Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Osmapentalyne and Osmapentalene Complexes Containing Boron Monofluoride Ligands: Structure, Bonding and Adaptive Aromaticity

Fangzhou Xu, Dandan Chen, Jie Zeng, and Jun Zhu*

State Key Laboratory of Physical Chemistry of Solid Surfaces and Collaborative Innovation Center of Chemistry for Energy Materials (iChEM), Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry and Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

The HOMA values were calculated using equation $HOMA=1-\frac{\alpha}{n}\sum_{i=1}^{n}(R_i-R_{opt})^2$, where n is the number of C-C bonds in the metallacycle, R_{opt} (1.388) is the optimal value for C-C bond, α (257.7) is an empirical constant that determines the range of HOMA index, and R_i corresponds to individual C-C bond lengths. Note that the HOMA method was originally developed for closed-shell systems, while in the T_1 state positive values do not necessarily indicate aromaticity (several instances have been reported for anti-aromatic systems)[1,2]. Given a specific electronic state, a larger HOMA value is supposed to arise from better equalization of C-C bond lengths. The variation of HOMA values (ΔHOMA) correlates well to the aromaticity change.

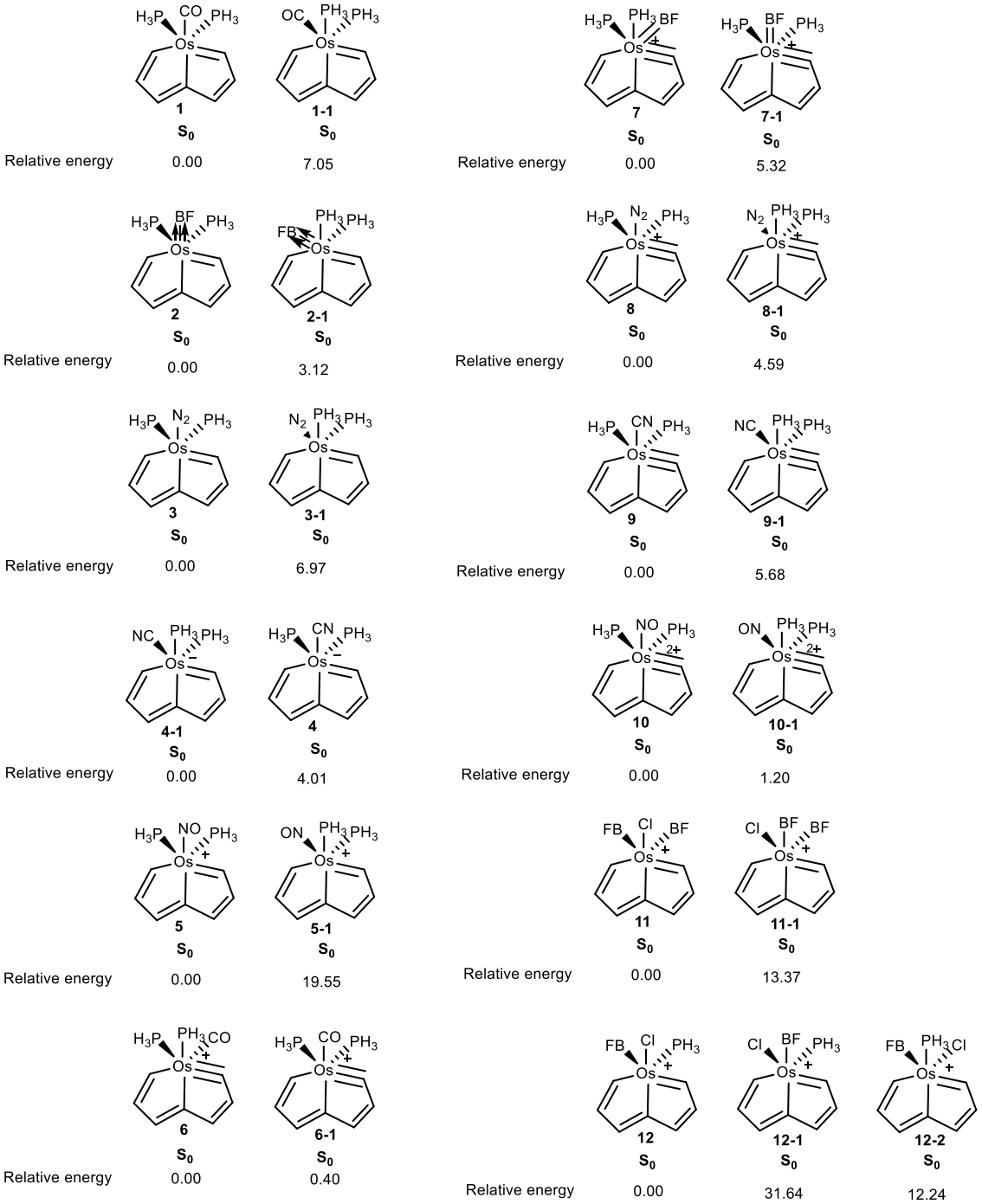


Figure S1. Relative electronic energy of the isomers of complexes **1-12** computed at the (U)B3LYP/6-311++G(d,p)-LanL2TZ(f) level.

Table S1. ΔE_{ST} values for complexes **1**-**12** computed at the (U)B3LYP/6-311++G(d,p)-Lanl2TZ(f) level.

Complexes	E (S_0, a.u.)	E (T_1, a.u.)	ΔE_{ST} (kcal mol^{-1})
1	-1161.235055	-1161.177448	-36.15
2	-1172.616086	-1172.557205	-36.95
3	-1157.398207	-1157.350332	-30.04
4	-1140.779736	-1140.736954	-26.85
5	-1177.615566	-1177.544495	-44.60
6	-1160.370424	-1160.297035	-45.65
7	-1171.763912	-1171.690301	-46.19
8	-1156.547826	-1156.474708	-45.88
9	-1140.087670	-1140.013634	-56.46
10	-1176.550729	-1176.519374	-19.68
11	-1070.986682	-1070.958984	-17.38
12	-1289.437594	-1289.401500	-22.65

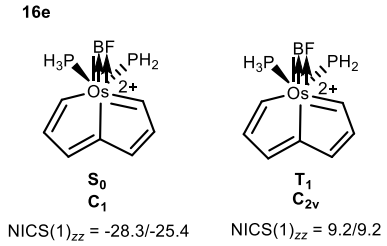


Figure S2. The $NICS(1)_{zz}$ values (ppm) of complexes **2** with two different symmetries in the S_0 and T_1 states.

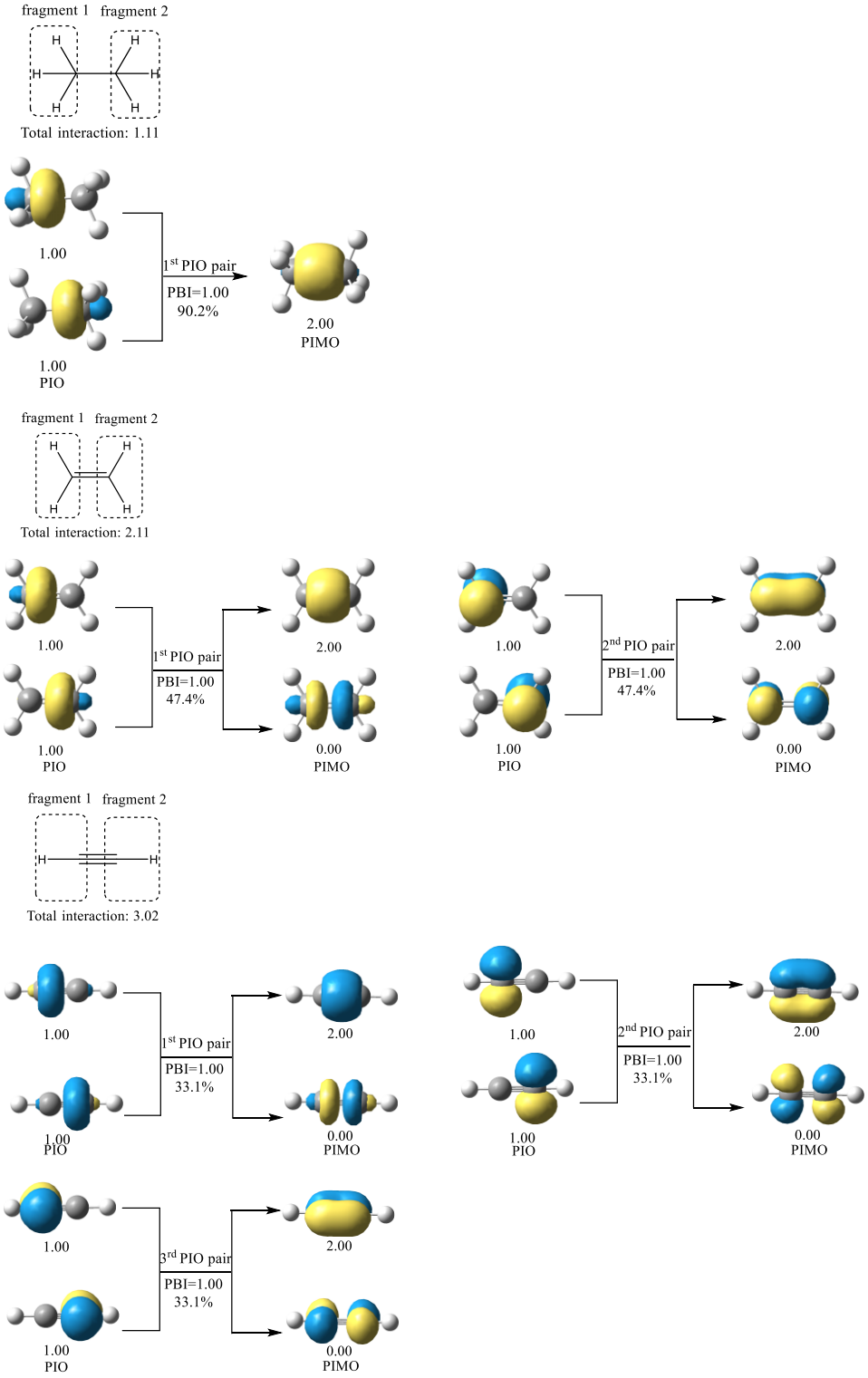


Figure S3. This structure presented in this paper is optimized using B3LYP/6-311++G (d, p) and all orbitals are computed based on the same level of theory. Principal interacting orbital (PIO) analysis on the C-C bonding interactions in ethane, ethylene, and acetylene. Isovalue: 0.10 a.u.

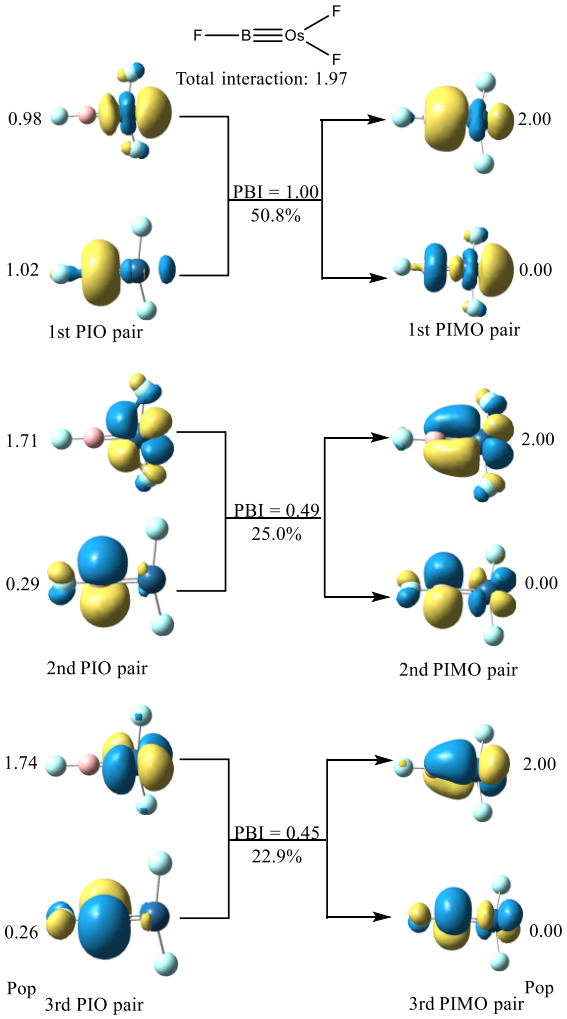


Figure S4. This structure presented in this paper is optimized using B3LYP/The 6-311++G(3df,3pd)[3] basis sets for B and F atoms and SDD effective core potential basis[4] for transition-metal atoms were used. all orbitals are computed based on the same level of theory. Principal interacting orbital (PIO) analysis with NBO 7.0 program on the Fe-BF bonding interactions. Isovalue: 0.05 a.u.

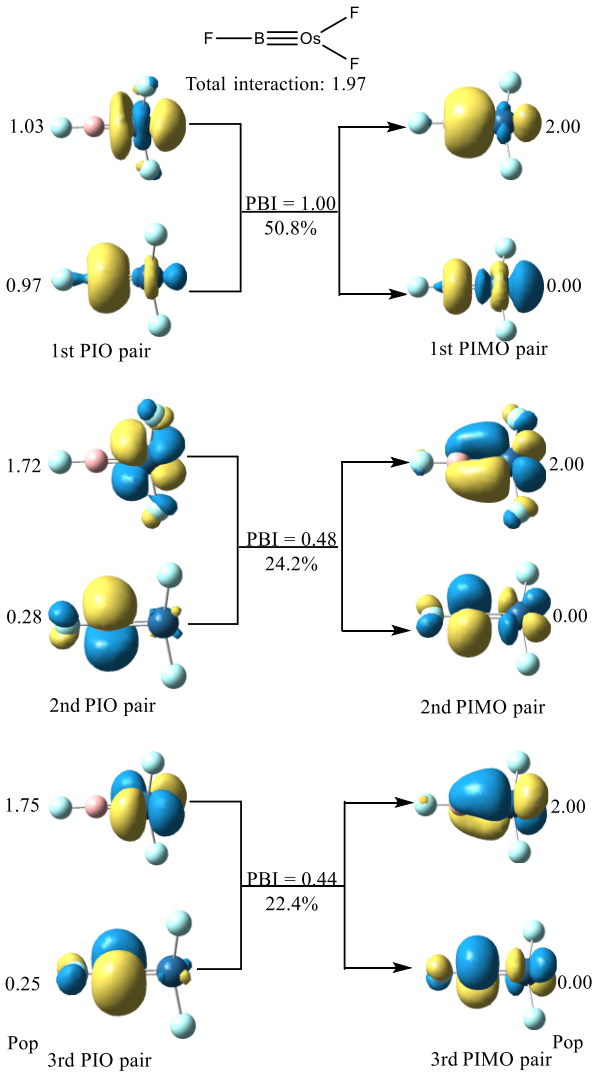


Figure S5. This structure presented in this paper is optimized using B3LYP/The 6-311++G(3df,3pd) basis sets for B and F atoms and SDD effective core potential basis for transition-metal atoms were used. all orbitals are computed based on the same level of theory. Principal interacting orbital (PIO) analysis with NBO 3.1 program[5] on the Fe-BF bonding interactions. Isovalue: 0.05 a.u.

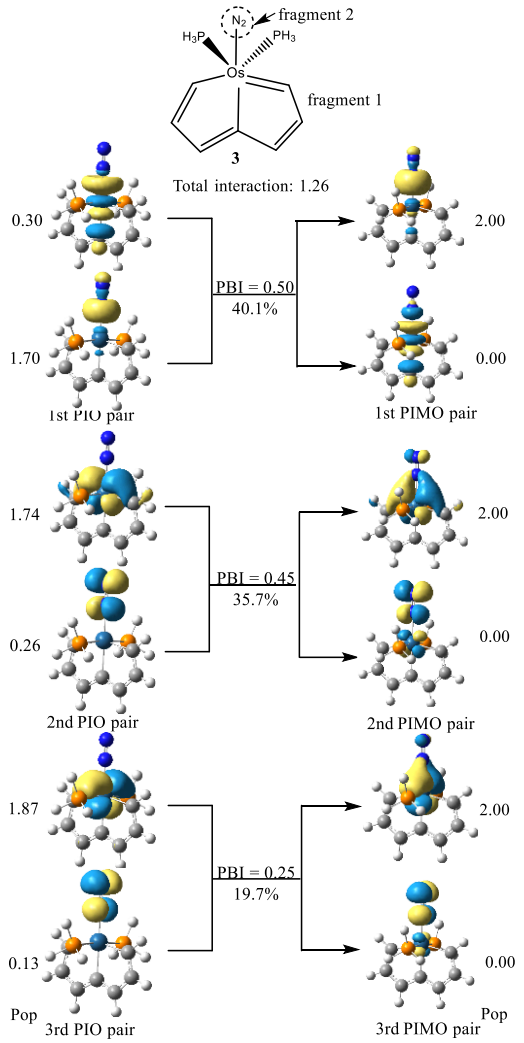


Figure S6. Principal interacting orbital (PIO) analysis on the Os-N_2 bonding interactions in complex **3**. Isovalue: 0.05 a.u.

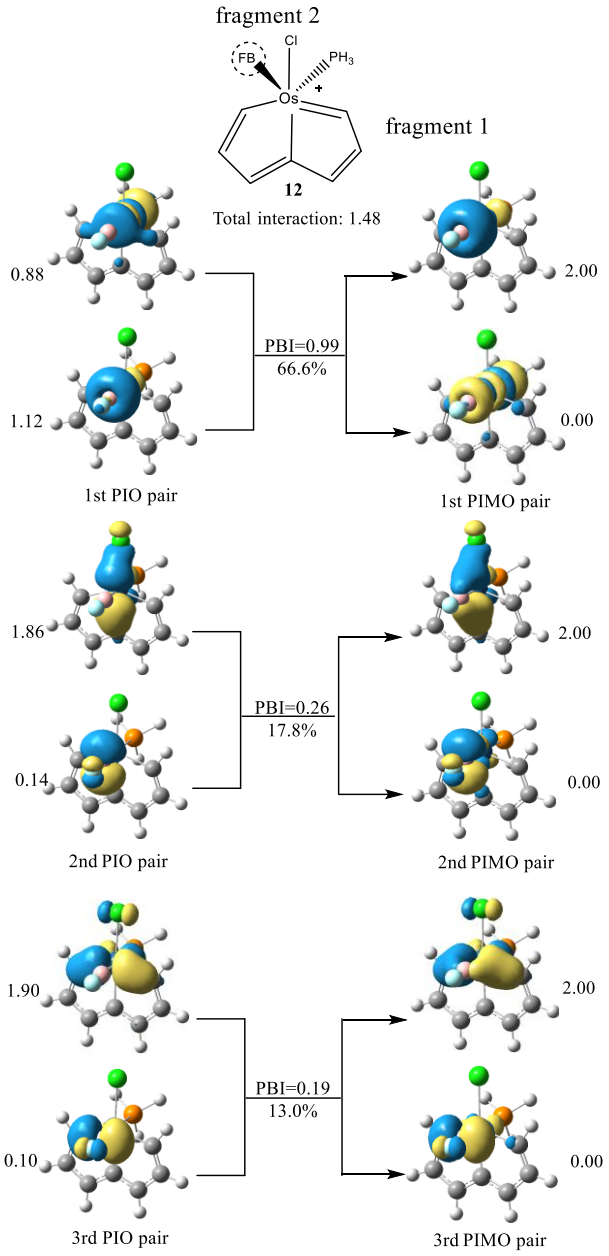


Figure S7. Principal interacting orbital (PIO) analysis on the Os-BF bonding interactions in complex **12**. Isovalue: 0.05 a.u.

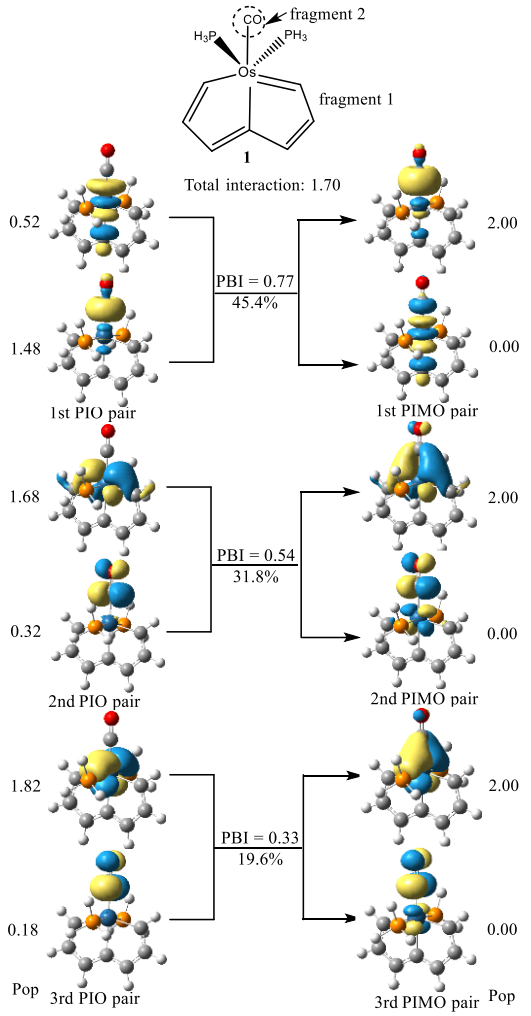


Figure S8. Principal interacting orbital (PIO) analysis on the Os-CO bonding interactions in complex **1**. Isovalue: 0.05 a.u.

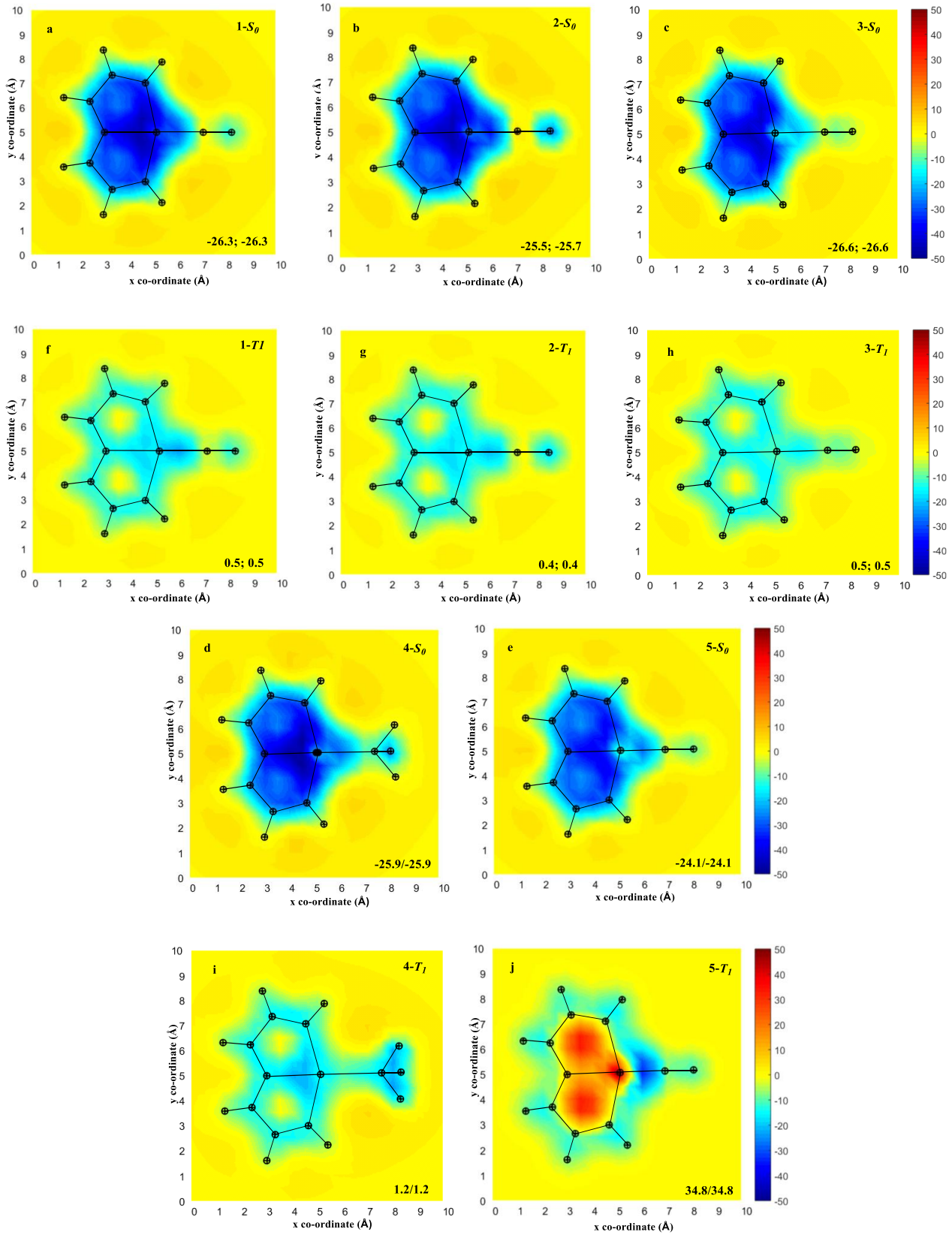


Figure S9. NICS(1)$_{zz}$ grids for complexes **1-5** in the S_0 and T_1 states. A fixed color scale (−50 to 50 ppm) is applied to all grids for easy comparison. NICS(1)$_{zz}$ values calculated at the ring centers (upper ring; lower ring) are commented on the bottom-right of each grid. **a–j** NICS(1)$_{zz}$ grids for **1-S$_0$**, **2-S$_0$**, **3-S$_0$**, **4-S$_0$**, **5-S$_0$**, **1-T$_1$**, **2-T$_1$**, **3-T$_1$**, **4-T$_1$** and **5-T$_1$**.

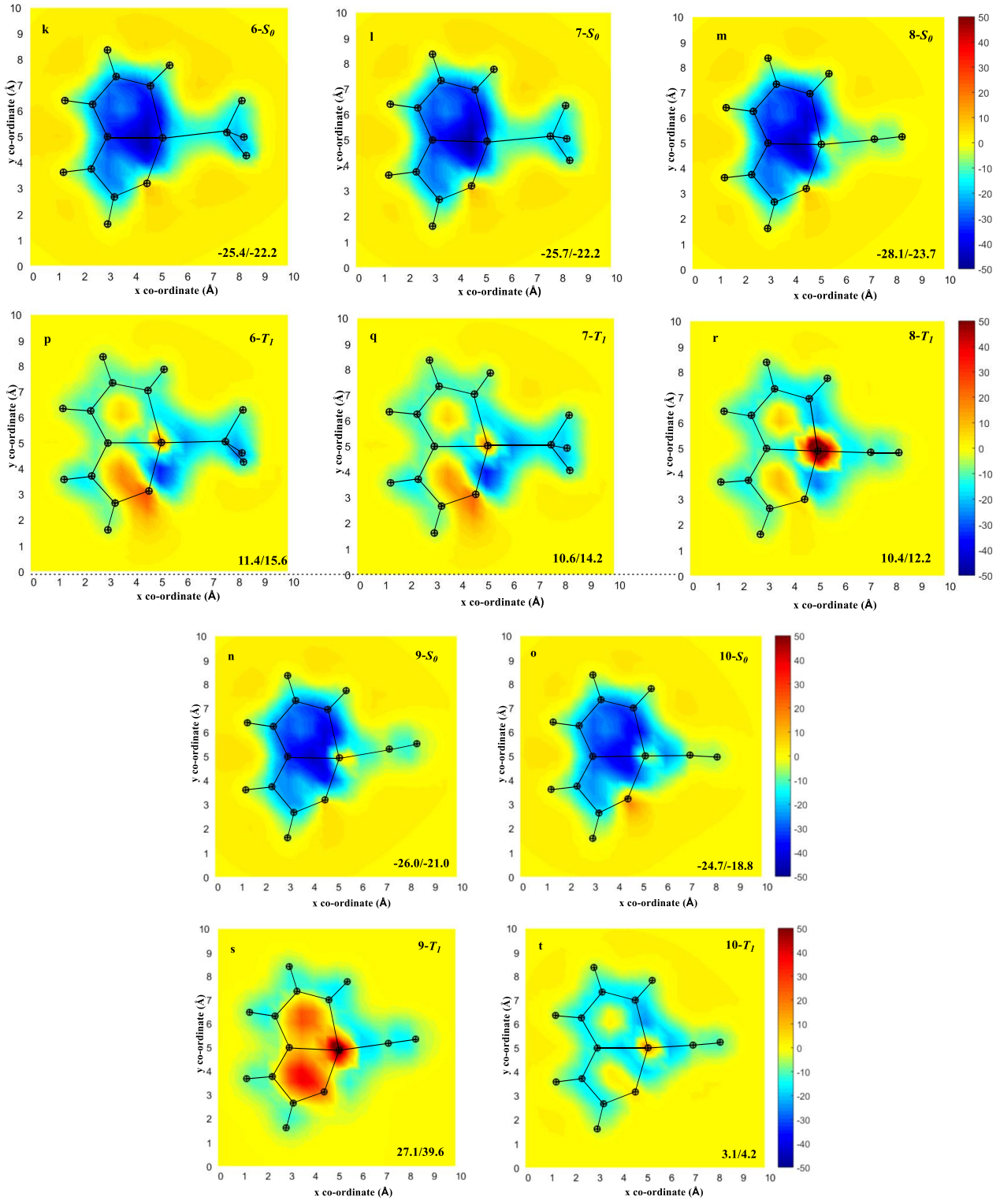
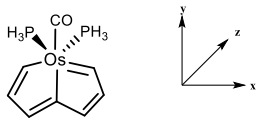


Figure S10. NICS(1)$_{zz}$ grids for complexes **6-10** in the S_0 and T_1 states. A fixed color scale (−50 to 50 ppm) is applied to all grids for easy comparison. NICS(1)zz values calculated at the ring centers (upper ring; lower ring) are commented on the bottom-right of each grid. **k-t** NICS(1)$_{zz}$ grids for **6-S$_0$**, **7-S$_0$**, **8-S$_0$**, **9-S$_0$**, **10-S$_0$**, **6-T$_1$**, **7-T$_1$**, **8-T$_1$**, **9-T$_1$** and **10-T$_1$**.

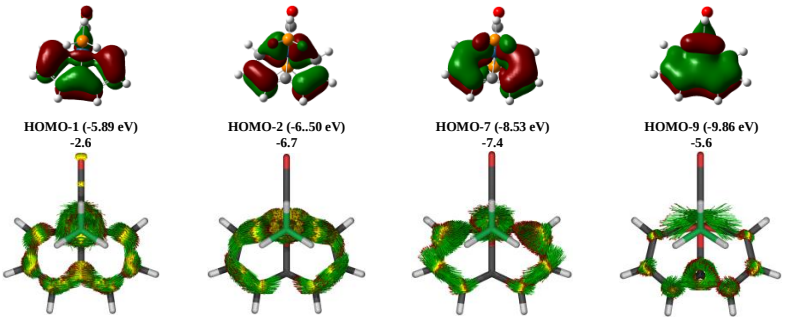
Table S2. NICS(1)$_{zz}$ values (ppm) for complexes **1**-**12**.

Complexes	S_0	T_1
1	-26.3/-26.3	0.5/0.5
2	-25.5/-25.7	0.4/0.4
3	-26.6/-26.6	0.5/0.5
4	-25.9/-25.9	1.2/1.2
5	-24.1/-24.1	34.8/34.8
6	-25.4/-22.2	11.4/15.6
7	-25.7/-22.2	10.6/14.2
8	-28.1/-23.7	10.4/12.2
9	-26.0/-21.0	27.1/39.6
10	-24.7/-18.8	3.1/4.2
11	-21.5/-21.5	-18.8/-18.8
12	-23.0/-23.0	-15.7/-15.7

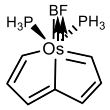
1-*S*$_0$



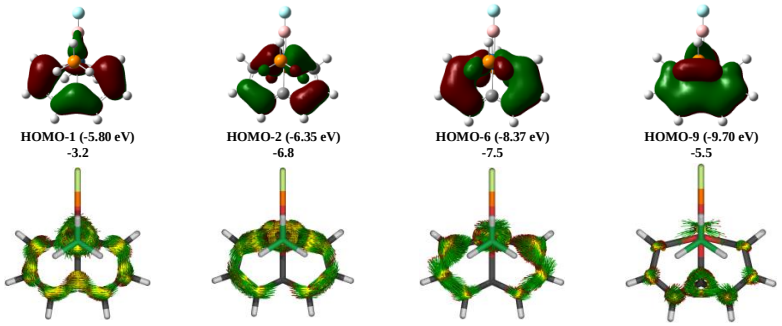
Orbitals	NICS(1)$_{zz}$
HOMO-1 HOMO-2	
HOMO-7 HOMO-9	-22.3
All σ Orbitals	-4.0
Total	-26.3



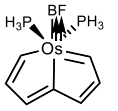
2-*S*$_0$ symmetry = C_{2v}



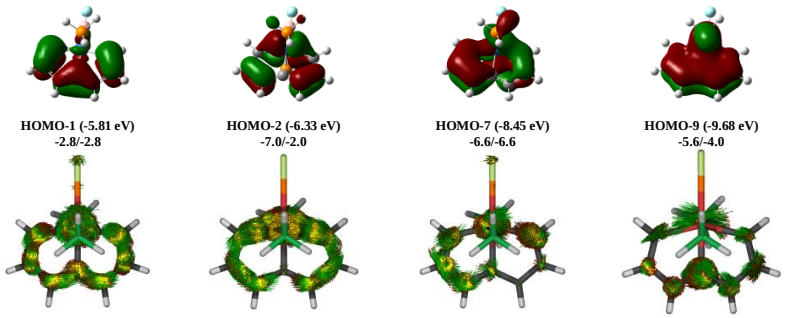
Orbitals	NICS(1)$_{zz}$
HOMO-1 HOMO-2	
HOMO-6 HOMO-9	-23.0
All σ Orbitals	-3.5
Total	-26.5



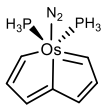
2-*S*$_0$ symmetry = C_1



Orbitals	NICS(1)$_{zz}$
HOMO-1 HOMO-2	
HOMO-7 HOMO-9	-22.0/-15.4
All σ Orbitals	-3.5/-10.3
Total	-25.5/-25.7



3-*S*$_0$



Orbitals	NICS(1)$_{zz}$
HOMO-1 HOMO-2	
HOMO-7 HOMO-9	-21.4
All σ Orbitals	-5.2
Total	-26.6

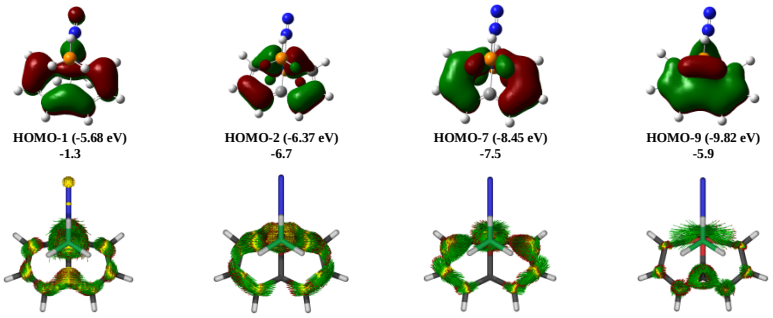
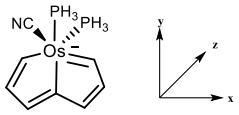
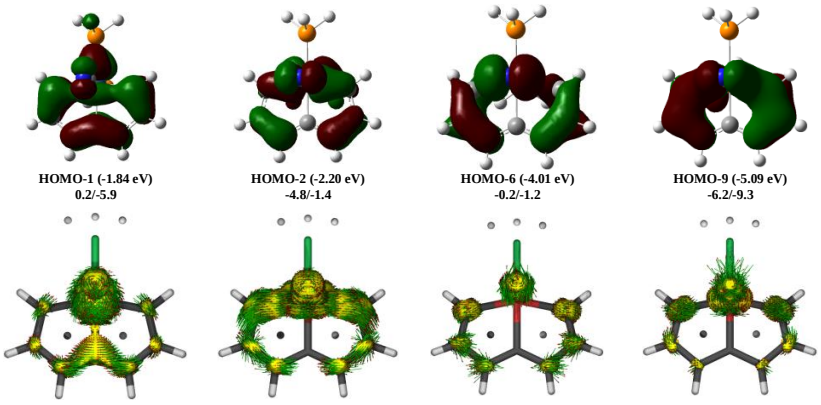


Figure S11**.** The NICS(1)$_{zz}$ values (ppm) given before and after the '/' are those computed at the geometrical centres of rings A and B, respectively. If the two ring NICS values are the same, then only one. ACID plots for individual molecular orbitals of compounds **1-3** in the singlet state. The isovalues for molecular orbitals and ACID surfaces are 0.03 and 0.024 a.u., respectively. The magnetic field vector is orthogonal with respect to the ring plane and points upward.

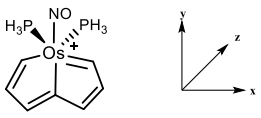
4-*S*$_0$



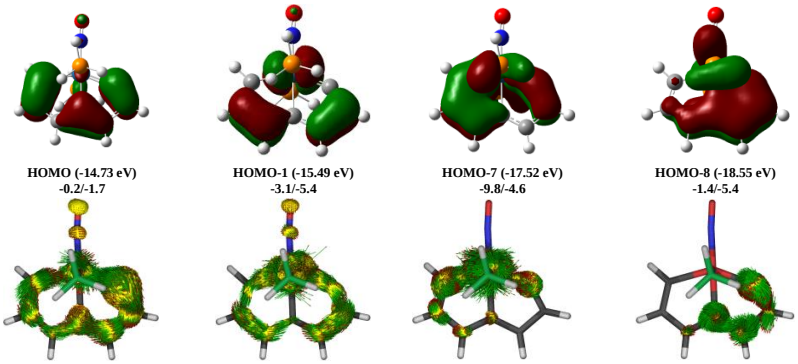
Orbitals	NICS(1)$_{zz}$
HOMO-1 HOMO-2	
HOMO-6 HOMO-9	-10.6/17.8
All σ Orbitals	-15.3/-8.1
Total	-25.9/-25.9



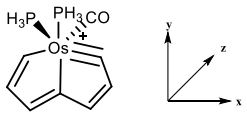
5-*S*$_0$



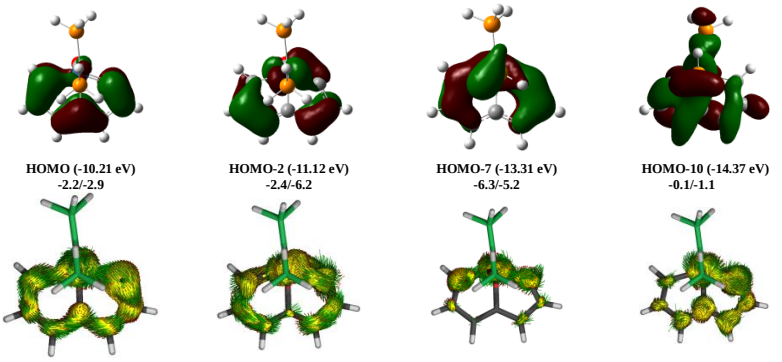
Orbitals	NICS(1)$_{zz}$
HOMO HOMO-1	
HOMO-7 HOMO-8	-14.5/-17.1
All σ Orbitals	-10.3/-1.6
Total	-24.8/-18.7



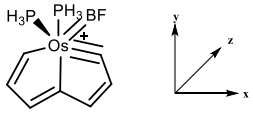
6-*S*$_0$



Orbitals	NICS(1)$_{zz}$
HOMO HOMO-2	
HOMO-7 HOMO-8	-11.0/-15.4
All σ Orbitals	-14.4/-6.6
Total	-25.4/-22.0



7-*S*$_0$



Orbitals	NICS(1)$_{zz}$
HOMO HOMO-2	
HOMO-7 HOMO-8	-16.9/-14.5
All σ Orbitals	-8.8/-7.7
Total	-25.7/-22.2

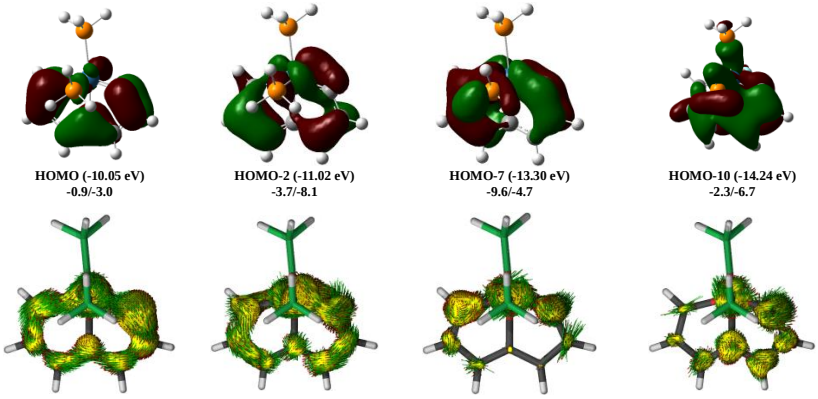
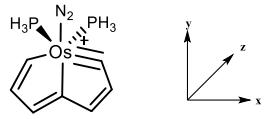
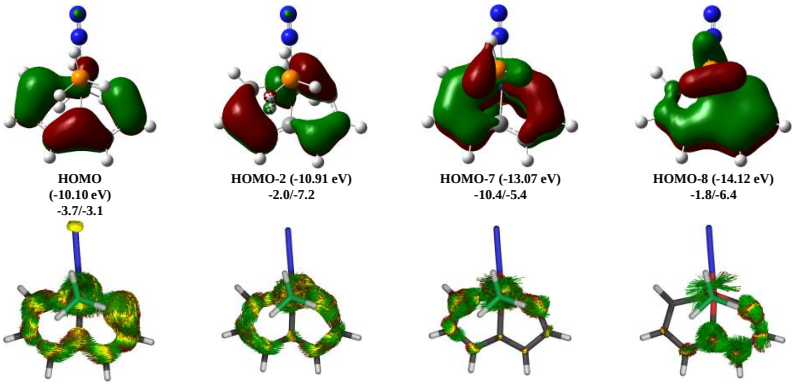


Figure S12. The NICS(1)$_{zz}$ values (ppm) given before and after the '/' are those computed at the geometrical centres of rings A and B, respectively. ACID plots for individual molecular orbitals of compounds **4-7** in the singlet state. If the two ring NICS values are the same, then only one. The isovalues for molecular orbitals and ACID surfaces are 0.03 and 0.024 a.u., respectively. The magnetic field vector is orthogonal with respect to the ring plane and points upward.

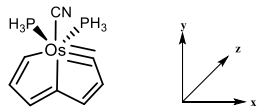
8-S_0



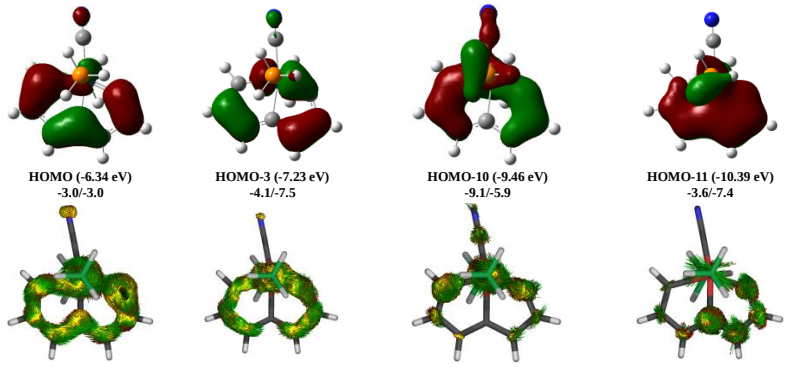
Orbitals	NICS(1)$_{zz}$
HOMO HOMO-2	
HOMO-7 HOMO-8	-17.9/-22.1
All σ Orbitals	-8.1/1.1
Total	-26.0/-21.0



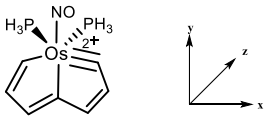
9-S_0



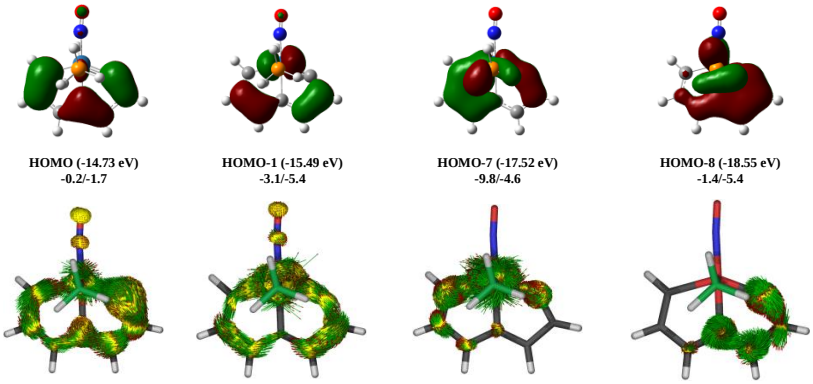
Orbitals	NICS(1)$_{zz}$
HOMO HOMO-3	
HOMO-10 HOMO-11	-16.5/-22.5
All σ Orbitals	-11.3/0.6
Total	-27.8/-21.9



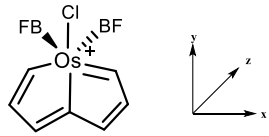
10-S_0



Orbitals	NICS(1)$_{zz}$
HOMO HOMO-1	
HOMO-7 HOMO-8	-14.8/-17.8
All σ Orbitals	-10.0/-0.9
Total	-24.8/-18.7



11-S_0



Orbitals	NICS(1)$_{zz}$
HOMO HOMO-2	
HOMO-9 HOMO-12	-21.9
All σ Orbitals	0.4
Total	-21.5

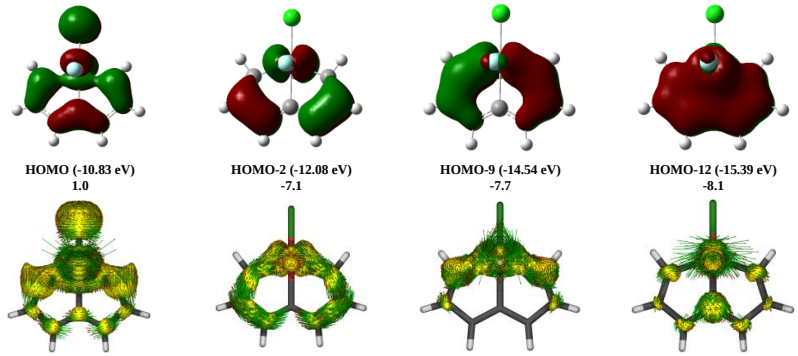
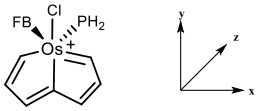


Figure S13. The NICS(1)$_{zz}$ values (ppm) given before and after the '/' are those computed at the geometrical centres of rings A and B, respectively. If the two ring NICS values are the same, then only one. ACID plots for individual molecular orbitals of compounds **8-11** in the singlet state. The isovalues for molecular orbitals and ACID surfaces are 0.03 and 0.024 a.u., respectively. The magnetic field vector is orthogonal with respect to the ring plane and points upward.

12-S_0



Orbitals		$NICS(1)_{zz}$
HOMO	HOMO-2	
HOMO-8	HOMO-11	-18.8
All σ Orbitals		-4.2
	Total	-23.0

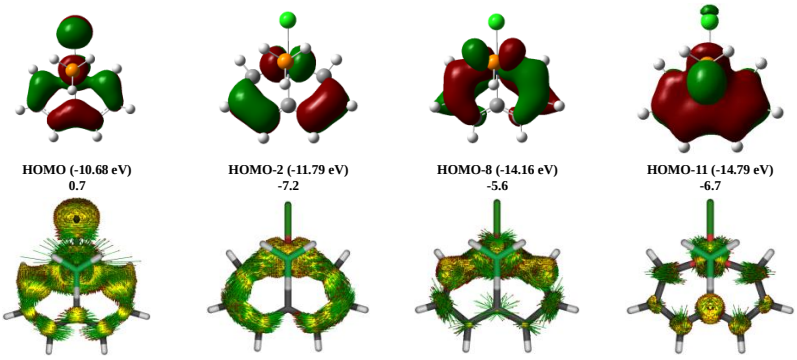


Figure S14. The $NICS(1)_{zz}$ values (ppm) given before and after the '/' are those computed at the geometrical centres of rings A and B, respectively. If the two ring NICS values are the same, then only one. ACID plots for individual molecular orbitals of compounds **12** in the singlet state. The isovalues for molecular orbitals and ACID surfaces are 0.03 and 0.024 a.u., respectively. The magnetic field vector is orthogonal with respect to the ring plane and points upward.

