

## Supporting Information

### **Why is the energy of the singly occupied orbital in some radicals below the highest occupied orbital energy?**

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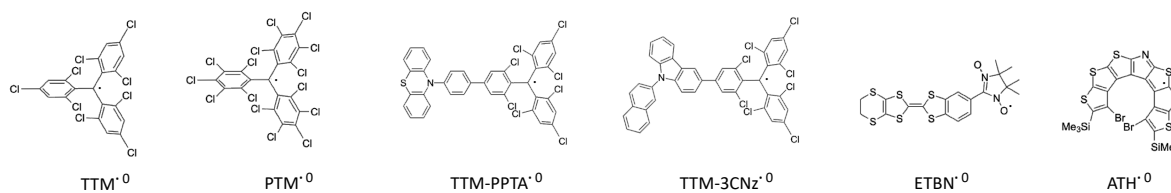


Figure S1: Chemical structures of the neutral radical systems studied in this work with the corresponding radical indicated by a dot in the structure:  $\text{TTM}^{\bullet 0}$ ,  $\text{PTM}^{\bullet 0}$ ,  $\text{TTM-PPTA}^{\bullet 0}$ ,  $\text{TTM-3CNz}^{\bullet 0}$ ,  $\text{ETBN}^{\bullet 0}$ ,  $\text{ATH}^{\bullet 0}$ . The labels are explained in the text.

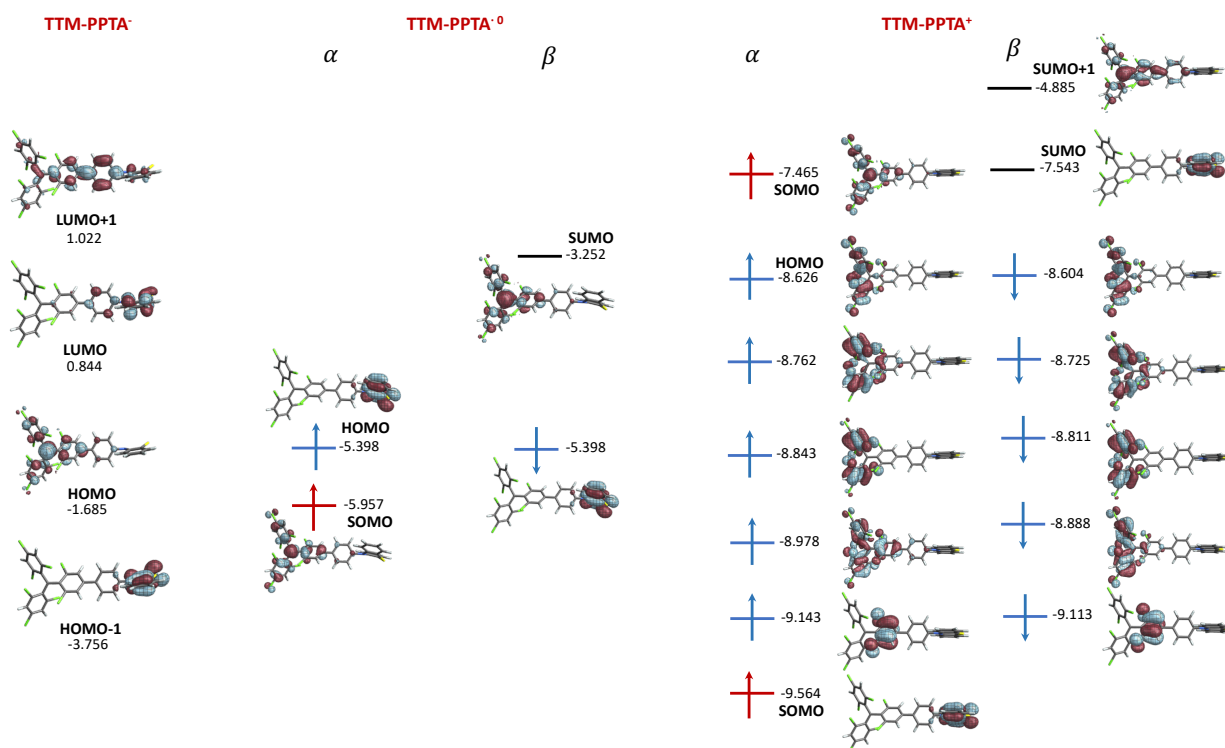


Figure S2: Orbital energies (in eV) and isosurfaces of selected molecular orbitals (MOs) ( $\pm 0.030$  au) for the TTM-PPTA system. From left to right: closed shell system, radical system, and bi-radical system.

