C	7.68901	-4.78237	-5.61427
C	-0.80923	4.73509	4.40059
C	-1.95216	6.66627	3.48070
C	-0.24617	2.23454	4.18700
C	-0.37679	5.98284	1.01124
C	4.93450	-0.91197	-6.53368
C	7.26993	-3.35242	-2.94460
C	6.19370	-1.43859	-5.84471
C	0.14735	3.67054	3.83190
C	5.92841	-1.95663	-4.43466
C	0.01773	3.96290	2.34001
C	2.20042	2.05883	-1.63211
C	3.01446	1.31045	-2.42737
C	3.66245	0.11150	-1.93632
C	4.46644	-0.63076	-2.74743
C	5.19365	-1.30788	-3.51386
C	3.40511	-0.25939	-0.56128
C	2.59568	0.49225	0.23556
C	1.96151	1.69973	-0.25120
C	1.20926	2.47563	0.57802
C	0.58957	3.22099	1.37452
H	5.94056	-3.35643	-6.84887
H	0.40183	1.52615	3.64995
H	-0.12699	2.05097	5.26758

H	-1.28784	2.02024	3.90118
H	-1.18370	6.71157	0.84935
H	0.58260	6.52473	1.12219
H	-0.31762	5.32956	0.13041
H	4.50991	-0.07778	-5.95443
H	5.16467	-0.54072	-7.54554
H	4.16346	-1.69356	-6.61095
H	8.09977	-2.64281	-2.76245
H	6.50762	-3.21218	-2.16675
H	7.65442	-4.37968	-2.87465
H	6.73445	-5.33090	-5.76157
H	8.23375	-5.24146	-4.77627
H	8.31069	-4.89971	-6.51436
H	-2.87685	6.09842	3.24247
H	-1.86443	7.51597	2.78778
H	-2.03841	7.08154	4.49537
H	1.72562	2.96185	-2.02255
H	3.20858	1.61400	-3.45886
H	3.87640	-1.16438	-0.17148
H	2.40191	0.19000	1.26751
H	-0.50687	5.10555	5.39115
C	7.27537	-0.34231	-5.76424
H	8.18345	-0.73320	-5.28199
H	7.54374	0.01238	-6.77355
H	6.91071	0.51277	-5.17657
C	1.60331	3.94326	4.25892
H	1.73559	3.72798	5.33328
H	2.29201	3.30195	3.69045
H	1.87506	4.99297	4.07057
H	7.45730	-2.51483	-7.31388
H	-1.83547	4.31705	4.47822

TTF derivative (20)
Energy: -2205.6547856
NImag: 0

C	1.85707	2.69257	1.69375
C	2.72969	1.91950	1.23267
C	3.66359	1.06348	0.71434
C	3.98726	-0.18685	1.36208
H	3.49728	-0.42361	2.30874
C	4.87534	-1.06503	0.81119
H	5.10549	-2.00647	1.31464
C	7.02518	-2.58811	-1.62269
C	6.33453	-1.71517	-1.04744
C	5.52379	-0.78977	-0.44962
C	5.24266	0.48409	-1.06989
H	5.74450	0.72543	-2.00934
C	4.35546	1.36290	-0.51836
H	4.13988	2.31110	-1.01537
C	0.91712	3.52312	2.17911
S	-0.01070	3.19117	3.65732
S	0.48830	5.06158	1.40008
C	-0.92229	4.68612	3.62021
C	-0.69573	5.53244	2.59990
H	-1.62976	4.86963	4.43053
H	-1.19560	6.49285	2.46628
C	7.73420	-3.53418	-2.26185
S	7.99209	-5.16496	-1.60740
S	8.47152	-3.27808	-3.85780
C	8.89660	-5.75298	-2.98628
C	9.11598	-4.90029	-4.00265
H	9.25537	-6.78301	-2.95577
H	9.66810	-5.14997	-4.91019