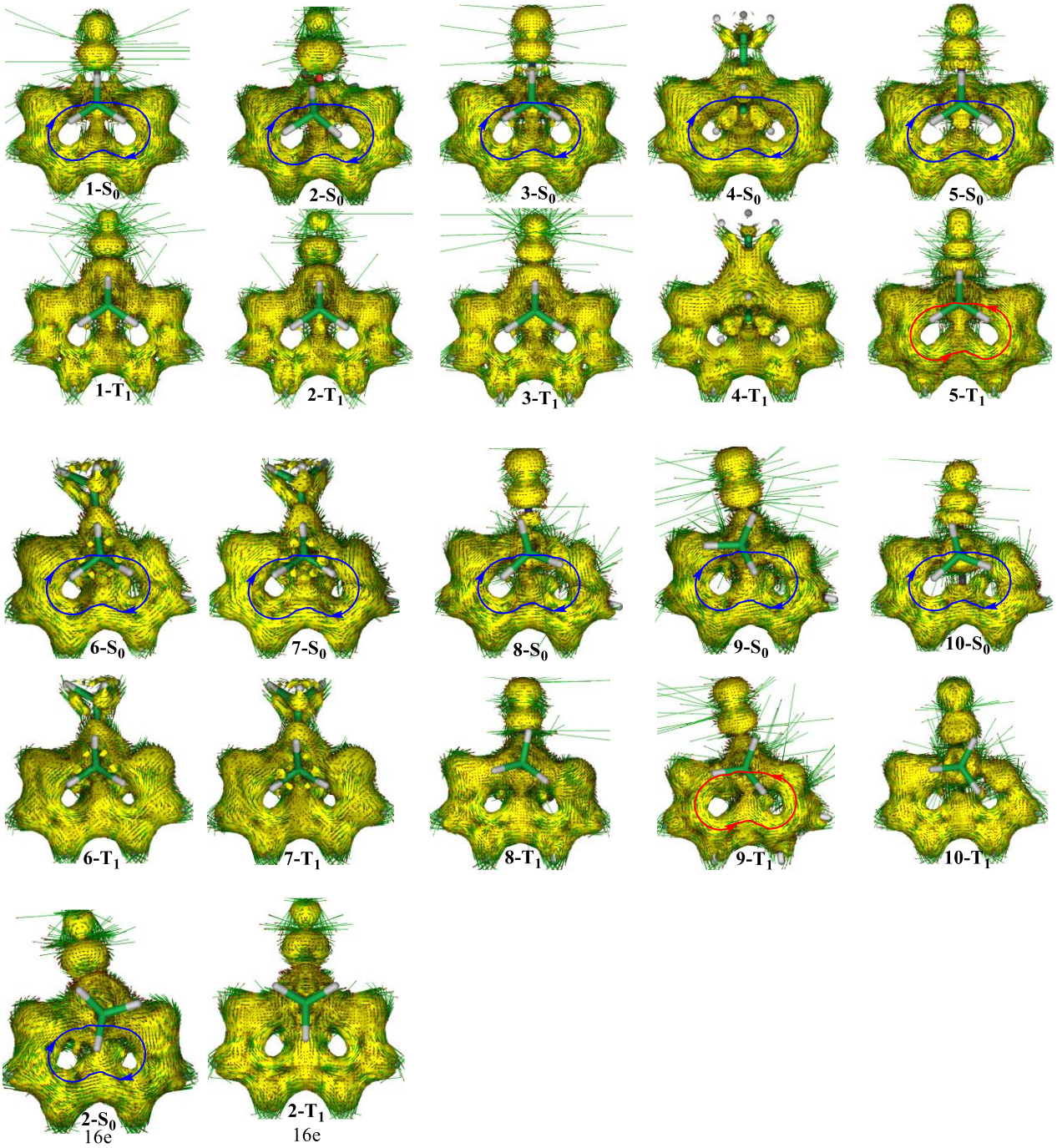


Figure S15. ACID plots of complexes **1**–**10** in the S_0 and T_1 states. The molecular planes are placed perpendicular to the magnetic field vector. Small green arrows are computed current density vectors. The isovalue for the surfaces is 0.035 a.u. The paratropic/diatropic ring currents indicate antiaromaticity and aromaticity, respectively

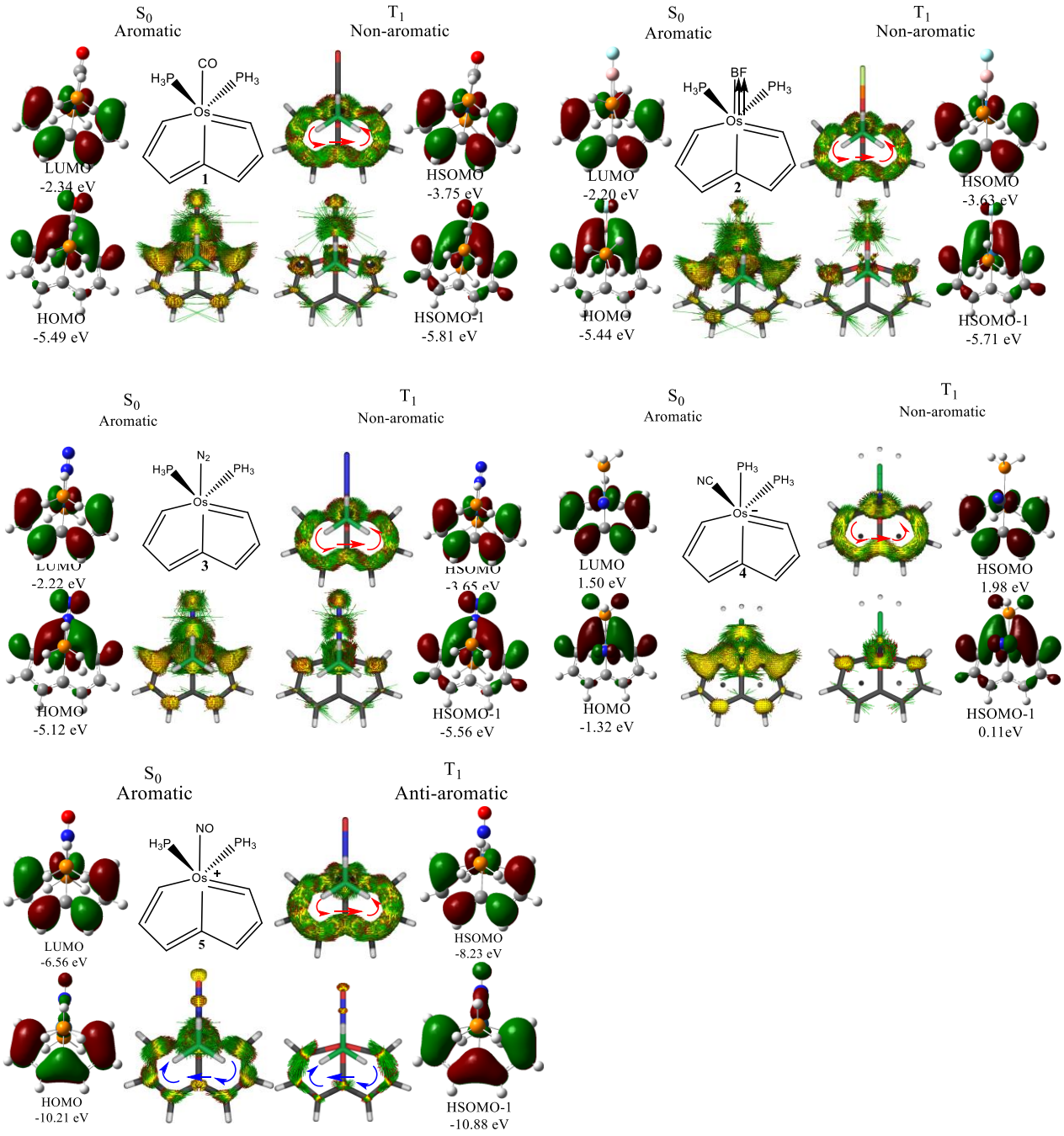


Figure S16. ACID plots for individual molecular orbitals of compounds **1**-**5**. The isovalues for molecular orbitals and ACID surfaces are 0.03 and 0.024 a.u., respectively. The magnetic field vector is orthogonal with respect to the ring plane and points upward.

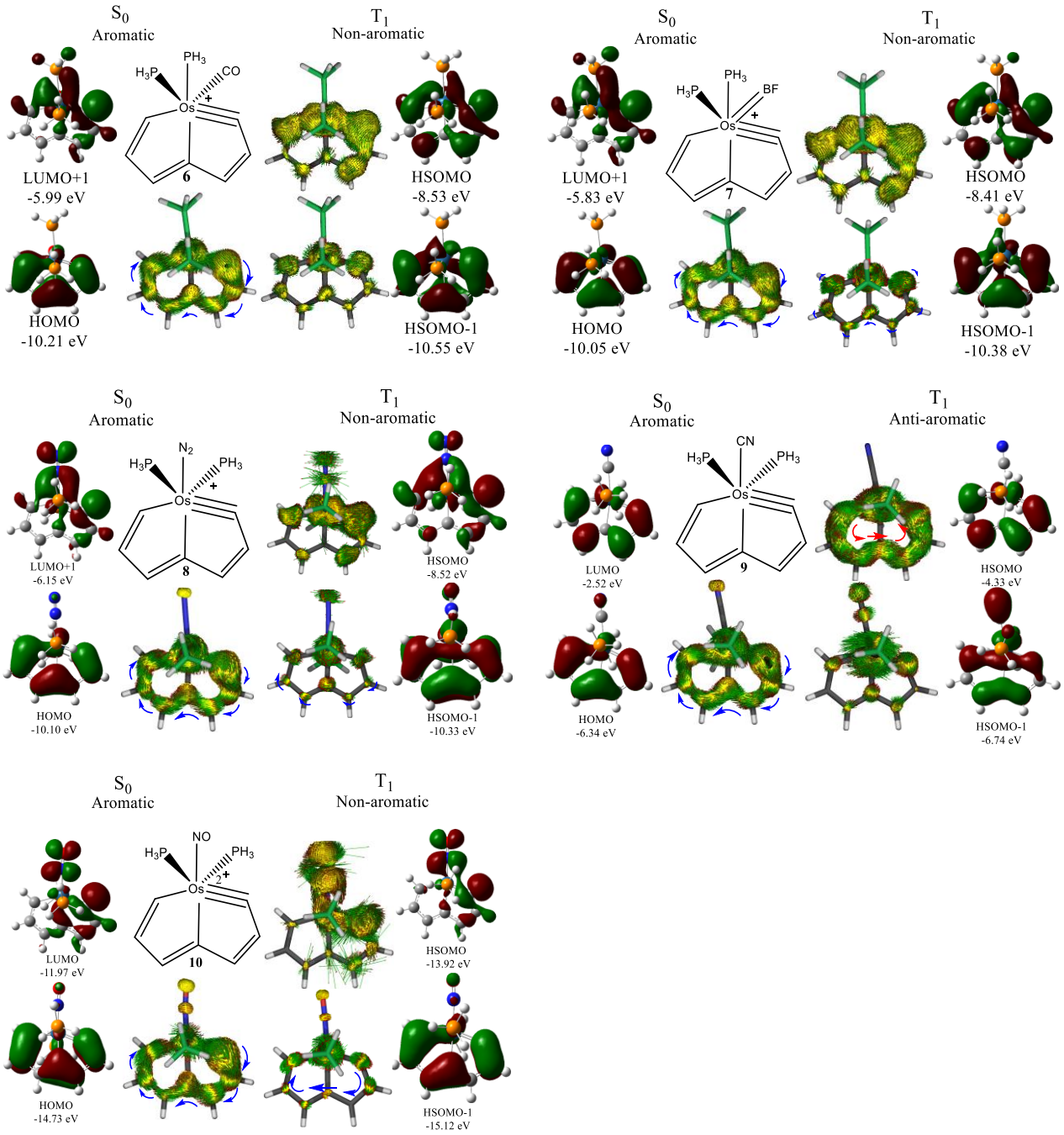


Figure S17. ACID plots for individual molecular orbitals of compounds **6**-**10**. The isovalues for molecular orbitals and ACID surfaces are 0.03 and 0.024 a.u., respectively. The magnetic field vector is orthogonal with respect to the ring plane and points upward.

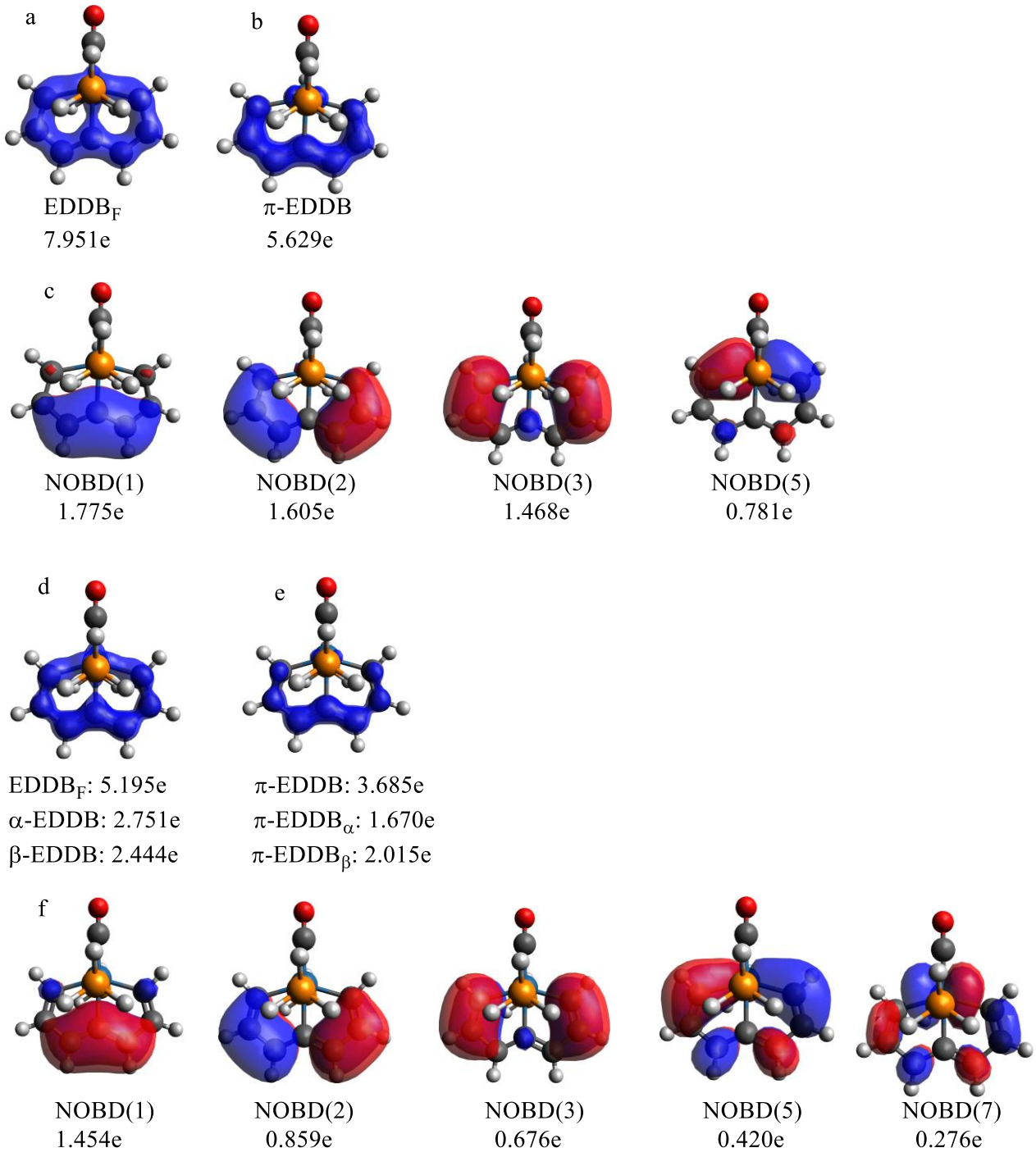


Figure S18. EDDB results of **1-S_0** and **1-T_1**. (a) delocalized electrons on the 8MR of **1-S_0**. (b) π contribution of **1-S_0**. (c) key NOBDs of **1-S_0**. (d) the whole system of **1-T_1**. (e) π contribution of **1-T_1**. (f) key NOBDs of **1-T_1**. Isovalues are 0.015.

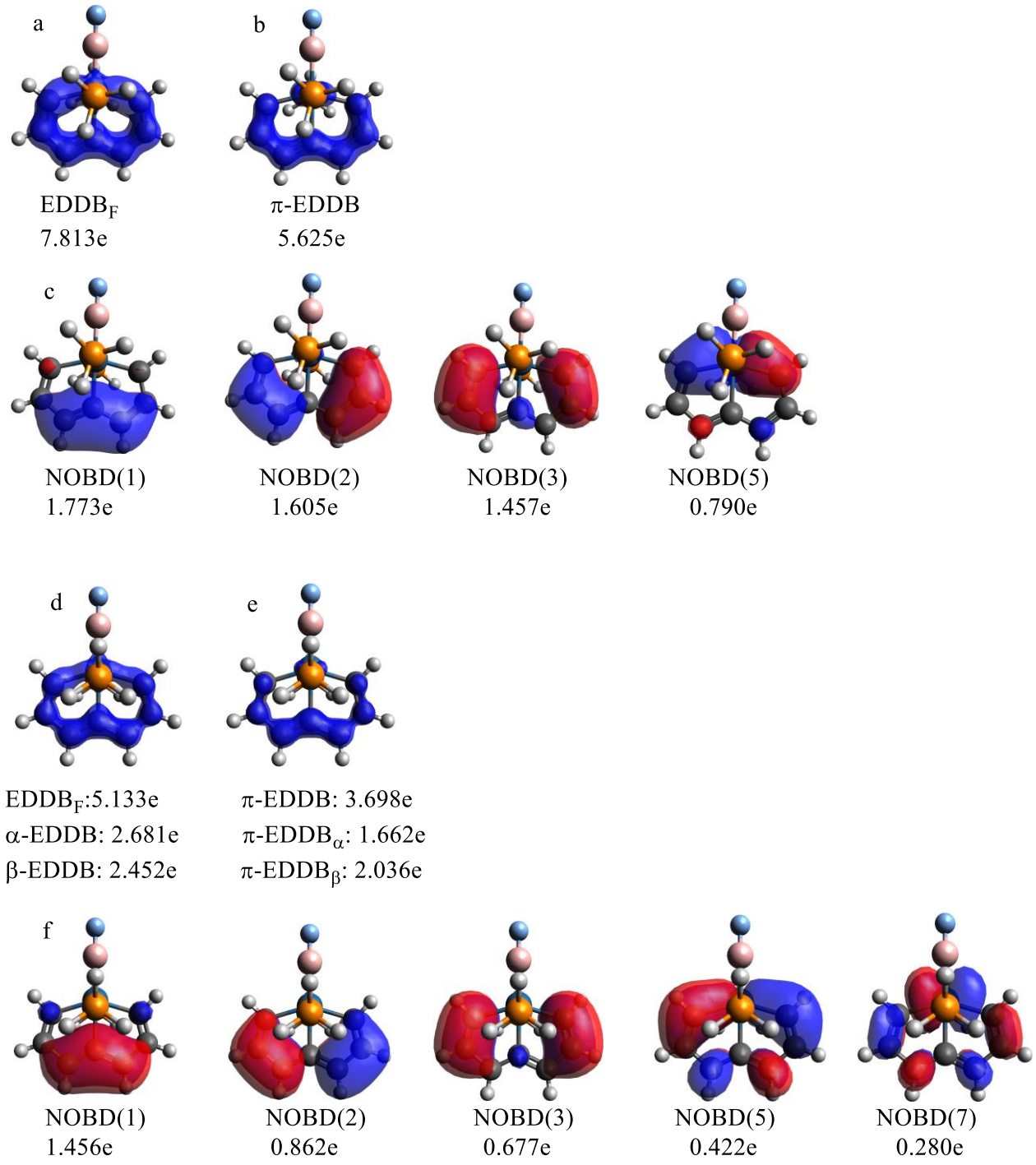


Figure S19. EDDB results of **2-S_0** and **2-T_1**. (a) delocalized electrons on the 8MR of **2-S_0**. (b) π contribution of **2-S_0**. (c) key NOBDs of **2-S_0**. (d) the whole system of **2-T_1**. (e) π contribution of **2-T_1**. (f) key NOBDs of **2-T_1**. Isovalues are 0.015.

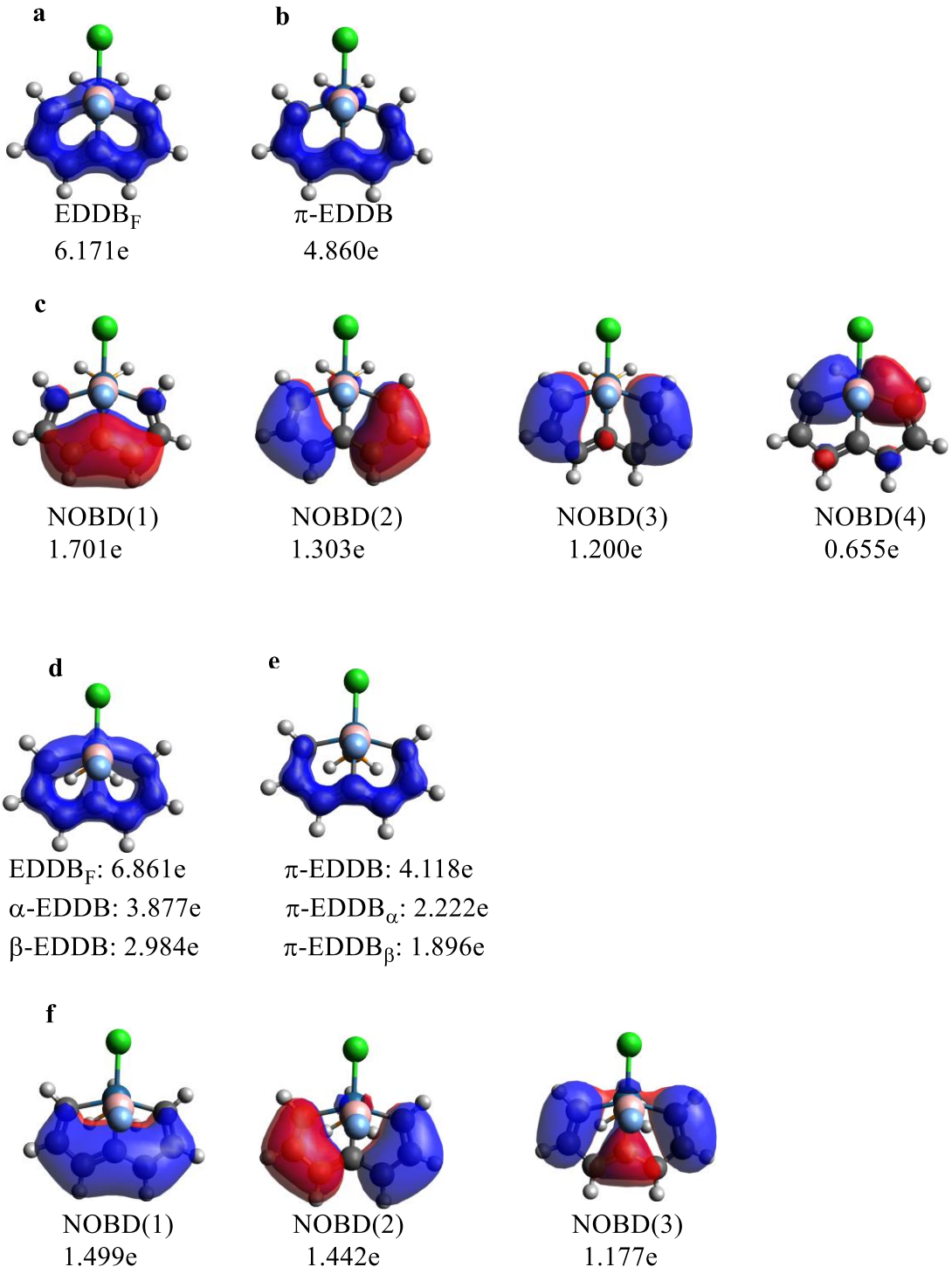


Figure S20. EDDB results of **12-*S*$_0$** and **12-*T*$_1$**. (a) delocalized electrons on the 8MR of **12-*S*$_0$**. (b) π contribution of **12-*S*$_0$**. (c) key NOBDs of **12-*S*$_0$**. (d) the whole system of **12-*T*$_1$**. (e) π contribution of **12-*T*$_1$**. (f) key NOBDs of **12-*T*$_1$**. Isovalues are 0.015.

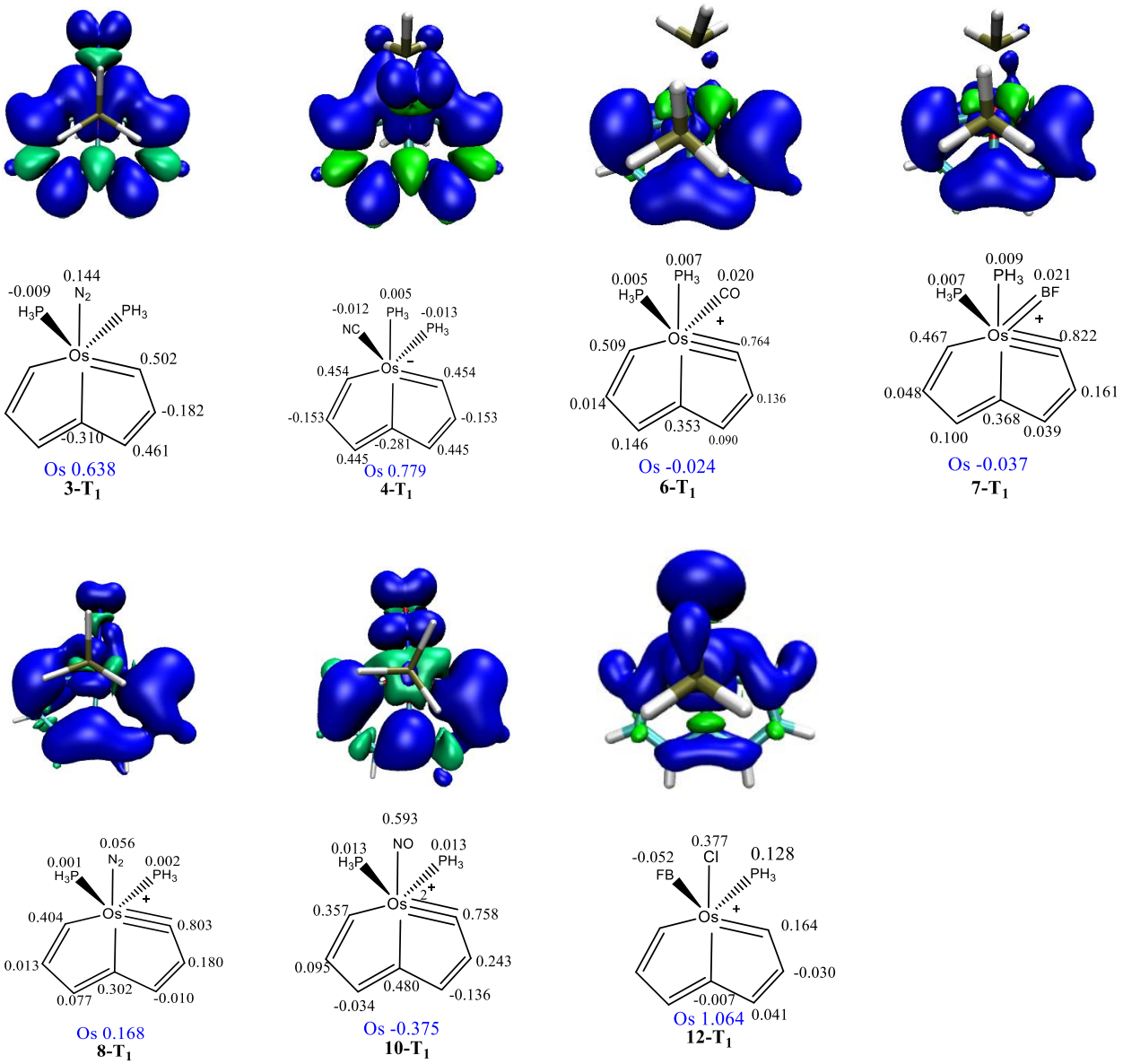


Figure S21. Spin density analyses for open-shell species. Density surfaces are presented with an isovalue 0.001 a.u. Specific values of the spin density are given at individual atoms and key ligands. The "-" sign simply refers to the β-spin.

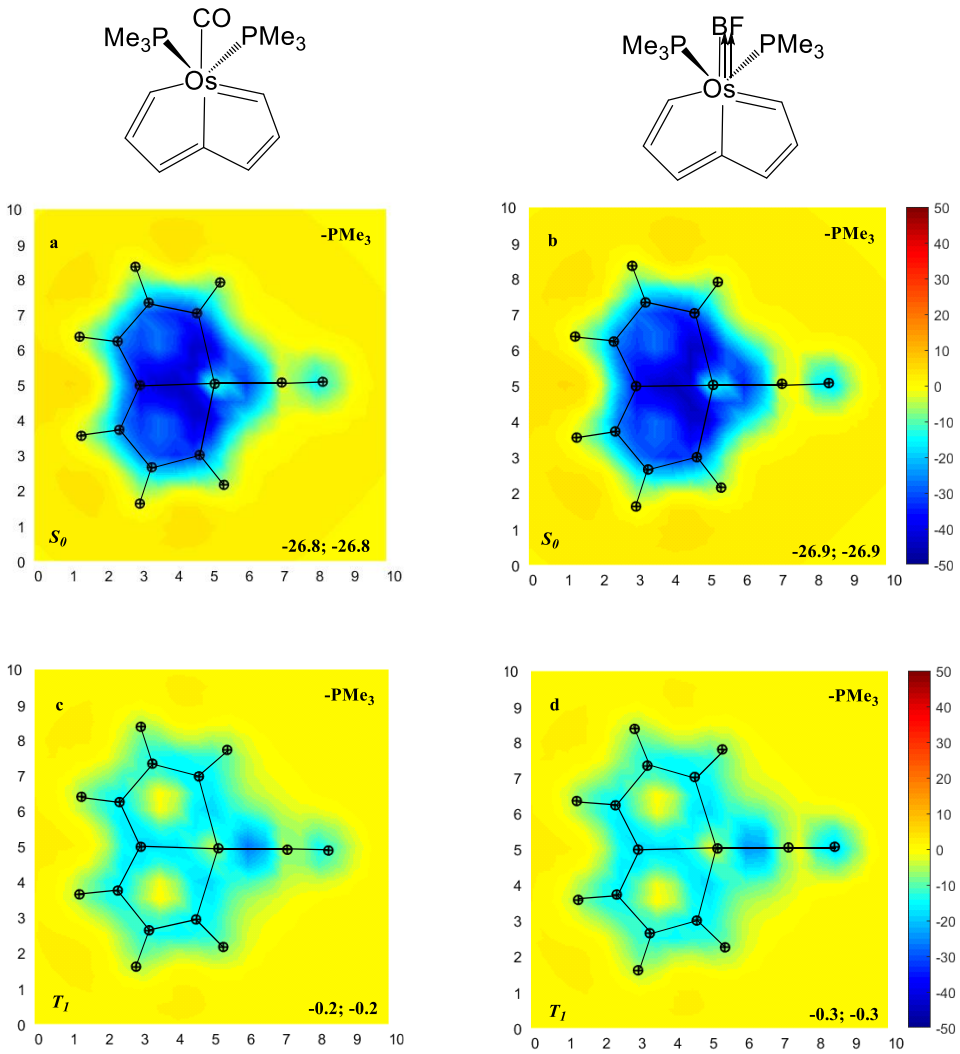


Figure S22. NICS(1)$_{zz}$ grids with PMe_3. Ring-center NICS(1)$_{zz}$ values (ppm) are commented on the bottomright of each grid. All values are given in p.p.m. **a-d**.

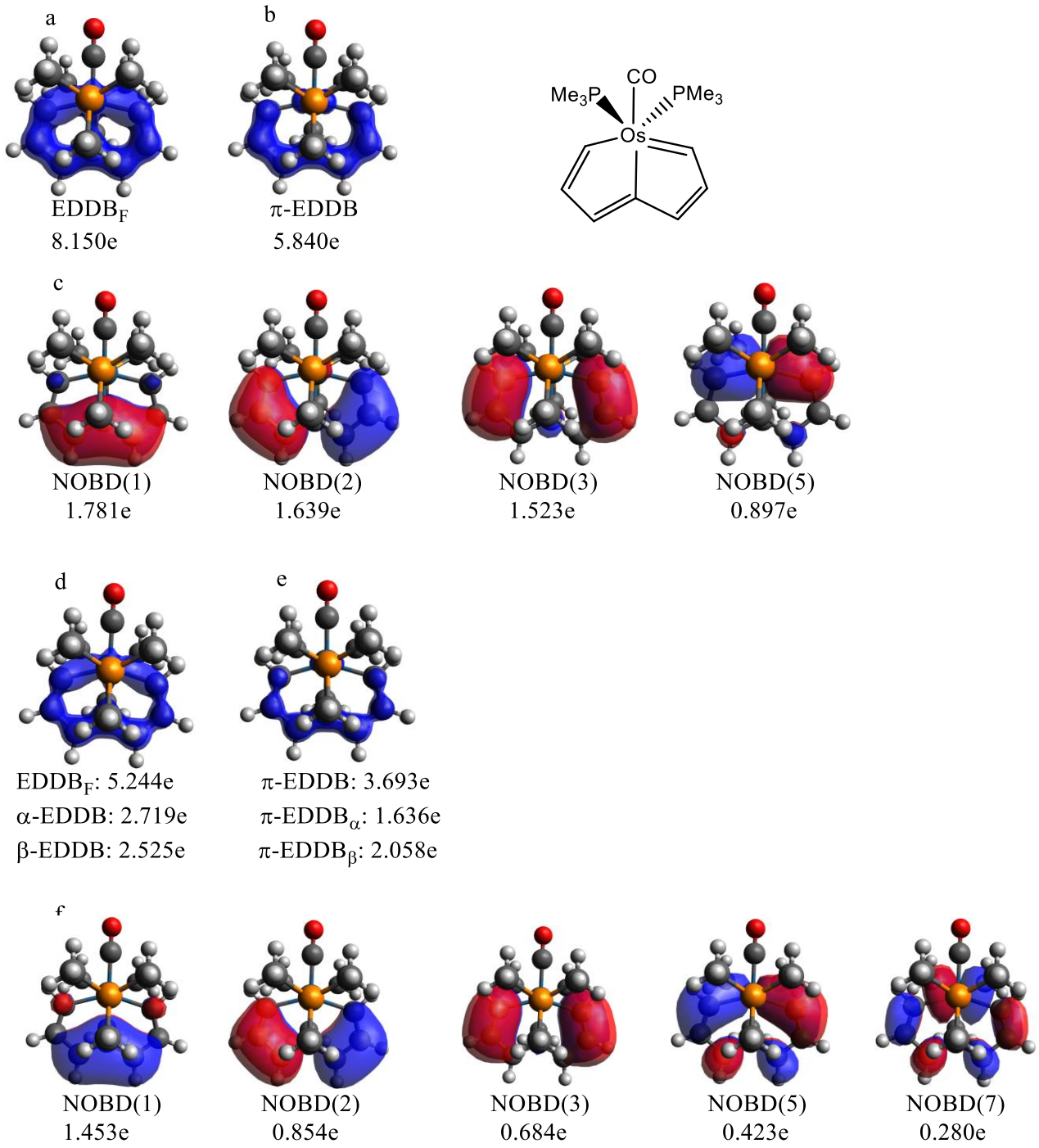


Figure S23. EDDB results of S_0 and T_1. (a) delocalized electrons on the 8MR of S_0. (b) π contribution of S_0. (c) key NOBDs of S_0. (d) the whole system of T_1. (e) π contribution of T_1. (f) key NOBDs of T_1. Isovalues are 0.015.

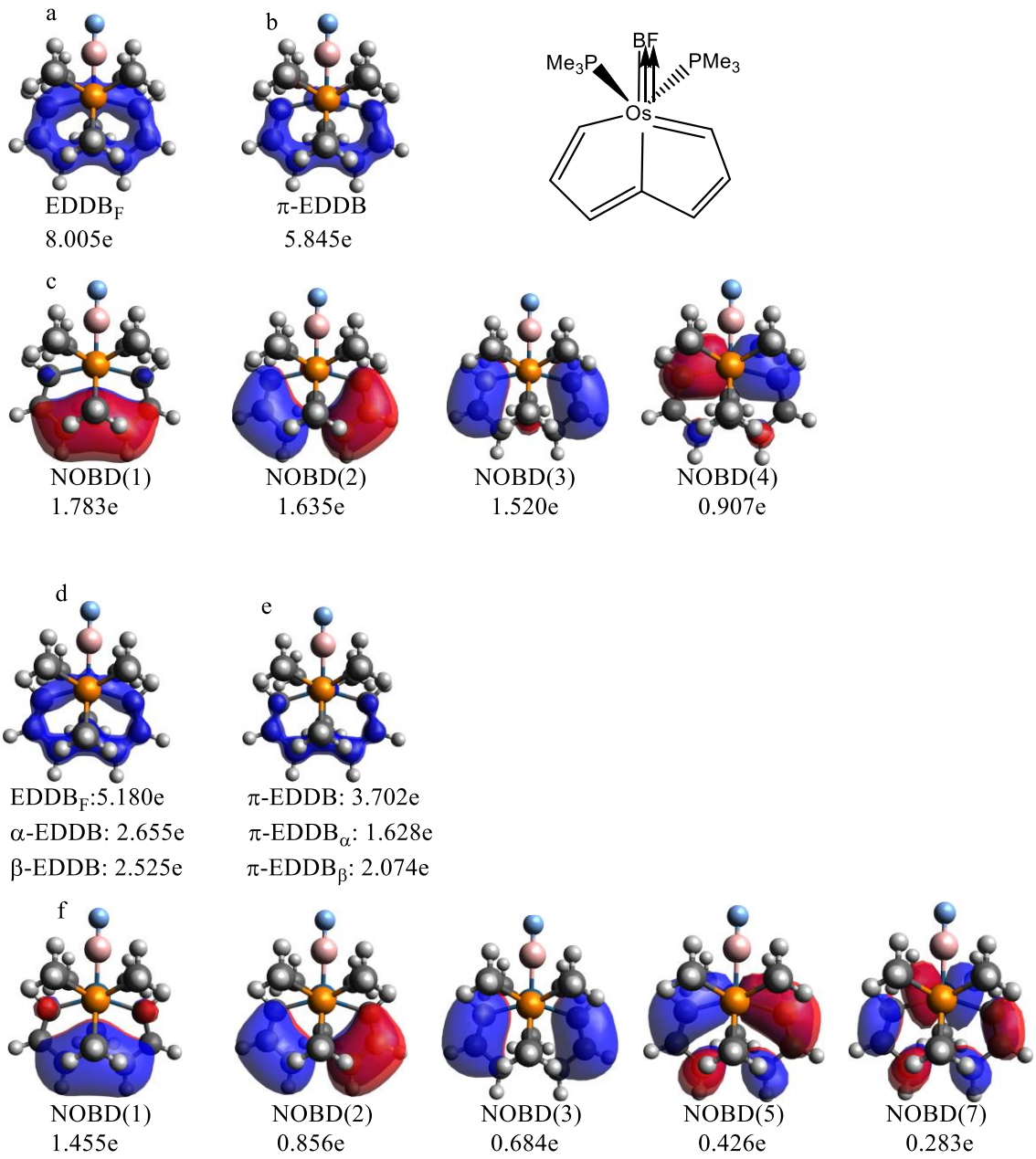


Figure S24. EDDB results of S_0 and T_1. (a) delocalized electrons on the 8MR of S_0. (b) π contribution of S_0. (c) key NOBDs of S_0. (d) the whole system of T_1. (e) π contribution of T_1. (f) key NOBDs of T_1. Isovalues are 0.015.

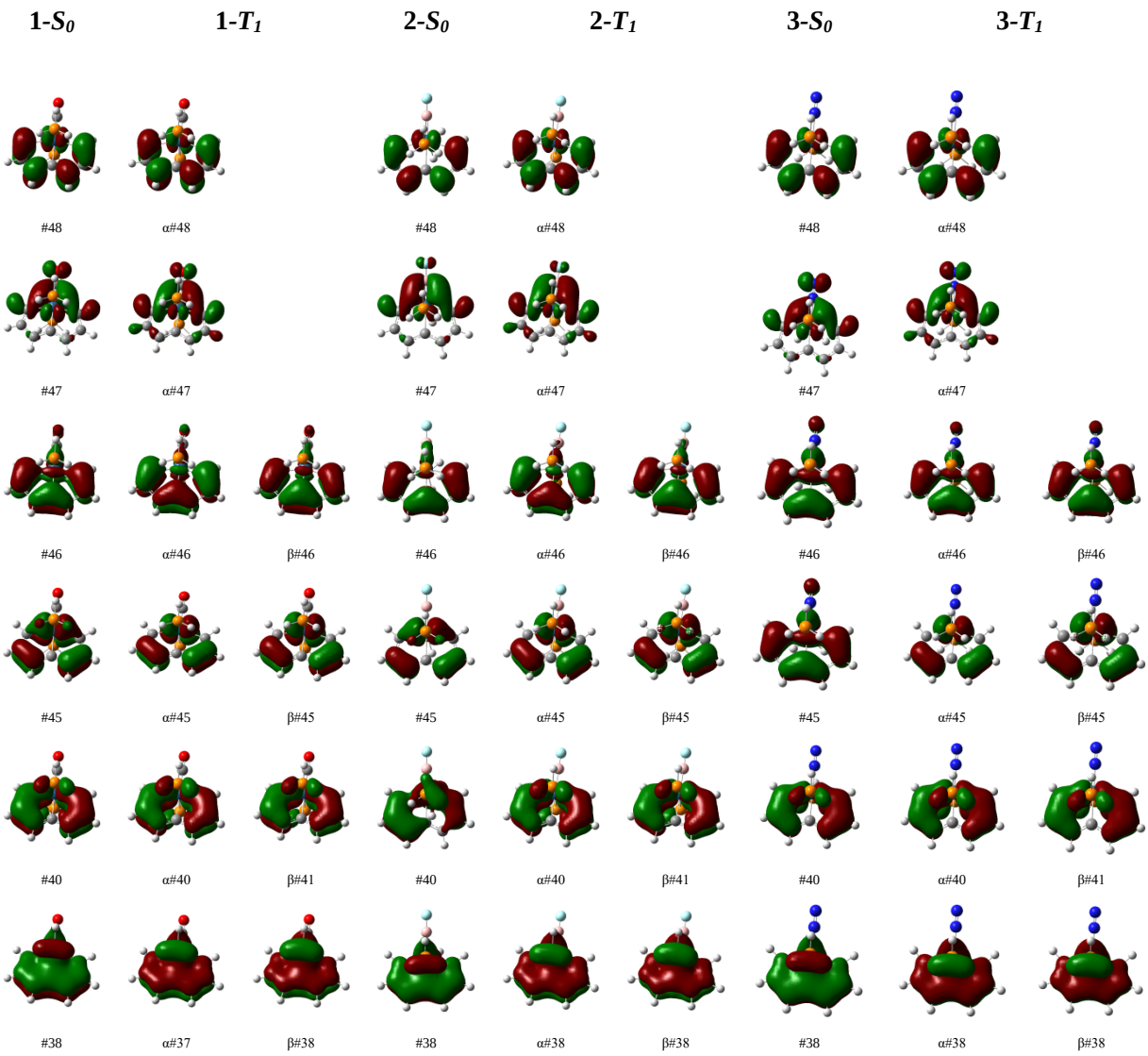


Figure S25. Key π molecular orbitals of compounds **1**-**3** in the S_0 and T_1 states. The isovalue is 0.03 a.u.

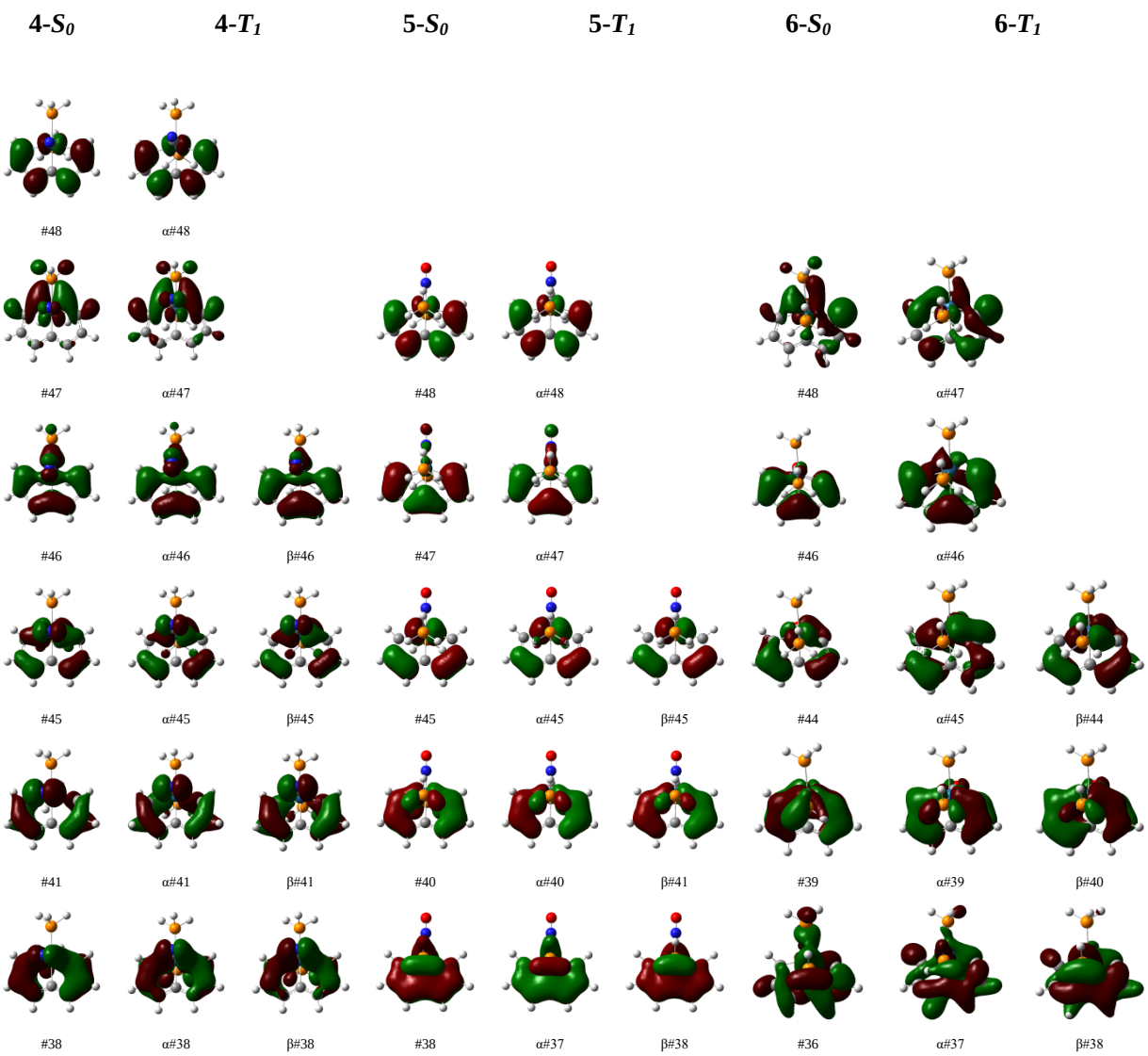


Figure S26. Key π molecular orbitals of compounds **4**-**6** in the S_0 and T_1 states. The isovalue is 0.03 a.u.