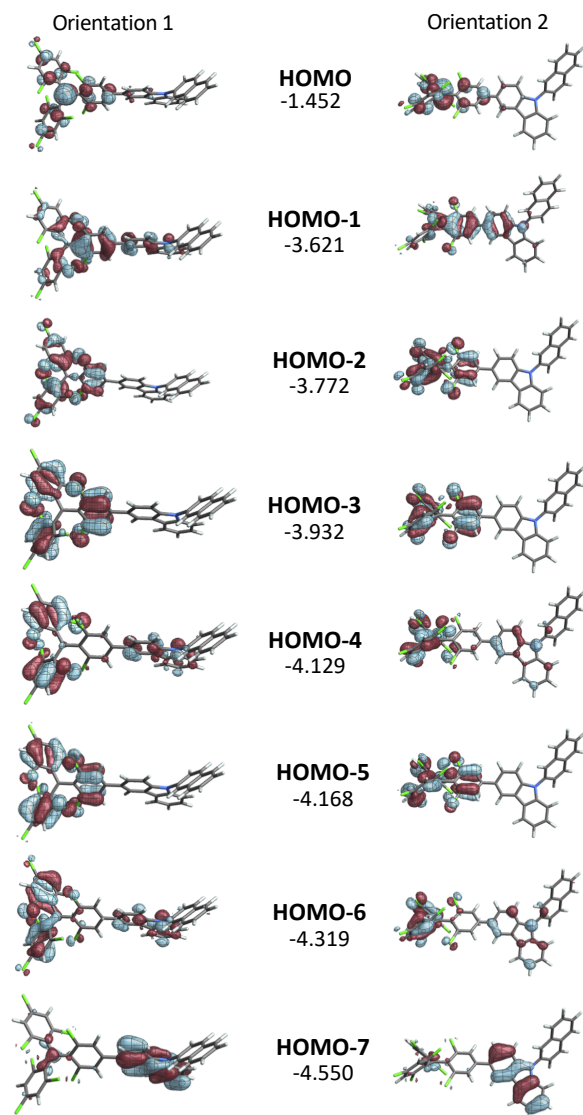


Figure S3: Orbital energies (in eV) and isosurfaces of molecular orbitals (MOs) ( $\pm 0.030$  au) for the TTM-3CNz system. Two orientations are plotted for the same system.

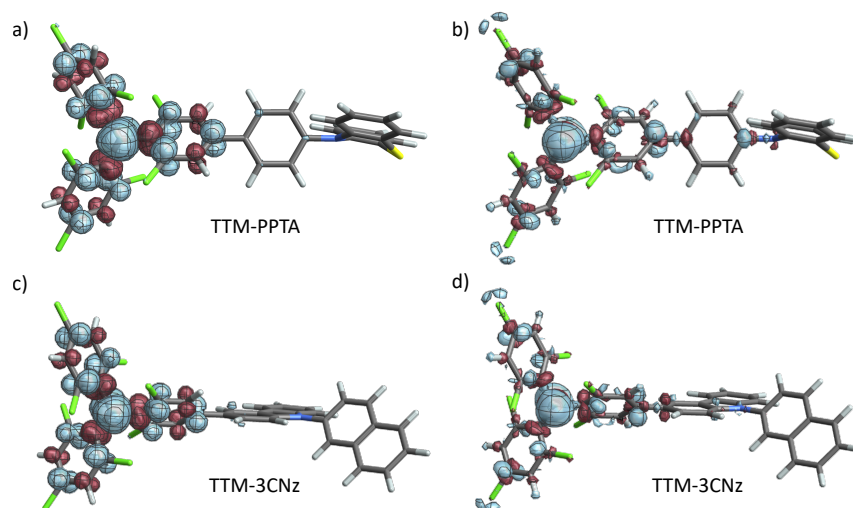


Figure S4: a) Isosurface ( $\pm 0.002$  a.u.) of the spin density of TTM-PPTA. b) Isosurface ( $\pm 0.002$  a.u.) of the density difference between the closed-shell parent and the radical (using the radical geometry) of TTM-PPTA. c) Isosurface ( $\pm 0.002$  a.u.) of the spin density of TTM-3CNz. d) Isosurface ( $\pm 0.002$  a.u.) of the density difference between the closed-shell parent and the radical (using the radical geometry) of TTM-3CNz.