NHC-CC- C_6H_4-CC-NHC (21)
Energy: -991.5951550
NImag: 0

C	1.94680	2.96870	1.30600
C	2.69250	2.10330	0.83060
C	3.52400	1.09090	0.40480
C	3.67060	-0.10520	1.21050
H	3.19890	-0.17040	2.03150
C	4.46280	-1.13270	0.82290
H	4.53150	-1.90110	1.37850
C	6.77620	-2.96870	-1.30600
C	6.03050	-2.10330	-0.83060
C	5.19900	-1.09090	-0.40480
C	5.05240	0.10520	-1.21050
H	5.52410	0.17040	-2.03150
C	4.26020	1.13270	-0.82290
H	4.19150	1.90110	-1.37850
C	0.94898	3.79837	2.13522
N	0.37405	3.40458	3.28514
N	0.51539	5.04597	1.81600
C	0.56358	2.12758	3.97286
C	-0.48662	4.50366	3.71800
C	0.92821	5.80454	0.62647
C	-0.34910	5.49056	2.74797
H	0.79143	1.36863	3.24884
H	1.37000	2.22124	4.67045
H	-0.33381	1.85798	4.50149
H	-1.09294	4.54493	4.59460
H	1.92385	5.51922	0.34449
H	0.25397	5.59741	-0.17676
H	0.90513	6.85320	0.84748
H	-0.84466	6.44396	2.74256
C	7.77402	-3.79837	-2.13522
N	8.22294	-5.02486	-1.81562
N	8.33549	-3.40168	-3.30730
C	7.87297	-5.81060	-0.63252
C	9.13801	-5.42444	-2.88289
C	8.08170	-2.11550	-3.97227
C	9.16019	-4.35802	-3.77514
H	7.63792	-5.14416	0.17540
H	7.02604	-6.42521	-0.85763
H	8.70071	-6.43659	-0.34889
H	9.67620	-6.34170	-2.96501
H	7.09014	-1.77784	-3.73776
H	8.79584	-1.39550	-3.63419

H	8.17679	-2.23841	-5.03288
H	9.73398	-4.30545	-4.68209

MIC-CC-C_6H_4-CC-MIC (22)
Energy: -1070.2218771
NImag: 0

C	1.94680	2.96870	1.30600
C	2.69250	2.10330	0.83060
C	3.52400	1.09090	0.40480
C	3.67060	-0.10520	1.21050
H	3.19890	-0.17040	2.03150
C	4.46280	-1.13270	0.82290
H	4.53150	-1.90110	1.37850
C	6.77620	-2.96870	-1.30600
C	6.03050	-2.10330	-0.83060
C	5.19900	-1.09090	-0.40480
C	5.05240	0.10520	-1.21050
H	5.52410	0.17040	-2.03150
C	4.26020	1.13270	-0.82290
H	4.19150	1.90110	-1.37850
C	0.94898	3.79837	2.13522
C	0.37405	3.40458	3.28514
N	0.51539	5.04597	1.81600
C	0.56358	2.12758	3.97286
N	-0.48662	4.50366	3.71800
C	0.92821	5.80454	0.62647
C	-0.34910	5.49056	2.74797
H	0.79143	1.36863	3.24884
H	1.37000	2.22124	4.67045
H	-0.33381	1.85798	4.50149
H	1.92385	5.51922	0.34449
H	0.25397	5.59741	-0.17676
H	0.90513	6.85320	0.84748
H	-0.84466	6.44396	2.74256
C	7.77402	-3.79837	-2.13522
N	8.22294	-5.02486	-1.81562
C	8.33549	-3.40168	-3.30730
C	7.87297	-5.81060	-0.63252
C	9.13801	-5.42444	-2.88289
N	9.16019	-4.35802	-3.77514
H	7.63792	-5.14416	0.17540
H	7.02604	-6.42521	-0.85763
H	8.70071	-6.43659	-0.34889
H	9.67620	-6.34170	-2.96501
C	-1.32270	4.55510	4.92598
H	-2.38910	4.56017	4.67325
H	-1.14118	3.69012	5.57402
H	-1.11866	5.45692	5.51437
C	9.94754	-4.28695	-5.01446
H	11.02302	-4.27656	-4.80389
H	9.74679	-5.14612	-5.66456
H	9.71398	-3.38030	-5.58414
C	8.05226	-2.04457	-3.97786
H	8.91607	-1.69715	-4.55598
H	7.20007	-2.10866	-4.66399
H	7.82047	-1.27302	-3.23484