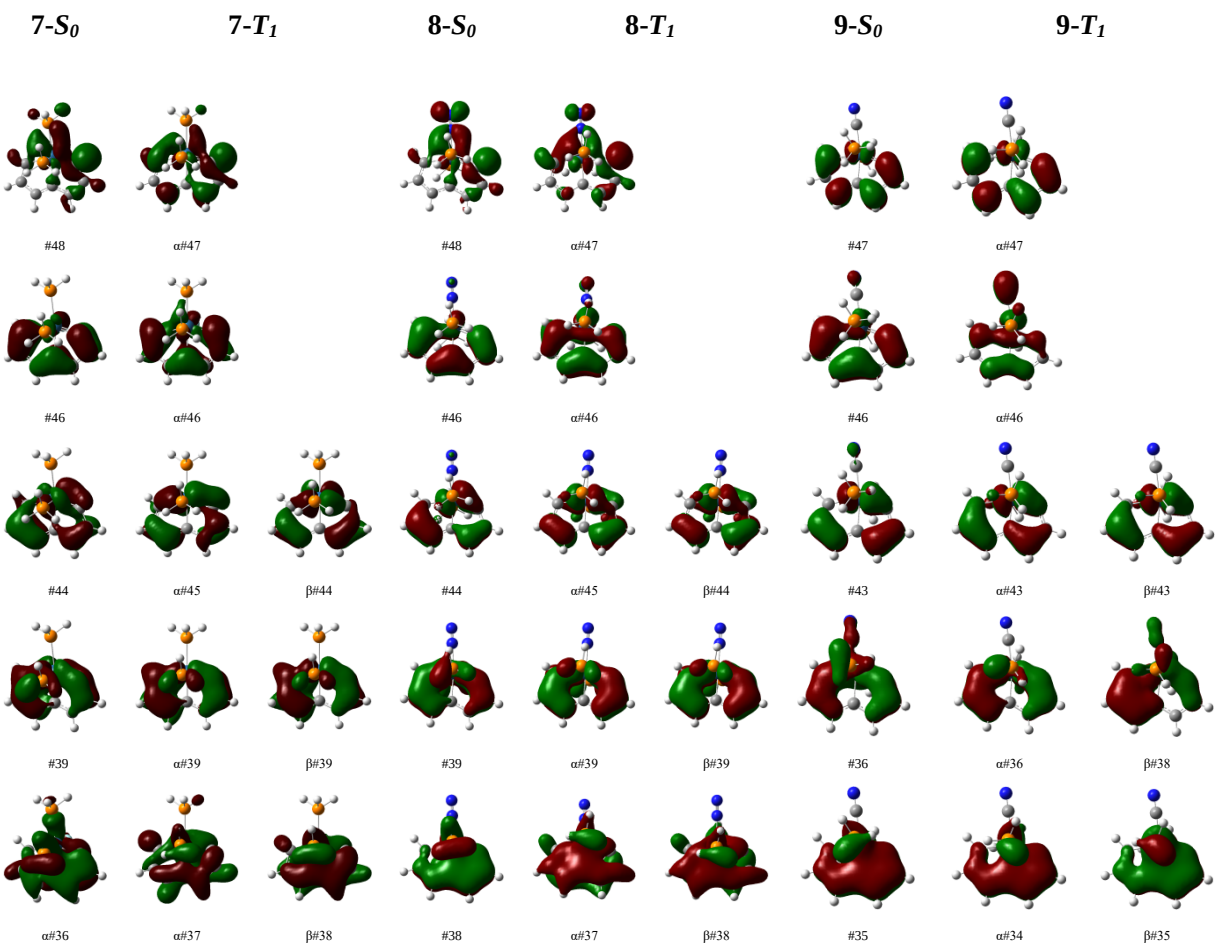


Figure 27. Key π molecular orbitals of compounds **7-9** in the S_0 and T_1 states. The isovalue is 0.03 a.u.

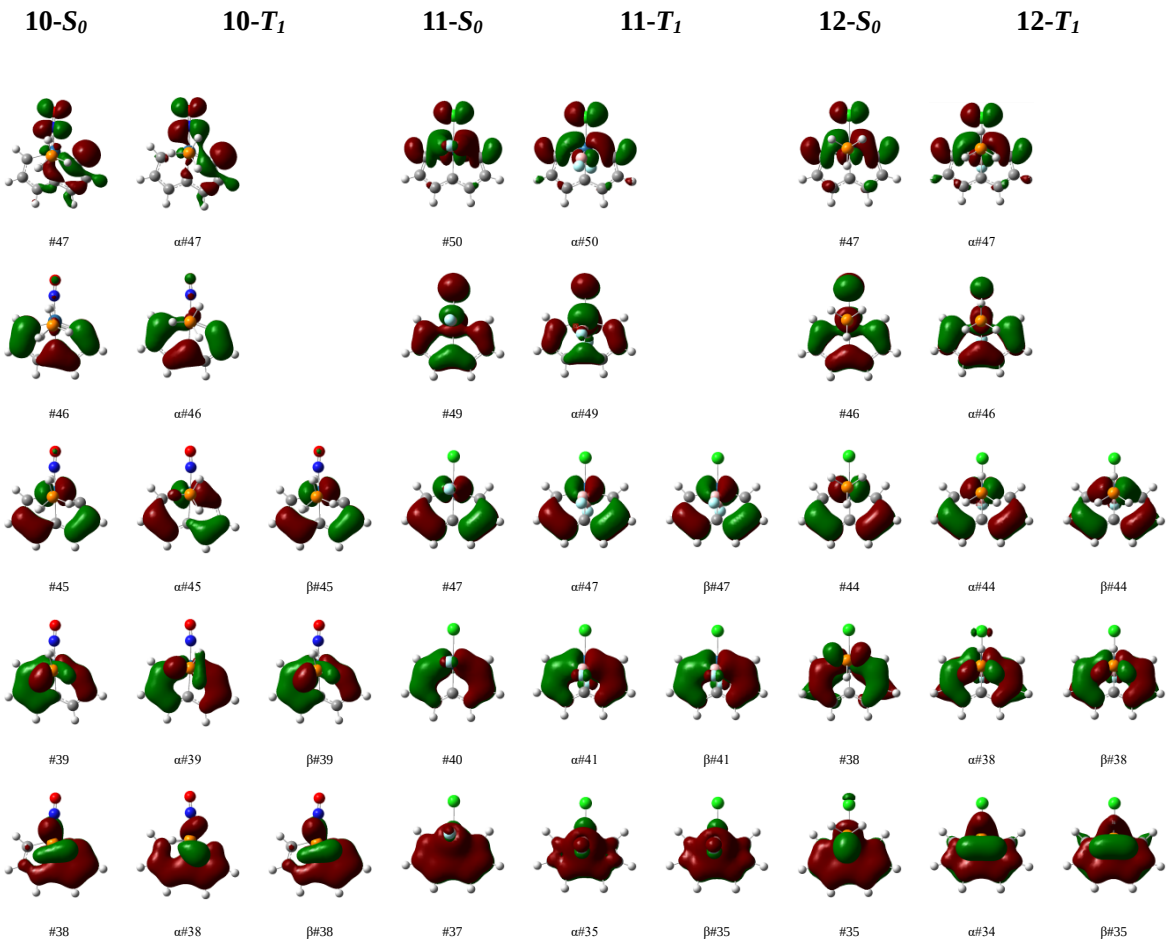


Figure S28. Key π molecular orbitals of compounds **10-12** in the S_0 and T_1 states. The isovalue is 0.03 a.u.

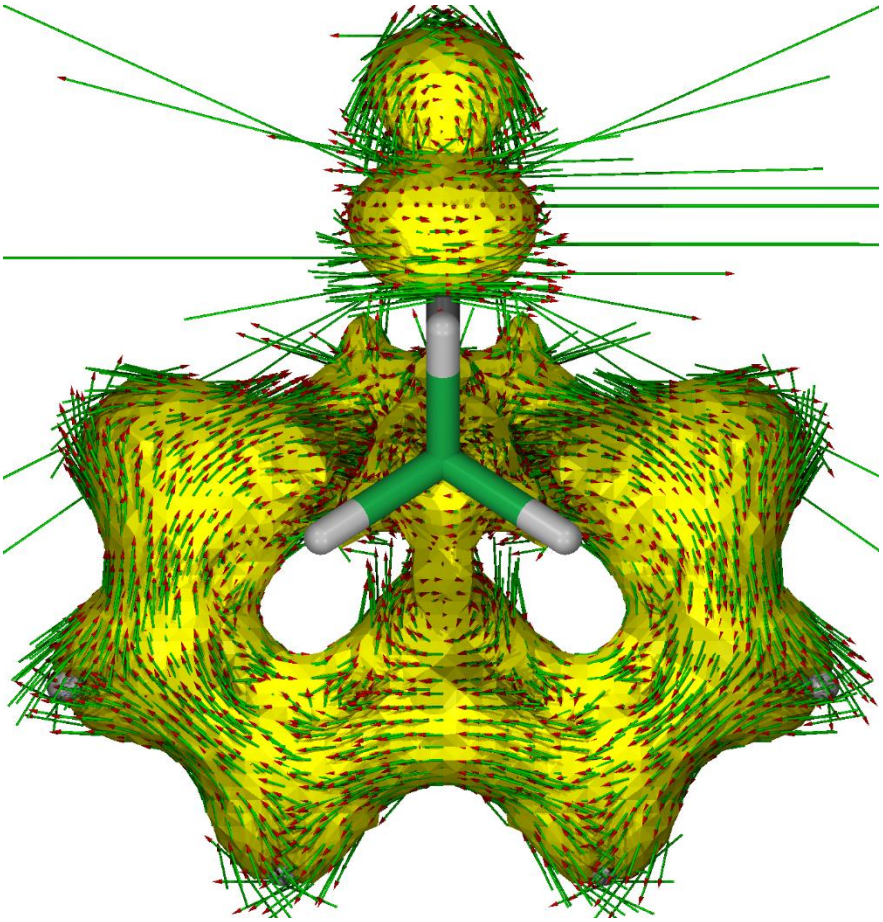


Figure S29. ACID plot of **1**-S_0. Isovalue: 0.035 a.u.

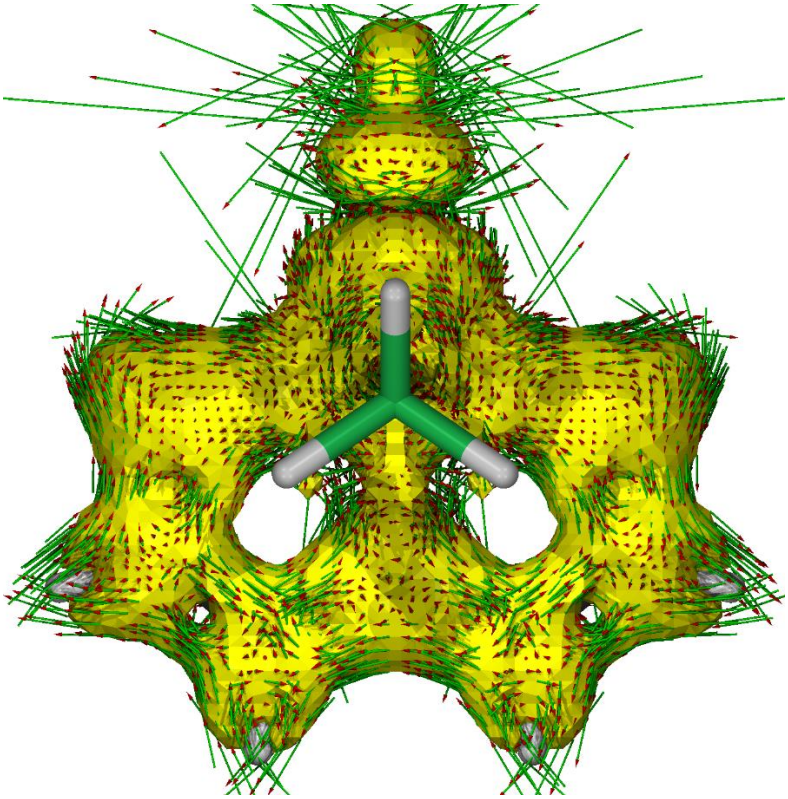


Figure S30. ACID plot of **1**-T_1. Isovalue: 0.035 a.u.

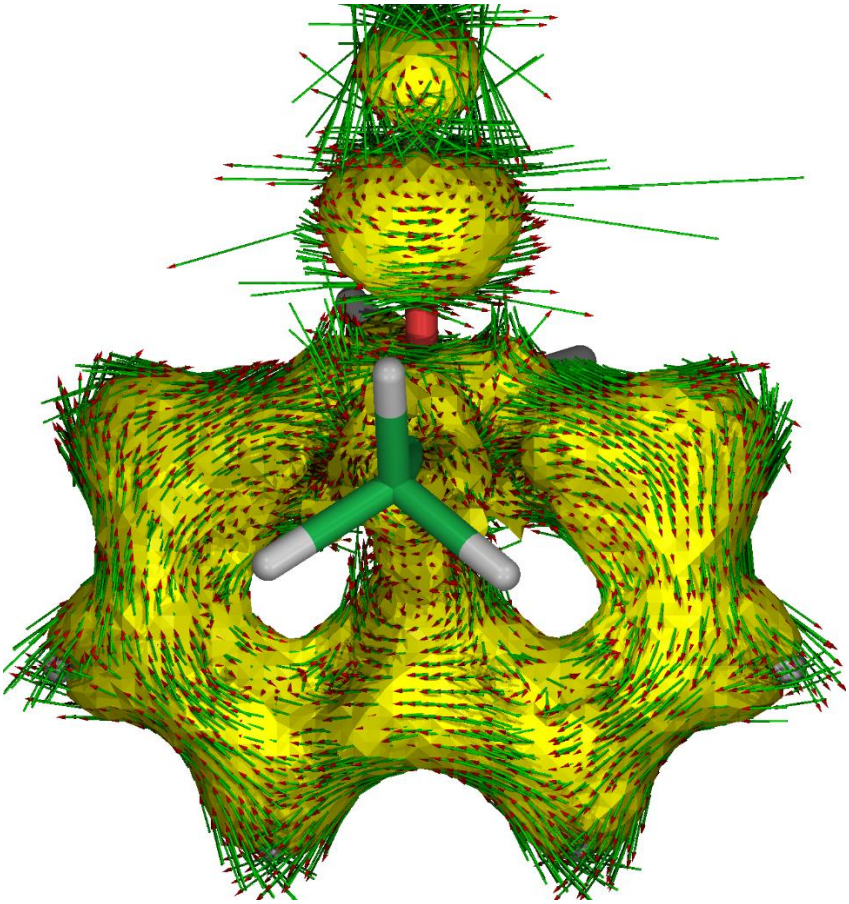


Figure 31. ACID plot of **2-S_0**. Isovalue: 0.035 a.u.

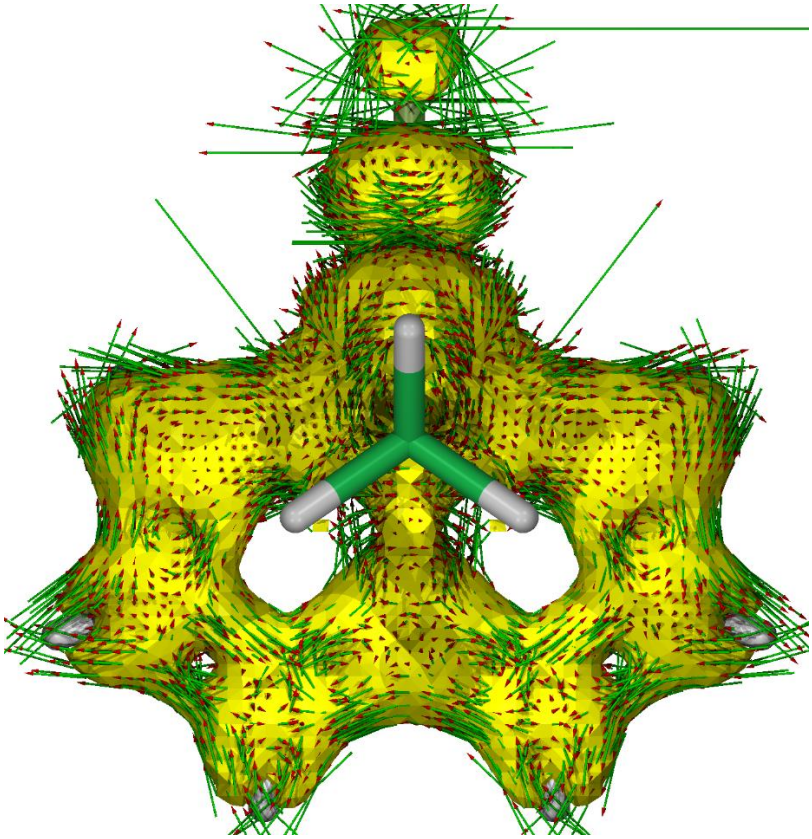


Figure S32. ACID plot of **2-T_1**. Isovalue: 0.035 a.u.

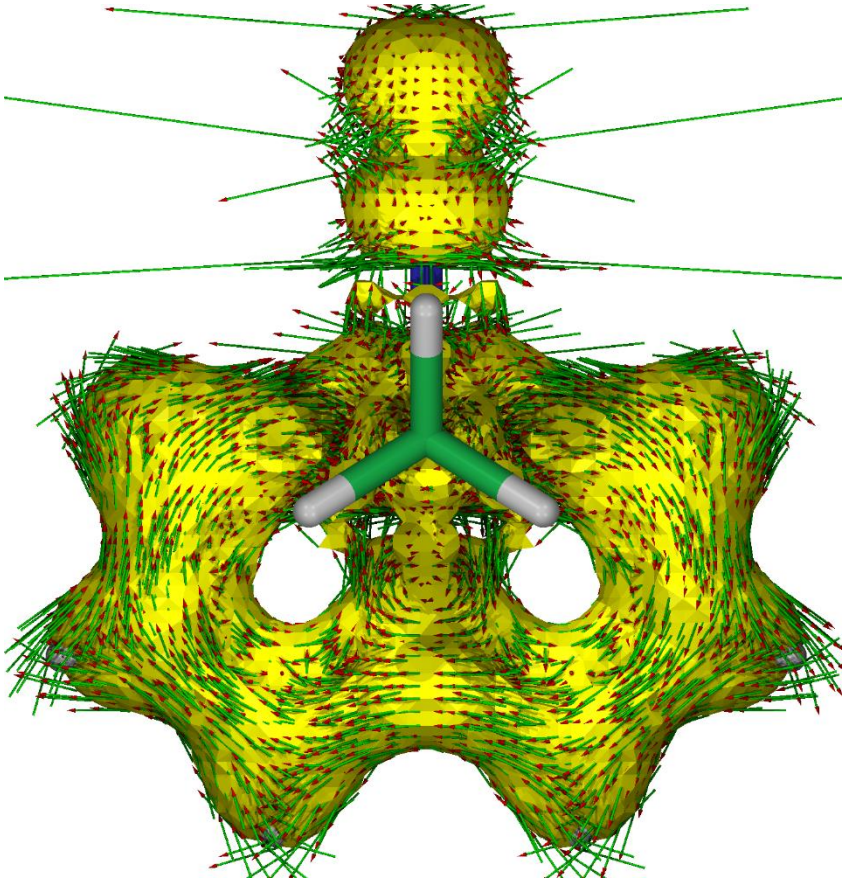


Figure S33. ACID plot of **3-S_0**. Isovalue: 0.035 a.u.

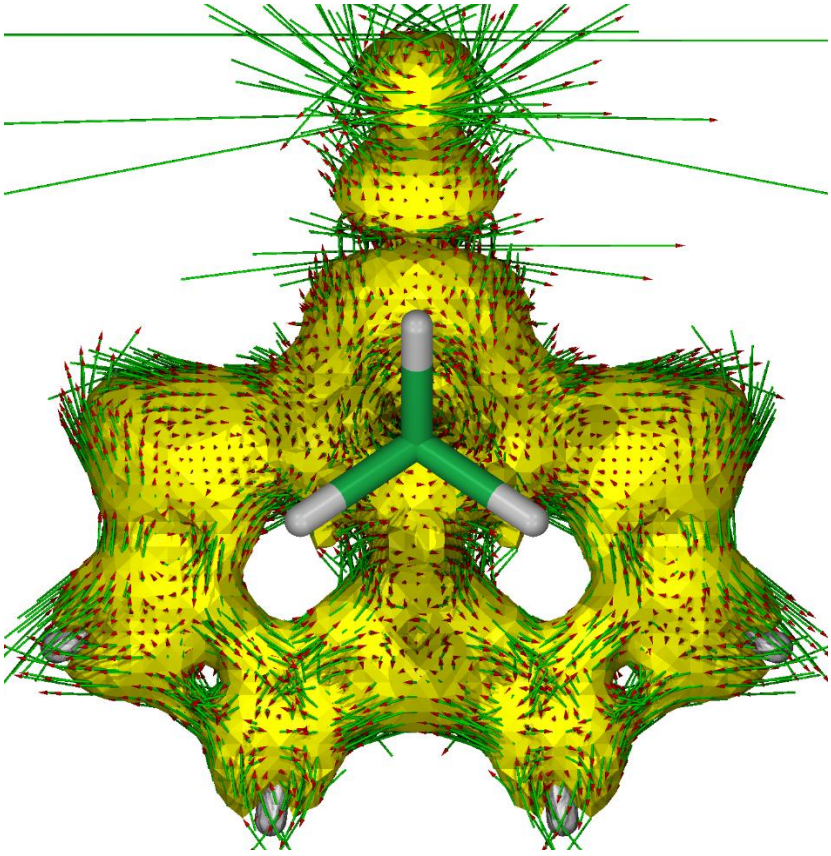


Figure S34. ACID plot of **3-T_1**. Isovalue: 0.035 a.u.

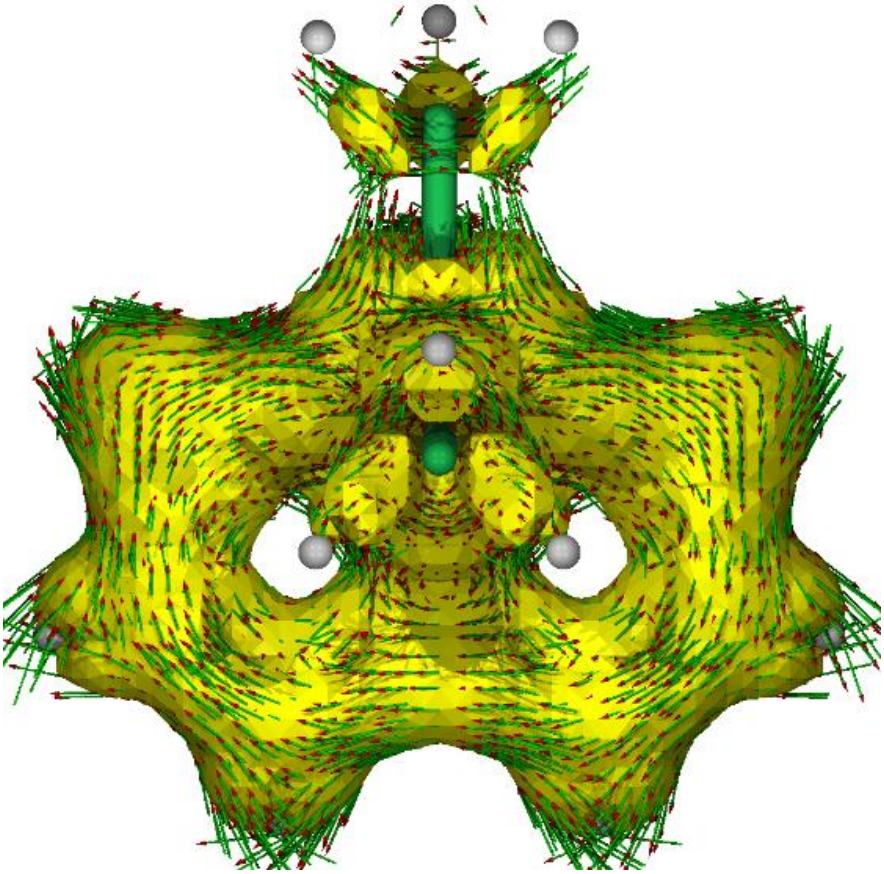


Figure S35. ACID plot of **4-S_0**. Isovalue: 0.035 a.u.

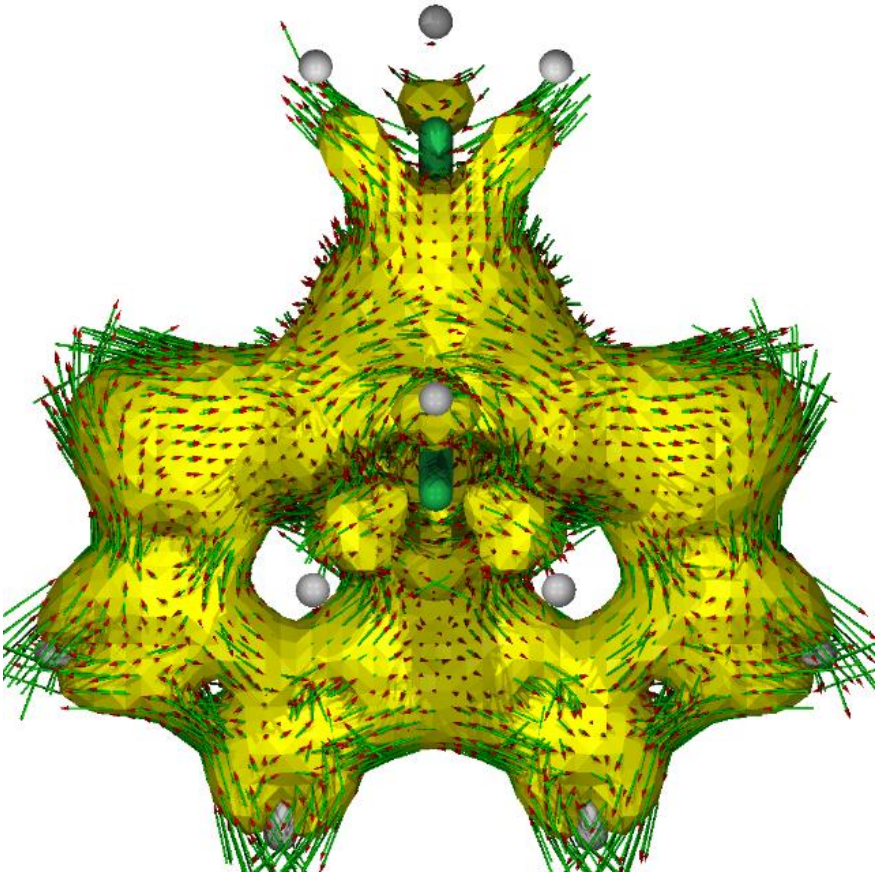


Figure S36. ACID plot of **4-T_1**. Isovalue: 0.035 a.u.

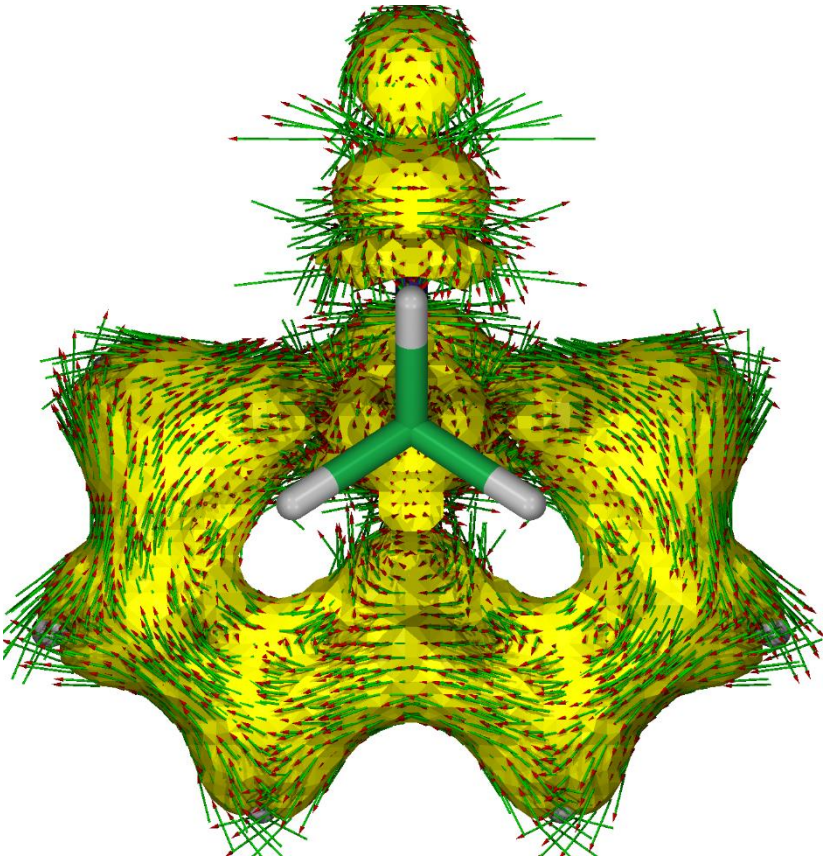


Figure S37. ACID plot of **5-S_0**. Isovalue: 0.035 a.u.

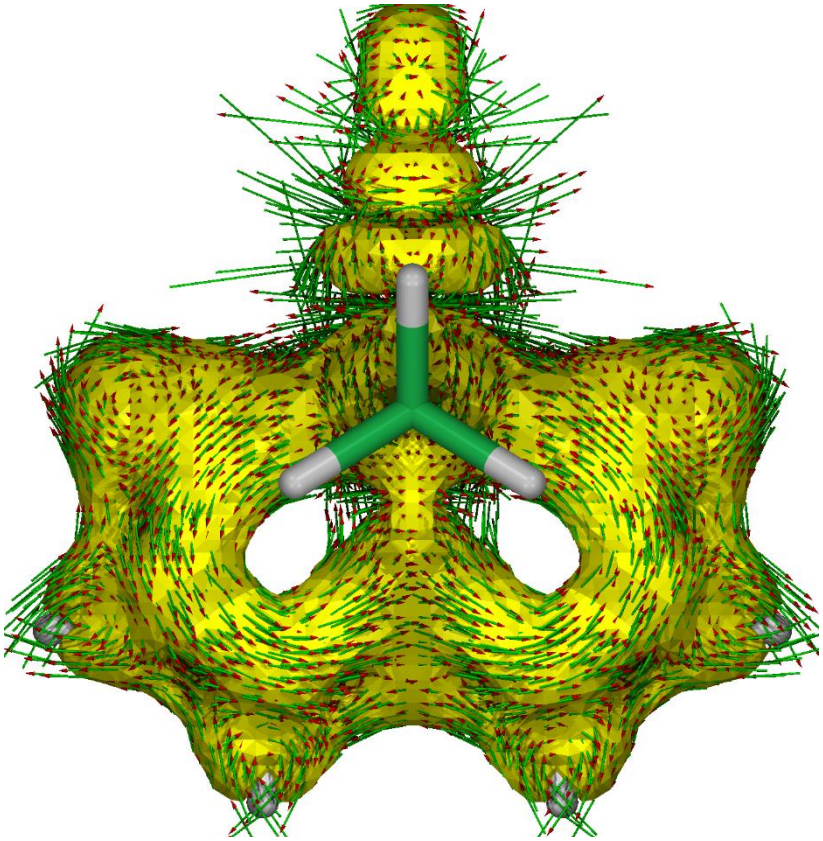


Figure S38. ACID plot of **5-T_1**. Isovalue: 0.035 a.u.

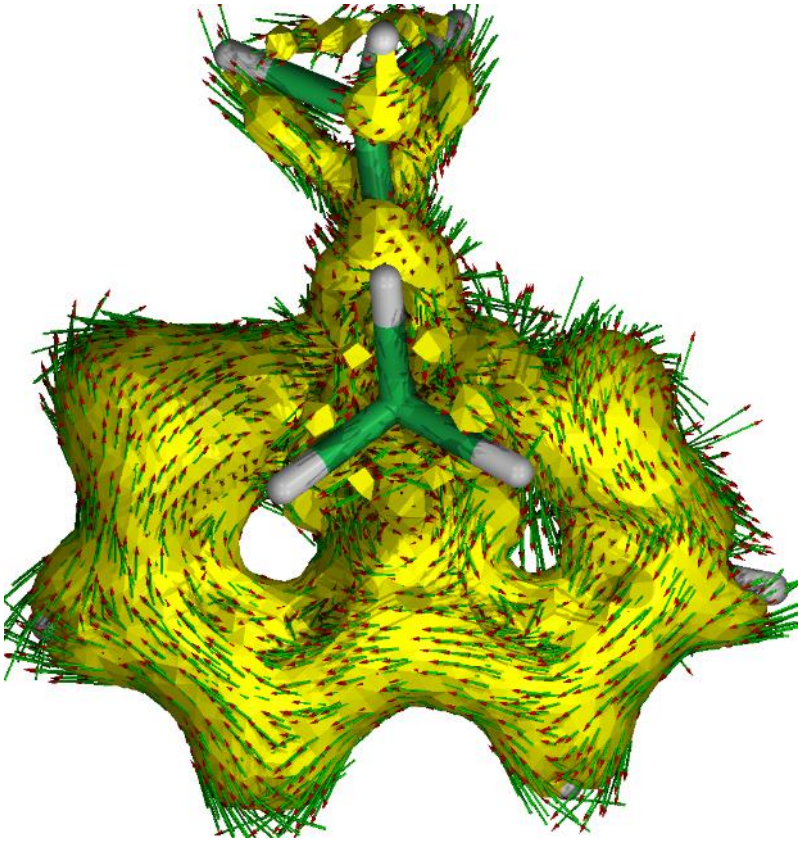


Figure S39. ACID plot of **6-S_0**. Isovalue: 0.035 a.u.

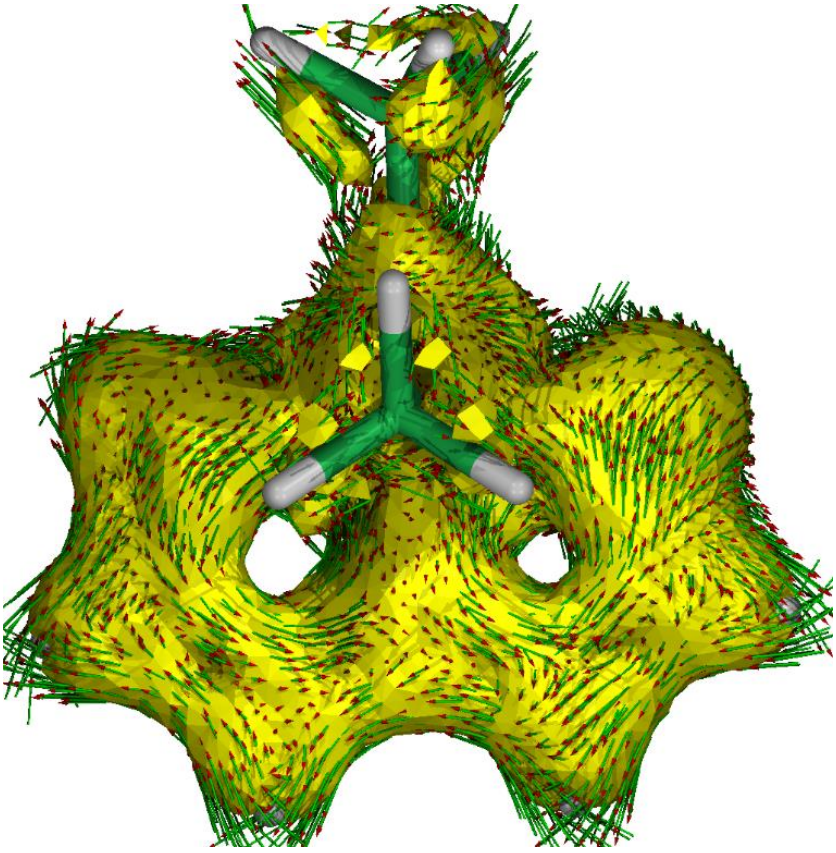


Figure S40. ACID plot of **6-T_1**. Isovalue: 0.035 a.u.

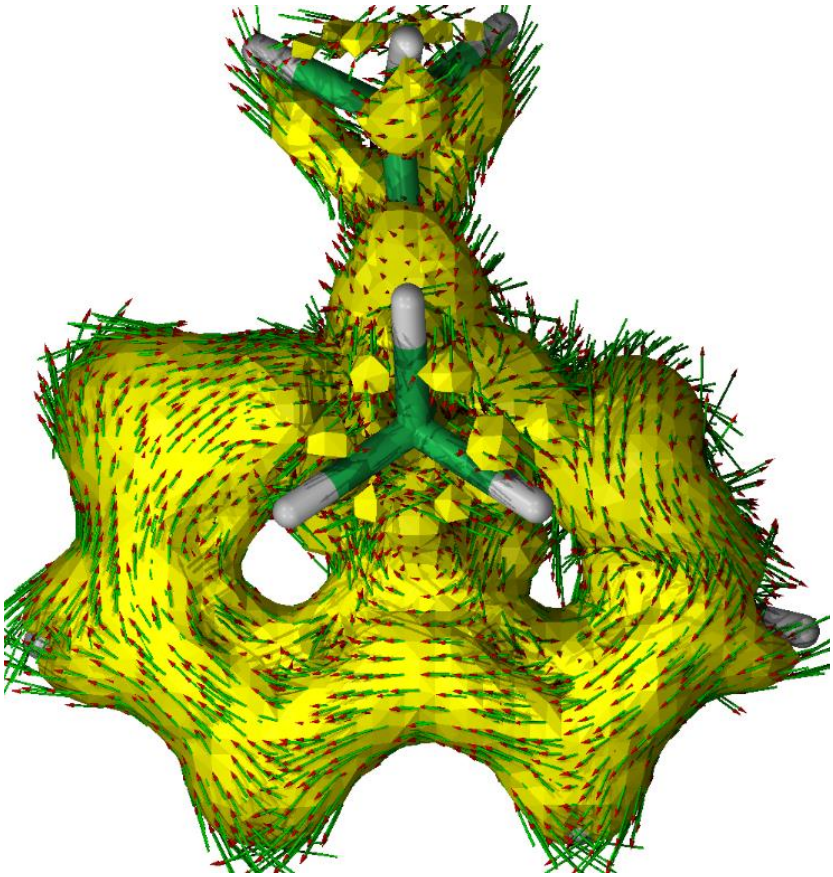


Figure S41. ACID plot of **7-S_0**. Isovalue: 0.035 a.u.

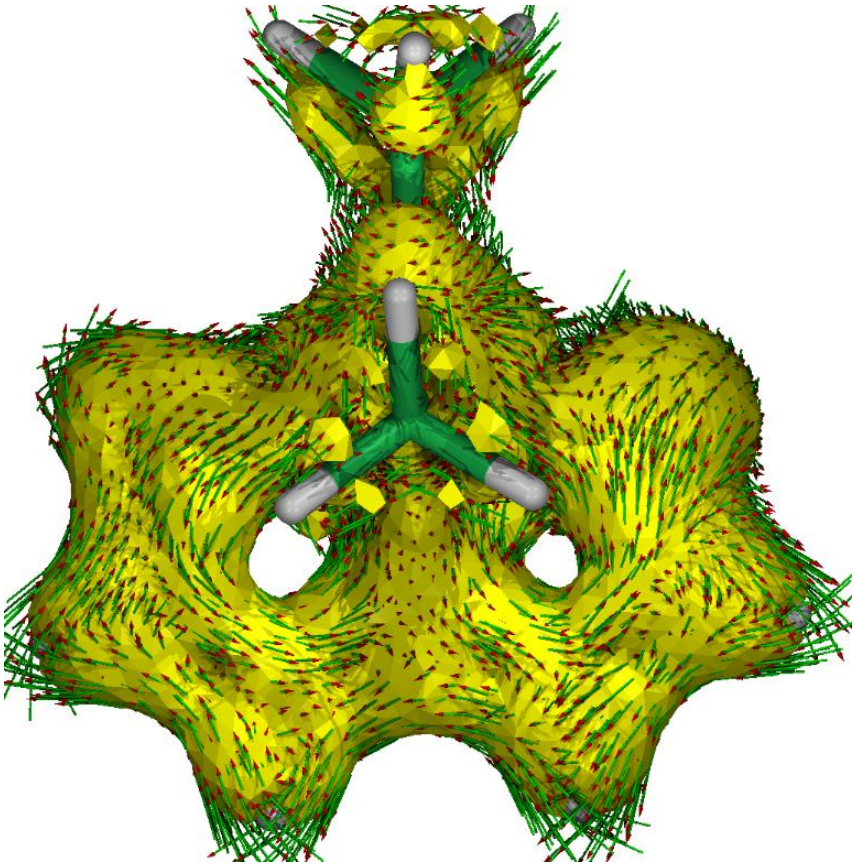


Figure S42. ACID plot of **7-T_1**. Isovalue: 0.035 a.u.

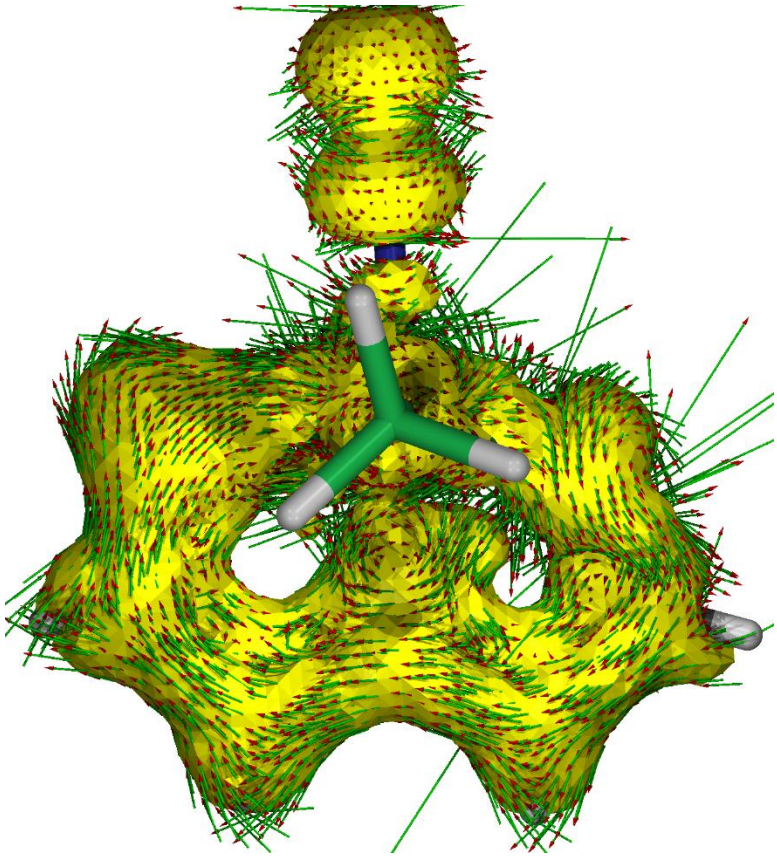


Figure S43. ACID plot of **8-S_0**. Isovalue: 0.035 a.u.

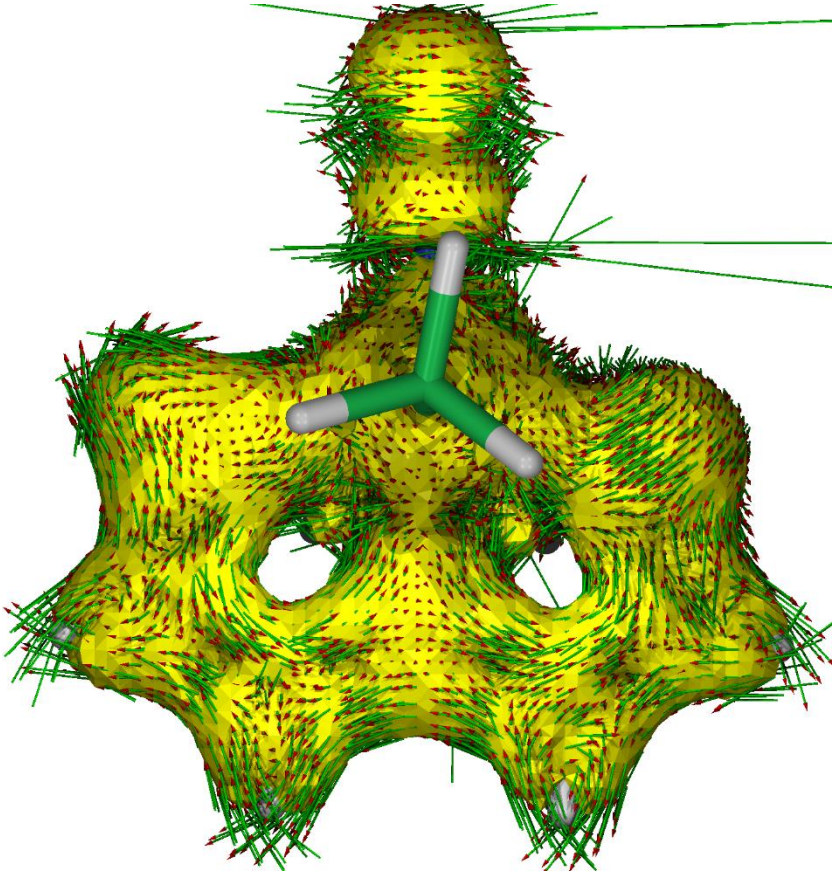


Figure S44. ACID plot of **8-T_1**. Isovalue: 0.035 a.u.

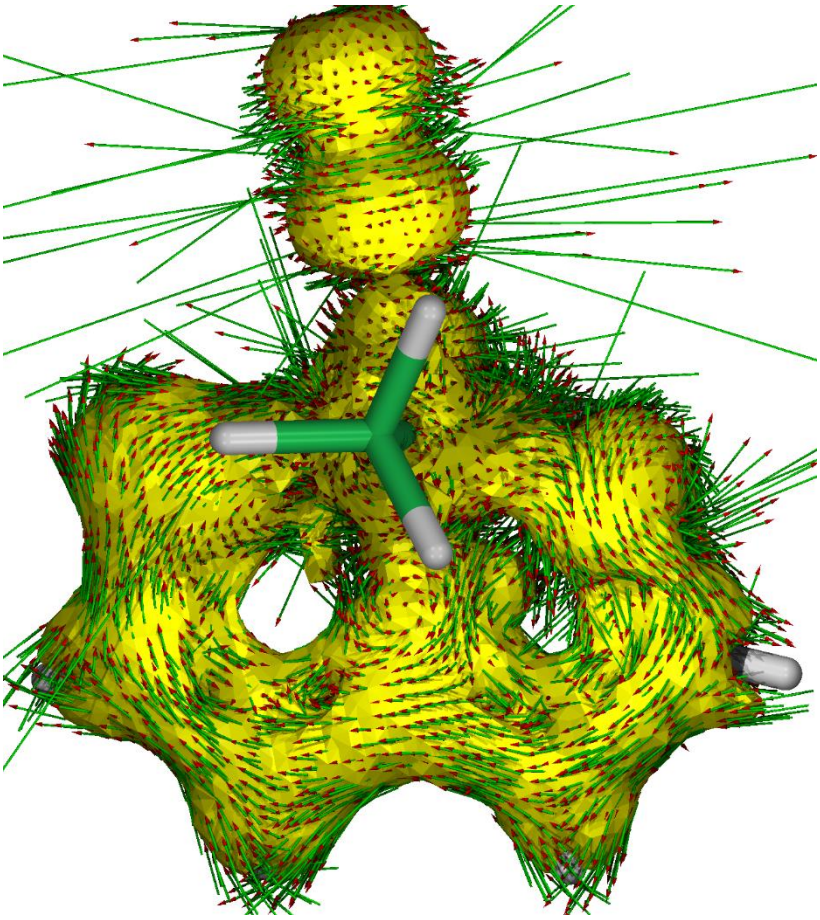


Figure S45. ACID plot of **9**-S_0. Isovalue: 0.035 a.u.

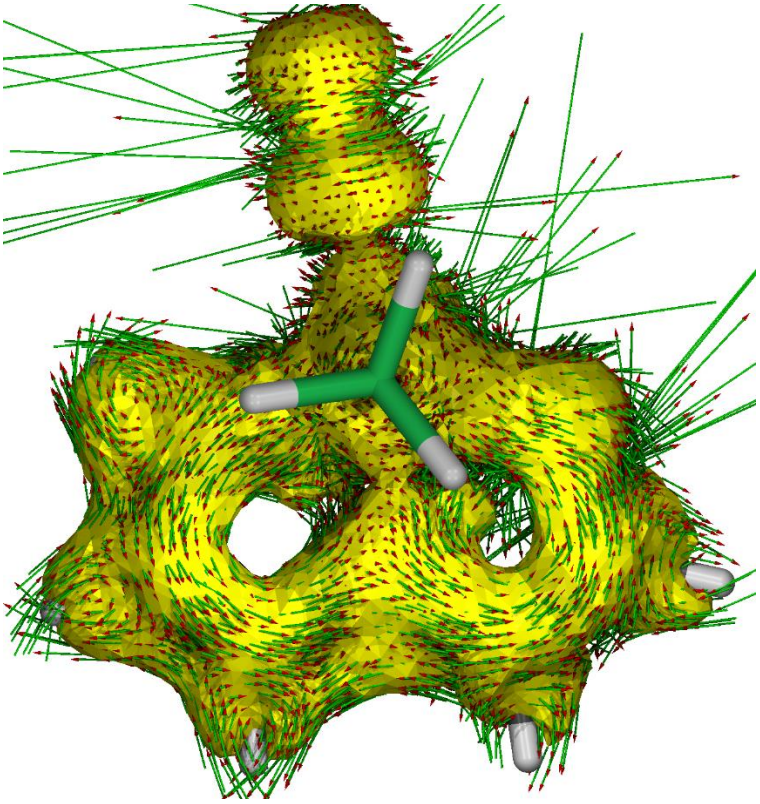


Figure S46. ACID plot of **9**-T_1. Isovalue: 0.035 a.u.