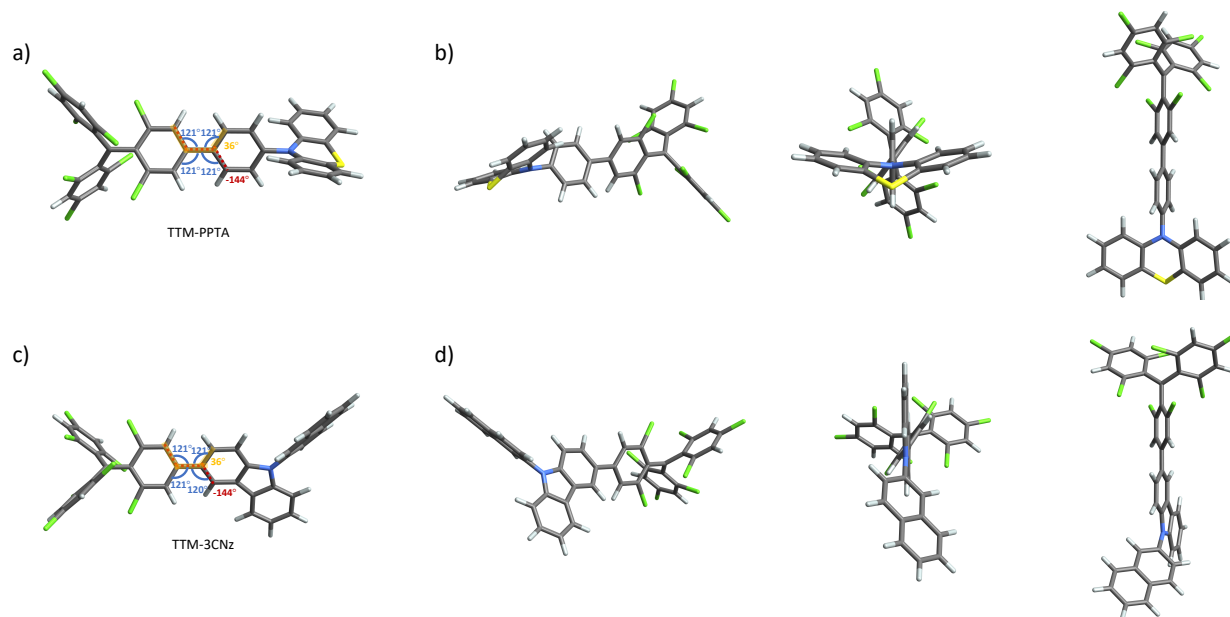


Figure S5: a) Structural parameters and b) different views of the DFT-optimized TTM-PPTA $^{\bullet 0}$  geometry. c) Structural parameters and d) different views of the DFT-optimized TTM-3CNz $^{\bullet 0}$  geometry. Angles (in blue) and dihedral angles (in orange and red) are indicated in the geometries.