Pyrazolin-CC-C_6H_4-CC-pyrazolin (23)
Energy: -1070.2179208
NImag: 0

N	6.66968	-3.16015	-4.29012
N	-0.43107	5.13858	2.02369
N	7.42379	-3.41754	-5.46250
N	-0.91245	5.84691	3.15042
C	6.95587	-2.53154	-6.42830
C	7.55917	-4.82702	-5.80452
C	-0.78109	4.98939	4.23683
C	-2.17089	6.54460	2.92798
C	0.29918	2.70645	4.76265
C	0.22738	5.94032	1.01134
C	5.39921	-0.47838	-6.56109
C	7.37676	-3.31944	-3.03333
C	6.06299	-1.64488	-5.90827
C	-0.12198	3.84592	3.89702
C	5.90298	-1.99900	-4.51432
C	0.15802	3.94112	2.48124
C	2.37307	1.97835	-1.34386
C	3.11482	1.24637	-2.22542
C	3.81014	0.04724	-1.81911
C	4.54912	-0.67806	-2.71749
C	5.20495	-1.33008	-3.55885
C	3.67954	-0.34257	-0.43463
C	2.93635	0.39008	0.44774
C	2.25263	1.59567	0.04417
C	1.53312	2.36468	0.92211
C	0.87636	3.10132	1.68931
H	7.32414	-2.61788	-7.45006
H	1.39469	2.57721	4.74059
H	-0.01478	2.85677	5.80619
H	-0.13650	1.76146	4.39848
H	-0.48182	6.64884	0.55766
H	1.08584	6.50039	1.42739
H	0.58942	5.26223	0.22789
H	5.63515	0.45196	-6.01780
H	5.72256	-0.36171	-7.60586
H	4.30150	-0.58621	-6.54240
H	8.18683	-2.57526	-2.91515
H	6.65319	-3.18619	-2.21836
H	7.80284	-4.33085	-2.96205
H	6.58131	-5.30639	-6.00169
H	8.06247	-5.36569	-4.98866
H	8.19101	-4.90839	-6.70080
H	-2.97051	5.85434	2.59852
H	-2.03765	7.32730	2.16765
H	-2.47167	7.03541	3.86503
H	1.85591	2.88048	-1.67969
H	3.19981	1.56610	-3.26695
H	4.19029	-1.24857	-0.09991
H	2.84584	0.06602	1.48753
H	-1.19420	5.28790	5.20011

Bisbentallene (24)
Energy: -1448.7633780
NImag: 0

C	1.94680	2.96870	1.30600
C	2.69250	2.10330	0.83060
C	3.52400	1.09090	0.40480
C	3.67060	-0.10520	1.21050
H	3.19890	-0.17040	2.03150
C	4.46280	-1.13270	0.82290
H	4.53150	-1.90110	1.37850
C	6.77620	-2.96870	-1.30600
C	6.03050	-2.10330	-0.83060
C	5.19900	-1.09090	-0.40480
C	5.05240	0.10520	-1.21050
H	5.52410	0.17040	-2.03150
C	4.26020	1.13270	-0.82290
H	4.19150	1.90110	-1.37850
C	0.94898	3.79837	2.13522
C	7.77402	-3.79837	-2.13522
N	-0.34910	5.49056	2.74797
N	-0.48662	4.50366	3.71800
N	9.16019	-4.35802	-3.77514
N	9.13801	-5.42444	-2.88289
C	0.51539	5.04597	1.81600
C	0.37405	3.40458	3.28514
C	8.33549	-3.40168	-3.30730
C	8.22294	-5.02486	-1.81562
O	7.88080	-5.79302	-0.65900
O	8.08860	-2.15049	-3.95418
O	0.91698	5.78391	0.65882
O	0.55934	2.15616	3.95747
C	-0.25227	2.12274	5.13436
H	-0.12968	1.18006	5.62550
H	0.04475	2.91035	5.79493
H	-1.27915	2.25281	4.86327
C	0.25374	7.05074	0.64663
H	0.51957	7.60097	1.52496
H	0.55062	7.60042	-0.22206
H	-0.80524	6.89874	0.62785
C	-1.21501	6.63596	3.06286
H	-0.83036	7.14901	3.91944
H	-1.23964	7.30463	2.22789
H	-2.20532	6.28798	3.27045
C	-0.37153	5.53269	4.76143
H	-1.32811	5.68995	5.21433
H	0.32654	5.20983	5.50531
H	-0.02924	6.44731	4.32415
C	10.52122	-4.81359	-4.09288
H	10.47546	-5.77464	-4.56105
H	10.98519	-4.11491	-4.75732
H	11.09369	-4.88281	-3.19156
C	9.03078	-6.35321	-4.01726
H	9.96406	-6.85836	-4.15408
H	8.26239	-7.07100	-3.81913
H	8.78784	-5.80630	-4.90427
C	8.59076	-7.03410	-0.68307
H	8.24708	-7.62570	-1.50574
H	9.63792	-6.84389	-0.79342
H	8.41851	-7.56134	0.23195
C	8.85154	-2.07859	-5.16152
H	9.89114	-2.18893	-4.93360
H	8.54641	-2.86197	-5.82343
H	8.68793	-1.13107	-5.63093