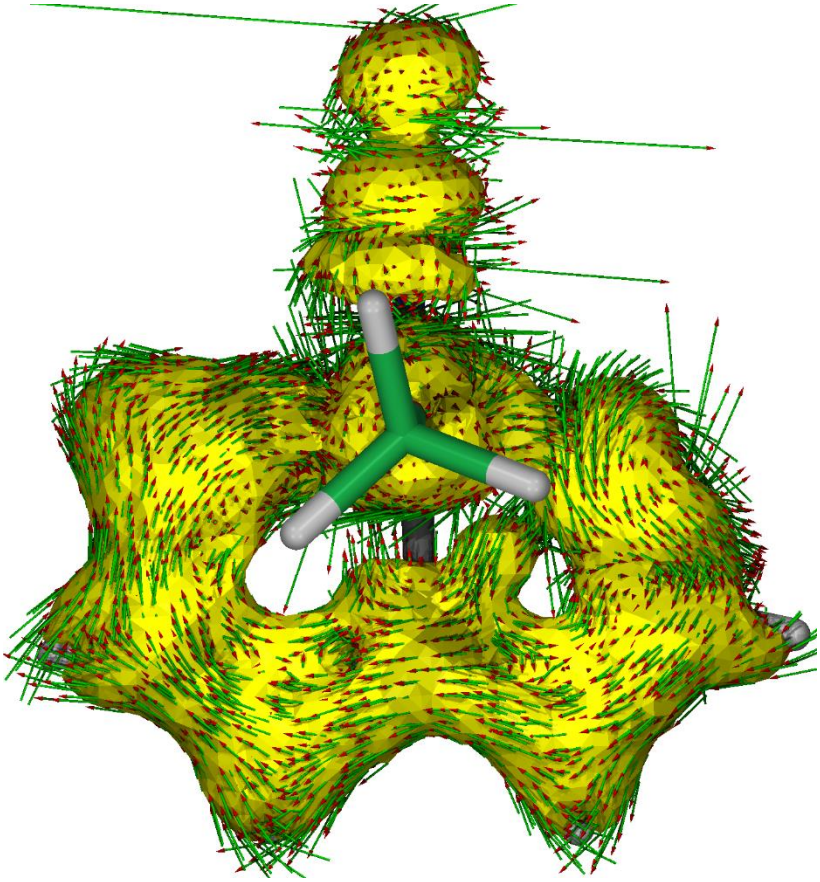


Figure S47. ACID plot of **10**-S_0. Isovalue: 0.035 a.u.

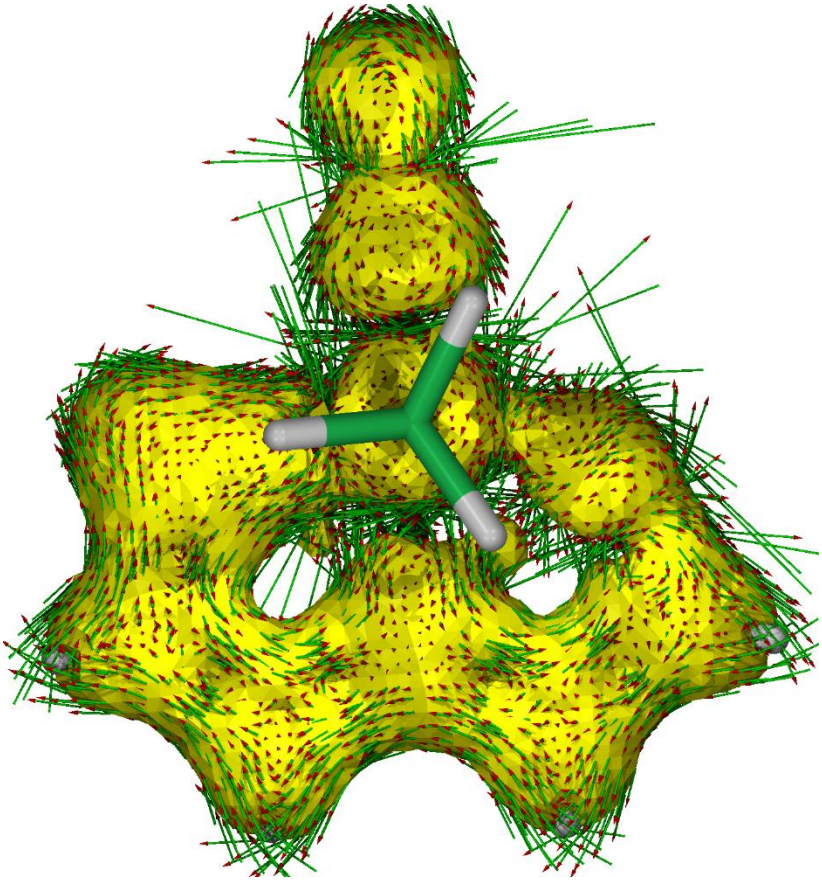


Figure S48. ACID plot of **10**-T_1. Isovalue: 0.035 a.u.

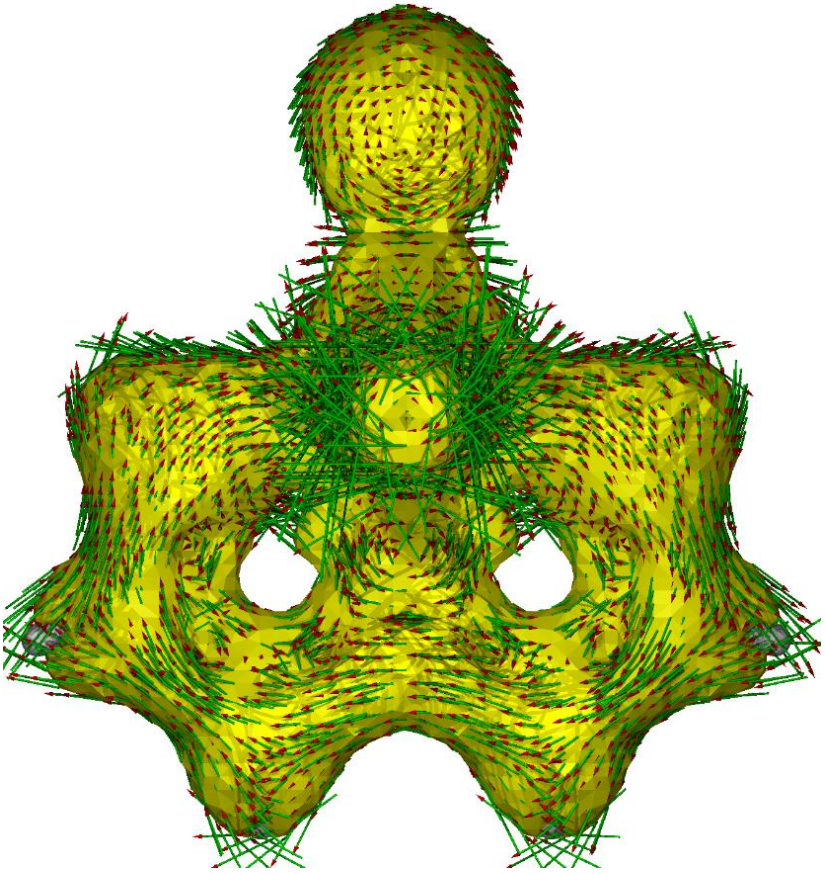


Figure S49. ACID plot of **11**-S_0. Isovalue: 0.035 a.u.

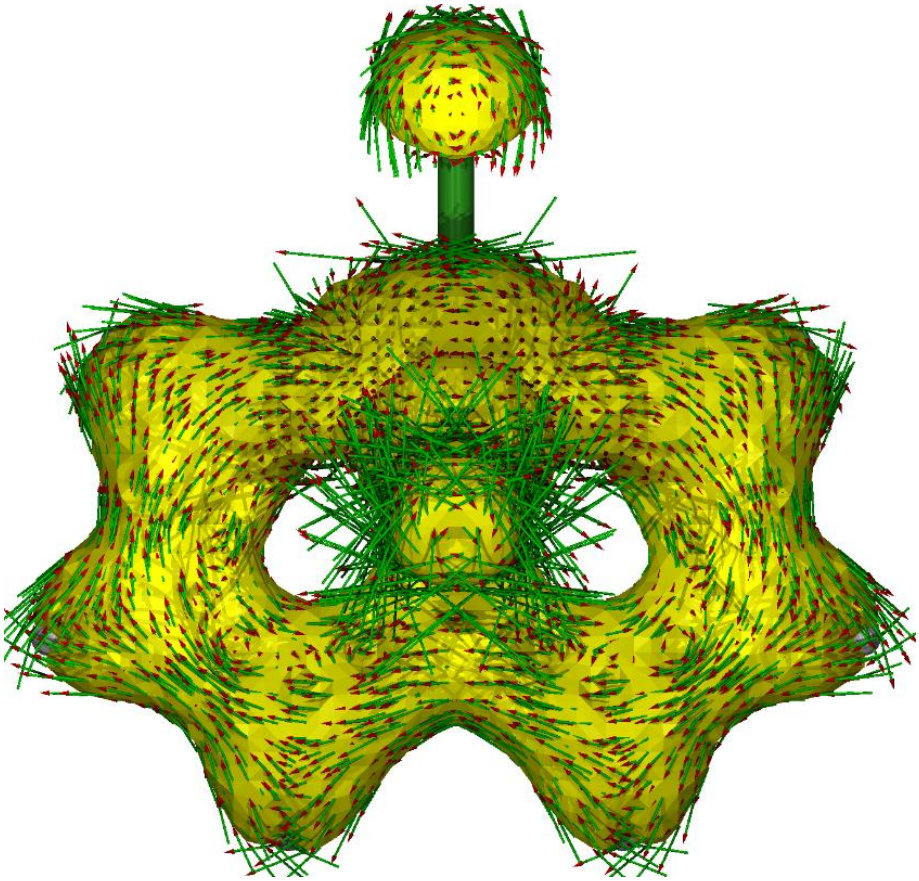


Figure S50. ACID plot of **11**-T_1. Isovalue: 0.035 a.u.

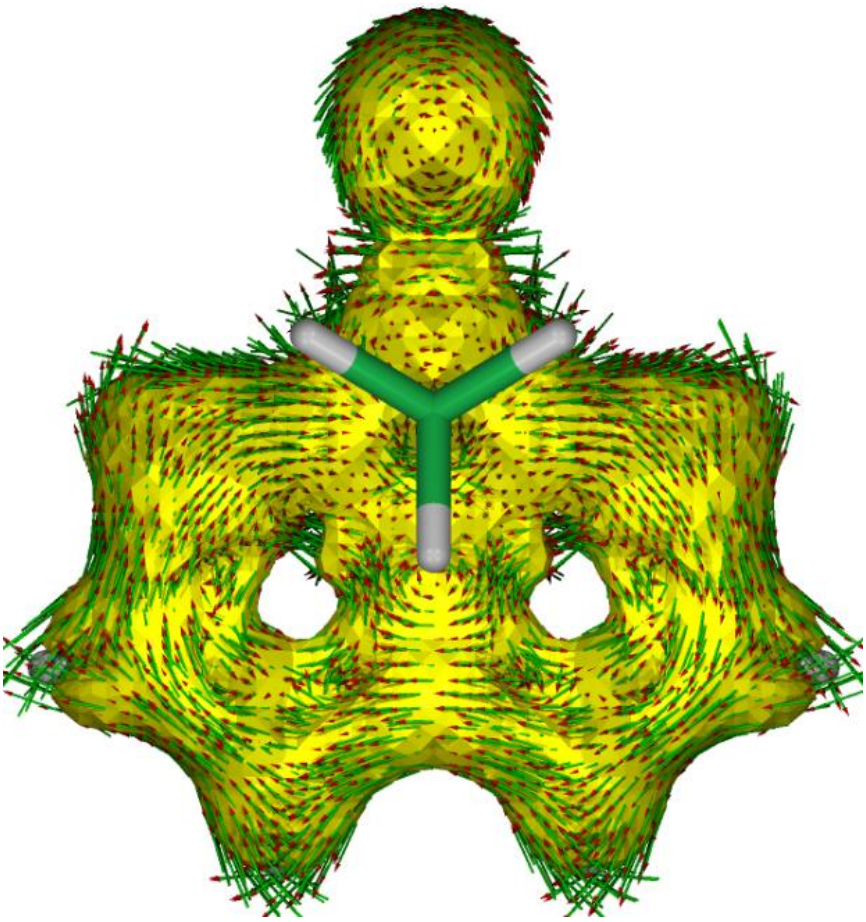


Figure S51. ACID plot of **12-S_0**. Isovalue: 0.035 a.u.

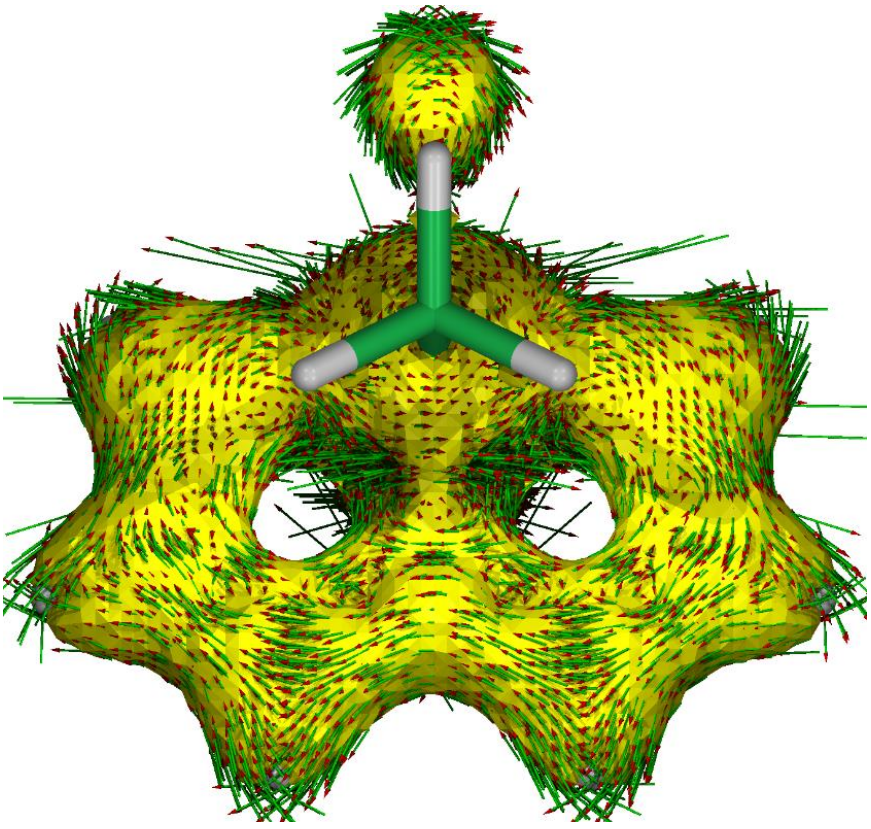


Figure S52. ACID plot of **12-T_1**. Isovalue: 0.035 a.u.

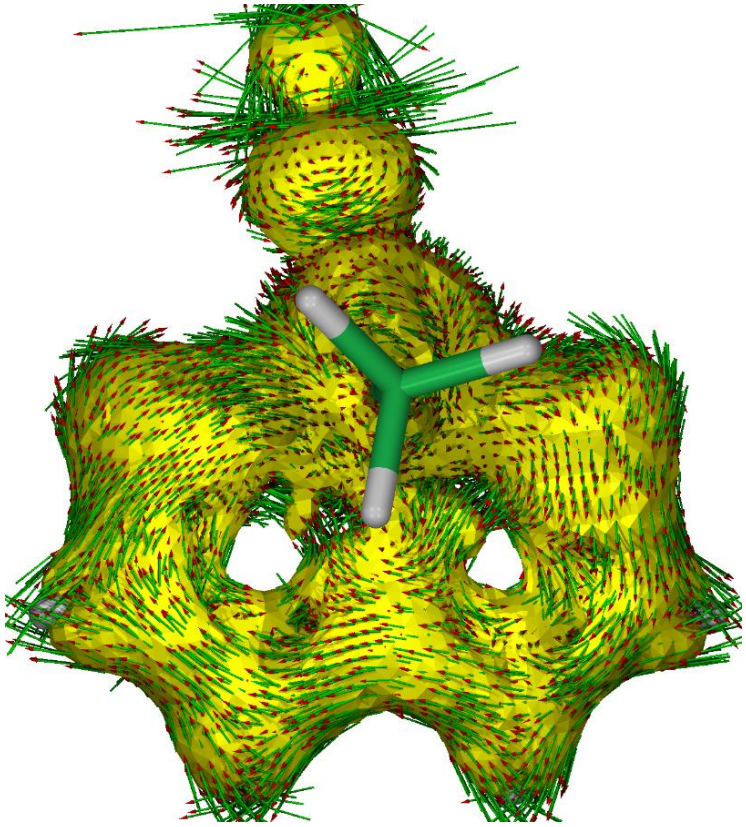


Figure S53. ACID plot of 16e of **2-S_0**. Isovalue: 0.035 a.u.

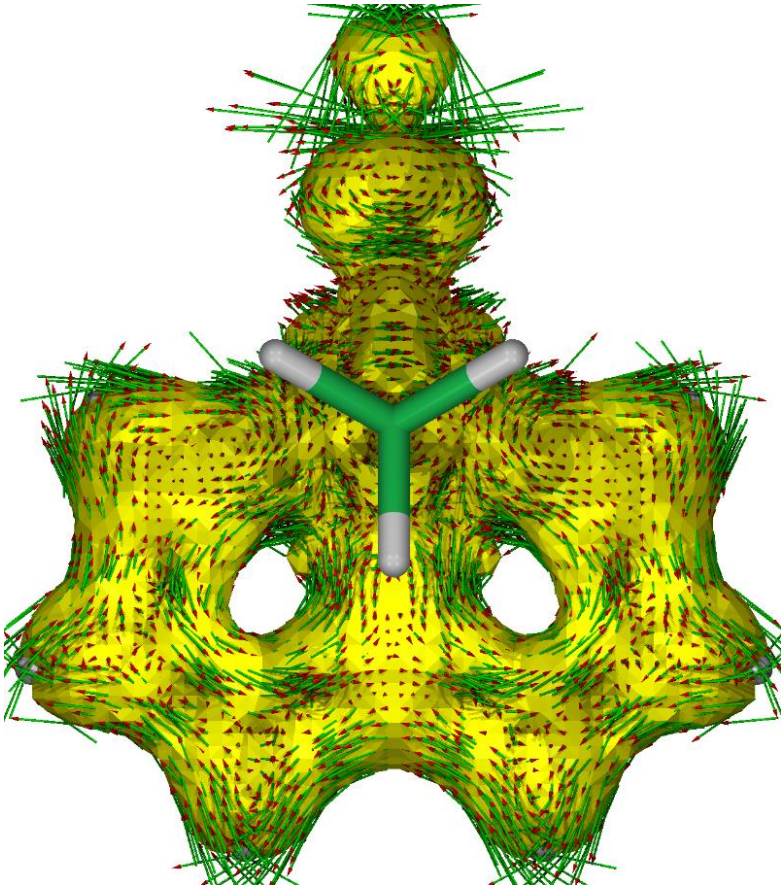


Figure 54. ACID plot of 16e of **2-T_1**. Isovalue: 0.035 a.u.

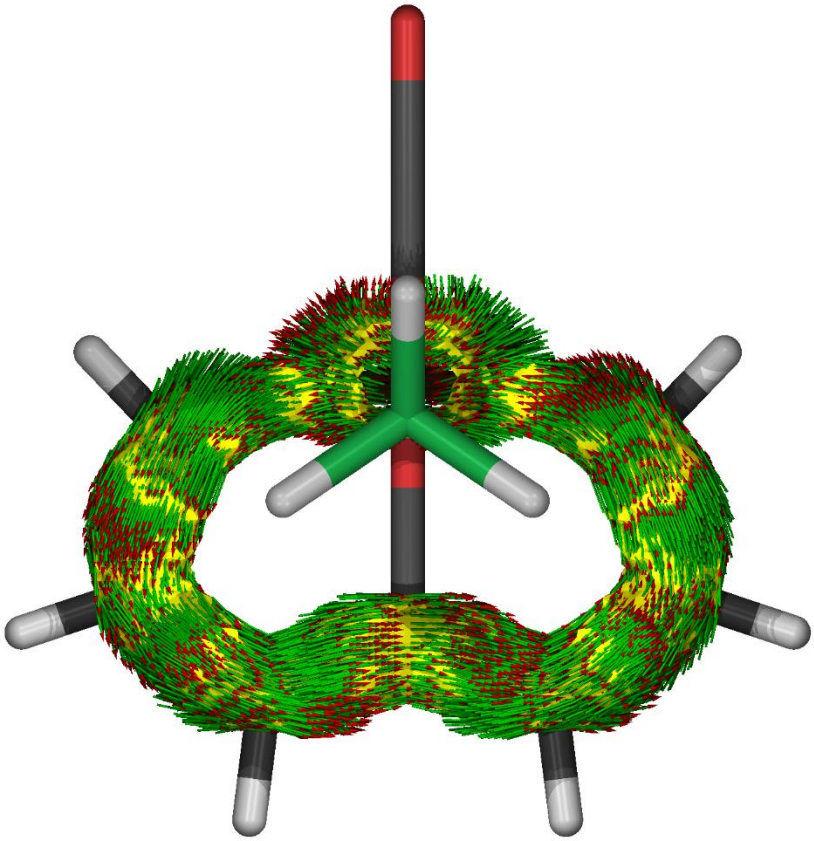


Figure S55. ACID plot of the HSOMO of **1**-T_1. Isovalue is 0.024 a.u.

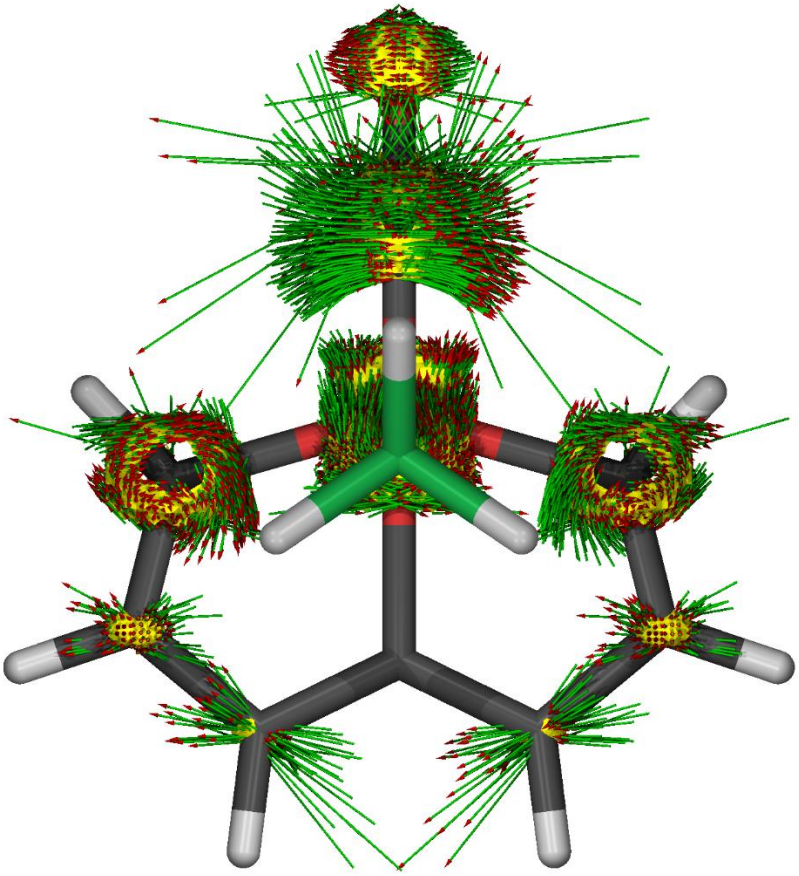


Figure S56. ACID plot of the HSOMO-1 of **1**-T_1. Isovalue is 0.024 a.u.

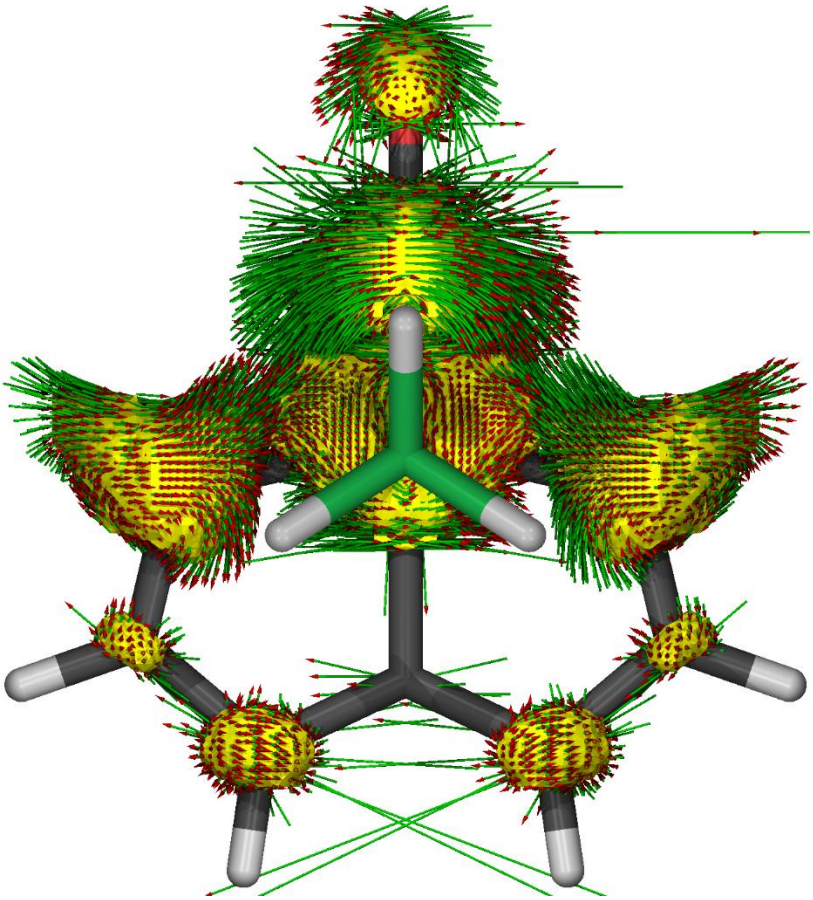


Figure S57. ACID plot of the HOMO of **1**-S_0. Isovalue is 0.024 a.u.

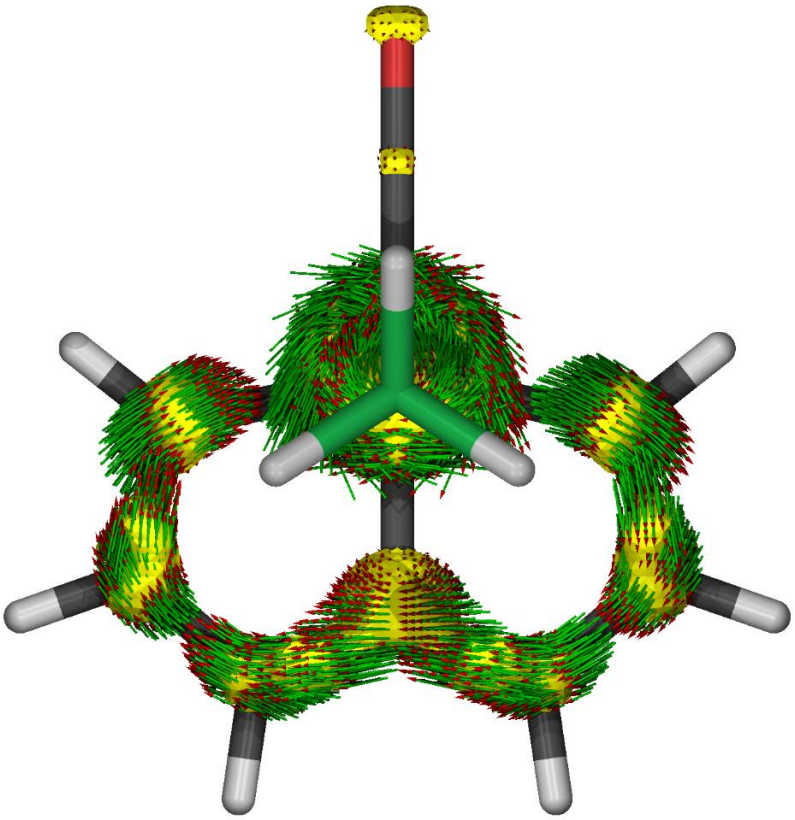


Figure S58. ACID plot of the HOMO-1 of **1**-S_0. Isovalue is 0.024 a.u.

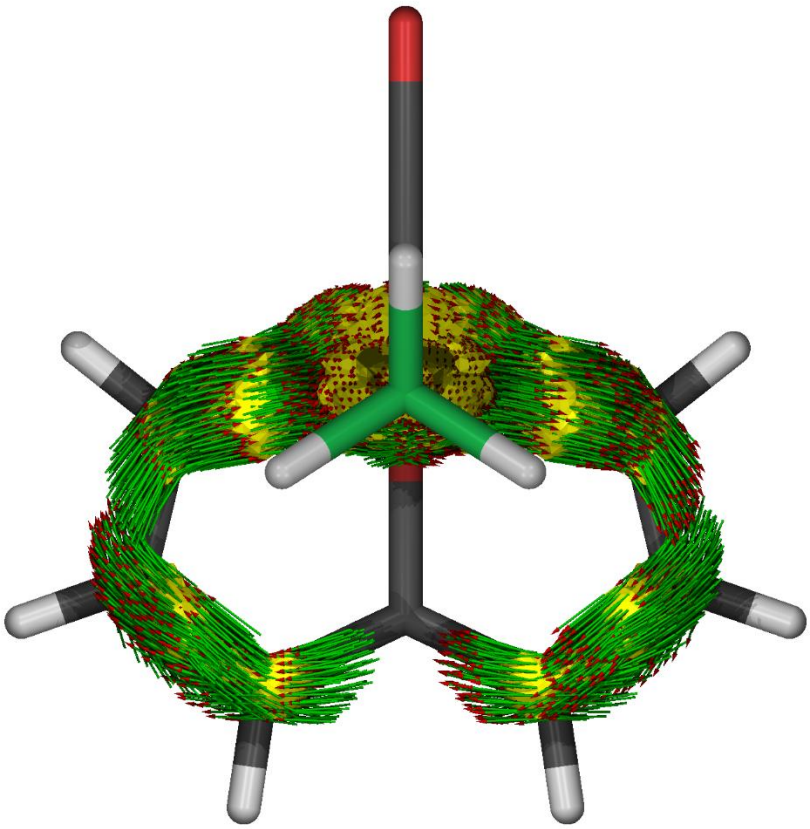


Figure S59. ACID plot of the HOMO-2 of **1**-S_0. Isovalue is 0.024 a.u.

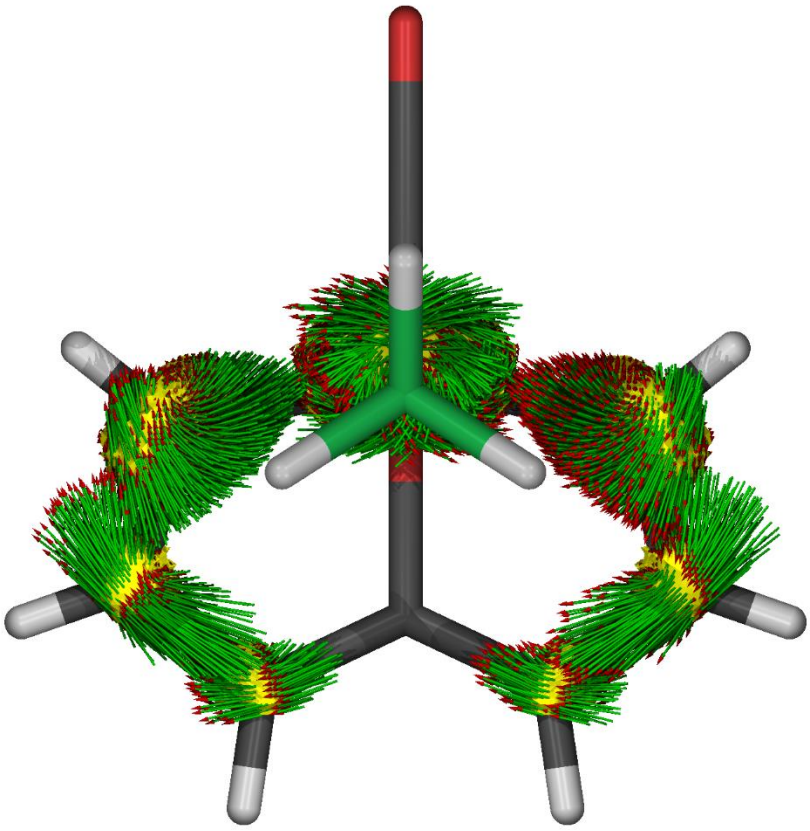


Figure S60. ACID plot of the HOMO-7 of **1**-S_0. Isovalue is 0.024 a.u.

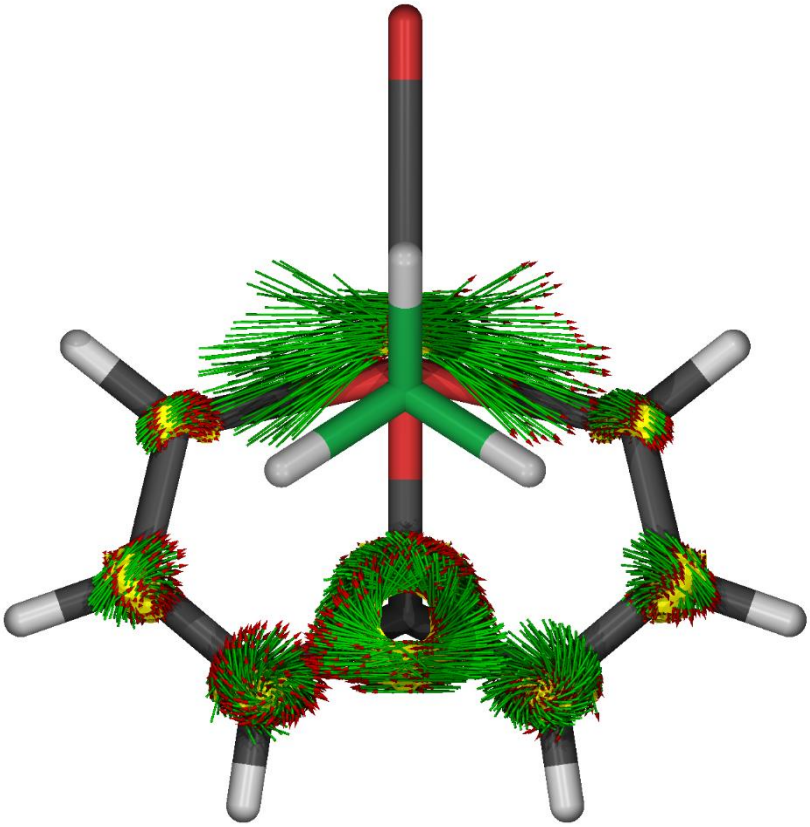


Figure S61. ACID plot of the HOMO-9 of **1**-S_0. Isovalue is 0.024 a.u.

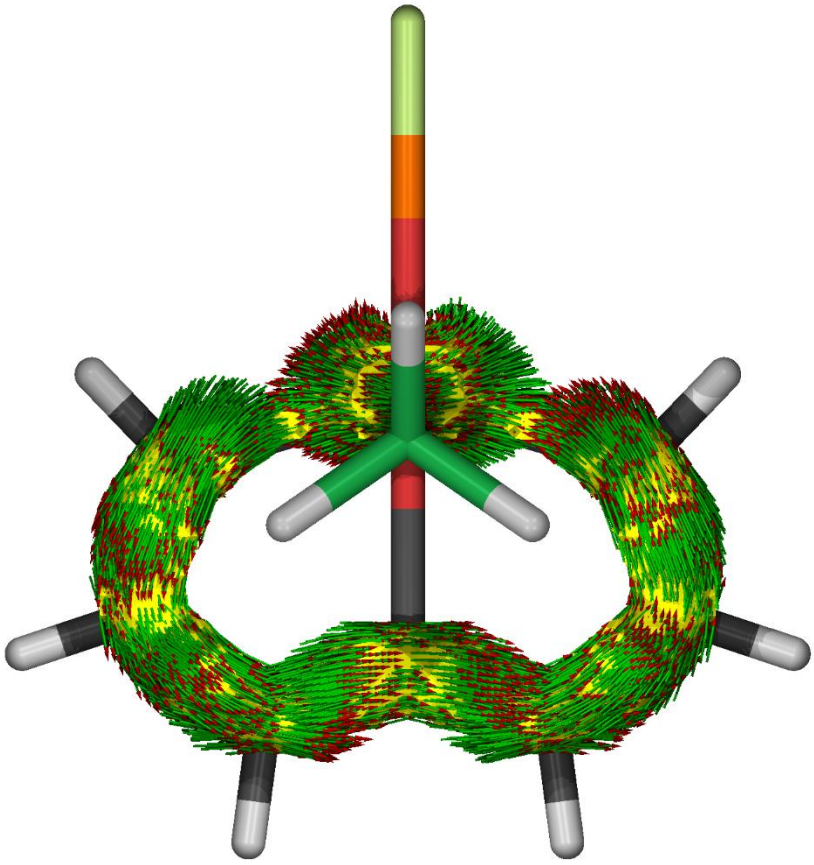


Figure S62. ACID plot of the HSOMO of **2**-T_1. Isovalue is 0.024 a.u.

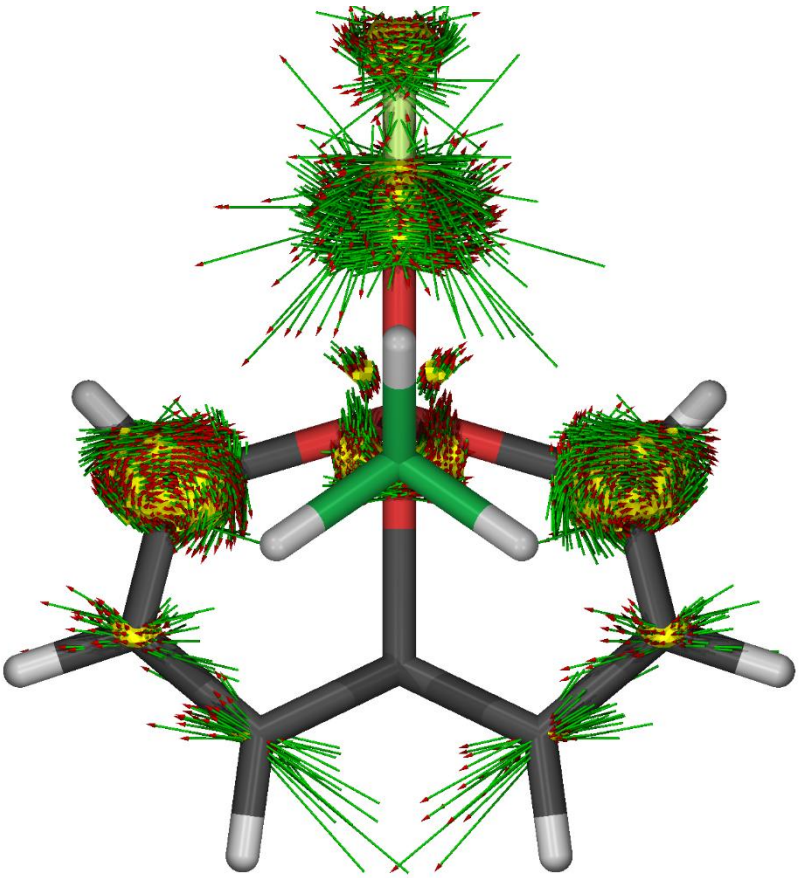


Figure S63. ACID plot of the HSOMO-1 of **2-*T*$_1$**. Isovalue is 0.024 a.u.

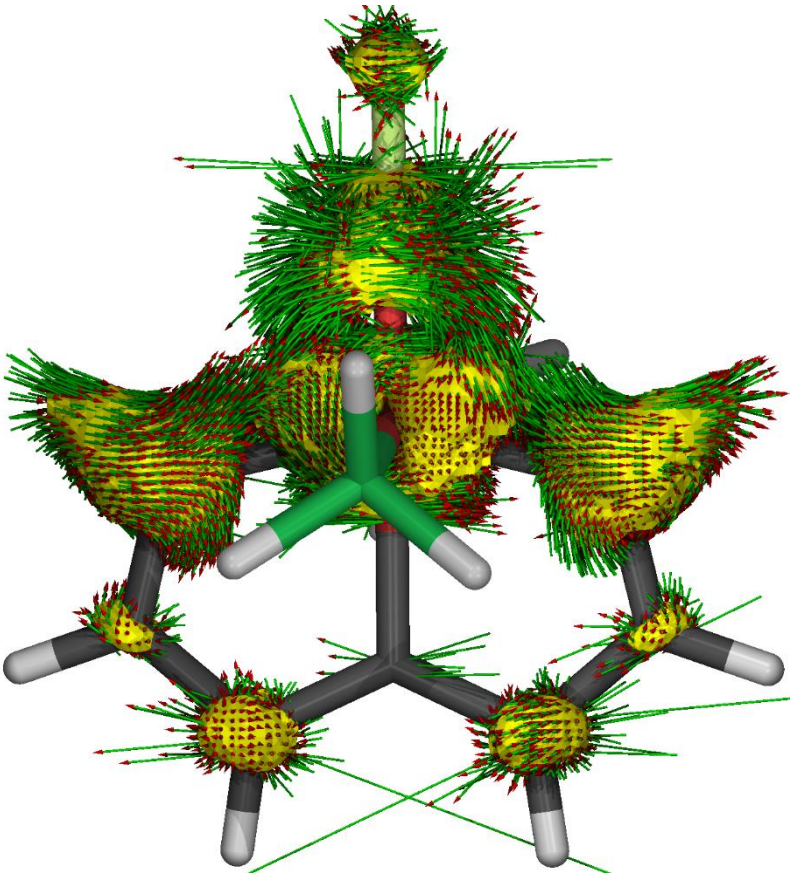


Figure S64. ACID plot of the HOMO of **2-*S*$_0$**. Isovalue is 0.024 a.u.

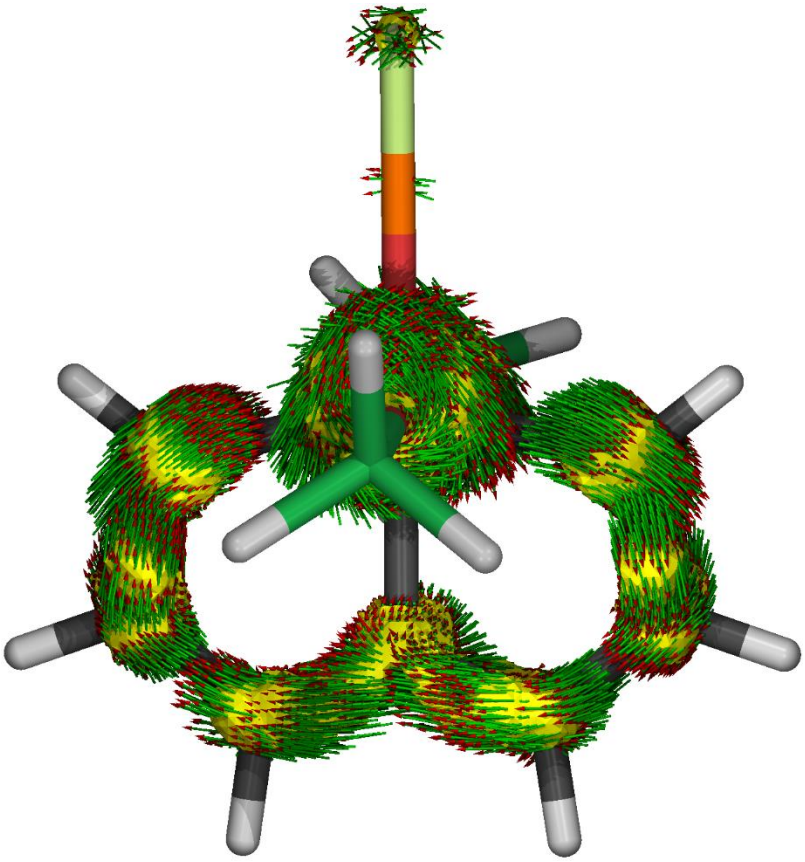


Figure S65. ACID plot of the HOMO-1 of **2-*S*$_0$**. Isovalue is 0.024 a.u.

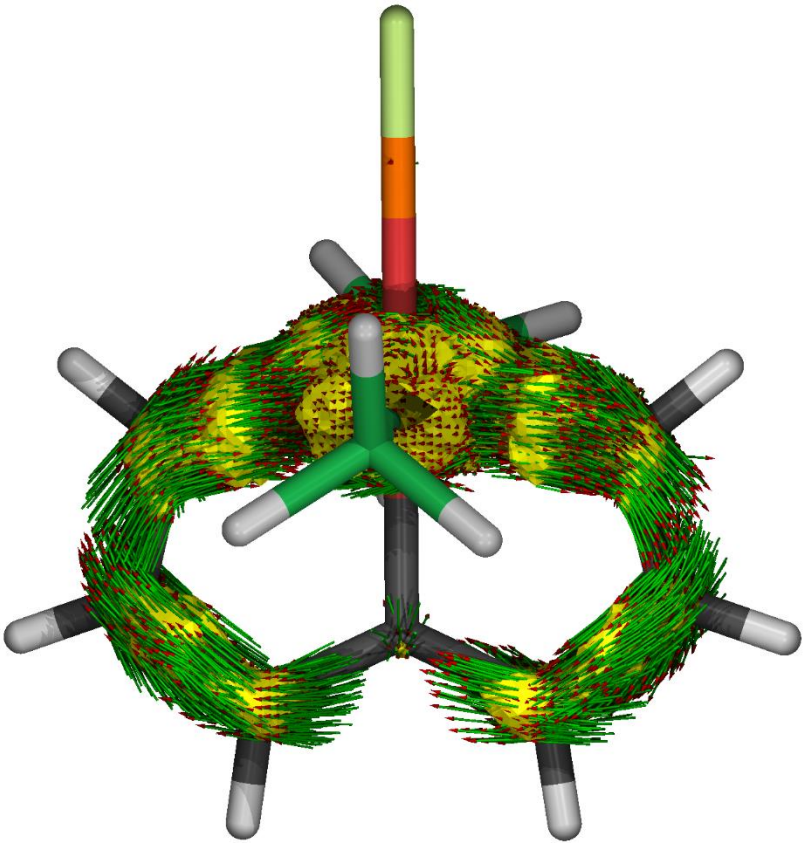


Figure S66. ACID plot of the HOMO-2 of **2-*S*$_0$**. Isovalue is 0.024 a.u.

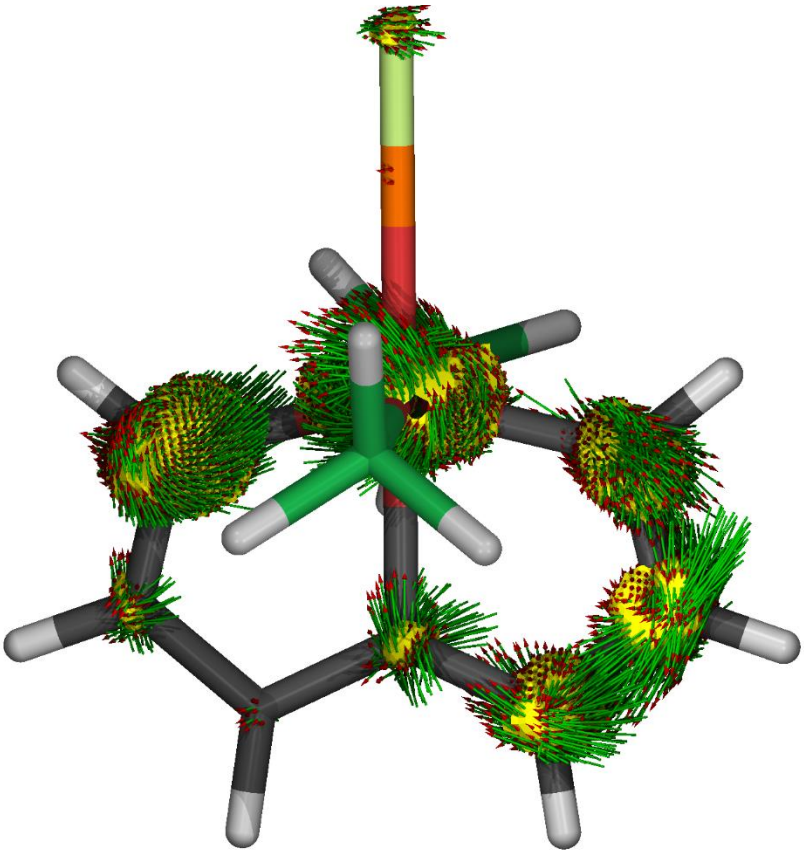


Figure S67. ACID plot of the HOMO-7 of **2-*S*$_0$**. Isovalue is 0.024 a.u.