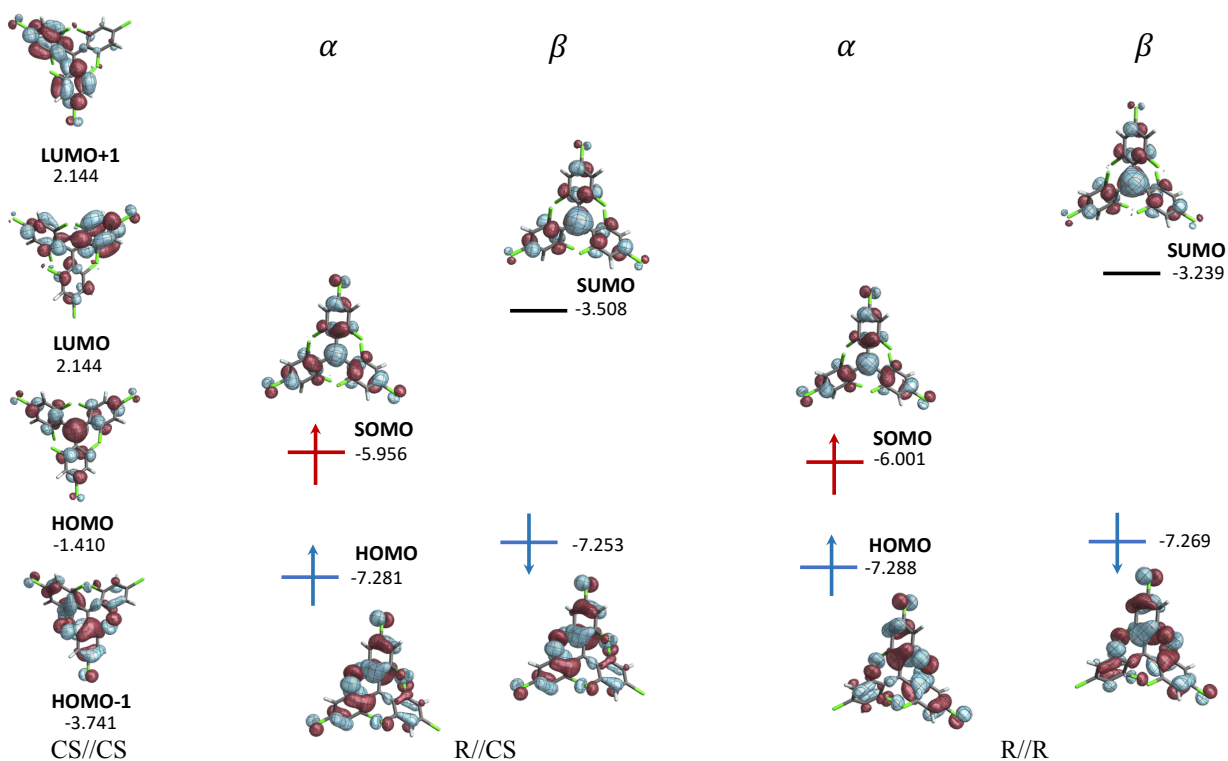


Figure S6: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of selected MOs of the TTM system. See Section 3.1 for a description of the labeling.

Table S1: MO energy contributions (in eV) for the TTM system.<sup>(a)</sup> The numbers are for the  $\alpha$  spin orbitals. See also Figure S6.

HOMO $\rightarrow$ SOMO	CS // CS	$\Delta \rightarrow$	$\tilde{R}$ // CS	$\Delta \rightarrow$	R // CS	$\Delta \rightarrow$	R // R
$T$	40.22	0.00	40.22	3.25	43.47	0.04	43.51
$V^{\text{nuc}}$	-1250 <sup>(b)</sup>	58.05	58.05	19.21	77.26	-11.11	66.15
$V^C$	+1250 <sup>(b)</sup>	-84.33	-6.42	-90.76	-19.96	-110.71	11.15
$V^{\text{XC}}$	-15.35	0.03	-15.32	-0.66	-15.97	-0.12	-16.09
total $\epsilon$	-1.41	-6.39	-7.80	1.84	-5.96	-0.04	-6.00
HOMO-1 $\rightarrow$ HOMO	CS // CS	$\Delta \rightarrow$	$\tilde{R}$ // CS	$\Delta \rightarrow$	R // CS	$\Delta \rightarrow$	R // R
$T$	49.16	0.00	49.16	1.57	50.73	-0.67	50.05
$V^{\text{nuc}}$	-1060 <sup>(c)</sup>	-101.25	0.00	-101.25	11.49	-89.76	4.79
$V^C$	+1060 <sup>(c)</sup>	64.84	-4.74	60.09	-11.77	48.33	-4.20
$V^{\text{XC}}$	-16.48	0.01	-16.47	-0.10	-16.57	0.08	-16.50
total $\epsilon$	-3.74	-4.74	-8.48	1.19	-7.28	-0.01	-7.29

<sup>(a)</sup> CS: Closed-shell system.  $\tilde{R}$ : Radical without SCF, using the MOs of the closed-shell system. R: Radical system. <sup>(b),(c)</sup> The listed number was subtracted from  $V^{\text{nuc}} / V^C$  to avoid large values in the other Table columns. Add it to get the full value of  $V^{\text{nuc}} / V^C$ .