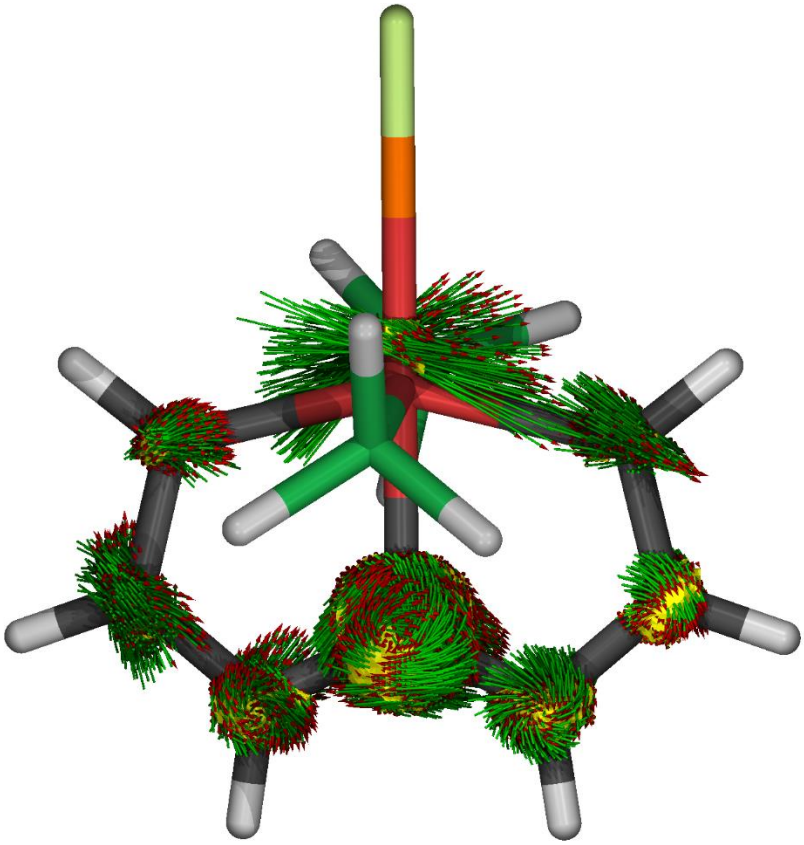


Figure S68. ACID plot of the HOMO-9 of **2-*S*$_0$**. Isovalue is 0.024 a.u.

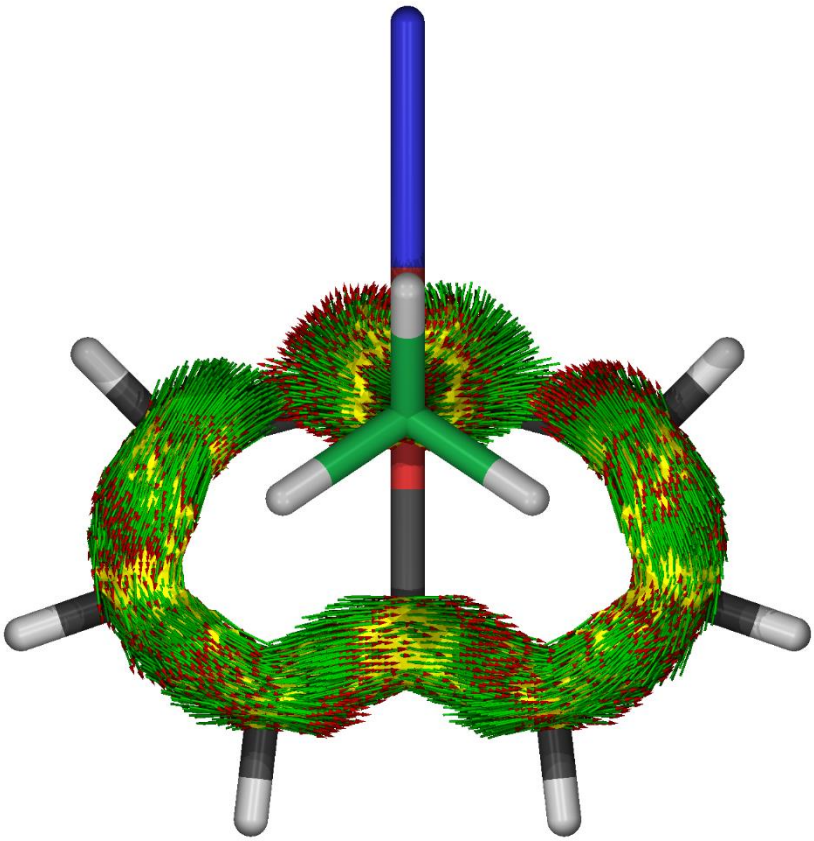


Figure S69. ACID plot of the HSOMO of **3-*T*$_1$**. Isovalue is 0.024 a.u.

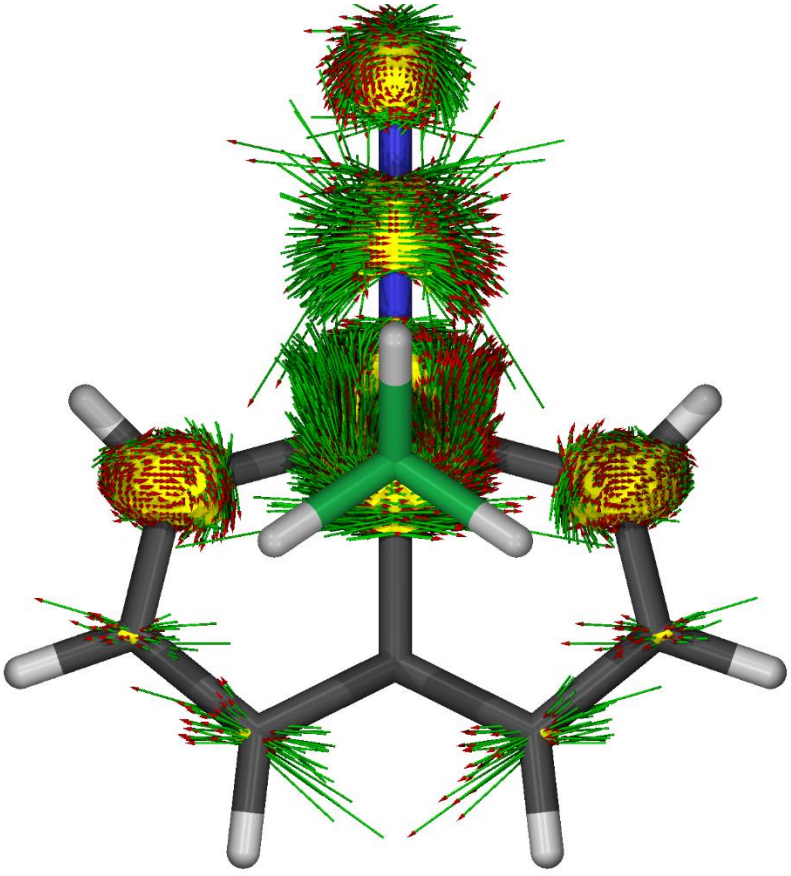


Figure S70. ACID plot of the HSOMO-1 of **3-*T*$_1$**. Isovalue is 0.024 a.u.

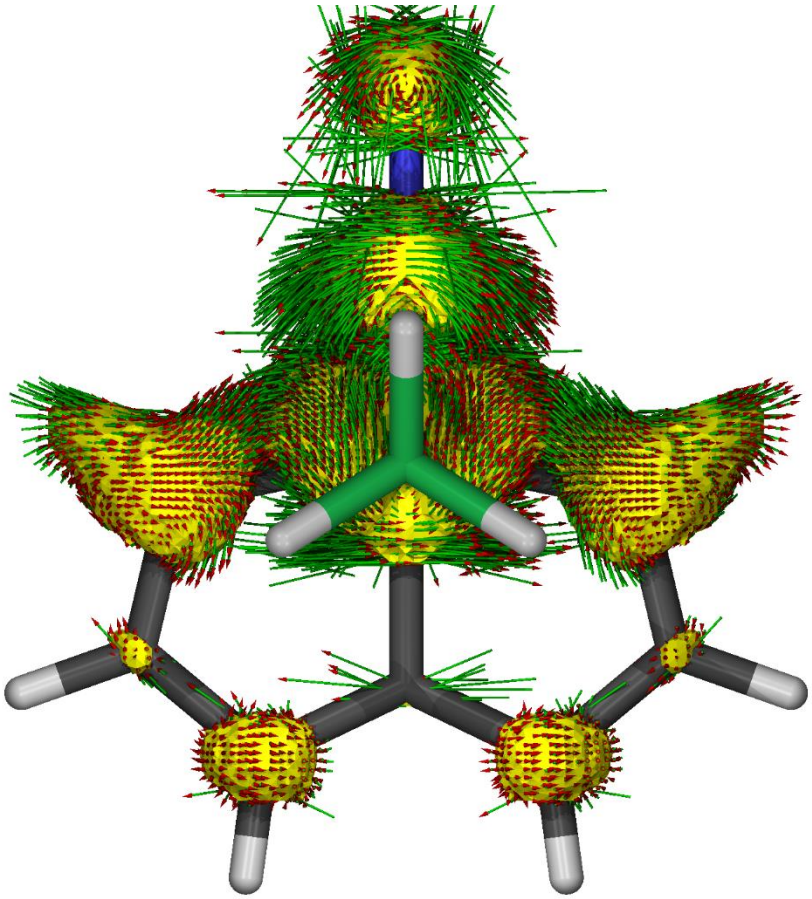


Figure S71. ACID plot of the HOMO of **3-S_0**. Isovalue is 0.024 a.u.

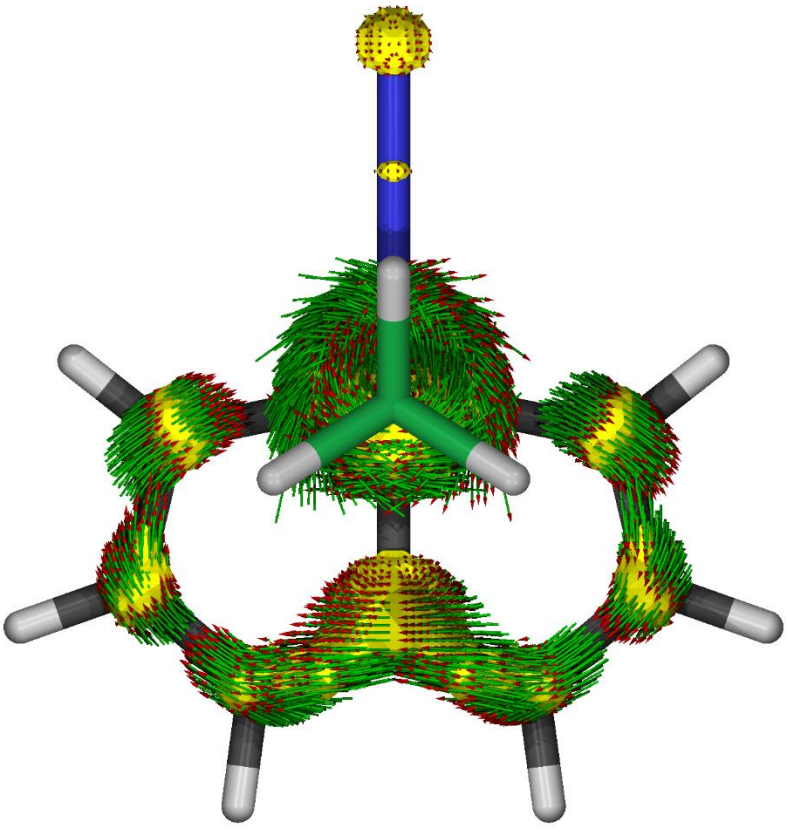


Figure S72. ACID plot of the HOMO-1 of **3-S_0**. Isovalue is 0.024 a.u.

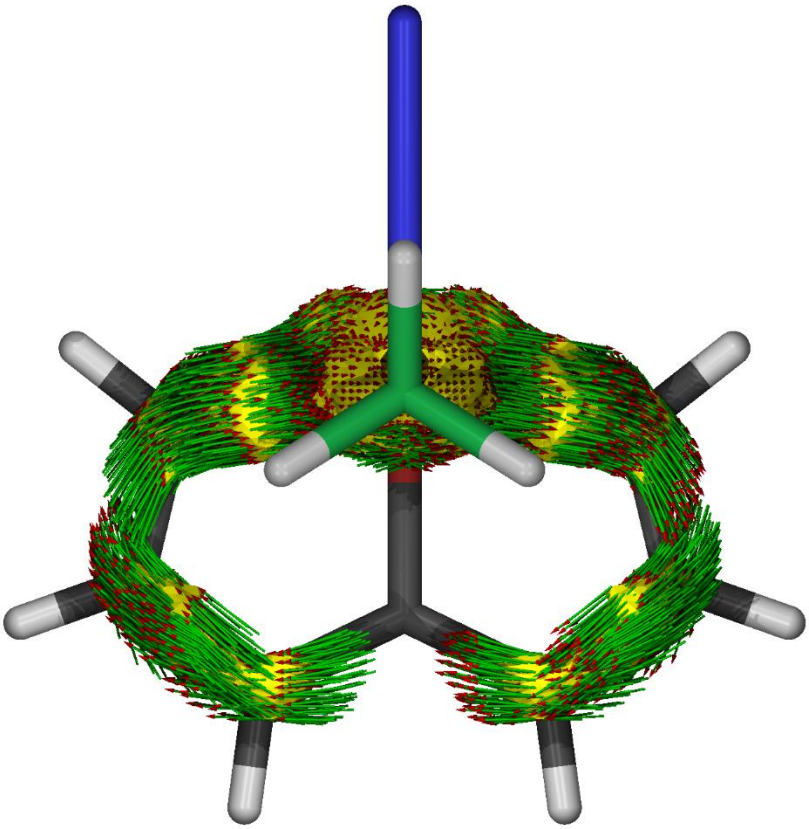


Figure S73. ACID plot of the HOMO-2 of **3**-S_0. Isovalue is 0.024 a.u.

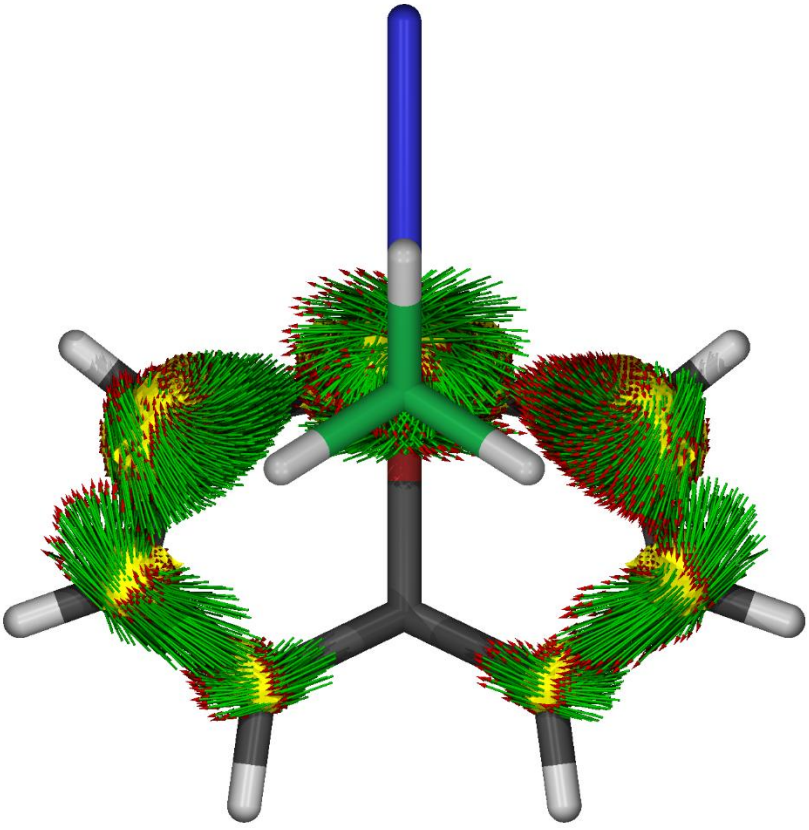


Figure S74. ACID plot of the HOMO-7 of **3**-S_0. Isovalue is 0.024 a.u.

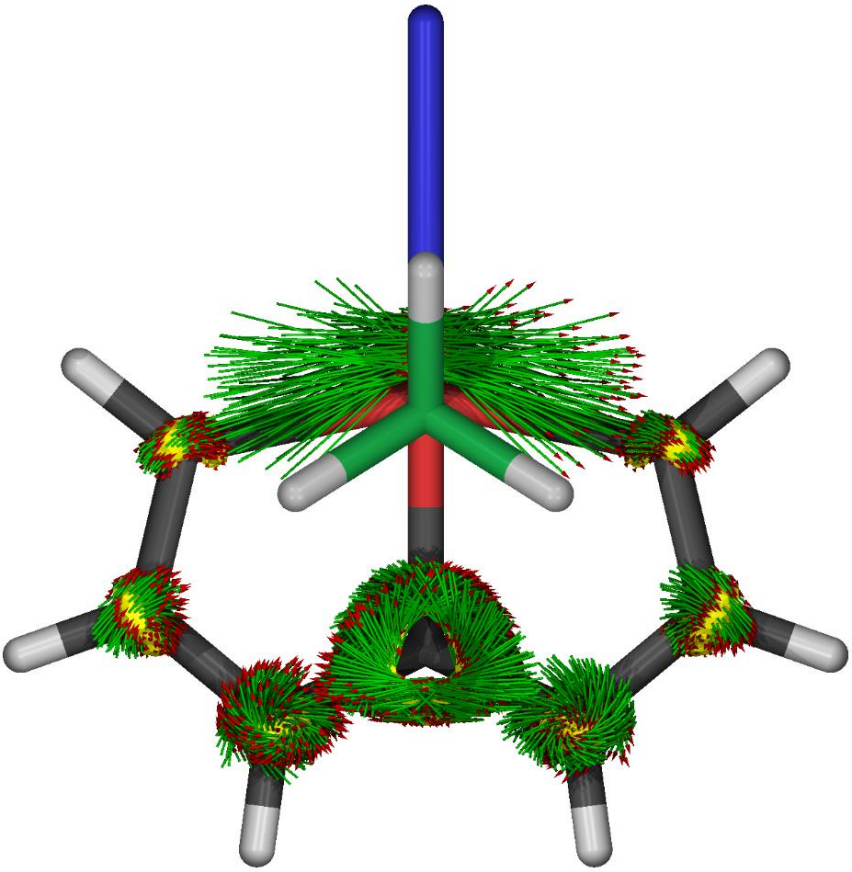


Figure S75. ACID plot of the HOMO-9 of **3**-S_0. Isovalue is 0.024 a.u.

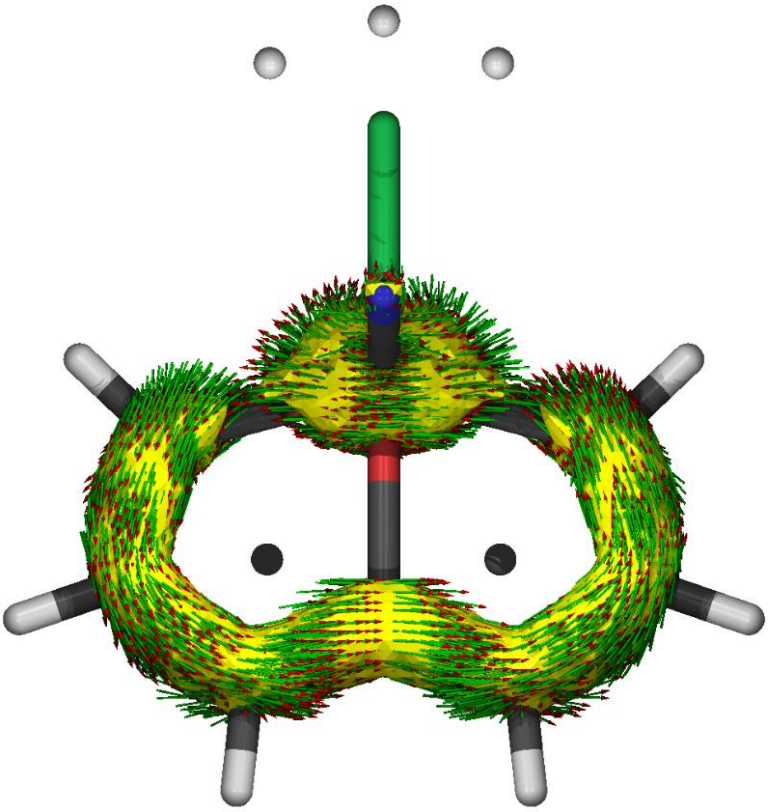


Figure S76. ACID plot of the HSOMO of **4**-T_1. Isovalue is 0.024 a.u.

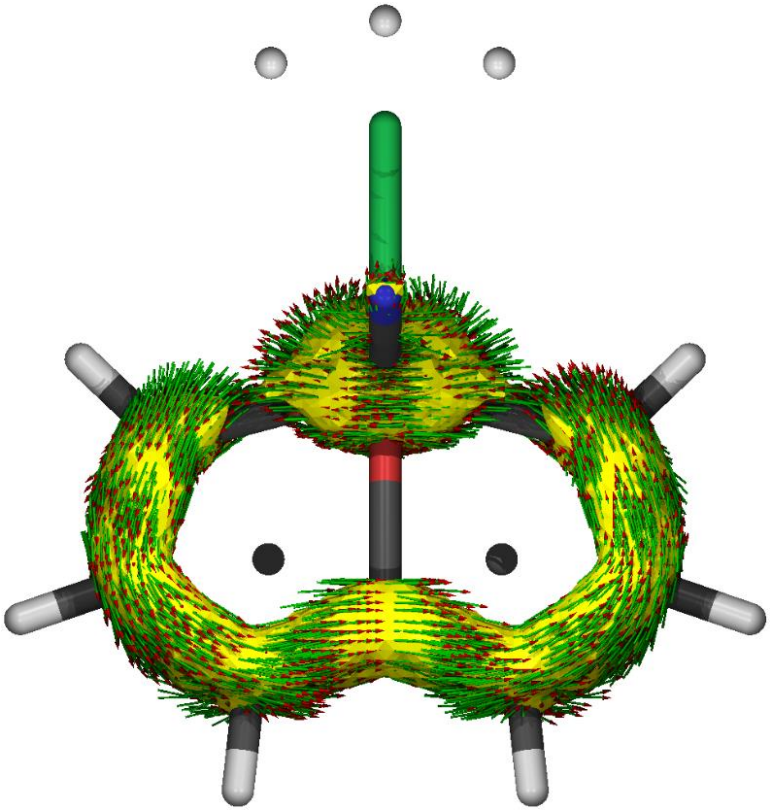


Figure S77. ACID plot of the HSOMO-1 of **4-*T*$_1$**. Isovalue is 0.024 a.u.

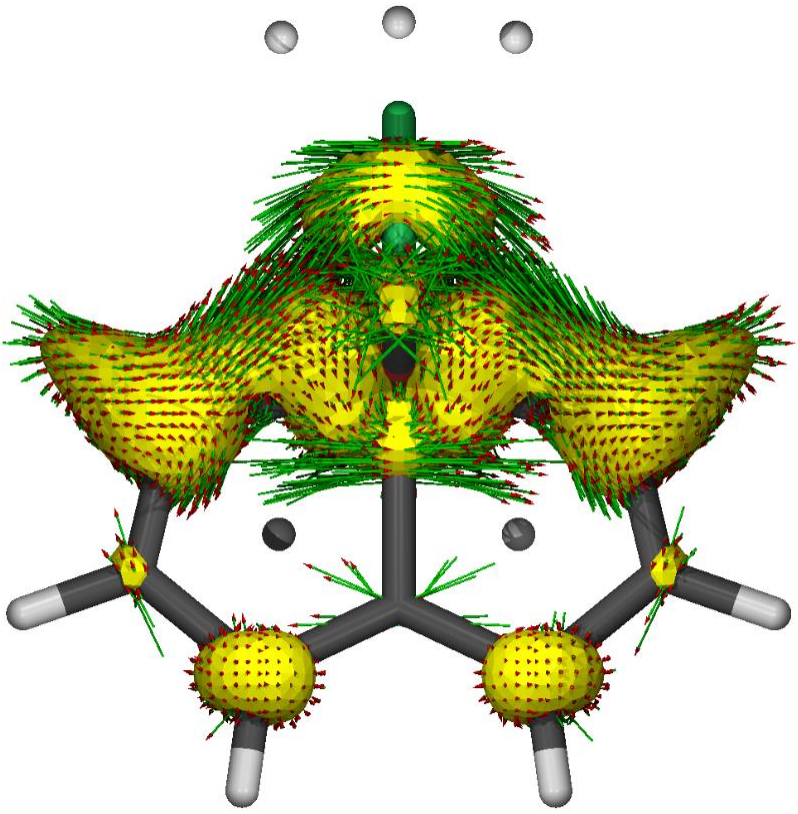


Figure S78. ACID plot of the HOMO of **4-*S*$_0$**. Isovalue is 0.024 a.u.

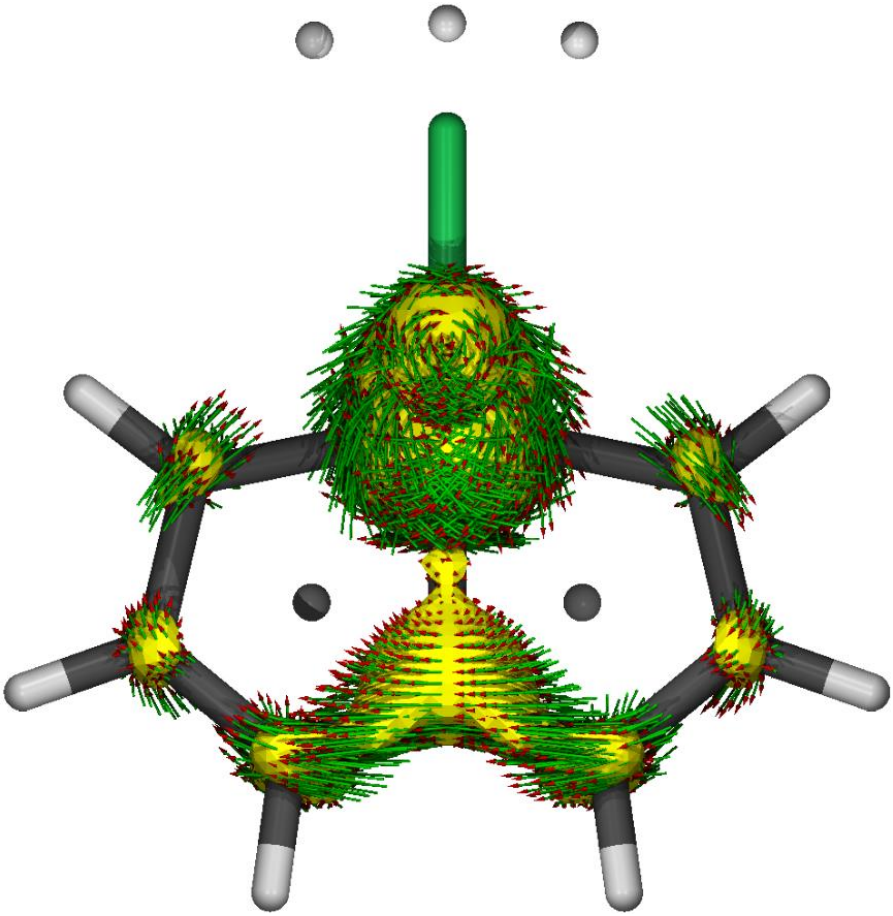


Figure S79. ACID plot of the HOMO-1 of **4-*S*$_0$**. Isovalue is 0.024 a.u.

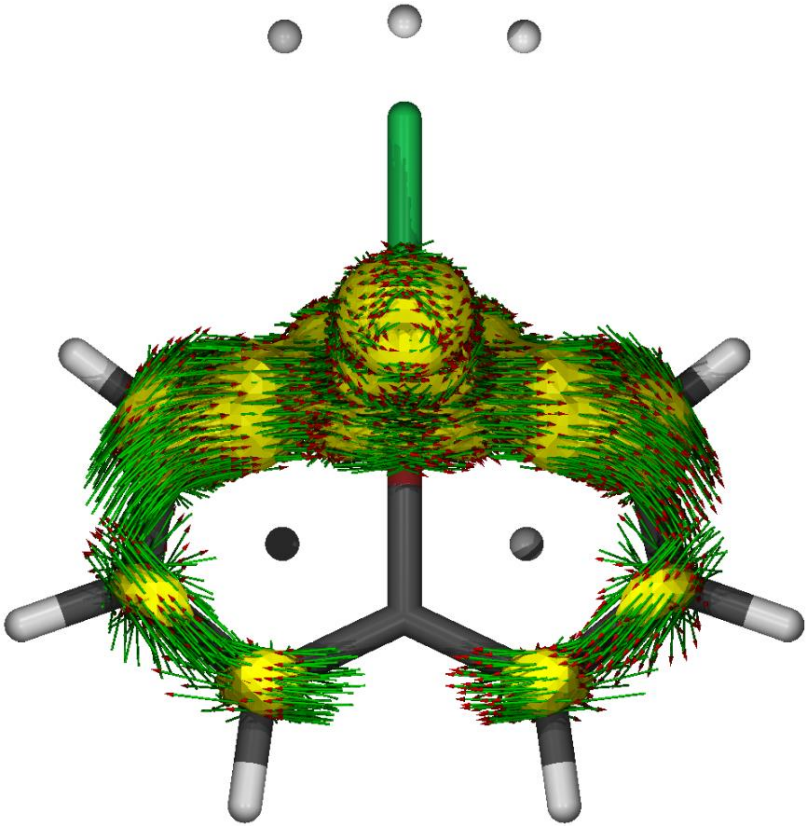


Figure S80. ACID plot of the HOMO-2 of **4-*S*$_0$**. Isovalue is 0.024 a.u.

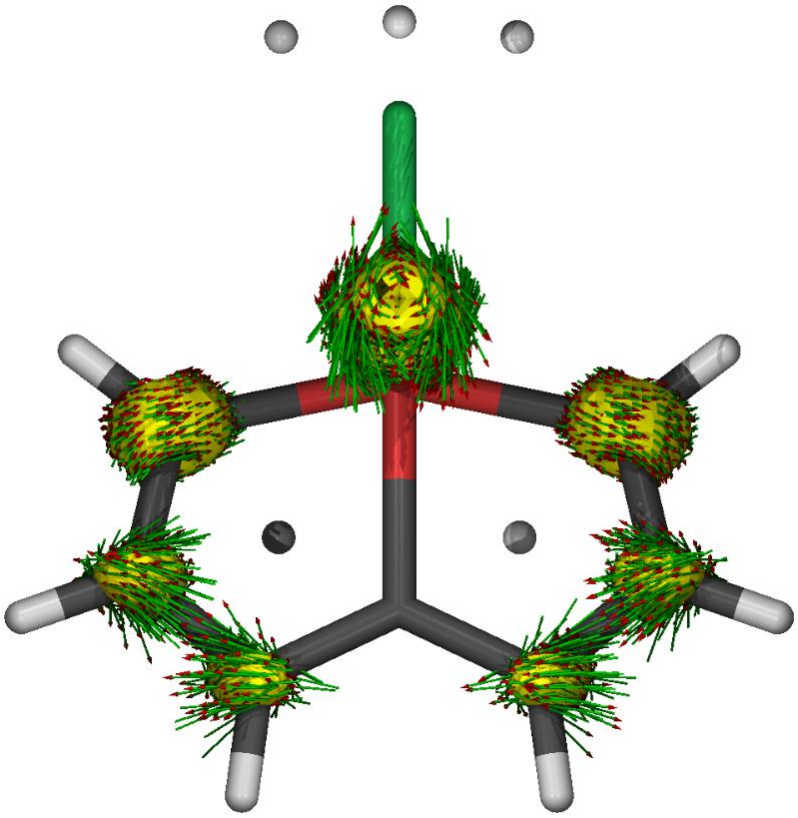


Figure S81. ACID plot of the HOMO-6 of **4**-S_0. Isovalue is 0.024 a.u.

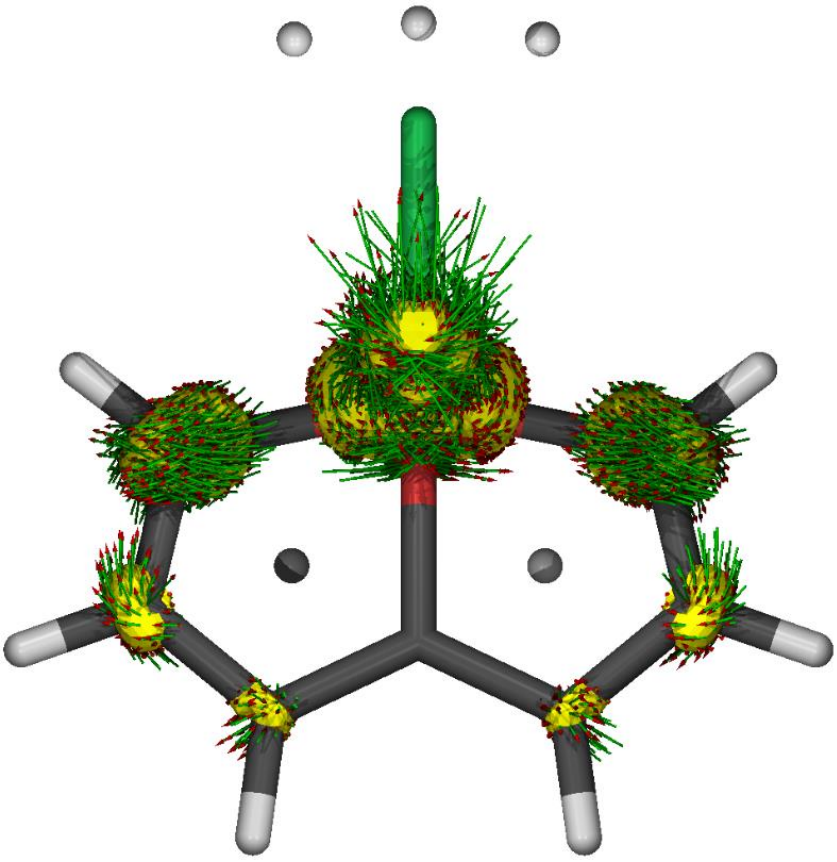


Figure S82. ACID plot of the HOMO-9 of **4**-S_0. Isovalue is 0.024 a.u.

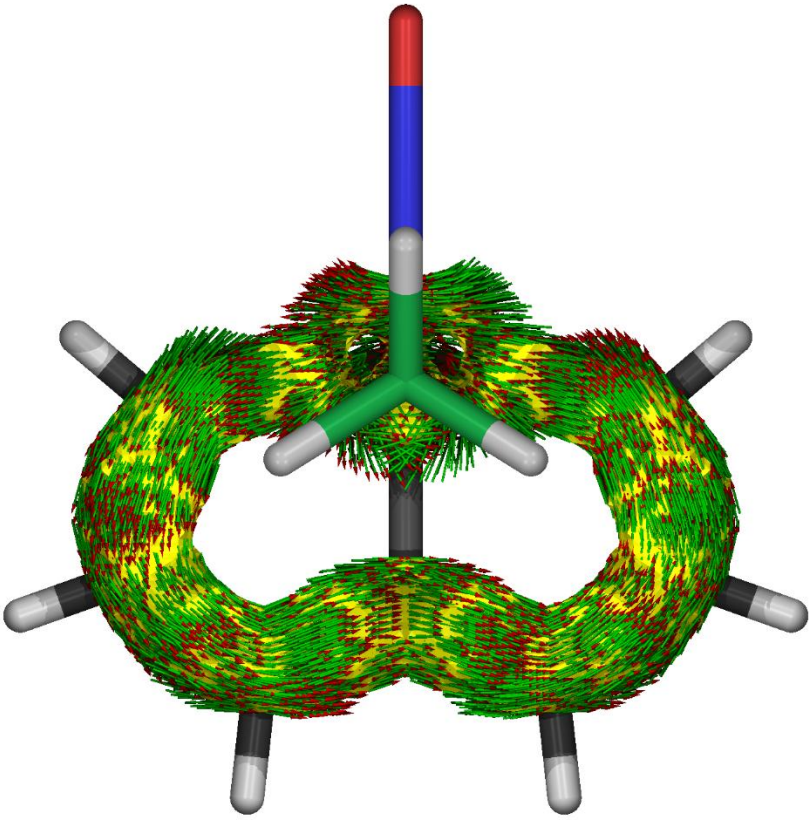


Figure S83. ACID plot of the HSOMO of **5-*T*$_1$**. Isovalue is 0.024 a.u.

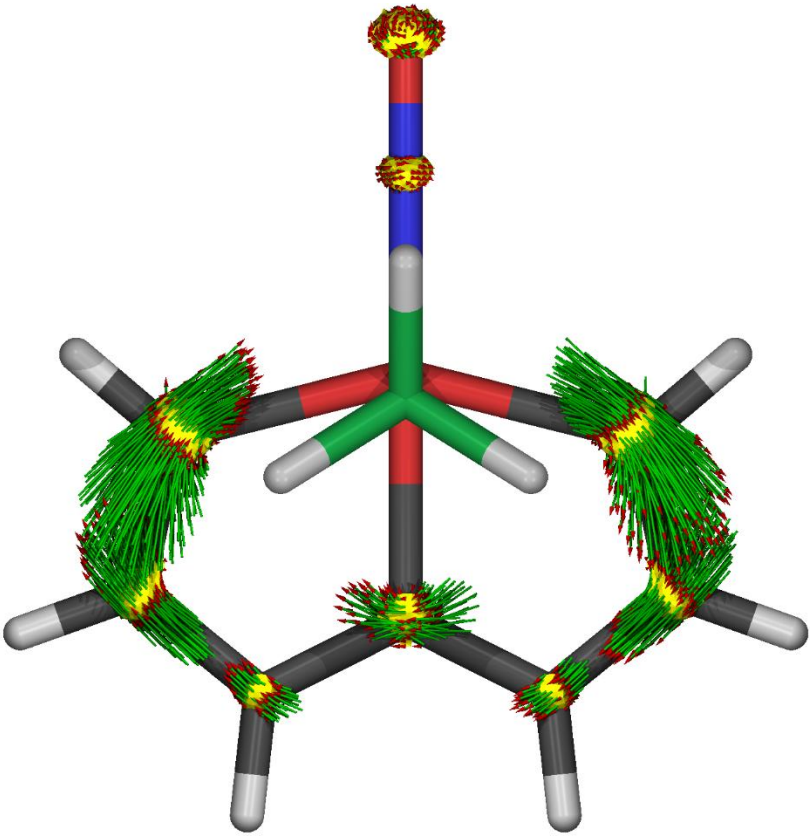


Figure S84. ACID plot of the HSOMO-1 of **5-*T*$_1$**. Isovalue is 0.024 a.u.

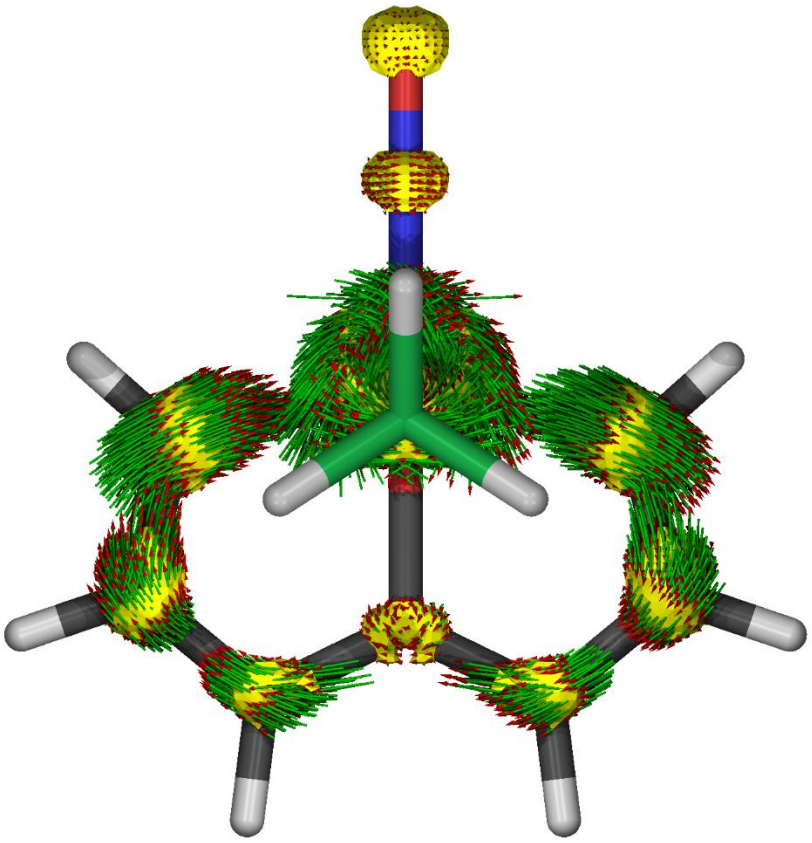


Figure S85. ACID plot of the HOMO of **5-*S*$_0$**. Isovalue is 0.024 a.u.

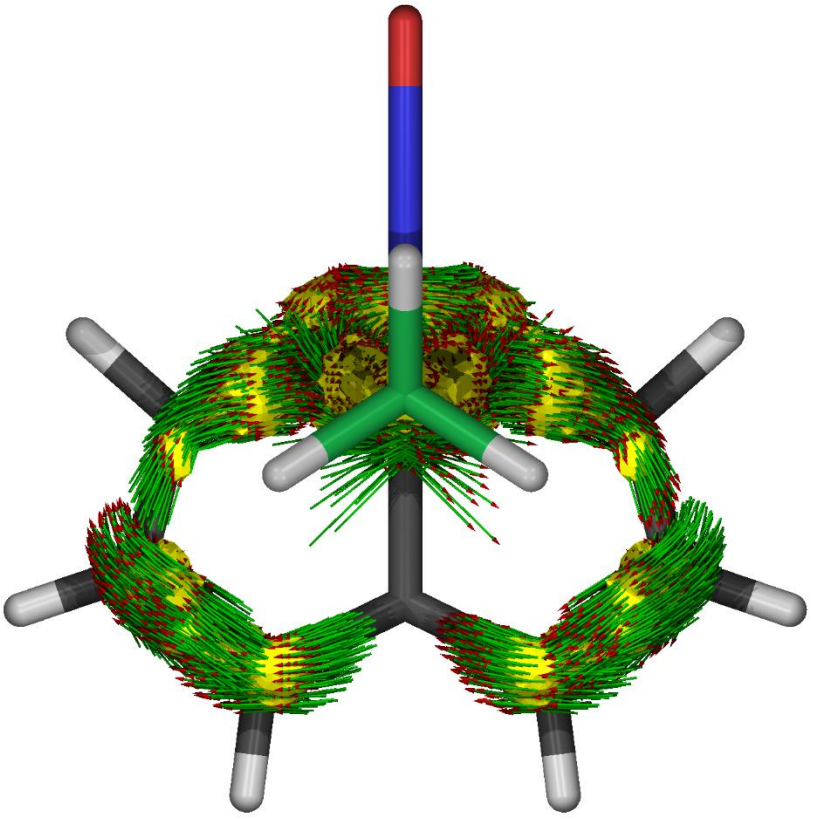


Figure S86. ACID plot of the HOMO-2 of **5-*S*$_0$**. Isovalue is 0.024 a.u.

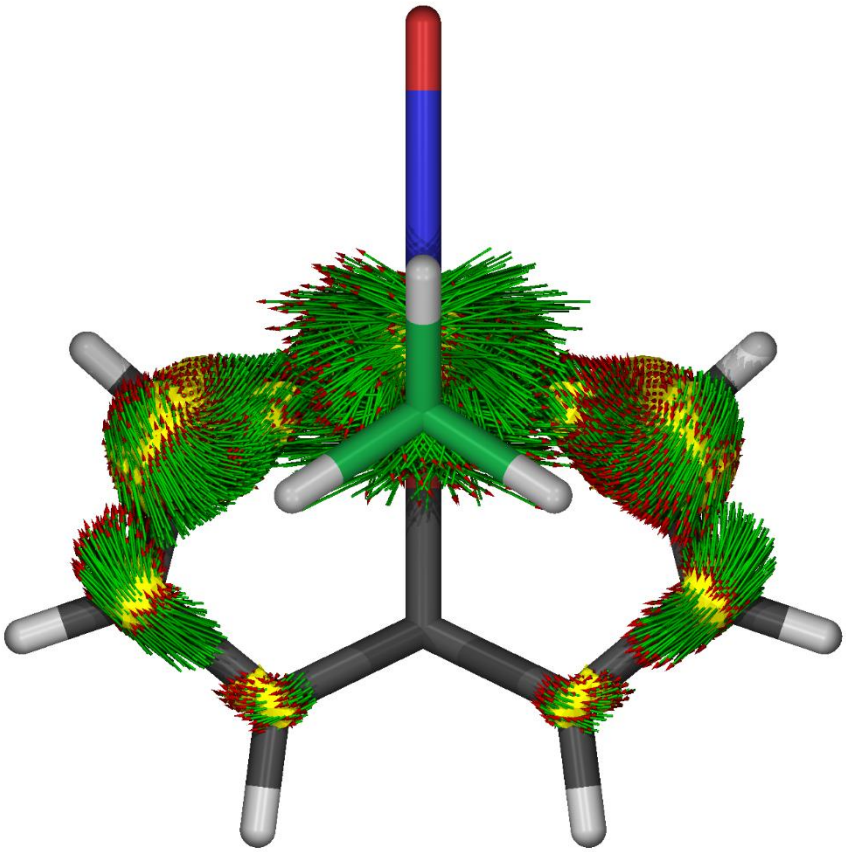


Figure S87. ACID plot of the HOMO-7 of **5**-S_0. Isovalue is 0.024 a.u.

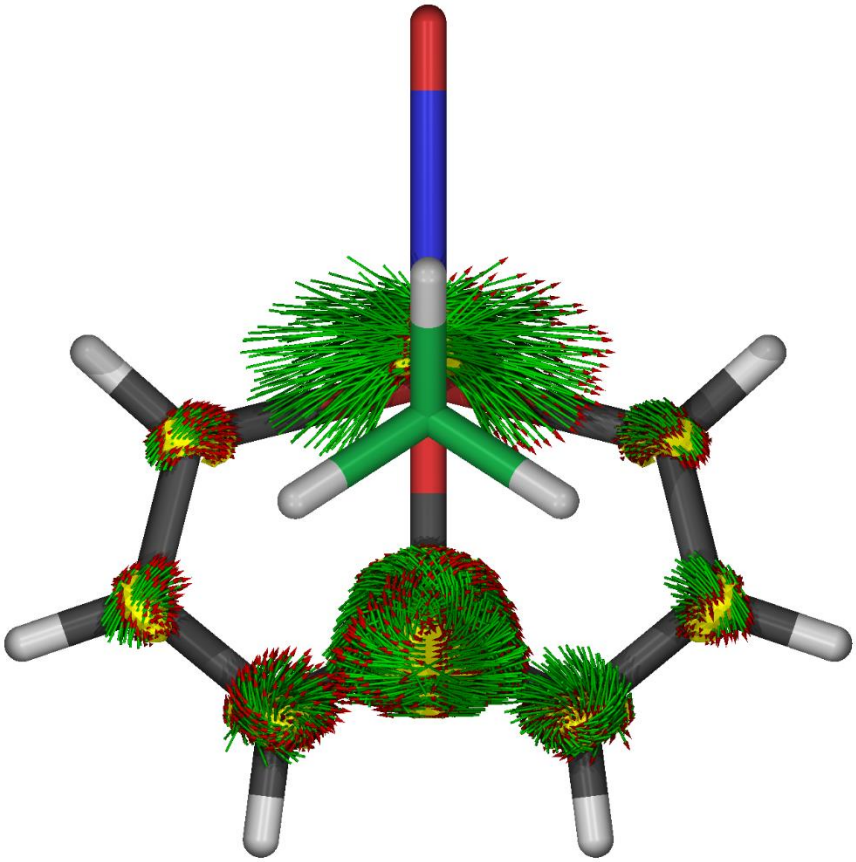


Figure S88. ACID plot of the HOMO-9 of **5**-S_0. Isovalue is 0.024 a.u.

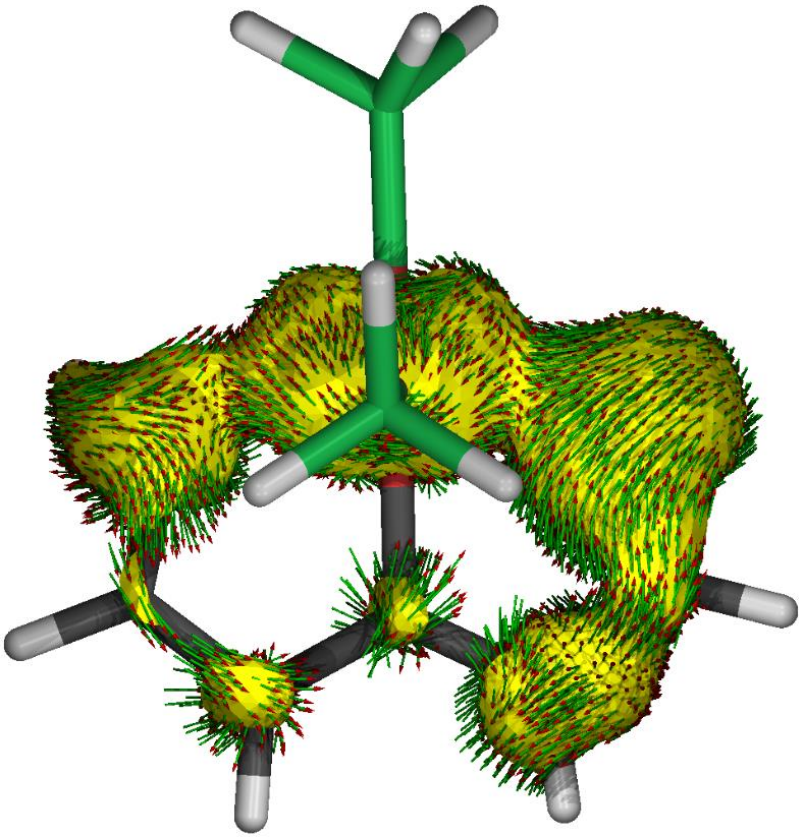


Figure S89. ACID plot of the HSOMO of **6**-T_1. Isovalue is 0.024 a.u.

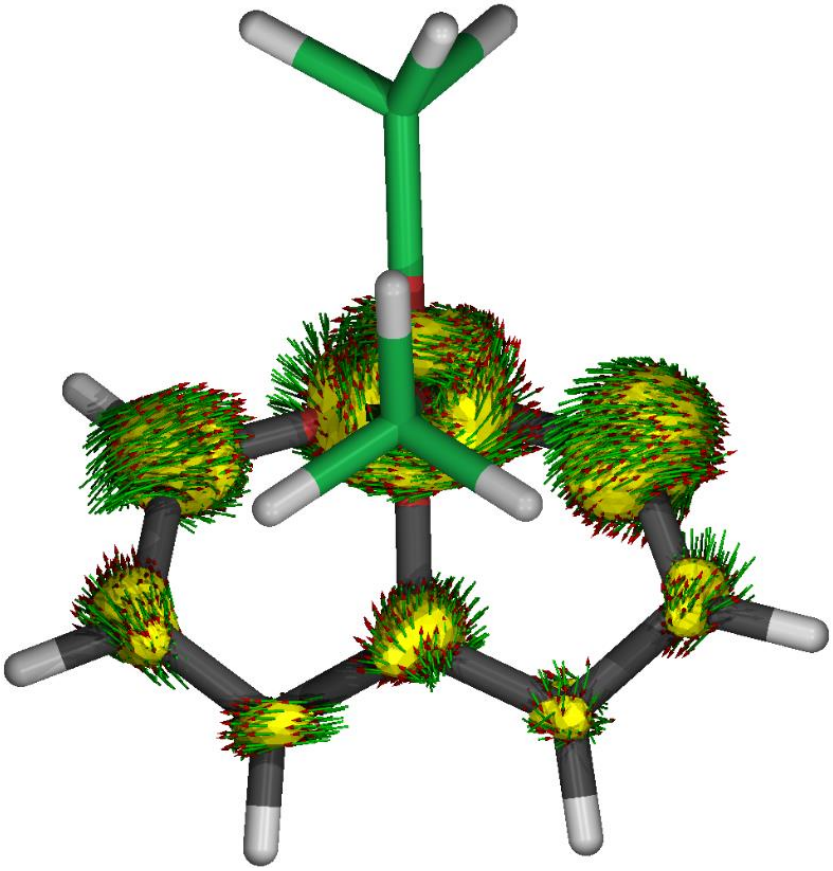


Figure S90. ACID plot of the HSOMO-1 of **6**-T_1. Isovalue is 0.024 a.u.

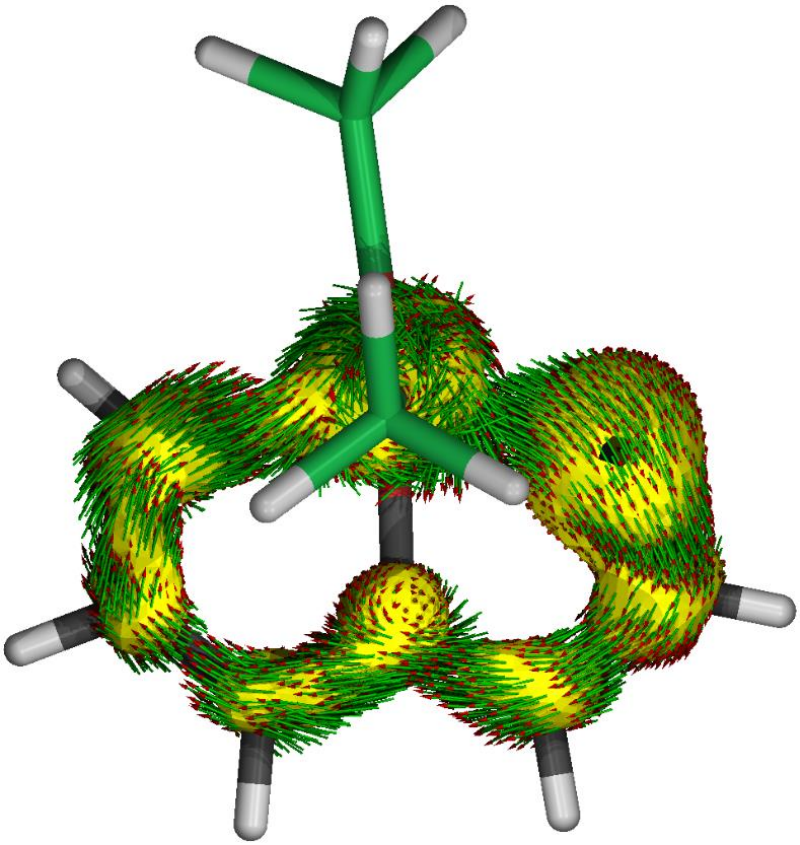


Figure S91. ACID plot of the HOMO of **6**-S_0. Isovalue is 0.024 a.u.

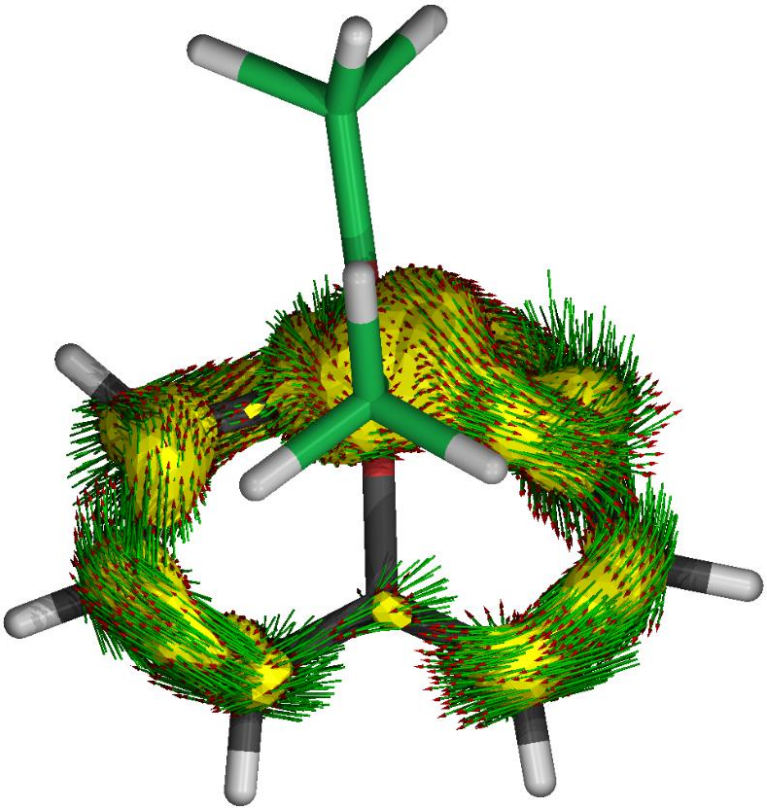


Figure S92. ACID plot of the HOMO-2 of **6**-S_0. Isovalue is 0.024 a.u.

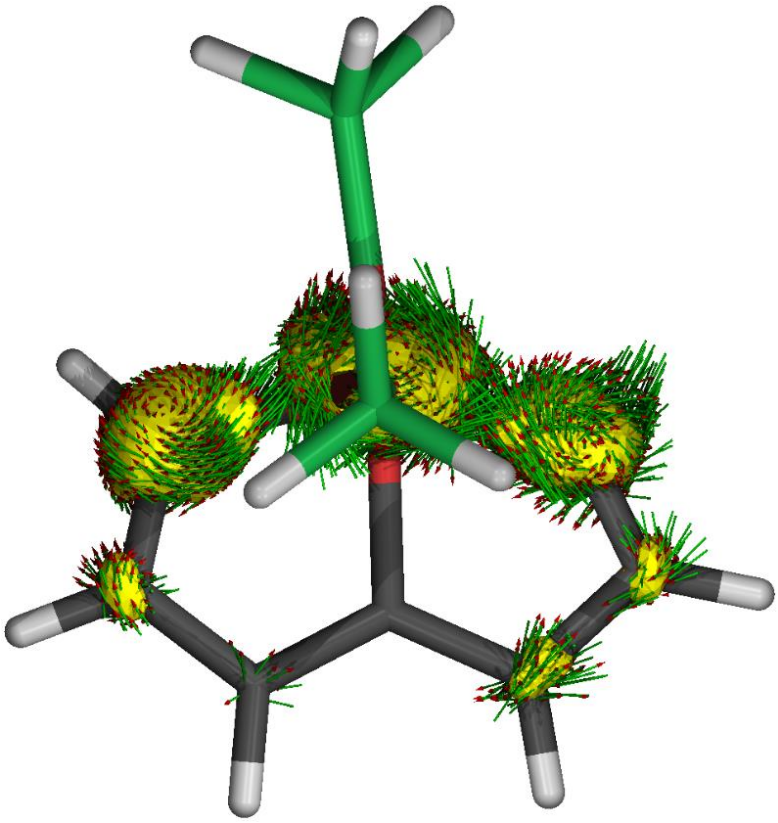


Figure S93. ACID plot of the HOMO-7 of **6**-S_0. Isovalue is 0.024 a.u.

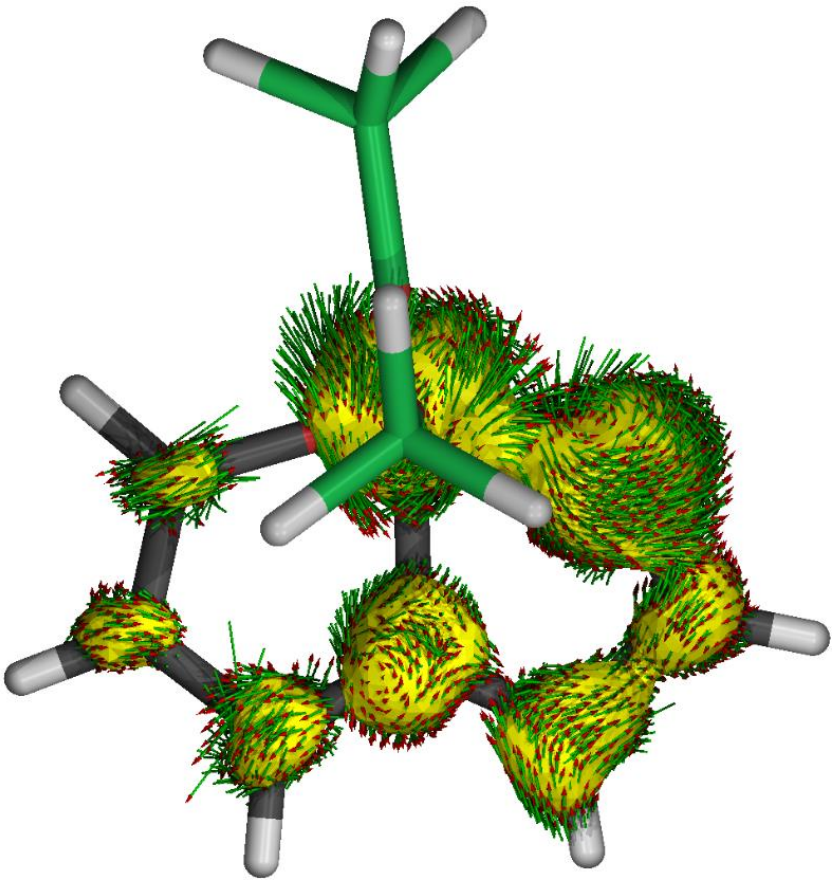


Figure S94. ACID plot of the HOMO-10 of **6**-S_0. Isovalue is 0.024 a.u.

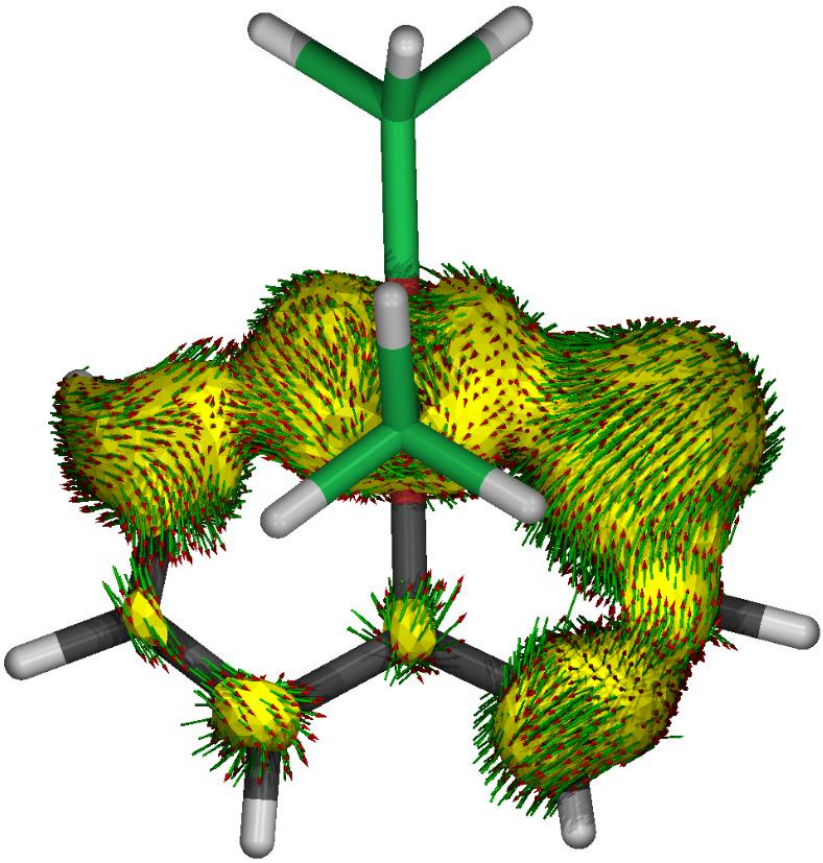


Figure S95. ACID plot of the HSOMO of **7-*T*$_1$**. Isovalue is 0.024 a.u.

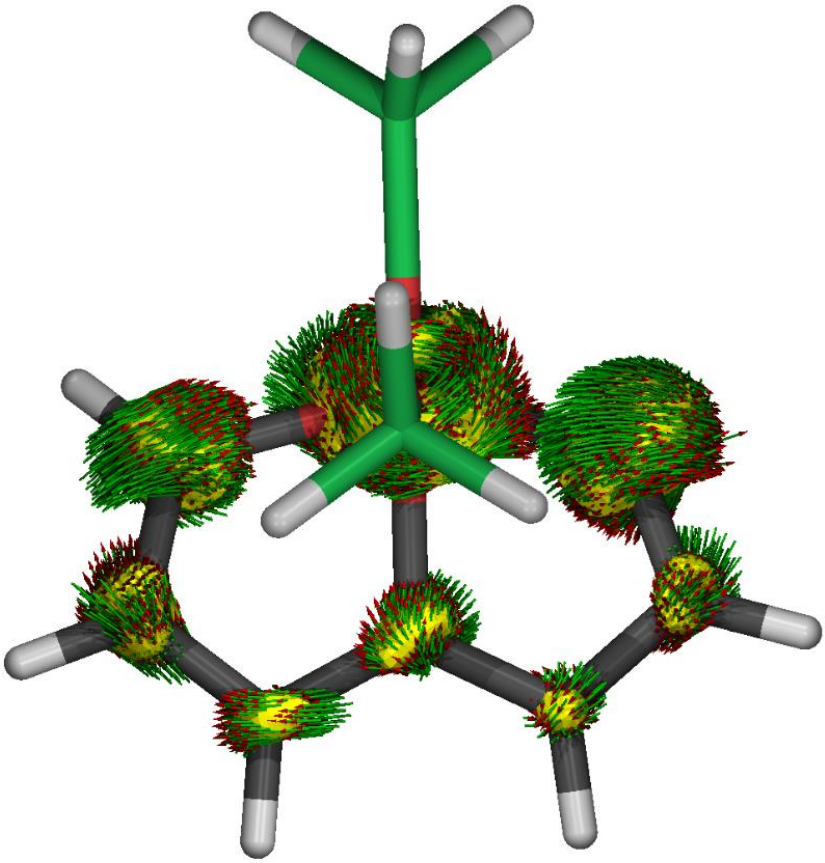


Figure S96. ACID plot of the HSOMO-1 of **7-*T*$_1$**. Isovalue is 0.024 a.u.

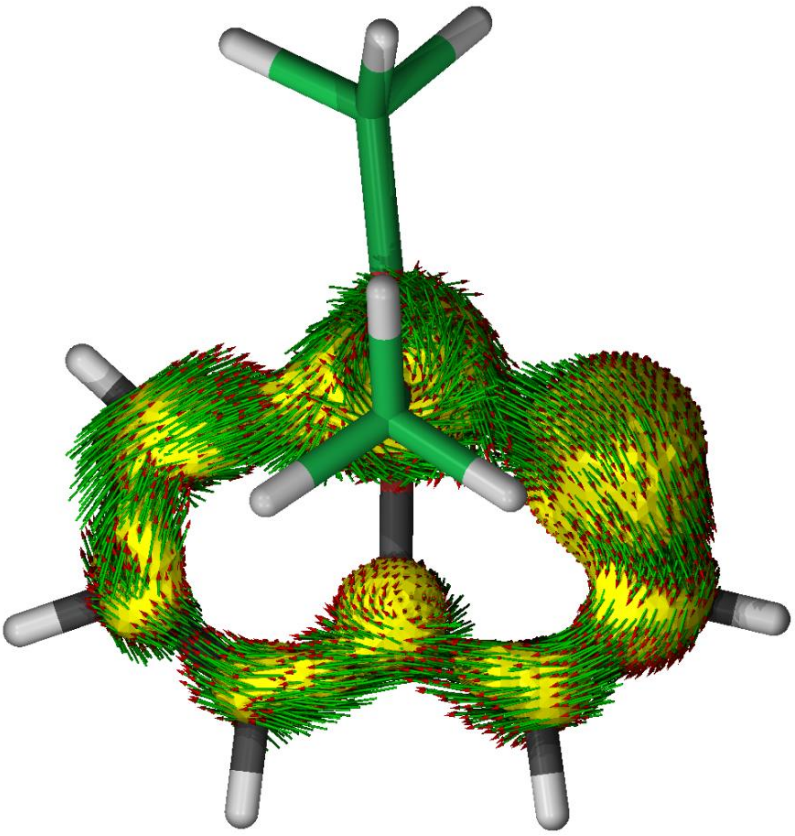


Figure S97. ACID plot of the HOMO of **7-*S*$_0$**. Isovalue is 0.024 a.u.

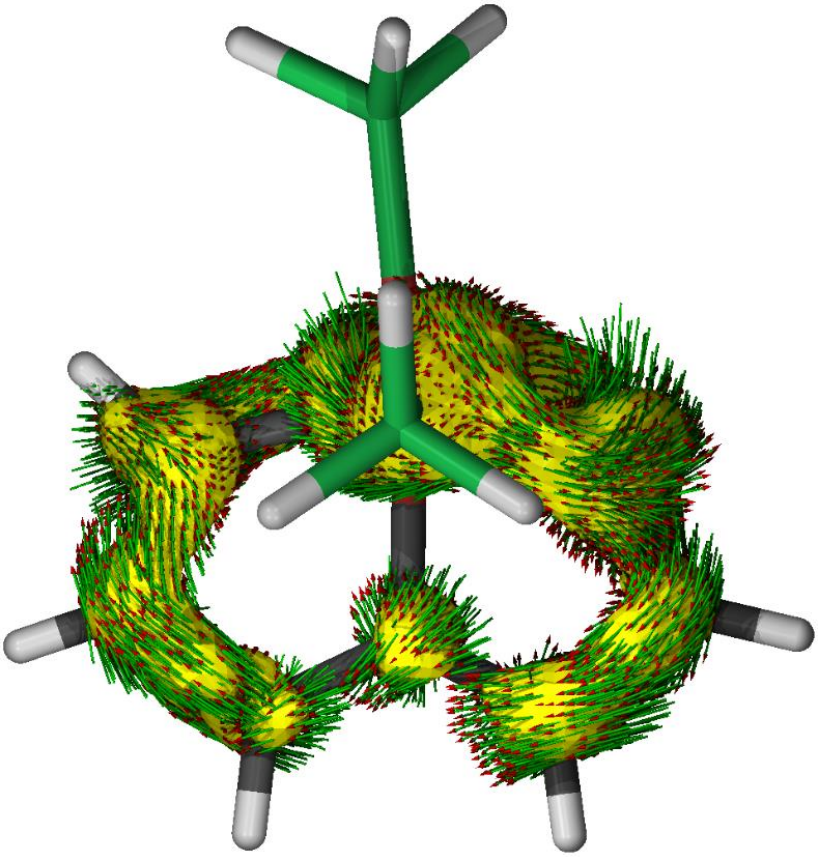


Figure S98. ACID plot of the HOMO-2 of **7-*S*$_0$**. Isovalue is 0.024 a.u.

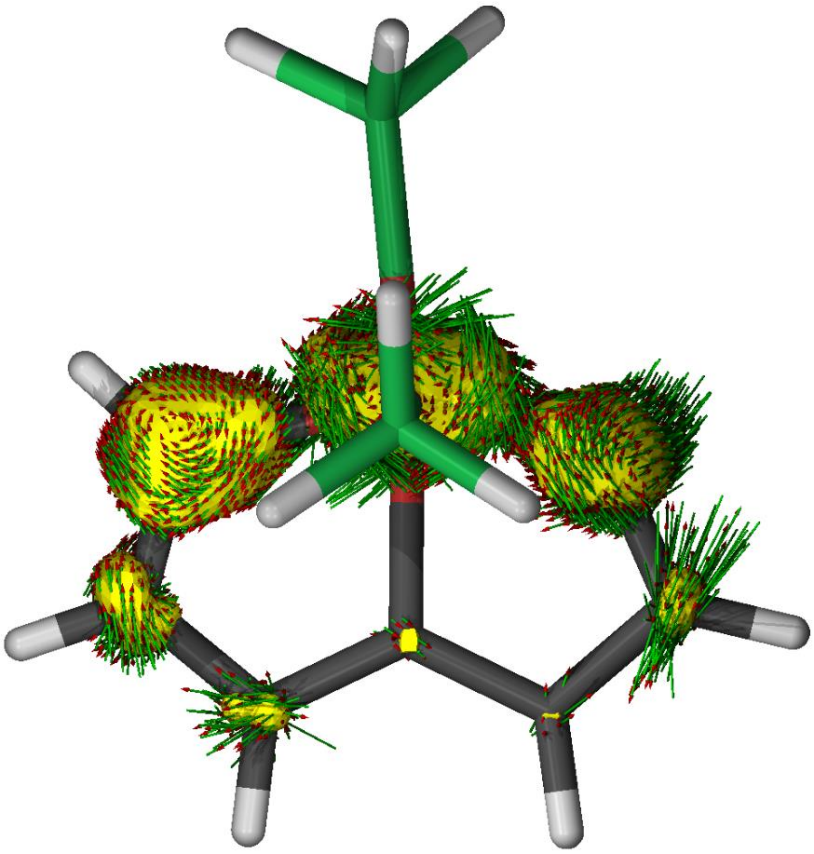


Figure S99. ACID plot of the HOMO-7 of **7-S_0**. Isovalue is 0.024 a.u.

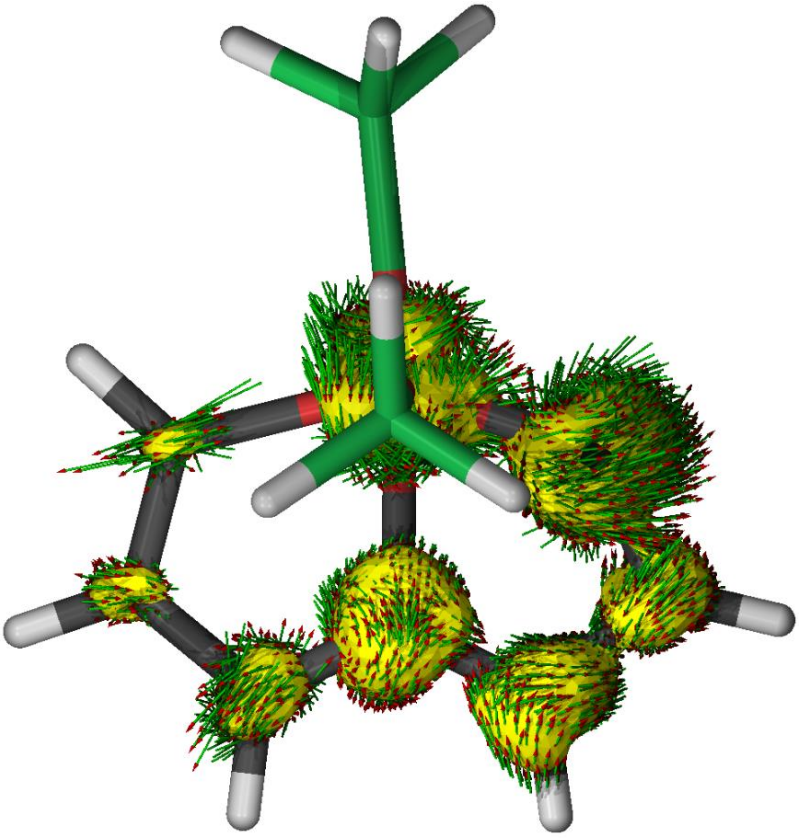


Figure S100. ACID plot of the HOMO-10 of **7-S_0**. Isovalue is 0.024 a.u.

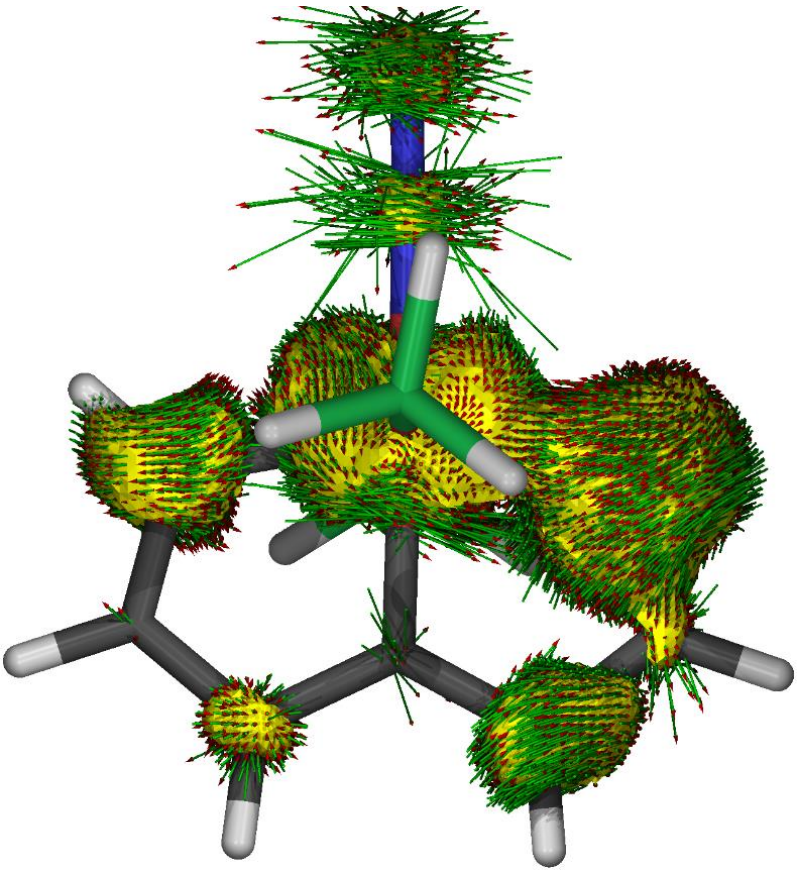


Figure S101. ACID plot of the HSOMO of **8**-T_1. Isovalue is 0.024 a.u.

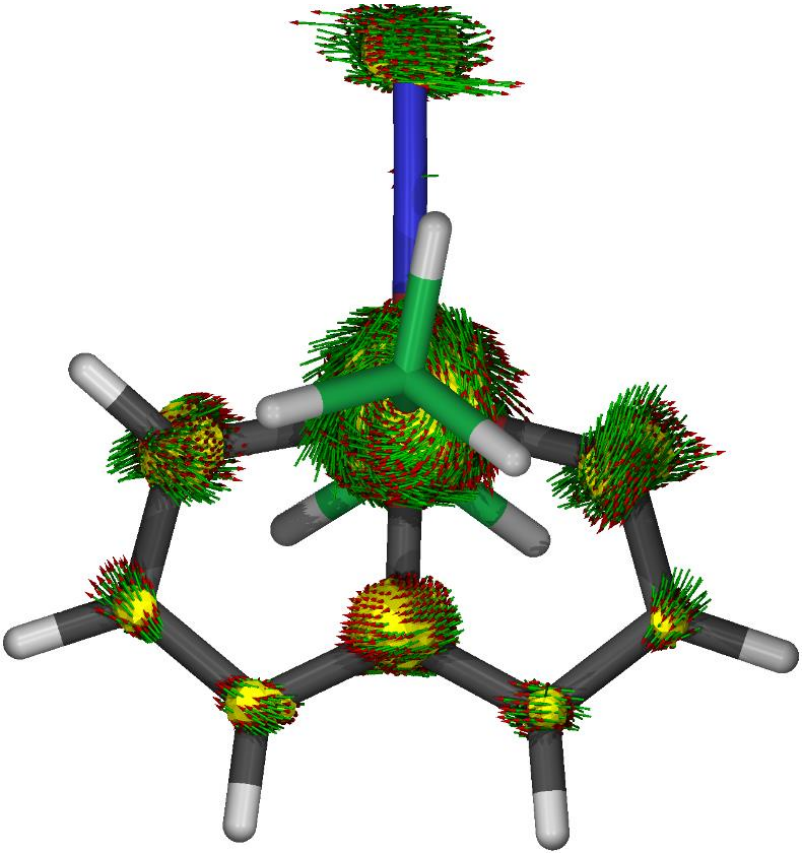


Figure S102. ACID plot of the HSOMO-1 of **8**-T_1. Isovalue is 0.024 a.u.

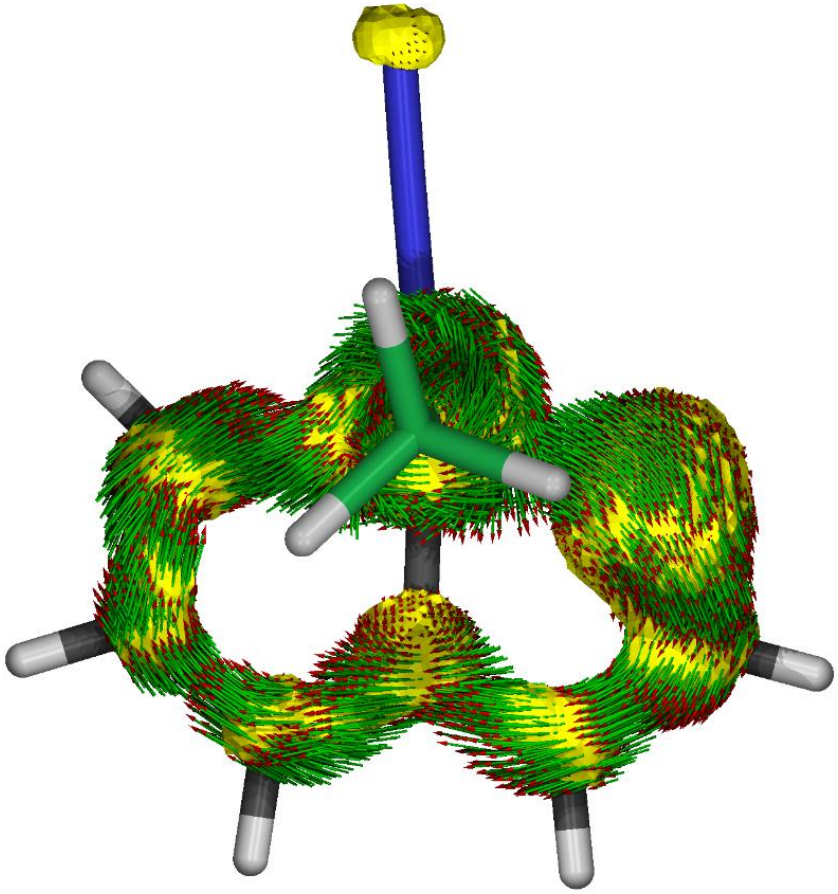


Figure S103. ACID plot of the HOMO of **8-S_0**. Isovalue is 0.024 a.u.

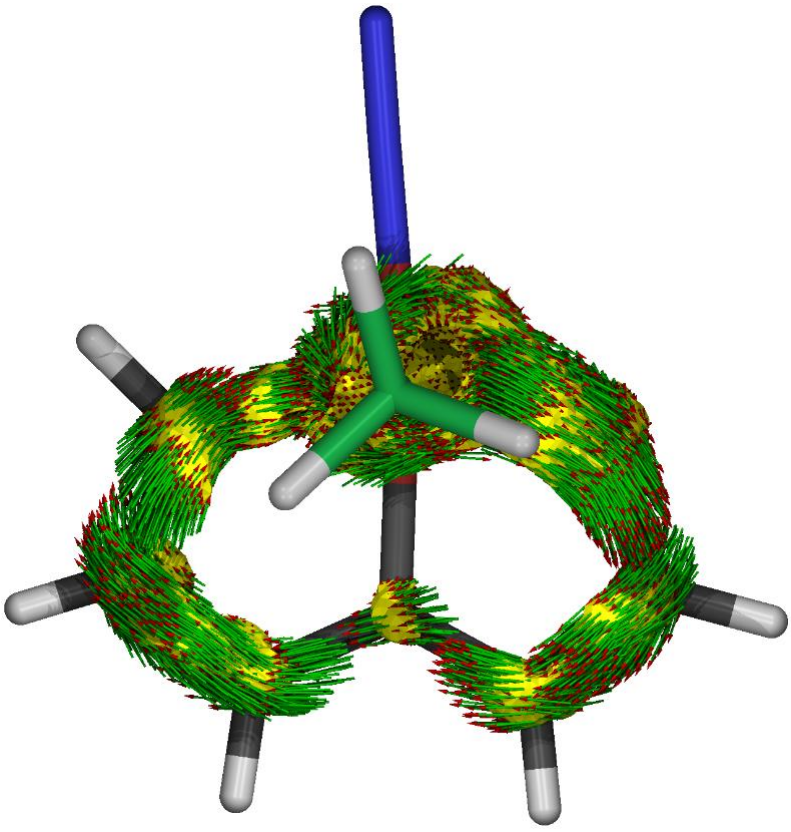


Figure S104. ACID plot of the HOMO-2 of **8-S_0**. Isovalue is 0.024 a.u.

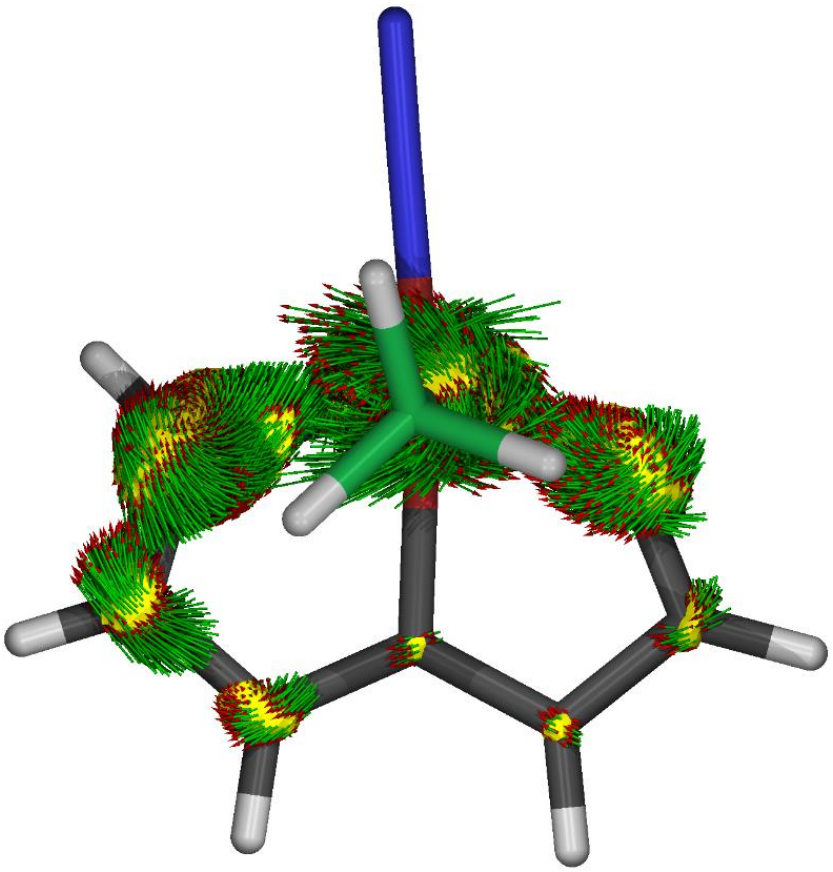


Figure S105 ACID plot of the HOMO-7 of **8-*S*$_0$**. Isovalue is 0.024 a.u.

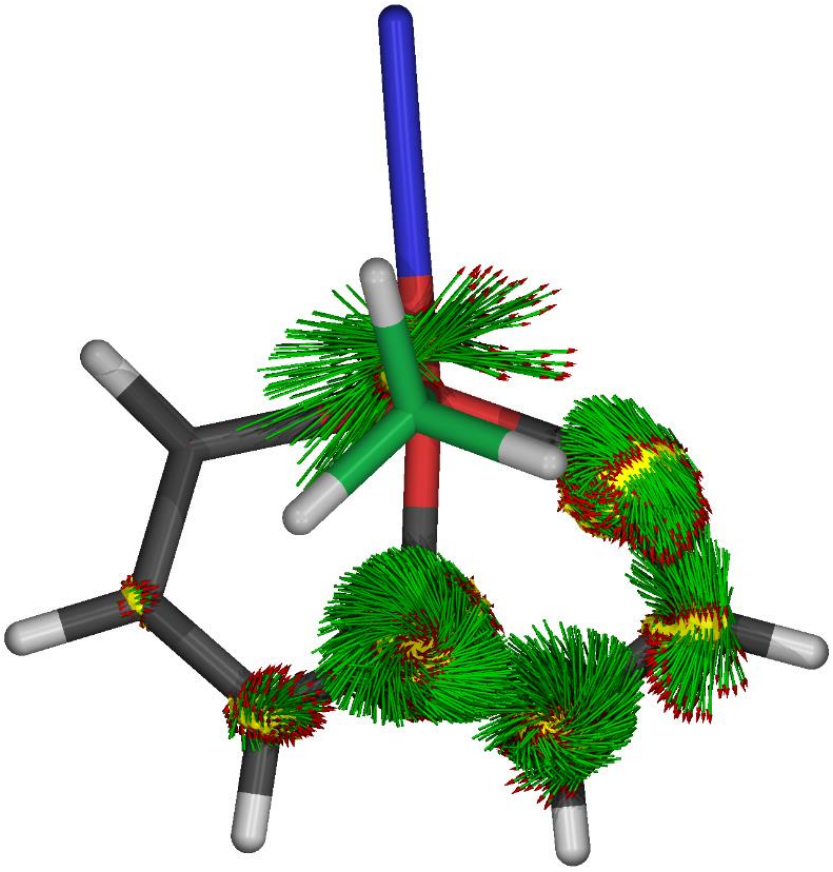


Figure S106 ACID plot of the HOMO-8 of **8-*S*$_0$**. Isovalue is 0.024 a.u.

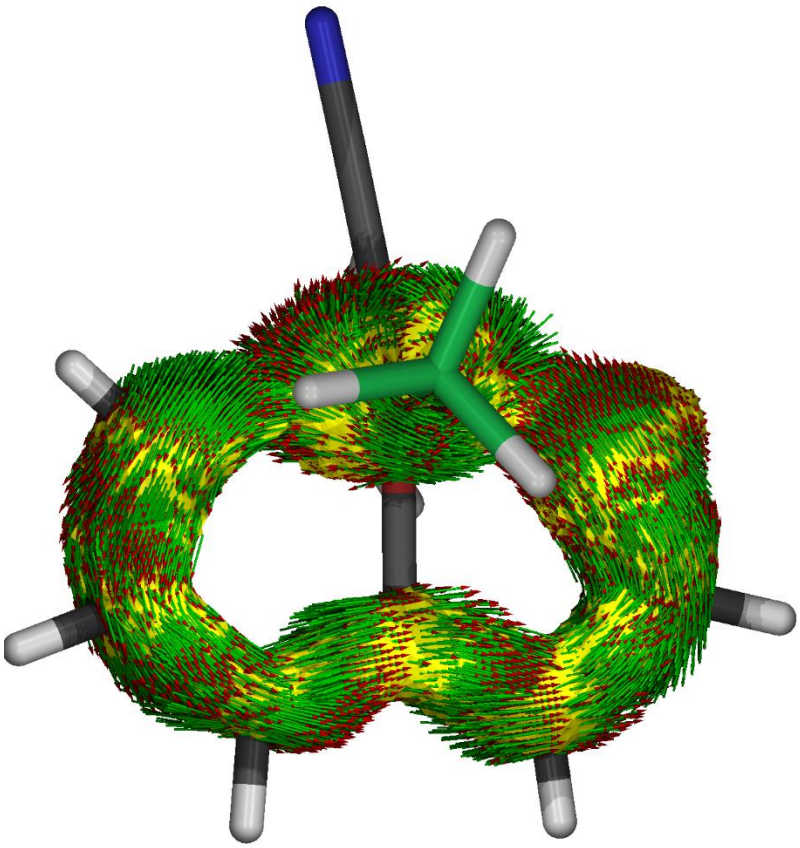


Figure S107 ACID plot of the HSOMO of **9**-T_1. Isovalue is 0.024 a.u.

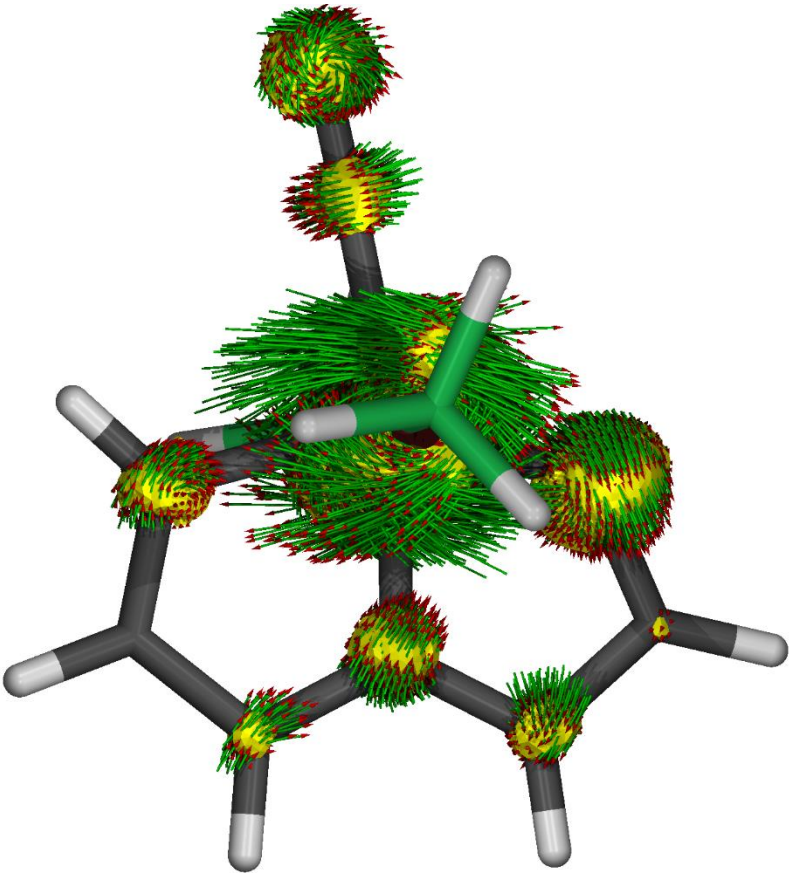


Figure S108 ACID plot of the HSOMO-1 of **9**-T_1. Isovalue is 0.024 a.u.

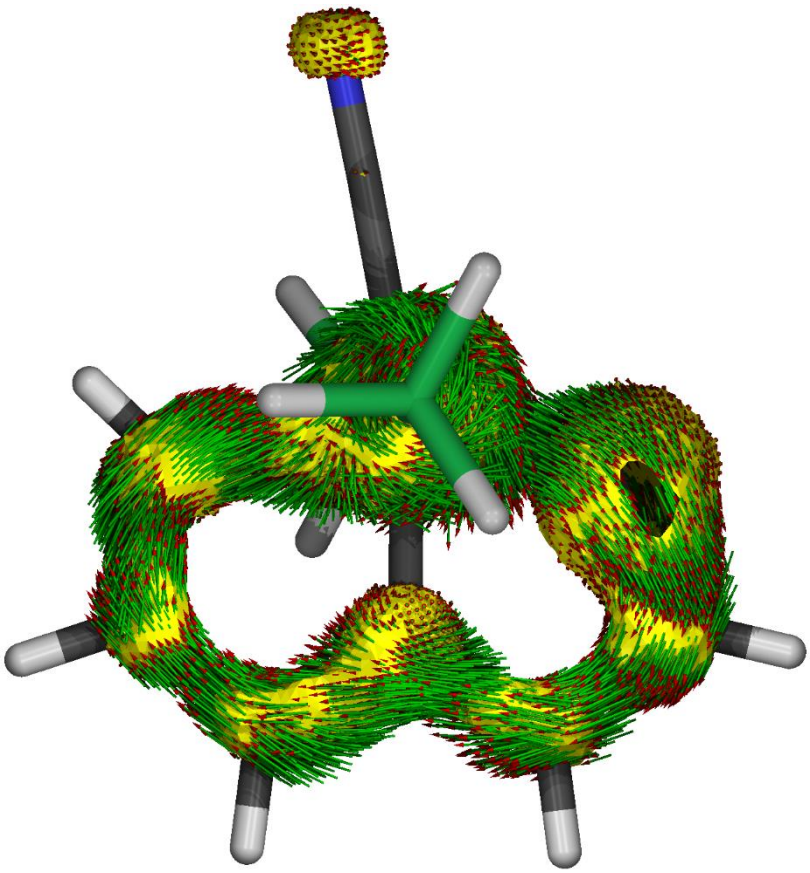


Figure S109 ACID plot of the HOMO of **9**-S_0. Isovalue is 0.024 a.u.

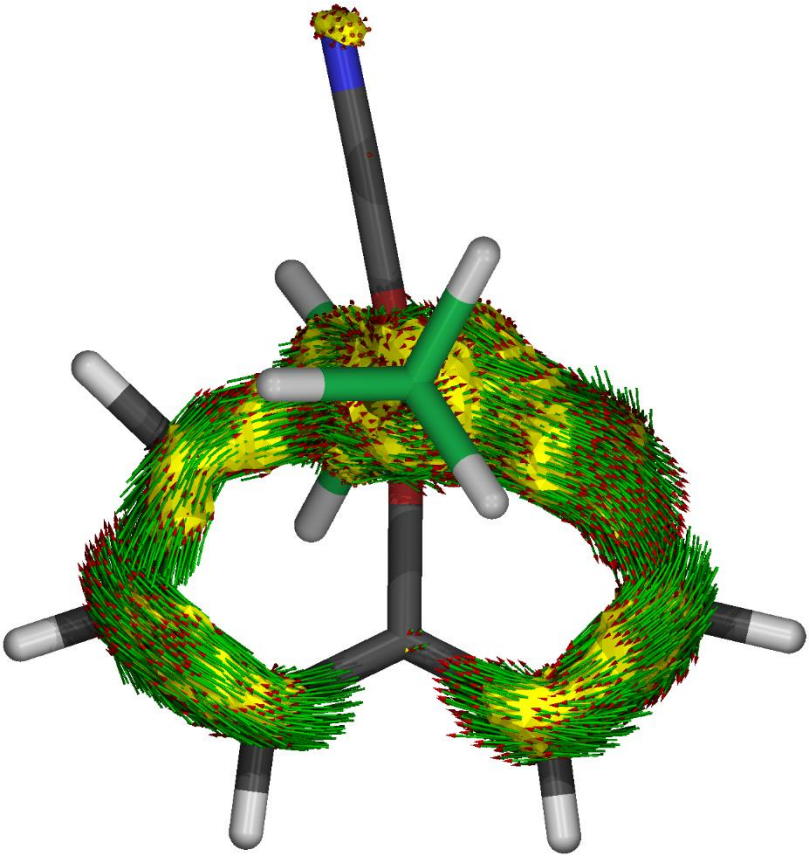


Figure S110CID plot of the HOMO-3 of **9**-S_0. Isovalue is 0.024 a.u.