Table S2: Selected Coulomb and exchange electron repulsion integrals (ERIs, in eV) for the closed-shell parent system of the TTM<sup>•0</sup>.

ERI Type	TTM
self-Coulomb <sup>(a)</sup> HOMO-1	4.938
Coulomb HOMO-1 / HOMO	4.743
self-Coulomb <sup>(a)</sup> HOMO	6.424
exchange HOMO-1 / HOMO	0.338

<sup>(a)</sup> This corresponds to the Coulomb repulsion between the  $\alpha$  spin and the  $\beta$  spin component of the MO.

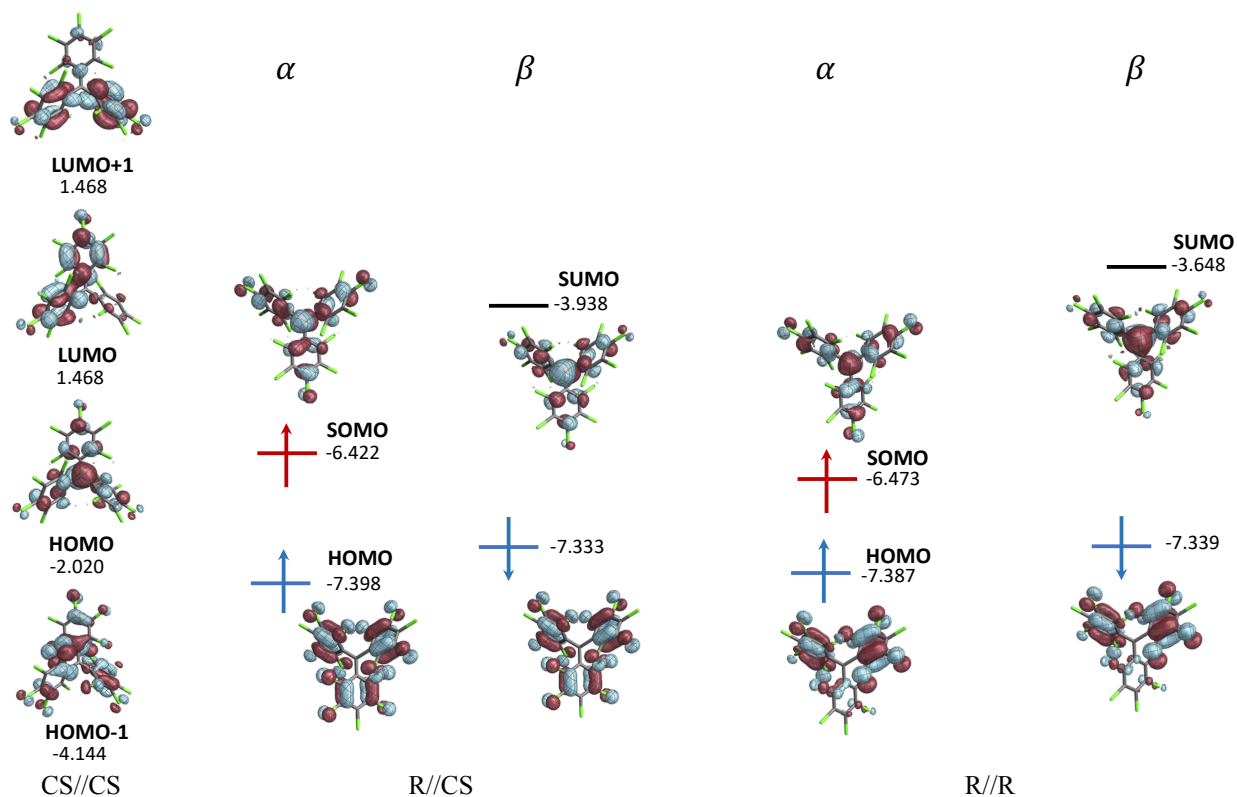


Figure S7: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of selected MOs of the PTM system. See Section 3.1 for a description of the labeling.