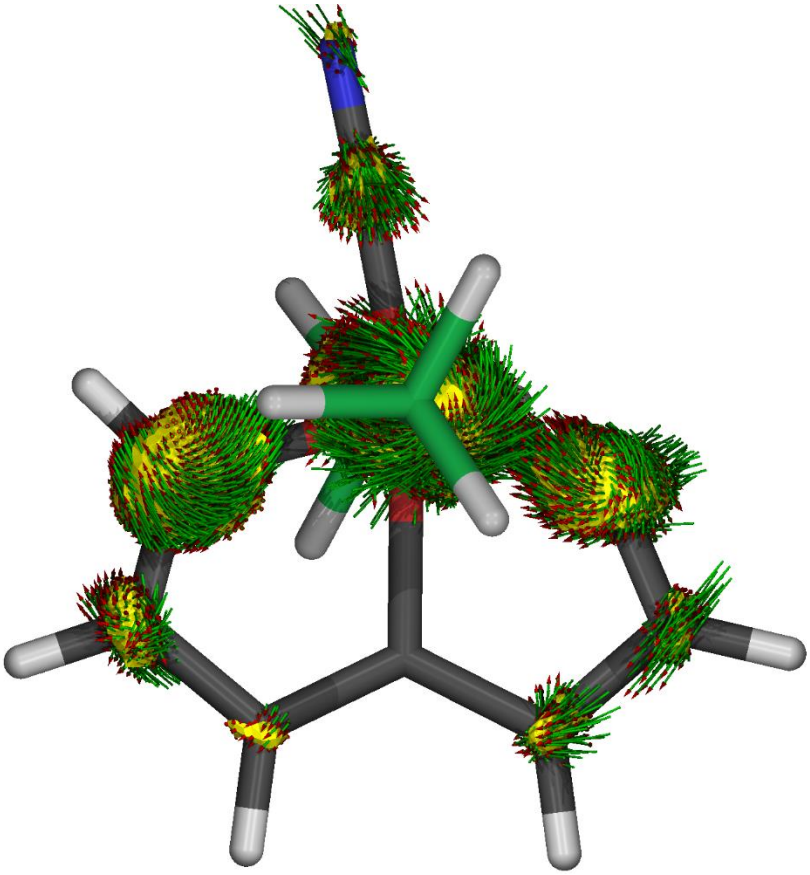


Figure S111ACID plot of the HOMO-10 of **9**-S_0. Isovalue is 0.024 a.u.

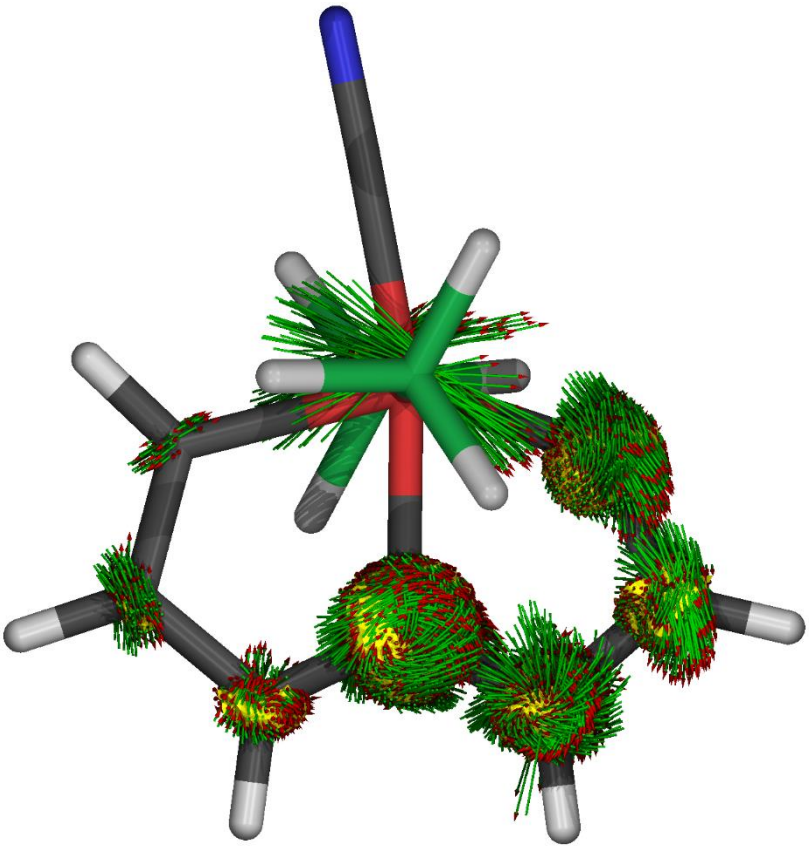


Figure S112ACID plot of the HOMO-11 of **9**-S_0. Isovalue is 0.024 a.u.

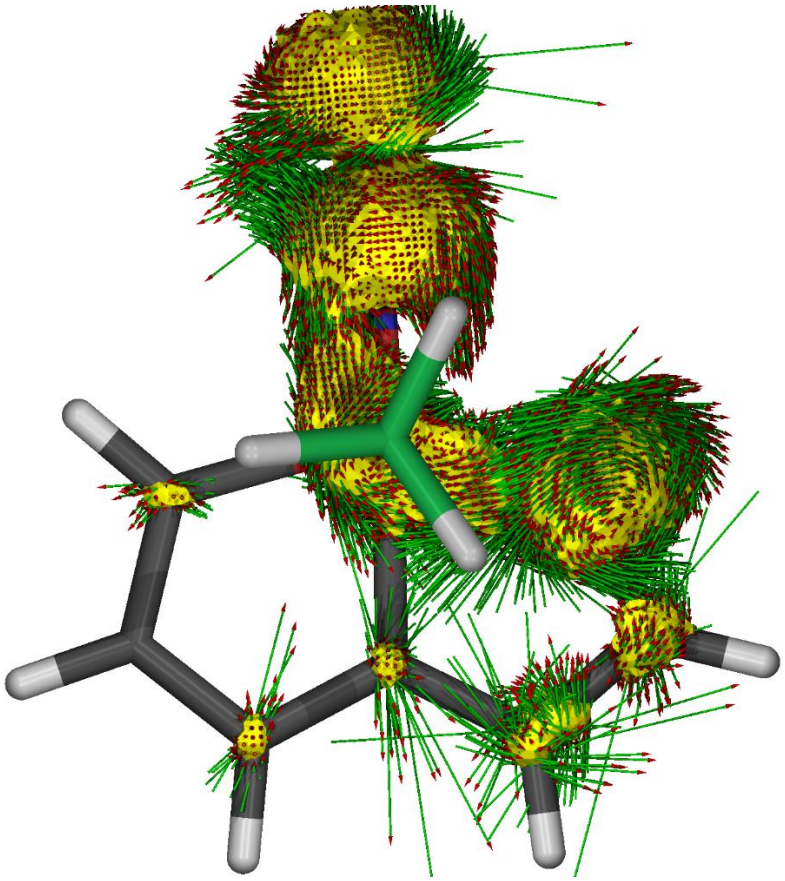


Figure S113 ACID plot of the HSOMO of **10**-T_1. Isovalue is 0.024 a.u.

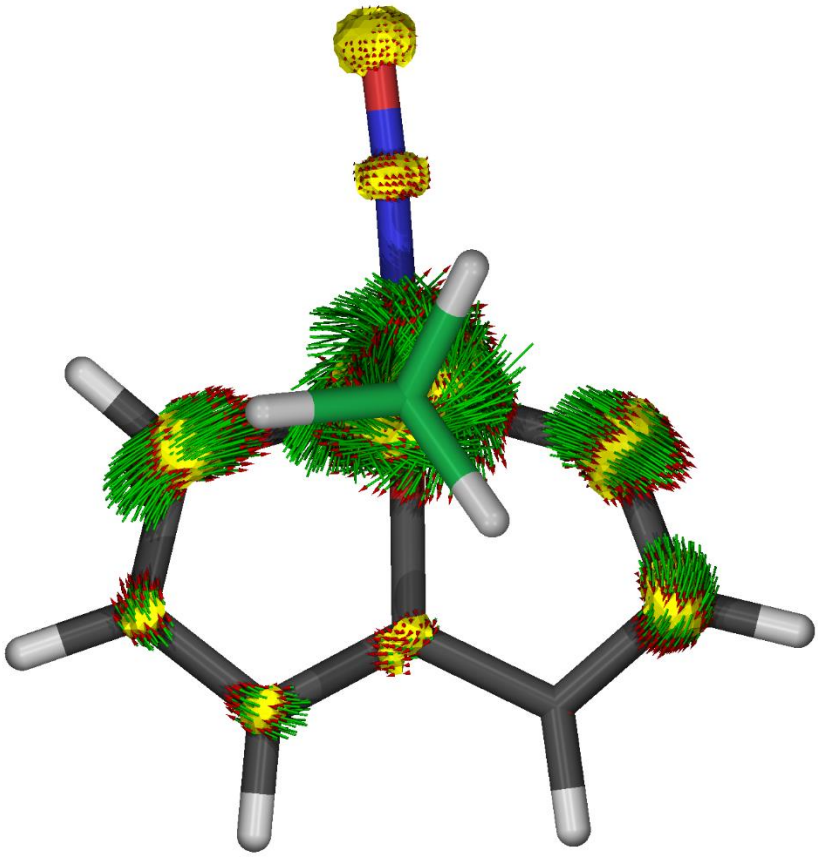


Figure S114 ACID plot of the HSOMO-1 of **10**-T_1. Isovalue is 0.024 a.u.

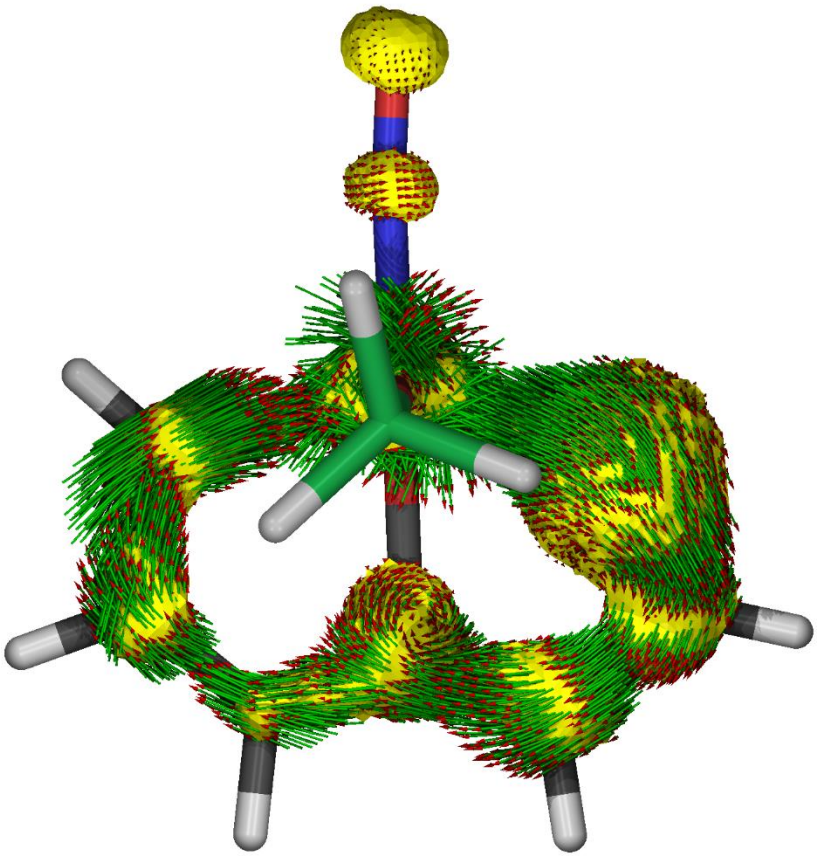


Figure S115 ACID plot of the HOMO of **10**-S_0. Isovalue is 0.024 a.u.

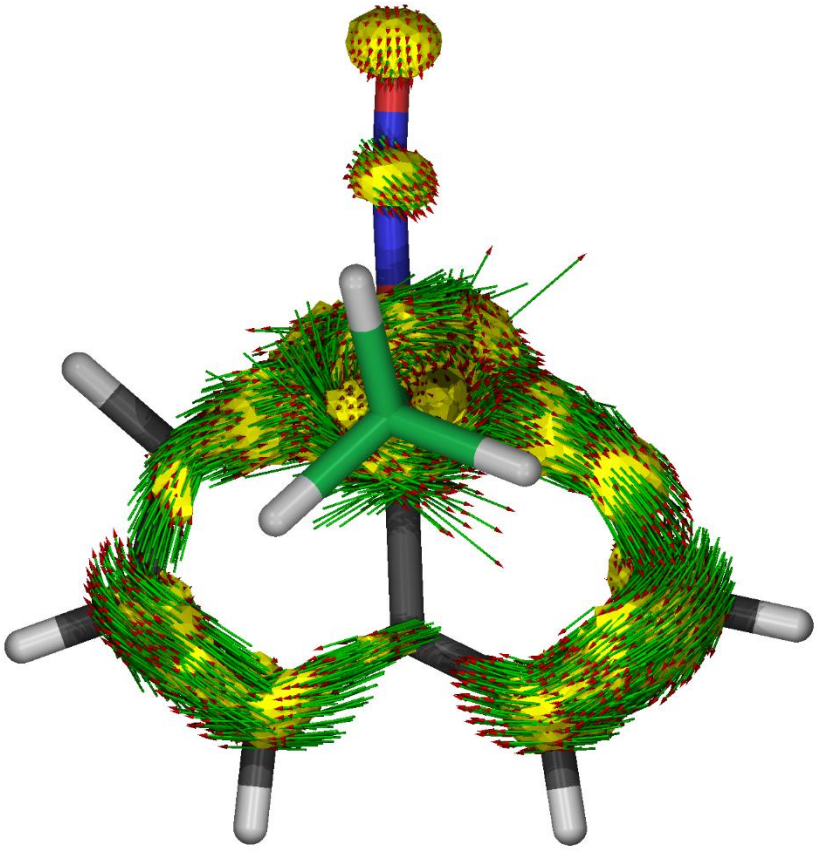


Figure S116 ACID plot of the HOMO-1 of **10**-S_0. Isovalue is 0.024 a.u.

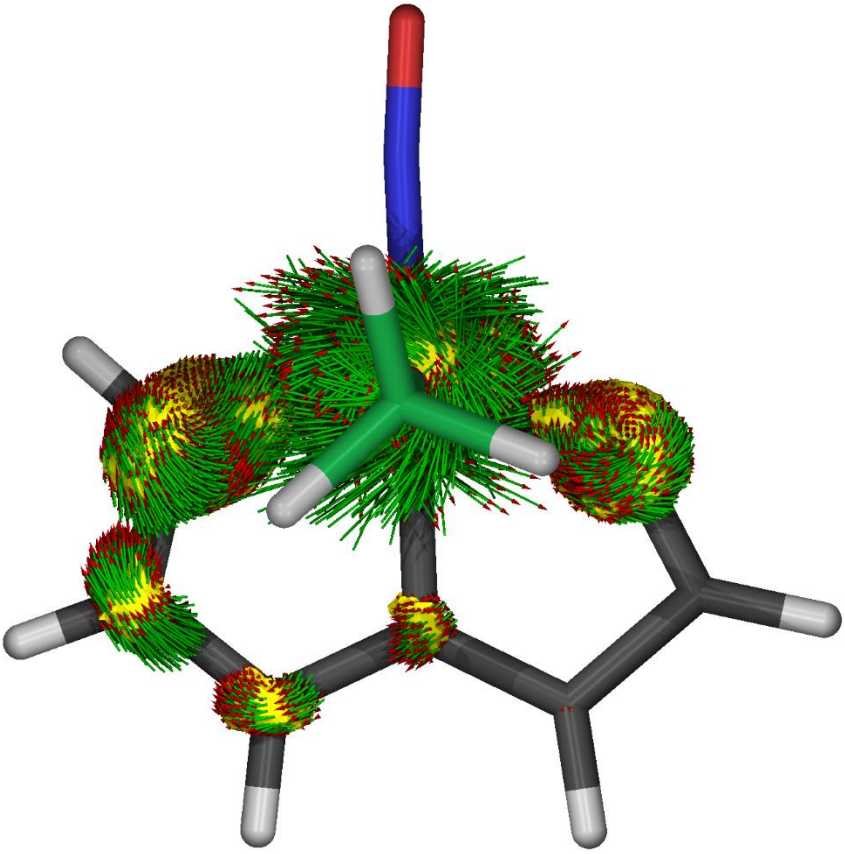


Figure S117 ACID plot of the HOMO-7 of **10**-S_0. Isovalue is 0.024 a.u.

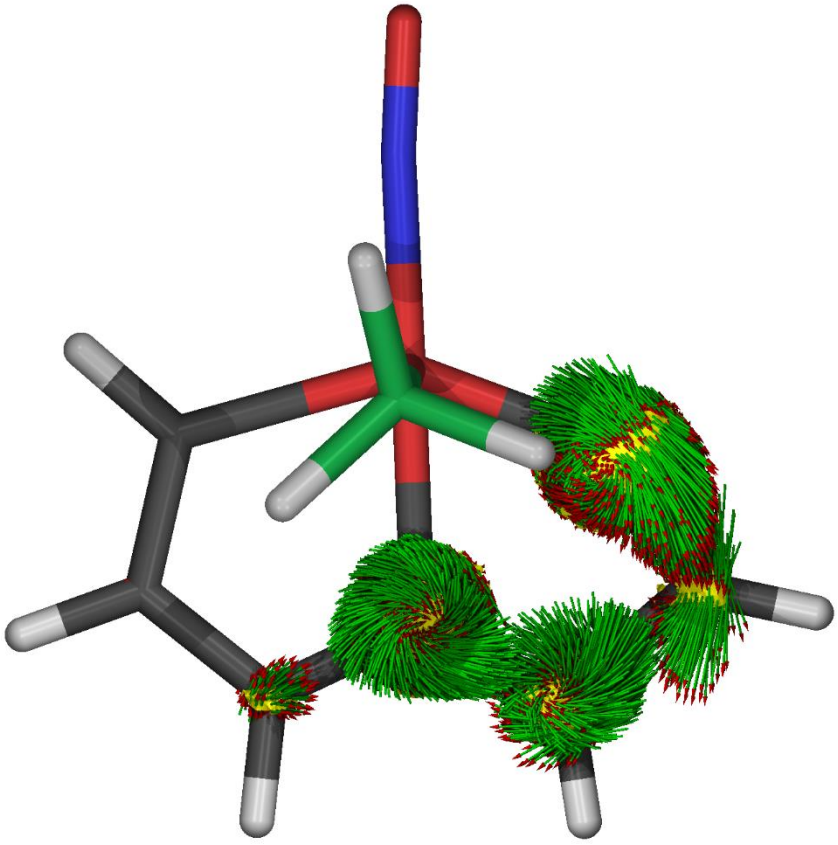


Figure S118 ACID plot of the HOMO-8 of **10**-S_0. Isovalue is 0.024 a.u.

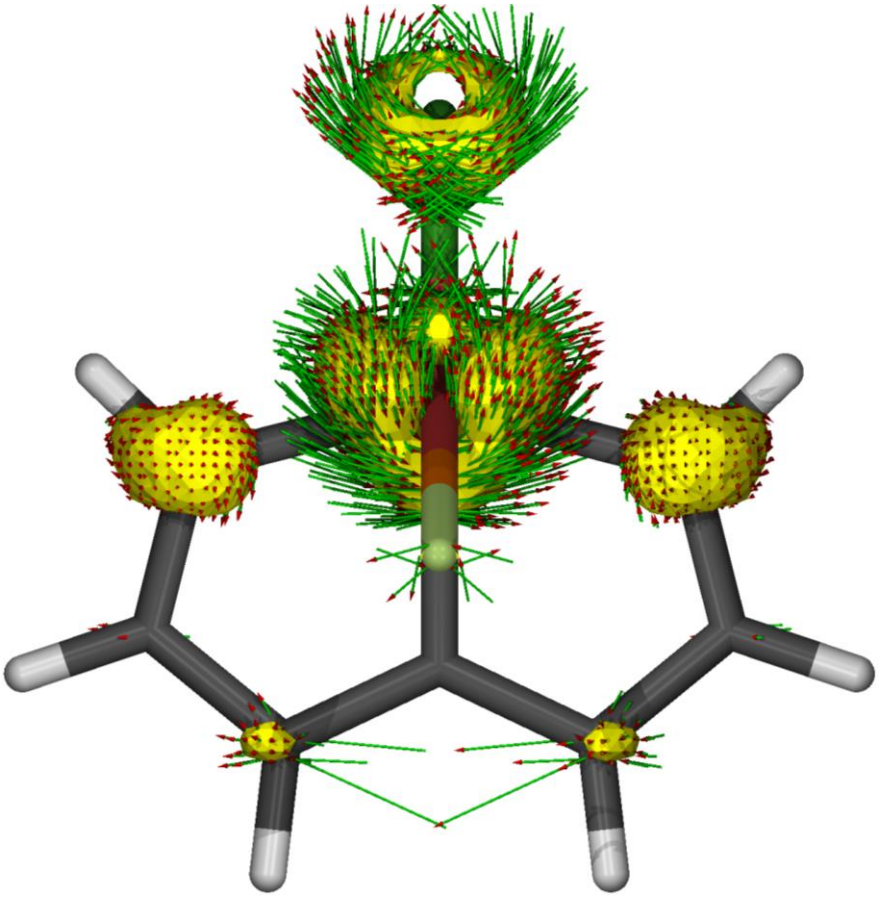


Figure S119 ACID plot of the HSOMO of **11**-T_1. Isovalue is 0.024 a.u.

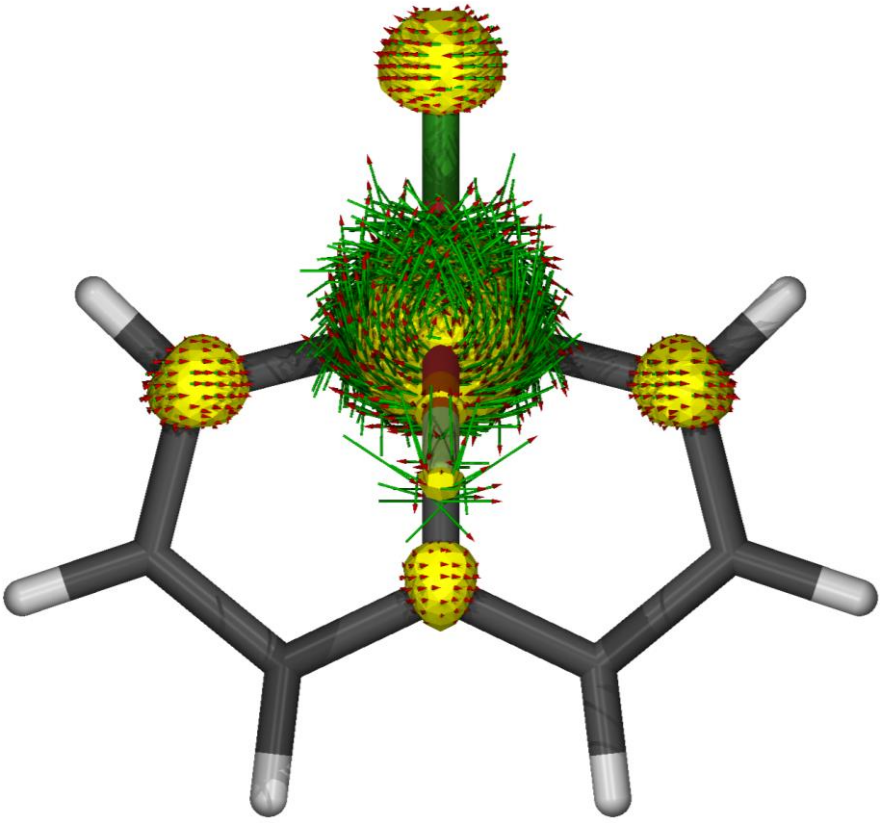


Figure S120 ACID plot of the HSOMO-1 of **11**-T_1. Isovalue is 0.024 a.u.

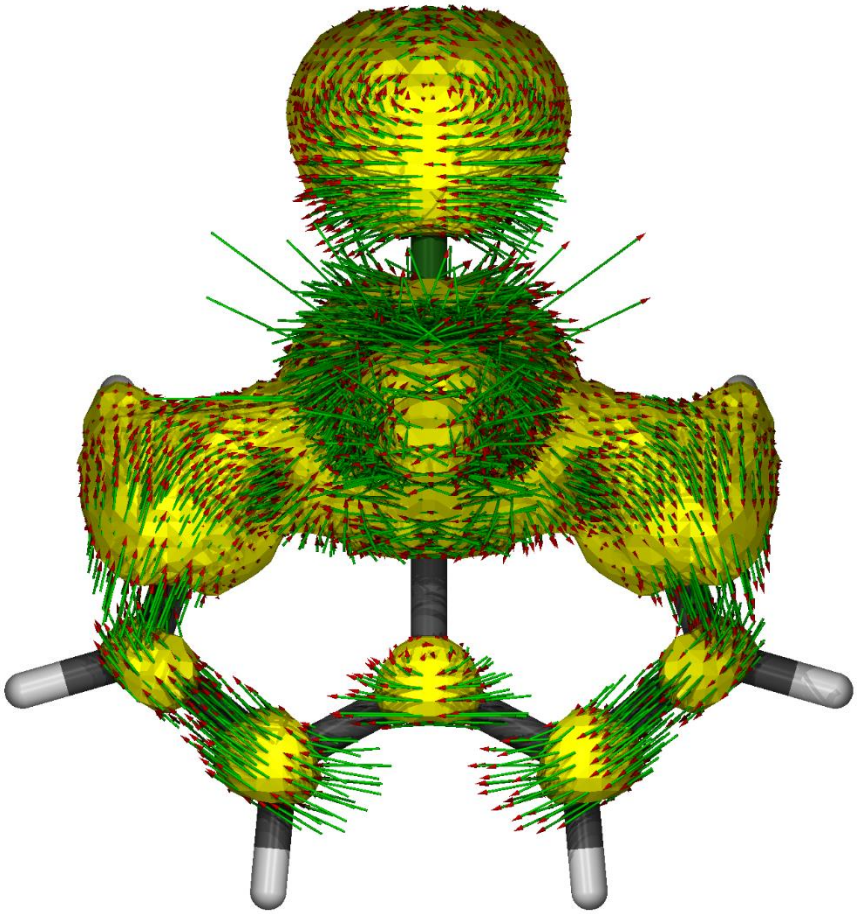


Figure S121 ACID plot of the HOMO of **11**-S_0. Isovalue is 0.024 a.u.

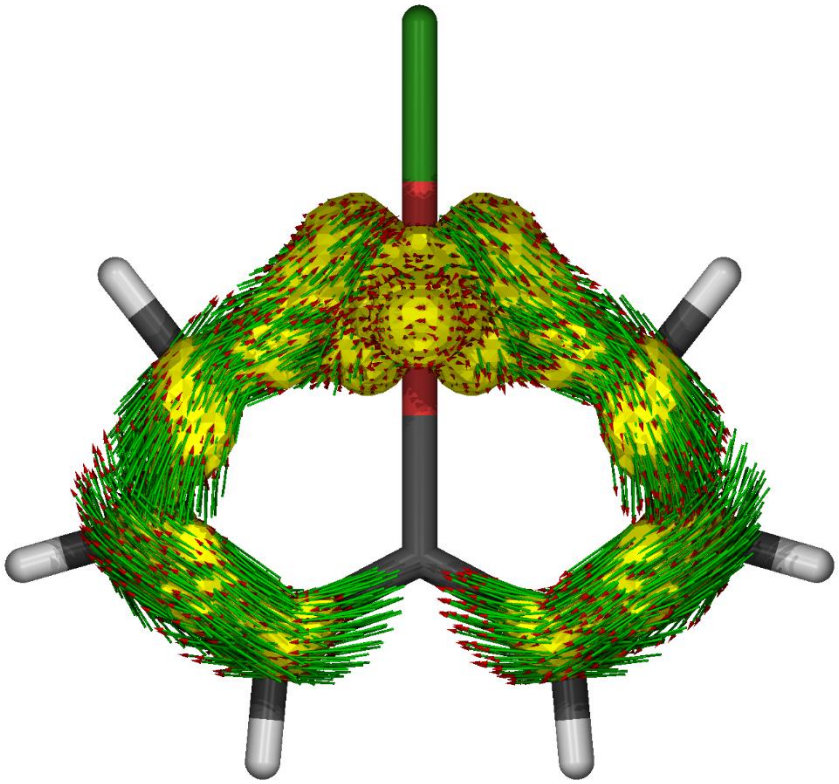


Figure S122. ACID plot of the HOMO-2 of **11**-S_0. Isovalue is 0.024 a.u.

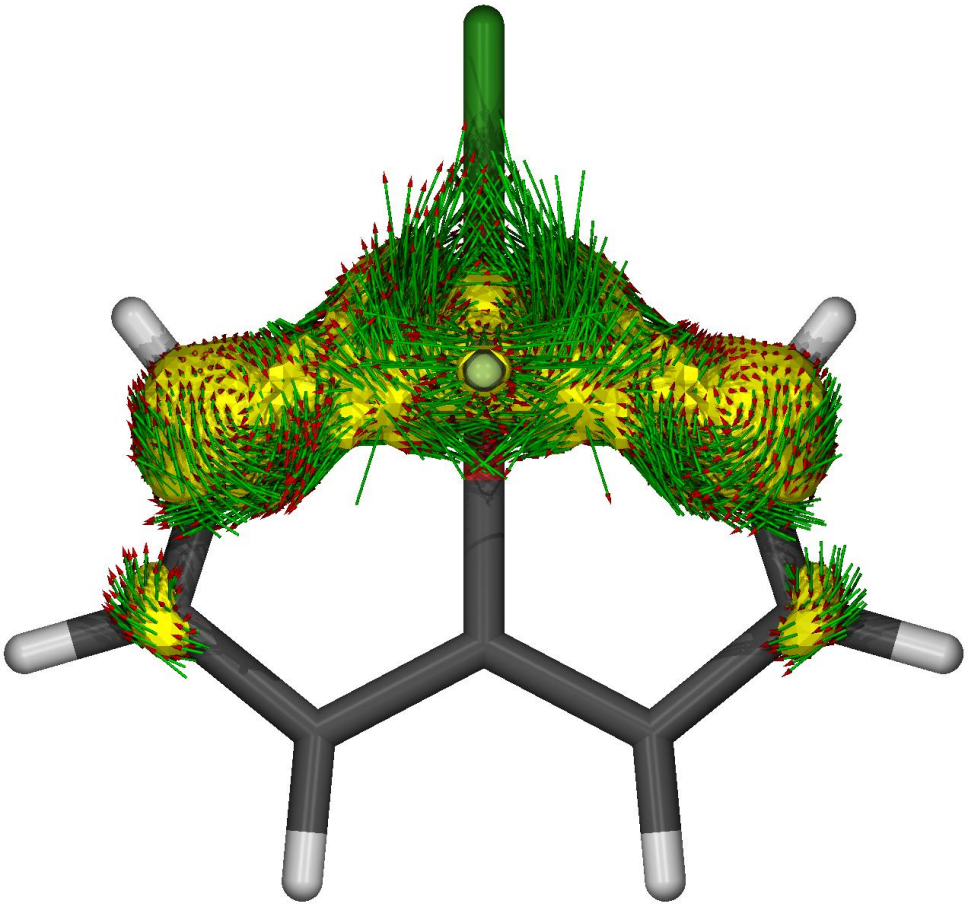


Figure S123. ACID plot of the HOMO-9 of **11**-S_0. Isovalue is 0.024 a.u.

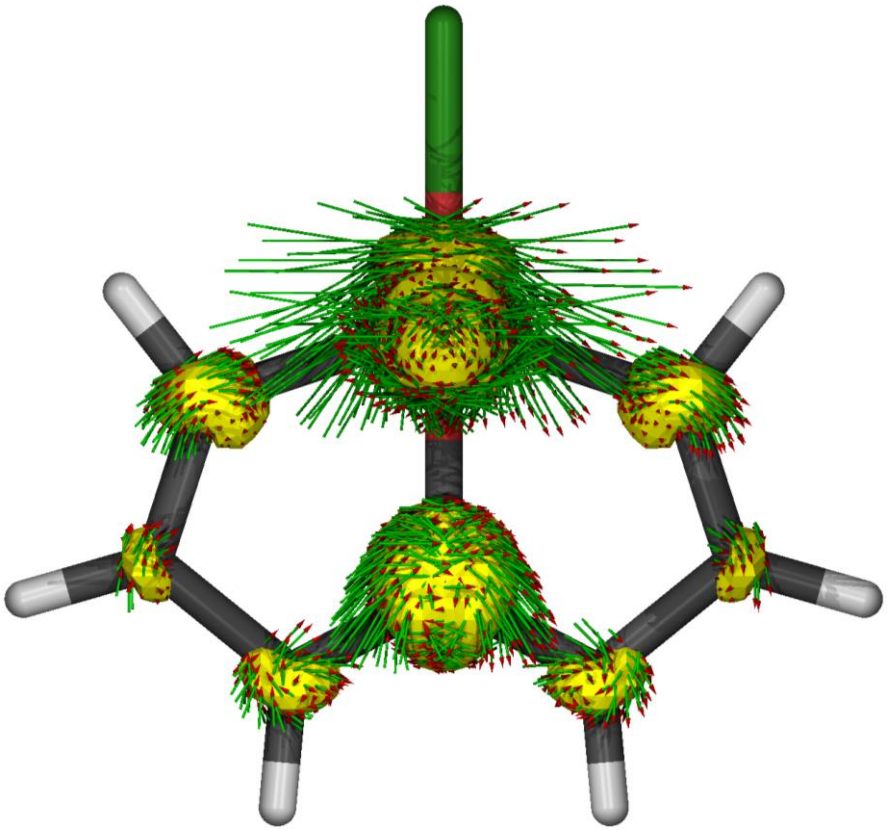


Figure S124. ACID plot of the HOMO-12 of **11**-S_0. Isovalue is 0.024 a.u.

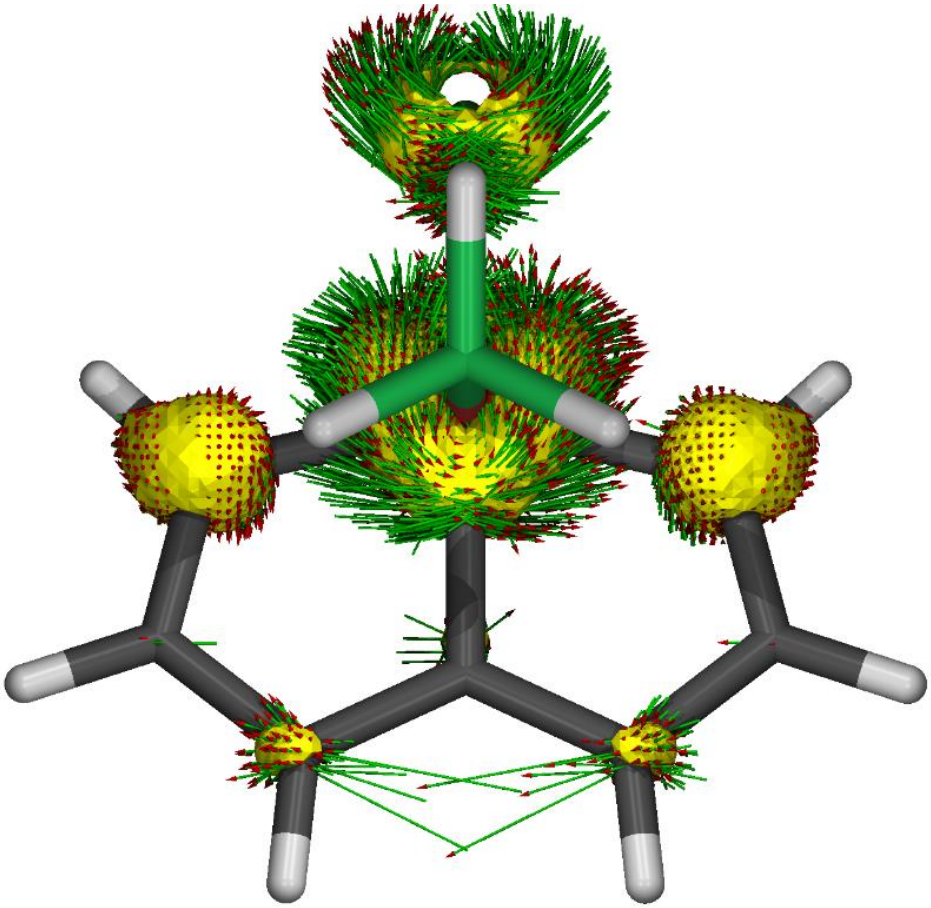


Figure S125. ACID plot of the HSOMO of **12-T_1**. Isovalue is 0.024 a.u.

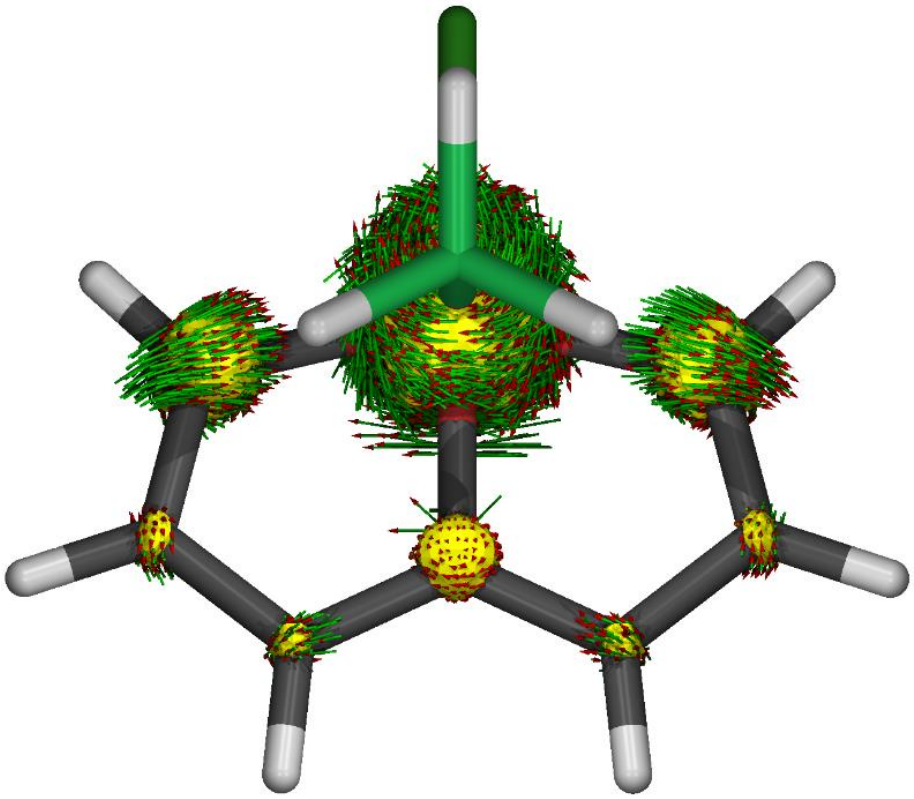


Figure S126. ACID plot of the HSOMO-1 of **12-T_1**. Isovalue is 0.024 a.u.

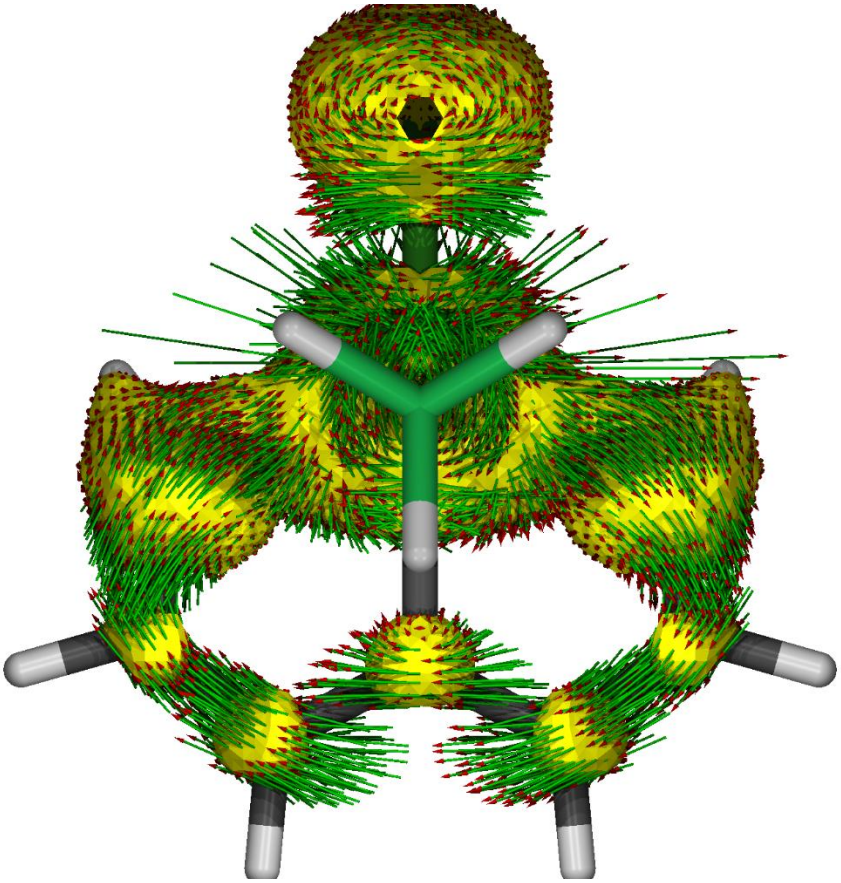


Figure S127. ACID plot of the HOMO of **12-S_0**. Isovalue is 0.024 a.u.

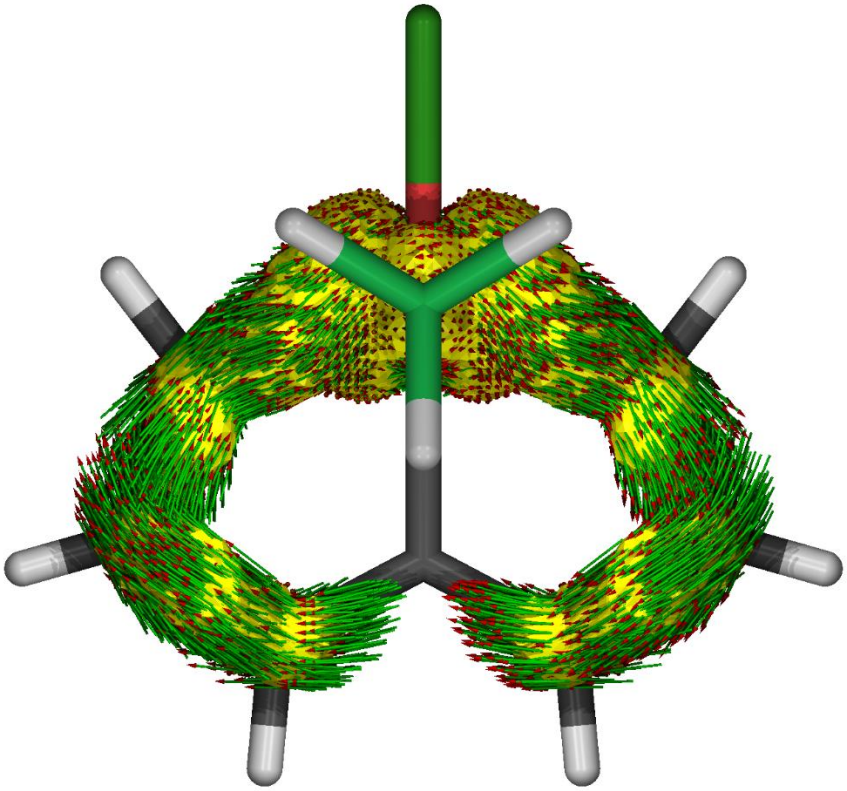


Figure S128. ACID plot of the HOMO-2 of **12-S_0**. Isovalue is 0.024 a.u.

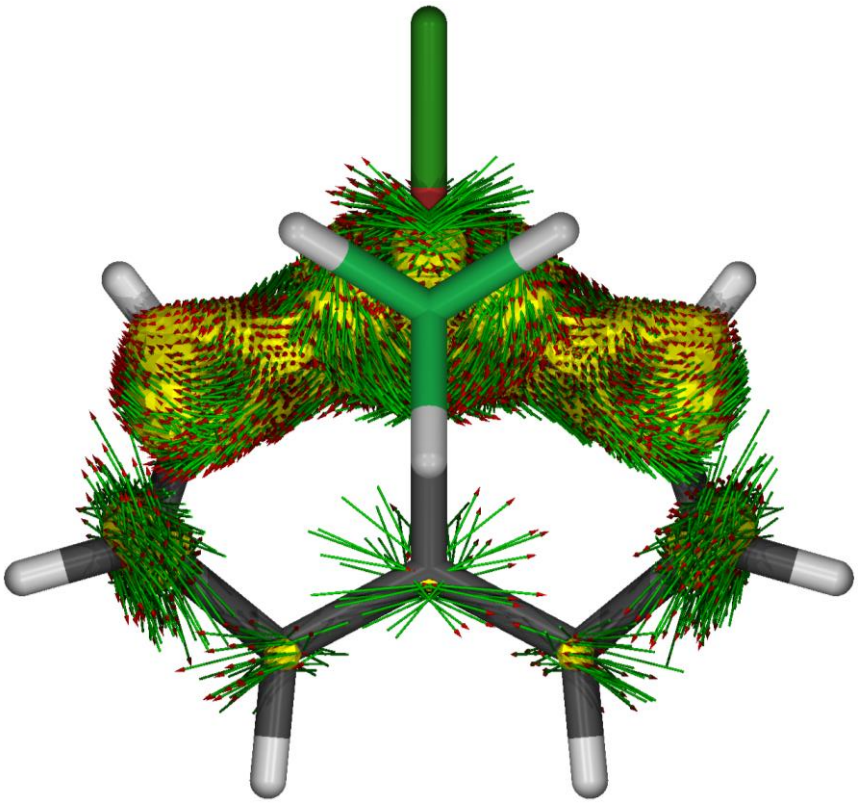


Figure S129. ACID plot of the HOMO-8 of **12-S_0**. Isovalue is 0.024 a.u.

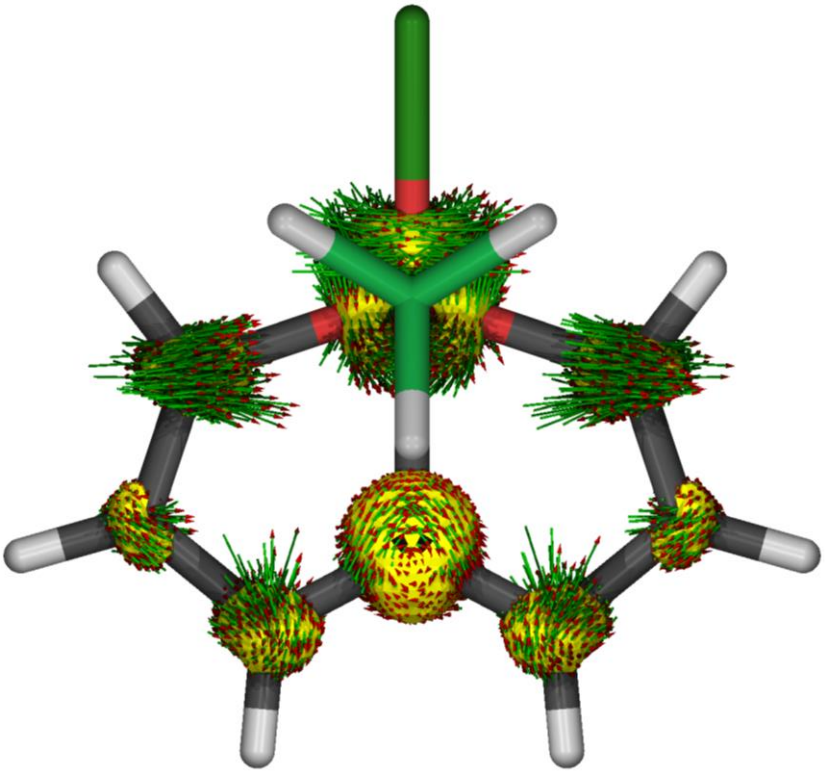


Figure S130. ACID plot of the HOMO-11 of **12-S_0**. Isovalue is 0.024 a.u.

1.singlet

E = -491.485922224 a.u.