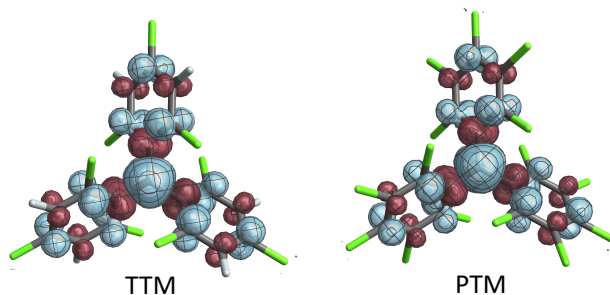


Figure S8: Isosurface ( $\pm 0.002$  a.u.) of the spin density for the TTM (left) and PTM (right) systems.

Table S3: MO energy contributions (in eV) for the PTM system.<sup>(a)</sup> The numbers are for the  $\alpha$  spin orbitals. See also Figure S7.

HOMO $\rightarrow$ SOMO		CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$		41.11	0.00	41.11	3.44	44.55	0.27	44.82
$V^{\text{nuc}}$	-1400 <sup>(b)</sup>	-66.09	0.00	-66.09	28.04	-38.04	-9.16	-47.20
$V^C$	+1400 <sup>(b)</sup>	38.43	-6.50	31.93	-28.76	3.17	8.97	12.14
$V^{\text{XC}}$		-15.47	0.04	-15.43	-0.66	-16.10	-0.14	-16.23
total $\epsilon$		-2.02	-6.47	-8.49	2.06	-6.42	-0.05	-6.47

HOMO-1 $\rightarrow$ HOMO		CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$		52.31	0.00	52.31	1.28	53.59	-0.22	53.37
$V^{\text{nuc}}$	-1350 <sup>(c)</sup>	-59.97	0.00	-59.97	30.30	-29.67	-3.63	-33.30
$V^C$	+1350 <sup>(c)</sup>	20.23	-4.44	15.78	-30.39	-14.61	3.82	-10.79
$V^{\text{XC}}$		-16.71	0.01	-16.71	0.00	-16.71	0.04	-16.67
total $\epsilon$		-4.14	-4.44	-8.58	1.18	-7.40	0.01	-7.39

<sup>(a)</sup> CS: Closed-shell system.  $\tilde{R}$ : Radical without SCF, using the MOs of the closed-shell system. R: Radical system. <sup>(b),(c)</sup> The listed number was subtracted from  $V^{\text{nuc}} / V^C$  to avoid large values in the other Table columns. Add it to get the full value of  $V^{\text{nuc}} / V^C$ .

Table S4: Selected Coulomb and exchange electron repulsion integrals (ERIs, in eV) for the closed-shell parent system of PTM $\cdot^0$ .

ERI Type	PTM
self-Coulomb <sup>(a)</sup> HOMO-1	4.317
Coulomb HOMO-1 / HOMO	4.444
self-Coulomb <sup>(a)</sup> HOMO	6.502
exchange HOMO-1 / HOMO	0.272

<sup>(a)</sup> This corresponds to the Coulomb repulsion between the  $\alpha$  spin and the  $\beta$  spin component of the MO.

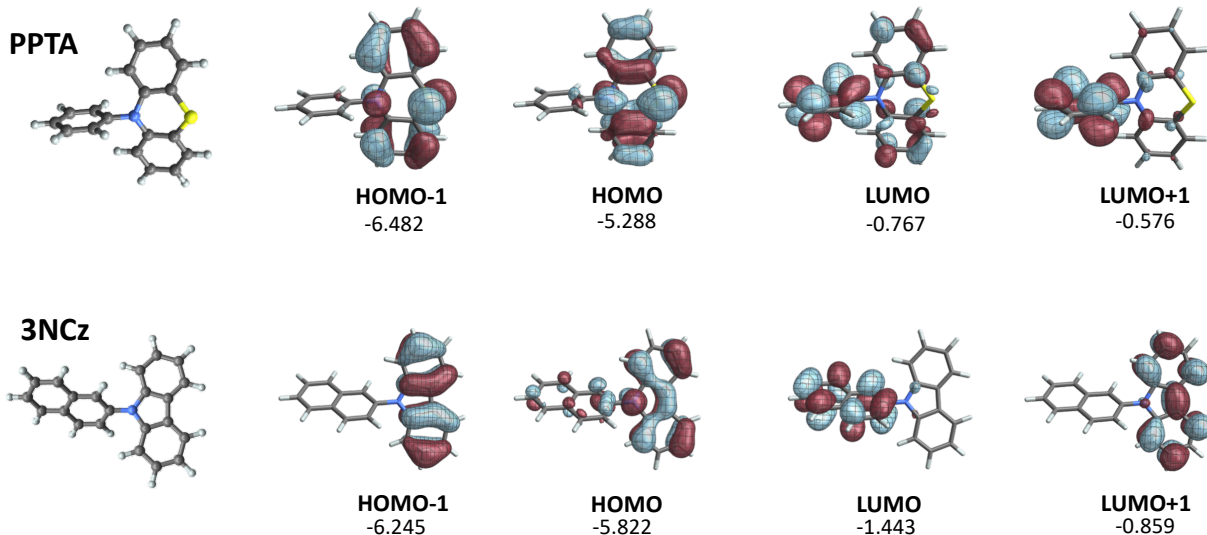


Figure S9: DFT-optimized structures of the PPTA and 3NCz systems, and their frontier molecular orbitals (MOs) with the corresponding isosurfaces ( $\pm 0.030$  a.u.) and orbital energies (in eV).

Table S5: MO energy contributions (in eV) for the ETBN system.<sup>(a)</sup> The numbers are for the  $\alpha$  spin orbitals. See also Figure S17.

HOMO $\rightarrow$ SOMO	CS // CS	$\Delta$ $\rightarrow$	$\tilde{R}$ // CS	$\Delta$ $\rightarrow$	R // CS	$\Delta$ $\rightarrow$	R // R
$T$	65.32	0.00	65.32	2.61	67.92	1.72	69.65
$V^{\text{nuc}}$	-1000 <sup>(b)</sup>	17.27	17.27	-10.27	7.00	-8.20	-1.20
$V^C$	+1000 <sup>(b)</sup>	-62.12	-9.20	-71.32	11.36	-59.96	7.47
$V^{\text{XC}}$		-20.53	0.05	-20.48	-0.90	-21.38	-0.15
total $\epsilon$		-0.07	-9.15	-9.21	2.80	-6.42	0.85
HOMO-4 $\rightarrow$ HOMO	CS // CS	$\Delta$ $\rightarrow$	$\tilde{R}$ // CS	$\Delta$ $\rightarrow$	R // CS	$\Delta$ $\rightarrow$	R // R
$T$	49.49	0.00	49.49	0.09	49.58	0.00	49.59
$V^{\text{nuc}}$	-1000 <sup>(b)</sup>	-16.69	0.00	-16.69	1.95	-14.74	-0.15
$V^C$	+1000 <sup>(b)</sup>	-19.63	-2.87	-22.51	-1.81	-24.32	0.18
$V^{\text{XC}}$		-16.06	0.01	-16.05	0.48	-15.57	-0.01
total $\epsilon$		-2.89	-2.87	-5.76	0.71	-5.05	0.03

<sup>(a)</sup> CS: Closed-shell system.  $\tilde{R}$ : Radical without SCF, using the MOs of the closed-shell system. R: Radical system. <sup>(b)</sup> The listed number was subtracted from  $V^{\text{nuc}} / V^C$  to avoid large values in the other Table columns. Add it to get the full value of  $V^{\text{nuc}} / V^C$ .