0 1

Os	0.00000000	0.00000000	0.31478800
P	-2.36430300	0.00000000	0.14548500
C	0.00000000	2.01980400	-0.14052400
C	0.00000000	2.34059000	-1.50401500
C	0.00000000	1.26210900	-2.41325900
H	0.00000000	1.41979100	-3.49211200
C	0.00000000	0.00000000	-1.81589900
C	0.00000000	-1.26210900	-2.41325900
H	0.00000000	-1.41979100	-3.49211200
H	-3.17981800	0.00000000	1.31478500
H	-2.97298600	1.08549700	-0.54970300
H	-2.97298600	-1.08549700	-0.54970300
C	0.00000000	-2.01980400	-0.14052400
C	0.00000000	-2.34059000	-1.50401500
H	0.00000000	-2.87685100	0.53665300
P	2.36430300	0.00000000	0.14548500
H	2.97298600	1.08549700	-0.54970300
H	3.17981800	0.00000000	1.31478500
H	2.97298600	-1.08549700	-0.54970300
H	0.00000000	3.36854600	-1.86307400
H	0.00000000	-3.36854600	-1.86307400
H	0.00000000	2.87685100	0.53665300
C	0.00000000	0.00000000	2.23040500
O	0.00000000	0.00000000	3.39055500

1-1.singlet

E = -491.476190432 a.u.

0 1

Os	-0.24743000	-0.03808000	-0.00012400
P	0.56789800	2.24483300	-0.00297500
C	0.17852100	-0.15681900	2.03215000
C	1.52699900	-0.34811600	2.34706800
C	2.41259900	-0.47858500	1.25900500
H	3.47895000	-0.65434600	1.39695700
C	1.81230600	-0.39627300	0.00110700
C	2.41351300	-0.48218800	-1.25608100
H	3.47995700	-0.65836800	-1.39279200
H	-0.34574500	3.34260700	-0.00411100
H	1.39436700	2.64815300	1.08529000
H	1.39427400	2.64593100	-1.09213900
C	0.17998400	-0.16279900	-2.03183900
C	1.52868100	-0.35491000	-2.34517800
H	-0.50190700	-0.18649000	-2.88671800
H	1.88690000	-0.42837000	3.37115100
H	1.88939000	-0.43811900	-3.36874600
H	-0.50402300	-0.17800500	2.88658900
C	-0.82115600	-1.85418600	0.00202800
O	-1.17769700	-2.94998500	0.00323700
P	-2.54240300	0.63568100	-0.00092700
H	-3.43423600	0.28330700	1.06614100
H	-2.84723300	2.03450900	-0.00380100
H	-3.43556400	0.27865200	-1.06530500

1.triplet

E = -491.427987592 a.u.

0 3

Os	0.00000000	0.00000000	0.37296100
P	-2.34058000	0.00000000	0.02807500
C	0.00000000	2.02368000	-0.20269100
C	0.00000000	2.35294700	-1.52353800
C	0.00000000	1.25406000	-2.43382000
H	0.00000000	1.38818000	-3.51313200
C	0.00000000	0.00000000	-1.81973600
C	0.00000000	-1.25406000	-2.43382000
H	0.00000000	-1.38818000	-3.51313200
H	-3.26789400	0.00000000	1.11332000
H	-2.86330300	1.09489500	-0.71549800
H	-2.86330300	-1.09489500	-0.71549800
C	0.00000000	-2.02368000	-0.20269100
C	0.00000000	-2.35294700	-1.52353800
H	0.00000000	-2.77832600	0.58631700
P	2.34058000	0.00000000	0.02807500
H	2.86330300	1.09489500	-0.71549800
H	3.26789400	0.00000000	1.11332000
H	2.86330300	-1.09489500	-0.71549800
H	0.00000000	3.38436100	-1.87051200
H	0.00000000	-3.38436100	-1.87051200
H	0.00000000	2.77832600	0.58631700
C	0.00000000	0.00000000	2.33278200
O	0.00000000	0.00000000	3.48563900

2.singlet symmetry = C_{2v}

E = -502.866594778 a.u.

0 1

Os	0.00000000	0.00000000	0.30982700
P	-2.35795500	0.00000000	0.12525200
C	0.00000000	2.01625400	-0.16923700
C	0.00000000	2.33784900	-1.53214600

C	0.00000000	1.26210200	-2.44425700
H	0.00000000	1.42531100	-3.52288800
C	0.00000000	0.00000000	-1.85272300
C	0.00000000	-1.26210200	-2.44425700
H	0.00000000	-1.42531100	-3.52288800
H	-3.21377900	0.00000000	1.26558400
H	-2.95688100	1.08328100	-0.58404800
H	-2.95688100	-1.08328100	-0.58404800
C	0.00000000	-2.01625400	-0.16923700
C	0.00000000	-2.33784900	-1.53214600
H	0.00000000	-2.87591900	0.50357600
P	2.35795500	0.00000000	0.12525200
H	2.95688100	1.08328100	-0.58404800
H	3.21377900	0.00000000	1.26558400
H	2.95688100	-1.08328100	-0.58404800
H	0.00000000	3.36680900	-1.88893000
H	0.00000000	-3.36680900	-1.88893000
H	0.00000000	2.87591900	0.50357600
B	0.00000000	0.00000000	2.24738200
F	0.00000000	0.00000000	3.54935600

2.singlet symmetry = C_1

E = -502.866688894 a.u.

0 1

Os	0.29829700	-0.02193600	0.00448800
P	0.53289100	2.31733200	0.19923400
C	-0.17115500	0.28529300	-1.99524900
C	-1.52820600	0.44021400	-2.30175900
C	-2.43813300	0.37732200	-1.22534500
H	-3.51188400	0.49836400	-1.37502000
C	-1.84993600	0.17101200	0.02085600
C	-2.44620500	0.07326500	1.27823900
H	-3.52186900	0.14455500	1.44478600
H	1.44894300	3.01293500	-0.64242800
H	-0.62199600	3.11667300	-0.05759700
H	0.91119300	2.89966000	1.44548900
C	-0.18052400	-0.17876600	2.01275600
C	-1.54111600	-0.11045800	2.34238700
H	0.49045700	-0.30439200	2.86491400
P	-0.20745400	-2.32043500	-0.24814600
H	-0.94528100	-2.69904600	-1.40859200
H	0.80559900	-3.32182700	-0.30544700
H	-1.03604600	-2.91307000	0.75021000
H	-1.88230600	0.60002500	-3.31919600
H	-1.89808800	-0.19276800	3.36797400
H	0.50324400	0.35623600	-2.85086000
B	2.21904100	-0.28420800	-0.01342300
F	3.50470700	-0.48998900	-0.02731600

2-1.singlet

E = -502.863393675 a.u.

0 1

C	0.16726300	0.17375200	2.02681300
C	1.49867300	0.46968200	2.34447900
C	2.36973000	0.67043700	1.25801300
H	3.41970400	0.92763400	1.39485500
C	1.77536200	0.54290200	-0.00016700
C	2.36968300	0.66984800	-1.25843300
H	3.41965200	0.92698100	-1.39543500
C	0.16718000	0.17282300	-2.02690000
C	1.49858200	0.46859200	-2.34476600
H	-0.51256300	0.13375300	-2.88294500
P	0.80043600	-2.22043100	0.00052300
H	1.66498500	-2.53997000	1.08820000
H	0.00823200	-3.41017300	0.00080100
H	1.66500400	-2.54048800	-1.08698800
H	1.85025200	0.57102800	3.36967600
H	1.85011300	0.56946700	-3.37002600
H	-0.51244100	0.13506000	2.88290500
Os	-0.25124300	0.00941300	-0.00000600
P	-2.45441700	-0.88039000	0.00011500
H	-3.38310600	-0.62204100	-1.06382600
H	-2.62878800	-2.30389500	0.00017400
H	-3.38310000	-0.62195200	1.06404300
B	-0.99946100	1.78046200	-0.00026700
F	-1.51503300	2.96233400	-0.00038000

2.triplet

E = -502.807344170 a.u.

0 3

Os	0.00000000	0.00000000	0.36894100
P	-2.33325300	0.00000000	-0.00317000
C	0.00000000	2.01597000	-0.22678300
C	0.00000000	2.35029600	-1.54647700
C	0.00000000	1.25616000	-2.46284600
H	0.00000000	1.39783500	-3.54158300
C	0.00000000	0.00000000	-1.85729300
C	0.00000000	-1.25616000	-2.46284600
H	0.00000000	-1.39783500	-3.54158300
H	-3.29391100	0.00000000	1.05288100
H	-2.84335100	1.09361400	-0.75855000

H	-2.84335100	-1.09361400	-0.75855000
C	0.00000000	-2.01597000	-0.22678300
C	0.00000000	-2.35029600	-1.54647700
H	0.00000000	-2.77193000	0.56054700
P	2.33325300	0.00000000	-0.00317000
H	2.84335100	1.09361400	-0.75855000
H	3.29391100	0.00000000	1.05288100
H	2.84335100	-1.09361400	-0.75855000
H	0.00000000	3.38347700	-1.88853100
H	0.00000000	-3.38347700	-1.88853100
H	0.00000000	2.77193000	0.56054700
B	0.00000000	0.00000000	2.36388300
F	0.00000000	0.00000000	3.65342100

3.singlet

E = -487.650352803 a.u.

0 1

Os	0.00000000	0.00000000	0.29904700
P	-2.36462200	0.00000000	0.16690900
C	0.00000000	2.02325100	-0.12382100
C	0.00000000	2.34332700	-1.48931200
C	0.00000000	1.26060100	-2.39136900
H	0.00000000	1.40542500	-3.47124100
C	0.00000000	0.00000000	-1.78355200
C	0.00000000	-1.26060100	-2.39136900
H	0.00000000	-1.40542500	-3.47124100
H	-3.15396100	0.00000000	1.35677400
H	-2.99224100	1.08417300	-0.51359900
H	-2.99224100	-1.08417300	-0.51359900
C	0.00000000	-2.02325100	-0.12382100
C	0.00000000	-2.34332700	-1.48931200
H	0.00000000	-2.88353500	0.55335900
P	2.36462200	0.00000000	0.16690900
H	2.99224100	1.08417300	-0.51359900
H	3.15396100	0.00000000	1.35677400
H	2.99224100	-1.08417300	-0.51359900
H	0.00000000	3.36952200	-1.85327900
H	0.00000000	-3.36952200	-1.85327900
H	0.00000000	2.88353500	0.55335900
N	0.00000000	0.00000000	2.29072200
N	0.00000000	0.00000000	3.40979800

3-1.singlet

E = -487.639474898 a.u.

0 1

Os	-0.24272100	0.04090100	-0.00004800
P	0.25134600	-2.25420200	0.00112500
C	0.18023700	0.10139300	-2.03323100
C	1.54020100	0.20385600	-2.34554200
C	2.43685600	0.26390300	-1.25831300
H	3.51303600	0.35918900	-1.39983100
C	1.83482400	0.21280300	-0.00002700
C	2.43672800	0.26528800	1.25825200
H	3.51289100	0.36074200	1.39978300
H	-0.80167100	-3.22000800	0.00111100
H	1.01936500	-2.76379200	-1.08610000
H	1.01854500	-2.76296300	1.08931800
C	0.18002000	0.10366000	2.03314100
C	1.53995000	0.20642900	2.34545900
H	-0.49138600	0.11345100	2.89788700
H	1.90756200	0.25318300	-3.36940700
H	1.90721300	0.25688700	3.36930600
H	-0.49111000	0.11026400	-2.89803000
N	-0.52437900	2.00953300	-0.00101600
N	-0.64371300	3.11436000	-0.00152300
P	-2.60861900	-0.31043500	0.00010100
H	-3.45797500	0.15138800	-1.06315400
H	-3.08922300	-1.65942500	-0.00015700
H	-3.45758900	0.15091300	1.06387700

3.triplet

E = -487.601869780 a.u.

0 3

Os	0.00000000	0.00000000	0.35842900
P	-2.34325200	0.00000000	0.05495900
C	0.00000000	2.03228000	-0.18767800
C	0.00000000	2.35787900	-1.51119900
C	0.00000000	1.25246700	-2.41217100
H	0.00000000	1.37257500	-3.49275200
C	0.00000000	0.00000000	-1.79031700
C	0.00000000	-1.25246700	-2.41217100
H	0.00000000	-1.37257500	-3.49275200
H	-3.25143100	0.00000000	1.15881700
H	-2.88339900	1.09373300	-0.67789700
H	-2.88339900	-1.09373300	-0.67789700
C	0.00000000	-2.03228000	-0.18767800
C	0.00000000	-2.35787900	-1.51119900
H	0.00000000	-2.80065100	0.58930400
P	2.34325200	0.00000000	0.05495900
H	2.88339900	1.09373300	-0.67789700
H	3.25143100	0.00000000	1.15881700

H	2.88339900	-1.09373300	-0.67789700
H	0.00000000	3.38601900	-1.86725300
H	0.00000000	-3.38601900	-1.86725300
H	0.00000000	2.80065100	0.58930400
N	0.00000000	0.00000000	2.37866100
N	0.00000000	0.00000000	3.49569500

4.singlet

E = -471.032036201 a.u.

-1 1

Os	-0.24226600	0.00542600	-0.00001100
P	0.35721300	-2.28541100	-0.00066800
C	0.16869200	0.08301300	-2.02123400
C	1.51934700	0.30164000	-2.34130500
C	2.40807500	0.45308500	-1.25993400
H	3.47385500	0.64209700	-1.40546600
C	1.81000000	0.35728400	0.00003500
C	2.40819200	0.45210100	1.26001500
H	3.47399100	0.64097600	1.40559400
H	-0.58083100	-3.37773900	-0.00012700
H	1.16912400	-2.78015300	-1.07500700
H	1.17045100	-2.78021100	1.07263400
C	0.16887700	0.08150100	2.02127800
C	1.51956500	0.29985300	2.34136600
H	-0.49255800	-0.00694600	2.89379400
H	1.88120100	0.37069600	-3.36919600
H	1.88152900	0.36812900	3.36927000
H	-0.49284400	-0.00479300	-2.89374100
P	-2.57503200	-0.29868100	-0.00008000
H	-3.29300400	-0.98968800	-1.05334200
H	-3.29268600	-0.99229700	1.05167000
H	-3.42826400	0.85426900	0.00144800
C	-0.62546500	2.01847700	0.00076900
N	-0.86487900	3.16041600	0.00122600

4-1.singlet

E = -471.027170145 a.u.

-1 1

P	-1.45044300	-1.92082600	-0.00037500
C	0.11769600	-0.20687500	-2.00864500
C	1.44947500	-0.51889600	-2.33993900
C	2.33727200	-0.71785400	-1.26414900
H	3.38367600	-0.99207900	-1.42111900
C	1.74430300	-0.58050300	0.00041800
C	2.33653900	-0.71806100	1.26527700
H	3.38280700	-0.99249200	1.42279000
H	-2.35195000	-2.19799800	-1.07890600
H	-0.79516100	-3.20020100	0.00245300
H	-2.35641700	-2.19531700	1.07504000
C	0.11663900	-0.20685700	2.00868000
C	1.44819000	-0.51904200	2.34062900
H	-0.59199000	-0.26790300	2.84686700
P	0.81087500	2.15857500	0.00001900
H	1.70164300	2.45708300	-1.08016400
H	0.06164000	3.37605800	-0.00038300
H	1.70092800	2.45742500	1.08070200
H	1.78543000	-0.65366300	-3.37050600
H	1.78361800	-0.65384100	3.37136300
H	-0.59053800	-0.26823300	-2.84715500
C	-2.15799600	0.92800700	-0.00008400
N	-3.22184200	1.41861200	-0.00000400
Os	-0.25421000	0.06414700	-0.00011500

4.triplet

E = -470.988989368 a.u.

-1 3

Os	-0.27086700	0.01575800	-0.00002200
P	0.52738900	-2.20509000	-0.00036600
C	0.26284500	0.09570800	-2.03524800
C	1.56872800	0.33252600	-2.35899600
C	2.45156300	0.49756300	-1.25128200
H	3.51773800	0.69160500	-1.36820100
C	1.83512400	0.41113900	0.00011500
C	2.45148800	0.49707800	1.25158300
H	3.51765700	0.69107000	1.36863900
H	-0.31349600	-3.37562800	-0.00033700
H	1.36943700	-2.61252100	-1.08416900
H	1.36974100	-2.61267600	1.08314000
C	0.26272400	0.09492300	2.03528000
C	1.56859200	0.33161400	2.35918400
H	-0.48907100	0.00758800	2.82629900
H	1.92424600	0.40759500	-3.38752700
H	1.92405600	0.40628700	3.38776200
H	-0.48891600	0.00867200	-2.82633400
P	-2.64725400	-0.47167200	-0.00008900
H	-3.23868100	-1.24356600	-1.06011000
H	-3.23847600	-1.24494500	1.05904000
H	-3.63097800	0.57174000	0.00067200
C	-0.75742700	1.99072300	0.00033000
N	-1.10017300	3.10728000	0.00054400

5.singlet

E = -507.864942469 a.u.

1 1

Os	0.00000000	0.00000000	0.34564200
P	0.00000000	-2.39934500	0.04590600
C	-2.00703600	0.00001600	-0.15606700
C	-2.34328600	0.00005100	-1.50211000
C	-1.25548100	0.00003900	-2.39875100
H	-1.38970700	0.00004700	-3.47828500
C	0.00000000	0.00000000	-1.78914200
C	1.25548100	-0.00003900	-2.39875100
H	1.38970700	-0.00004700	-3.47828500
H	0.00010400	-3.20872000	1.21299700
H	-1.10435500	-2.93252800	-0.66722800
H	1.10426700	-2.93248700	-0.66739400
C	2.00703600	-0.00001600	-0.15606700
C	2.34328600	-0.00005100	-1.50211000
H	2.82318600	-0.00003500	0.56590600
P	0.00000000	2.39934500	0.04590600
H	-1.10426700	2.93248700	-0.66739400
H	-0.00010400	3.20872000	1.21299700
H	1.10435500	2.93252800	-0.66722800
H	-3.37097500	0.00007300	-1.85184300
H	3.37097500	-0.00007300	-1.85184300
H	-2.82318600	0.00003500	0.56590600
O	0.00000000	0.00000000	3.30823000
N	0.00000000	0.00000000	2.15398600

5-1.singlet

E = -507.835206673 a.u.

1 1

Os	0.24259400	0.09988600	0.00013500
P	-0.69273000	-2.18011900	-0.00292200
C	-0.23224700	0.10991400	2.04528300
C	-1.56327400	0.32342700	2.35421600
C	-2.42644300	0.52394700	1.25377200
H	-3.48961200	0.71800700	1.37769500
C	-1.81819600	0.46608300	0.00073300
C	-2.42658400	0.52733400	-1.25206700
H	-3.48977000	0.72171200	-1.37534700
H	0.22406900	-3.26712400	-0.00438900
H	-1.50822500	-2.52519200	1.10516800
H	-1.50822000	-2.52218400	-1.11194300
C	-0.23249100	0.11543100	-2.04497800
C	-1.56353000	0.32984000	-2.35316500
H	0.47499100	0.11009600	-2.87409100
H	-1.92989800	0.37730800	3.37486600
H	-1.93028100	0.38650300	-3.37362000
H	0.47530100	0.10230200	2.87432600
N	0.99948000	1.71783400	0.00194100
O	1.56070400	2.72273700	0.00295400
P	2.49232500	-0.91208900	-0.00101100
H	2.88112500	-1.74705800	1.08436400
H	2.88087200	-1.74518200	-1.08791600
H	3.58314000	0.00000700	-0.00035500

5.triplet

E = -507.793896521 a.u.

1 3

Os	0.00000000	0.00000000	0.33126300
P	0.00000000	-2.40808600	0.13175200
C	-2.05981900	0.00001700	-0.18458300
C	-2.35675900	0.00002600	-1.55831600
C	-1.27369200	0.00001500	-2.44103600
H	-1.39197900	0.00001800	-3.51993500
C	0.00000000	0.00000000	-1.80196200
C	1.27369200	-0.00001500	-2.44103600
H	1.39197900	-0.00001800	-3.51993500
H	0.00005300	-3.15418900	1.34009500
H	-1.09819500	-2.99167000	-0.55250100
H	1.09815300	-2.99164800	-0.55258600
C	2.05981900	-0.00001700	-0.18458300
C	2.35675900	-0.00002600	-1.55831600
H	2.88988500	-0.00001600	0.51856100
P	0.00000000	2.40808600	0.13175200
H	-1.09815300	2.99164800	-0.55258600
H	-0.00005300	3.15418900	1.34009500
H	1.09819500	2.99167000	-0.55250100
H	-3.38050200	0.00004000	-1.92339500
H	3.38050200	-0.00004000	-1.92339500
H	-2.88988500	0.00001600	0.51856100
O	0.00000000	0.00000000	3.29000000
N	0.00000000	0.00000000	2.13571300

6.singlet

E = -490.622769489 a.u

1 1

C	-0.49535600	0.04722400	-1.80242800
C	-1.79460300	0.12257100	-2.22972800
C	-2.60649600	0.17622400	-1.07280400
H	-3.69177900	0.23449100	-1.11605600
C	-1.87383500	0.15001700	0.12308200

C	-2.34979900	0.20745400	1.42198700
H	-3.41033100	0.26939900	1.65283500
C	-1.35221700	0.19321800	2.42316400
C	-0.05558500	0.12331500	1.95780000
H	0.75181900	0.14401600	2.69163900
P	-0.12751100	-2.37356900	0.04105400
H	-2.14454000	0.13294200	-3.25408400
H	-1.60235400	0.24180800	3.47799600
H	-0.93148800	-2.93696600	-0.98495900
H	0.97981000	-3.26576400	0.01304600
H	-0.79704600	-2.82523700	1.20798700
Os	0.24938400	0.04968300	-0.09317500
P	2.75006100	-0.16932000	-0.08118900
H	3.44549000	0.20960000	1.10022200
H	3.33330500	-1.44780900	-0.29845100
H	3.46654300	0.59142200	-1.04248900
C	0.37357000	1.98687400	-0.06565100
O	0.40438000	3.12227300	-0.03710800

6-1.singlet

E = -490.620583497 a.u

1 1

C	1.48910700	-1.09974200	0.00000000
C	1.40574900	-2.46872400	0.00000000
C	0.02855800	-2.79025300	0.00000000
H	-0.33626800	-3.81510200	0.00000000
C	-0.79740600	-1.65264300	0.00000000
C	-2.18277200	-1.58974200	0.00000000
H	-2.81215400	-2.47681100	0.00000000
C	-2.72150300	-0.28335100	0.00000000
C	-1.79649400	0.74663400	0.00000000
H	-2.17859900	1.76824700	0.00000000
P	0.02855800	0.16282800	2.41240600
P	0.02855800	0.16282800	-2.41240600
H	2.22910000	-3.17173100	0.00000000
H	-3.79350800	-0.11255700	0.00000000
H	0.92216500	-0.70447100	-3.09479200
H	0.19622600	1.35846200	-3.16004200
H	-1.22735900	-0.28667500	-2.89584700
H	0.92216500	-0.70447100	3.09479200
H	0.19622600	1.35846200	3.16004200
H	-1.22735900	-0.28667500	2.89584700
Os	0.20753000	0.25540100	0.00000000
C	1.00279600	2.10003800	0.00000000
O	1.48901900	3.12558200	0.00000000

6.triplet

E = -490.549088210 a.u.

1 3

C	-0.26068400	0.13016500	-1.92271700
C	-1.59185900	0.15684000	-2.36747000
C	-2.46734500	0.37031500	-1.30441000
H	-3.52988200	0.55871900	-1.43192400
C	-1.82472200	0.31802900	-0.02707300
C	-2.47437600	0.38557300	1.24090200
H	-3.54590800	0.52494900	1.34668900
C	-1.61380300	0.29444900	2.32263600
C	-0.23596100	0.23547000	1.99680300
H	0.44915200	0.56168700	2.78234300
P	-0.31639800	-2.36392000	0.07400700
H	-1.90005900	0.07662100	-3.40513700
H	-1.97005000	0.35675700	3.34683900
H	-1.10801800	-2.88170100	-0.98642500
H	0.72978700	-3.32612600	0.09985700
H	-1.07779400	-2.78207500	1.19759500
Os	0.23660300	0.03608600	-0.03200200
P	2.69427700	-0.39581900	-0.02263100
H	3.42031500	-0.22249600	1.18908500
H	3.15862800	-1.69187300	-0.38170100
H	3.49716700	0.38942100	-0.89353100
C	0.64977000	1.91684400	-0.05611400
O	0.89256100	3.03044800	-0.06218600

7.singlet

E = -502.016309112 a.u

1 1

C	-0.48131300	-0.05124900	-1.80527700
C	-1.78518000	-0.04171000	-2.24007000
C	-2.59994000	0.04487500	-1.09208400
H	-3.68658600	0.05916500	-1.13771700
C	-1.86821700	0.11135700	0.10635800
C	-2.34808100	0.20705300	1.40182300
H	-3.41056500	0.23818600	1.62986700
C	-1.35256100	0.27331200	2.40199200
C	-0.05159000	0.22959100	1.93978700
H	0.75089000	0.30988500	2.67478200
P	-0.09071100	-2.42270000	0.17066900
H	-2.13043700	-0.10305200	-3.26413800
H	-1.60497500	0.35409100	3.45434200
H	-0.90515900	-3.05448400	-0.80743000
H	1.01420200	-3.31978900	0.18436400

H	-0.74664500	-2.81213200	1.36836700
Os	0.26187400	0.04621600	-0.10582100
P	2.74854400	-0.14920000	-0.08723600
H	3.44986200	0.37408900	1.03412400
H	3.35484200	-1.43484800	-0.15480400
H	3.45141800	0.49870000	-1.13684300
B	0.29068800	1.99592900	-0.11210500
F	0.24012500	3.25969700	-0.08540300

7-1.singlet

E = -502.005935421 a.u

1 1

C	1.77490400	-0.47351600	0.00000000
C	2.24122800	-1.76583900	0.00000000
C	1.10207700	-2.60103000	0.00000000
H	1.17136200	-3.68701000	0.00000000
C	-0.10466300	-1.87778500	0.00000000
C	-1.40760100	-2.34178000	0.00000000
H	-1.65756500	-3.40095200	0.00000000
C	-2.40739200	-1.33852800	0.00000000
C	-1.95932800	-0.02924000	0.00000000
H	-2.71377200	0.75727500	0.00000000
P	-0.10466300	0.17061600	2.40199400
P	-0.10466300	0.17061600	-2.40199400
H	3.27533400	-2.08596500	0.00000000
H	-3.46205500	-1.59700900	0.00000000
H	1.08599100	0.04059900	-3.16620700
H	-0.74237800	1.23239400	-3.09492200
H	-0.85571200	-0.93753800	-2.87421400
H	1.08599100	0.04059900	3.16620700
H	-0.74237800	1.23239400	3.09492200
H	-0.85571200	-0.93753800	2.87421400
Os	0.08720300	0.30415400	0.00000000
B	0.25420900	2.31788900	0.00000000
F	0.46855100	3.56504600	0.00000000

7.triplet

E = -501.942197451 a.u.

1 3

C	-0.22584300	0.30548700	-1.90591600
C	-1.56371500	0.43384200	-2.34413100
C	-2.44214100	0.56556500	-1.27634900
H	-3.50047400	0.78367400	-1.39311400
C	-1.81316100	0.38328000	-0.00456900
C	-2.46974900	0.36627100	1.26137500
H	-3.53876200	0.51999500	1.37435700
C	-1.61797700	0.16655600	2.33211500
C	-0.23485200	0.09488700	2.00273300
H	0.44812500	0.31950700	2.82498300
P	-0.43061000	-2.39881000	-0.11437000
H	-1.86619100	0.46573600	-3.38639700
H	-1.97484200	0.15098800	3.35788000
H	-1.19815000	-2.80629600	-1.23939800
H	0.56215900	-3.41737700	-0.11179900
H	-1.26488100	-2.85906200	0.94015300
Os	0.23932600	0.01983900	-0.01795900
P	2.64772200	-0.53778600	-0.03322800
H	3.43444800	-0.23543300	1.11396900
H	3.03315000	-1.89849900	-0.20358400
H	3.46941600	0.04929000	-1.03461200
B	0.73394000	1.89452200	0.05099800
F	1.05394000	3.12230100	0.07665300

8. singlet

E = -486.799836142 a.u.

1 1

C	0.47444000	-0.00025600	-1.79483000
C	1.79063800	-0.00028400	-2.19444700
C	2.57333900	-0.00014300	-1.02147500
H	3.66066500	-0.00008900	-1.03318400
C	1.80095100	0.00004200	0.15541100
C	2.25326700	0.00032400	1.46727000
H	3.31008100	0.00043600	1.72157700
C	1.23303900	0.00049500	2.44350800
C	-0.05403900	0.00030900	1.93884000
H	-0.88408000	0.00050300	2.64868300
P	-0.17628100	2.41253700	0.00245400
P	-0.17632700	-2.41279500	0.00300900
H	2.16283900	-0.00040500	-3.21095600
H	1.45739000	0.00069000	3.50531500
H	-1.37291300	-3.15219100	0.21046900
H	0.63885400	-2.92548700	1.04550900
H	0.35541100	-3.08715100	-1.12777900
H	0.35697900	3.08621000	-1.12802700
H	-1.37321600	3.15196500	0.20781300
H	0.63735700	2.92597800	1.04578000
Os	-0.29712600	-0.00001500	-0.10710800
N	-2.41398700	0.00001500	-0.11791400
N	-3.51579500	0.00021900	-0.13816900

8-1. singlet

E = -486.792746173 a.u.

1 1

C	-0.48603700	0.05952900	-1.79826100
C	-1.78668600	0.13709200	-2.22707000
C	-2.60364300	0.18321000	-1.07379400
H	-3.68805200	0.25320500	-1.12056200
C	-1.87390800	0.14088800	0.12368600
C	-2.35423000	0.19770300	1.42080800
H	-3.41421600	0.27033500	1.65079900
C	-1.35669200	0.16649500	2.42243800
C	-0.06072600	0.08188400	1.95542500
H	0.74585000	0.06751300	2.69135100
P	-0.10895900	-2.31289200	0.00918900
H	-2.13326200	0.16434600	-3.25245400
H	-1.60721900	0.21326900	3.47748900
H	-0.88821200	-2.86200100	-1.04284700
H	1.00895700	-3.19182500	-0.01098500
H	-0.79717400	-2.78291800	1.15758100
Os	0.24415500	0.03450500	-0.08716300
P	2.75548900	-0.13647000	-0.07725000
H	3.42397000	-0.22380700	1.17601600
H	3.34525600	-1.24929400	-0.73606400
H	3.50418000	0.91609400	-0.67120900
N	0.37521800	2.07355000	-0.05566100
N	0.39303500	3.17535600	-0.03194100

8.triplet

E = -486.725978053 a.u.

1 3

C	0.20420500	-0.12096800	-1.94000000
C	1.57554900	-0.20187700	-2.31937900
C	2.41994600	-0.31031700	-1.22739400
H	3.49315400	-0.46431600	-1.31304100
C	1.73631700	-0.20523500	0.03353700
C	2.35346400	-0.22841200	1.32490900
H	3.42432700	-0.34793600	1.46500600
C	1.46557700	-0.10565400	2.38265800
C	0.09560100	-0.02899500	2.01549000
H	-0.62075600	-0.13429900	2.83393400
P	0.11003900	2.42496600	-0.06944000
P	-0.56758100	-2.36473400	-0.01594100
H	1.92526300	-0.20930100	-3.34776800
H	1.80093400	-0.12209700	3.41529800
H	-1.87837700	-2.85103300	-0.26940000
H	-0.24746300	-3.07643800	1.17197200
H	0.17820400	-3.10137500	-0.97435300
H	0.89392800	2.92613000	-1.14290500
H	-1.02014400	3.28328000	-0.14217800
H	0.79622500	2.98135200	1.04314700
Os	-0.27069100	0.03423400	-0.03165200
N	-2.33700500	0.27950900	-0.05162500
N	-3.43637200	0.40899600	-0.04442800

9. singlet

E = -470.338594149 a.u.

0 1

C	0.60574900	-0.30815700	-1.73695100
C	1.96404100	-0.39761500	-2.03240000
C	2.68554700	-0.19067500	-0.84932400
H	3.77415100	-0.20141100	-0.79754700
C	1.83837400	0.02971600	0.25964300
C	2.21630700	0.27183900	1.56899500
H	3.25502000	0.32809400	1.89007100
C	1.13357200	0.44176500	2.46530700
C	-0.11967400	0.33635500	1.89350800
H	-0.99639600	0.44980800	2.53287900
P	-0.31222200	2.35285900	-0.36855600
P	-0.36428700	-2.37139400	0.24385700
H	2.39031000	-0.58904400	-3.01039000
H	1.29122800	0.63301500	3.52364000
H	-1.37563000	-3.11076400	-0.42795500
H	-0.56605200	-2.83454000	1.57360100
H	0.77908700	-3.14354200	-0.10839500
H	-0.20489600	2.92511100	-1.66728700
H	-1.46891300	3.03157000	0.10085300
H	0.70354800	3.09092000	0.30305200
Os	-0.26998000	-0.01816100	-0.13399400
N	-3.52575800	0.00160600	-0.08269800
C	-2.36308500	-0.00526300	-0.11537800

9-1. singlet

E = -470.331019424 a.u.

0 1

C	-0.48994100	0.21387700	-1.78630400
C	-1.78070700	0.50148500	-2.19523000
C	-2.57090300	0.59699800	-1.03938300
H	-3.63375400	0.83119000	-1.05887300
C	-1.83868800	0.37997200	0.14412000
C	-2.30851200	0.42403100	1.44435500
H	-3.34747900	0.63737000	1.68653600
C	-1.32521400	0.19117500	2.43147600
C	-0.05559500	-0.03350200	1.93889200

H	0.75022200	-0.18042700	2.66247400
P	-0.35372800	-2.35350200	-0.07142700
H	-2.11842400	0.64909800	-3.21317100
H	-1.56141900	0.21357000	3.49171600
H	-0.94985300	-2.93703000	-1.22798700
H	0.61954200	-3.36777700	0.18328400
H	-1.31800300	-2.74343500	0.90224300
Os	0.23060100	-0.01134700	-0.10309800
P	2.70658200	-0.23022200	-0.09464600
H	3.38656600	0.23636200	1.06640500
H	3.40373400	-1.46653600	-0.25818100
H	3.39196000	0.53865200	-1.07316800
C	0.67272200	1.97842700	0.06333700
N	0.96278400	3.09891600	0.16538700

9.triplet

E = -470.264457007 a.u.

0 3

C	0.55009300	-0.00062800	-1.80875800
C	1.89635400	-0.00066000	-2.13497000
C	2.64574800	0.00011800	-0.92381800
H	3.73294100	0.00037000	-0.88979900
C	1.80301400	0.00057900	0.21314200
C	2.24513600	0.00135200	1.59916200
H	3.29602900	0.00211400	1.87409700
C	1.21260500	0.00113300	2.53268100
C	-0.08541500	0.00048700	2.02015000
H	-0.93928800	0.00040000	2.69505200
P	-0.32931900	2.37867800	-0.05721000
P	-0.32789800	-2.37879600	-0.05576500
H	2.31254200	-0.00120200	-3.13569100
H	1.41938200	0.00146600	3.60064000
H	-1.42388700	-3.04024900	-0.67348900
H	-0.36087900	-2.99441600	1.22676100
H	0.75734800	-3.09372700	-0.63793800
H	0.75490100	3.09404400	-0.64075500
H	-1.42630200	3.03912000	-0.67425000
H	-0.36151000	2.99493900	1.22503800
Os	-0.27137900	-0.00006700	-0.13851500
N	-3.52753800	-0.00092400	-0.03535500
C	-2.36511500	-0.00063500	-0.08099300

10. singlet

E = -506.800881055 a.u.

2 1

C	1.80450800	-0.47831600	0.00000000
C	2.31775600	-1.71511900	0.00000000
C	1.14912300	-2.55125100	0.00000000
H	1.22173200	-3.63725000	0.00000000
C	-0.04685300	-1.83160700	0.00000000
C	-1.35730200	-2.31665600	0.00000000
H	-1.56676500	-3.38504900	0.00000000
C	-2.37772300	-1.34925200	0.00000000
C	-1.95635900	-0.02820300	0.00000000
H	-2.71353200	0.75539800	0.00000000
P	-0.04685300	0.10406500	2.46291300
P	-0.04685300	0.10406500	-2.46291300
H	3.35406500	-2.03295100	0.00000000
H	-3.42647600	-1.62685200	0.00000000
H	1.10208400	-0.46477100	-3.06774300
H	-0.22711600	1.31064200	-3.18631500
H	-1.11187500	-0.71177900	-2.91653800
H	1.10208400	-0.46477100	3.06774300
H	-0.22711600	1.31064200	3.18631500
H	-1.11187500	-0.71177900	2.91653800
Os	0.06034100	0.34619100	0.00000000
O	0.28396900	3.31236700	0.00000000
N	0.13626000	2.19279200	0.00000000

10-1. singlet

E = -506.799550650 a.u.

2 1

C	0.48840500	0.04461500	-1.83378400
C	1.75325700	-0.01097600	-2.29137700
C	2.59058600	-0.11811300	-1.12828600
H	3.67580600	-0.16037100	-1.20320300
C	1.89245000	-0.13811500	0.07793700
C	2.39121400	-0.21409500	1.37246200
H	3.45866000	-0.26205200	1.57763800
C	1.42048300	-0.22815000	2.40467800
C	0.11301600	-0.17004900	1.98926500
H	-0.68451100	-0.24438500	2.72831600
P	0.17273000	2.35346600	0.12259900
H	2.09628000	0.04483300	-3.31851400
H	1.70357400	-0.29138700	3.45045300
H	1.02364000	2.89252200	-0.87387000
H	-0.96253600	3.20030500	0.04512200
H	0.77399200	2.74396200	1.34401100
Os	-0.24382600	-0.09723000	-0.08613200
O	-0.54806800	-3.02494900	-0.07061800
N	-0.44927700	-1.90197800	-0.09415700

P	-2.75999400	0.35441900	-0.07415600
H	-3.17725700	1.56458500	-0.68343700
H	-3.53955400	-0.61070500	-0.76207000
H	-3.39534800	0.41666100	1.19360300

10.triplet

E = -506.769368994 a.u.

2 3

C	1.85442300	-0.37683800	0.00000000
C	2.24300600	-1.74199800	0.00000000
C	1.12330400	-2.56075700	0.00000000
H	1.17636200	-3.64703900	0.00000000
C	-0.10254500	-1.82397600	0.00000000
C	-1.40921800	-2.38159000	0.00000000
H	-1.60048200	-3.45148500	0.00000000
C	-2.42077900	-1.43285900	0.00000000
C	-1.97459300	-0.08453000	0.00000000
H	-2.74319500	0.69022900	0.00000000
P	0.05803800	0.23280200	2.47974700
P	0.05803800	0.23280200	-2.47974700
H	3.27175900	-2.09005100	0.00000000
H	-3.47336200	-1.69834400	0.00000000
H	0.70672400	-0.89651600	-3.03914700
H	0.72175800	1.32251000	-3.09775800
H	-1.20717400	0.22018300	-3.11887500
H	0.70672400	-0.89651600	3.03914700
H	0.72175800	1.32251000	3.09775800
H	-1.20717400	0.22018300	3.11887500
Os	0.05534300	0.29671400	0.00000000
O	0.05803800	3.31840600	0.00000000
N	0.09045900	2.17685900	0.00000000

11. singlet

E = -625.702971513 a.u.

1 1

Os	0.00000000	0.00000000	0.31426000
C	0.00000000	1.90389200	-0.32231200
C	0.00000000	2.32193400	-1.62297500
C	0.00000000	1.23168000	-2.50813900
H	0.00000000	1.33004600	-3.58973700
C	0.00000000	0.00000000	-1.86248000
C	0.00000000	-1.23168000	-2.50813900
H	0.00000000	-1.33004600	-3.58973700
Cl	0.00000000	0.00000000	2.67857900
C	0.00000000	-1.90389200	-0.32231200
C	0.00000000	-2.32193400	-1.62297500
H	0.00000000	-2.57682400	0.54147900
H	0.00000000	3.36282400	-1.92325200
H	0.00000000	-3.36282400	-1.92325200
H	0.00000000	2.57682400	0.54147900
B	2.05069800	0.00000000	0.24427600
B	-2.05069800	0.00000000	0.24427600
F	-3.29855300	0.00000000	0.14981300
F	3.29855300	0.00000000	0.14981300

11.triplet

E = -625.674052596 a.u.

1 3

Os	0.00000000	0.00000000	0.45064100
C	0.00000000	2.01344900	-0.06494200
C	0.00000000	2.35104000	-1.41433800
C	0.00000000	1.26628300	-2.30370500
H	0.00000000	1.39002900	-3.38321100
C	0.00000000	0.00000000	-1.70219400
C	0.00000000	-1.26628300	-2.30370500
H	0.00000000	-1.39002900	-3.38321100
Cl	0.00000000	0.00000000	2.74503600
C	0.00000000	-2.01344900	-0.06494200
C	0.00000000	-2.35104000	-1.41433800
H	0.00000000	-2.80247700	0.68697700
H	0.00000000	3.37850500	-1.76141300
H	0.00000000	-3.37850500	-1.76141300
H	0.00000000	2.80247700	0.68697700
B	1.89057500	0.00000000	-0.21990700
B	-1.89057500	0.00000000	-0.21990700
F	-3.01115900	0.00000000	-0.78838700
F	3.01115900	0.00000000	-0.78838700

11-1. singlet

E = -625.682664958 a.u.

1 1

Os	-0.03397600	0.28498300	0.00000000
C	0.15742500	-0.35723000	1.90084800
C	0.15742500	-1.65388700	2.31142400
C	0.05731000	-2.55284700	1.22864600
H	0.03885300	-3.63228800	1.35154500
C	-0.02107600	-1.91312200	0.00000000
C	0.05731000	-2.55284700	-1.22864600
H	0.03885300	-3.63228800	-1.35154500
C	0.15742500	-0.35723000	-1.90084800
C	0.15742500	-1.65388700	-2.31142400
H	0.05950300	0.50713200	-2.56589100

H	0.17436500	-1.94734900	3.35518300
H	0.17436500	-1.94734900	-3.35518300
H	0.05950300	0.50713200	2.56589100
B	0.01206500	2.37946200	0.00000000
F	0.07568000	3.62846600	0.00000000
Cl	-2.42133900	0.36854300	0.00000000
B	1.91122500	0.28757600	0.00000000
F	3.17360900	0.27511200	0.00000000

12. singlet

E = -509.288165786 a.u.

1 1

Os	0.07197300	0.29372000	0.00000000
C	0.09373100	-0.33733500	1.88919100
C	0.09416400	-1.63659200	2.31761000
C	0.09416400	-2.52457500	1.22986300
H	0.09549600	-3.60595700	1.32955200
C	0.09183900	-1.87463500	0.00000000
C	0.09416400	-2.52457500	-1.22986300
H	0.09549600	-3.60595700	-1.32955200
Cl	-0.16427000	2.64209400	0.00000000
C	0.09373100	-0.33733500	-1.88919100
C	0.09416400	-1.63659200	-2.31761000
H	0.08135100	0.53178700	-2.55577000
P	-2.49263000	0.28140700	0.00000000
H	-3.11569900	0.93829900	1.09319600
H	-3.11569900	0.93829900	-1.09319600
H	-3.17700900	-0.96311100	0.00000000
H	0.09111200	-1.93153400	3.36004700
H	0.09111200	-1.93153400	-3.36004700
H	0.08135100	0.53178700	2.55577000
B	2.02478700	0.25945100	0.00000000
F	3.28054500	0.17456700	0.00000000

12-1. singlet

E = -509.236148 a.u.

1 1

Os	-0.29021900	0.02716200	0.00001700
C	0.35917900	-0.05389900	1.87677700
C	1.64693700	0.08844200	2.30625800
C	2.53293000	0.28968900	1.23011800
H	3.60218000	0.43444500	1.35720400
C	1.88849800	0.28962300	-0.00010500
C	2.53286800	0.28953900	-1.23037000
H	3.60212800	0.43415800	-1.35752900
C	0.35905200	-0.05385800	-1.87679900
C	1.64678700	0.08825300	-2.30642600
H	-0.52208200	-0.03111300	-2.52934500
H	1.93227900	0.10171800	3.35221800
H	1.93204100	0.10138400	-3.35241100
H	-0.52185500	-0.03151100	2.52946200
B	-2.37307600	-0.25108800	0.00041100
F	-3.61534800	-0.41678000	0.00057200
Cl	-0.68706500	2.37011200	-0.00019000
P	0.10776000	-2.33758000	-0.00008000
H	-0.38505400	-3.09629300	1.09493300
H	-0.38598900	-3.09632600	-1.09464800
H	1.47269500	-2.72928300	-0.00066500

12-2. singlet

E = -509.269597 a.u.

1 1

Os	-0.21323200	0.07800000	-0.00007900
C	0.42780600	0.03981300	1.87444200
C	1.68303000	-0.25409000	2.31499000
C	2.53797300	-0.50510400	1.22903600
H	3.58600000	-0.76937500	1.33172800
C	1.90249000	-0.38730300	0.00036000
C	2.53854200	-0.50507900	-1.22803400
H	3.58663700	-0.76926600	-1.33025800
C	0.42862500	0.03962100	-1.87429500
C	1.68405000	-0.25414000	-2.31435800
H	-0.45771600	0.15008900	-2.51176900
H	1.96208400	-0.32163700	3.35935900
H	1.96353600	-0.32166800	-3.35861200
H	-0.45868500	0.15060500	2.51163400
Cl	-0.88611900	-2.24228600	-0.00035500
P	-2.79276700	0.36264700	0.00003900
H	-3.42561200	-0.28485700	-1.09236400
H	-3.42561800	-0.28494200	1.09238900
H	-3.45362700	1.62114700	0.00007100
B	0.22548400	1.96649000	-0.00005400
F	0.54906900	3.18958700	-0.00036500

12.triplet

E = -509.250828104 a.u.

1 3

Os	-0.31769200	-0.15947800	-0.00000800
C	0.14582900	-0.01781400	-2.01160600
C	1.42952800	0.39233500	-2.35341500
C	2.27088600	0.64744500	-1.26065300
H	3.29587200	0.99140700	-1.37376800

C	1.68665300	0.43551800	-0.00042500
C	2.27240700	0.64422400	1.25962800
H	3.29752000	0.98792500	1.37241100
Cl	-2.55451400	-0.77315800	-0.00022000
C	0.14825400	-0.02306500	2.01147900
C	1.43236500	0.38628700	2.35274900
H	-0.56079200	-0.26935900	2.80330100
P	-0.73453100	2.31386200	0.00303800
H	-2.08419000	2.75472800	0.00370900
H	-0.19287800	3.02233200	1.10637000
H	-0.19318100	3.02466500	-1.09893700
H	1.76349200	0.50808400	-3.37907800
H	1.76756200	0.49940900	3.37830200
H	-0.56434800	-0.26207400	-2.80303500
B	0.66552600	-1.87004900	-0.00194200
F	1.37967300	-2.90449000	-0.00303500

2 16e singlet

E = -502.222842207 a.u.

2 1

P	-0.02366500	2.44804200	0.17984200
C	-0.01859600	-0.21460900	1.85749900
C	1.18725400	-0.49976800	2.45477400
C	2.26246200	-0.37861800	1.56026000
H	3.29975200	-0.48596500	1.86662500
C	1.87644100	-0.09404200	0.25498500
C	2.72709900	0.09943500	-0.83604300
H	3.81150700	0.10495200	-0.76746800
H	-0.92549500	3.29043400	-0.51989000
H	-0.12066900	2.94647100	1.50542400
H	1.23707600	2.93731300	-0.24581700
C	0.67081400	0.15940000	-1.79422700
C	2.01510900	0.29160500	-2.03217700
H	-0.10788200	-0.05914200	-2.54884400
P	-0.31836200	-2.43247900	-0.33493100
H	0.87615000	-3.06042800	0.10101400
H	-1.31494800	-3.15140700	0.37182000
H	-0.46247600	-2.94215600	-1.65242300
H	1.29250500	-0.74028300	3.50770000
H	2.45294800	0.47732800	-3.00735800
H	-0.90554200	0.05012700	2.44454300
B	-2.42072300	0.13278800	-0.03639500
F	-3.66293000	0.20320600	-0.03669000
Os	-0.30600000	0.02271200	-0.09220000

2 16e triplet

E = -502.201883005 a.u.

2 3

P	-0.28524000	2.45519200	0.00003600
C	0.30290700	-0.00006600	1.93795200
C	1.67035900	-0.00009600	2.32552500
C	2.54750700	-0.00007300	1.25871500
H	3.62823700	-0.00009100	1.37242100
C	1.88293500	-0.00002500	0.00002700
C	2.54754600	0.00000300	-1.25864100
H	3.62828100	-0.00000100	-1.37231200
H	-0.92090500	3.08405200	-1.10095000
H	-0.92072800	3.08401600	1.10114600
H	0.99047100	3.07754200	-0.00005900
C	0.30296900	0.00003600	-1.93794700
C	1.67043200	0.00003400	-2.32547900
H	-0.45194800	0.00005600	-2.73161800
P	-0.28535600	-2.45518100	-0.00006300
H	0.99031900	-3.07760200	-0.00009200
H	-0.92095500	-3.08401000	1.10097900
H	-0.92098300	-3.08396000	-1.10111800
H	1.98406100	-0.00013400	3.36474800
H	1.98416700	0.00005400	-3.36469200
H	-0.45203100	-0.00008600	2.73160100
B	-2.34007200	0.00004300	-0.00000300
F	-3.59289300	0.00007500	0.00000200
Os	-0.28382300	0.00000300	-0.00000700

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