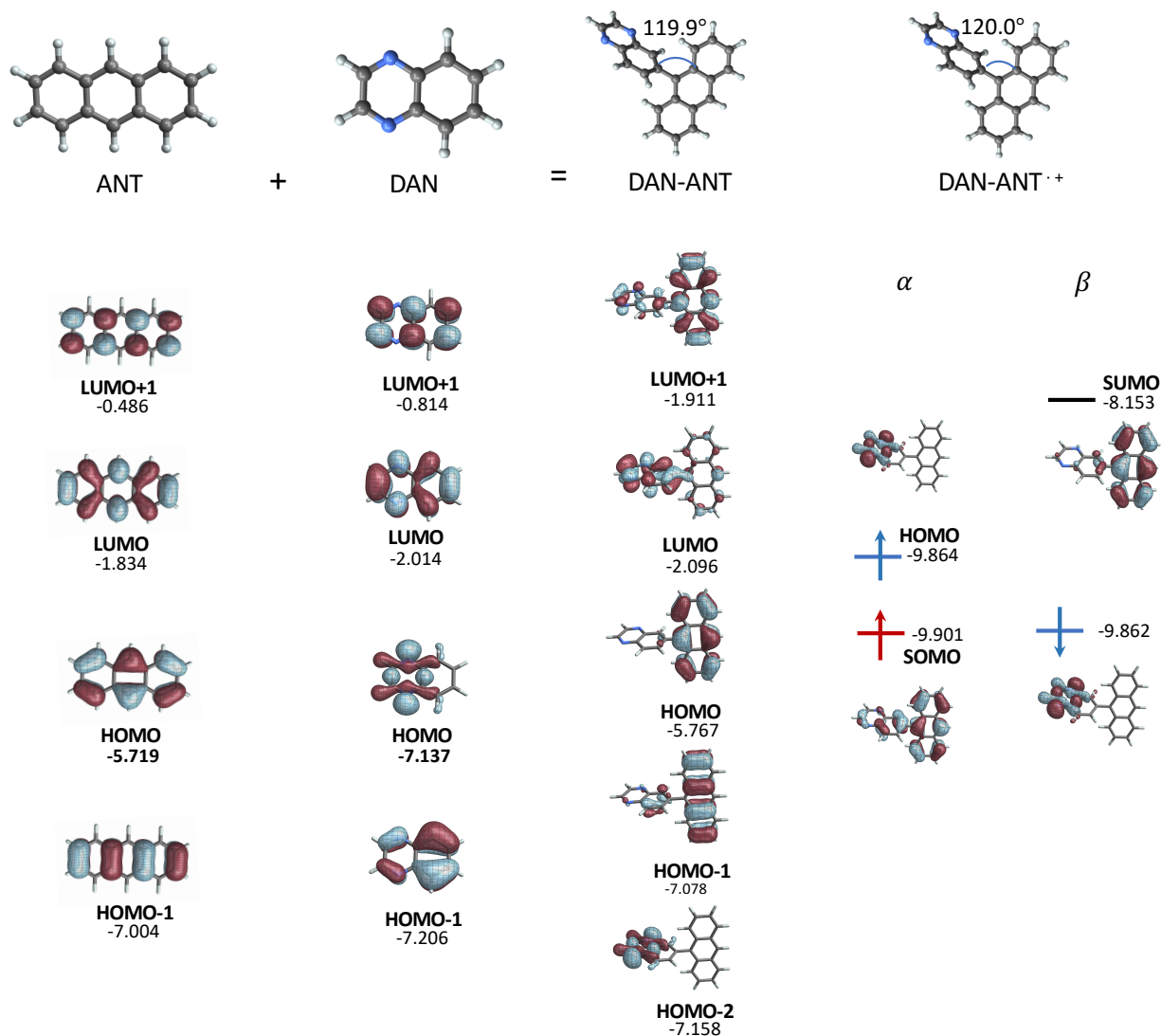


Figure S10: Isosurfaces ( $\pm 0.030$  au) of frontier molecular orbitals (MOs) of the ANT, DAN and DAN-ANT systems. The latter is shown in its closed-shell configuration and in the radical cation form.

Table S6: Selected Coulomb and exchange electron repulsion integrals (ERIs, in eV) for the closed-shell parent system of  $\text{ETBN}^{\cdot 0}$ .

ERI Type	ETBN
self-Coulomb <sup>(a)</sup> HOMO-4	4.925
self-Coulomb <sup>(a)</sup> HOMO-1	7.605
Coulomb HOMO-4 / HOMO	2.875
Coulomb HOMO-1 / HOMO	7.740
self-Coulomb <sup>(a)</sup> HOMO	9.196
exchange HOMO-1 / HOMO	2.460

<sup>(a)</sup> This corresponds to the Coulomb repulsion between the  $\alpha$  spin and the  $\beta$  spin component of the MO.

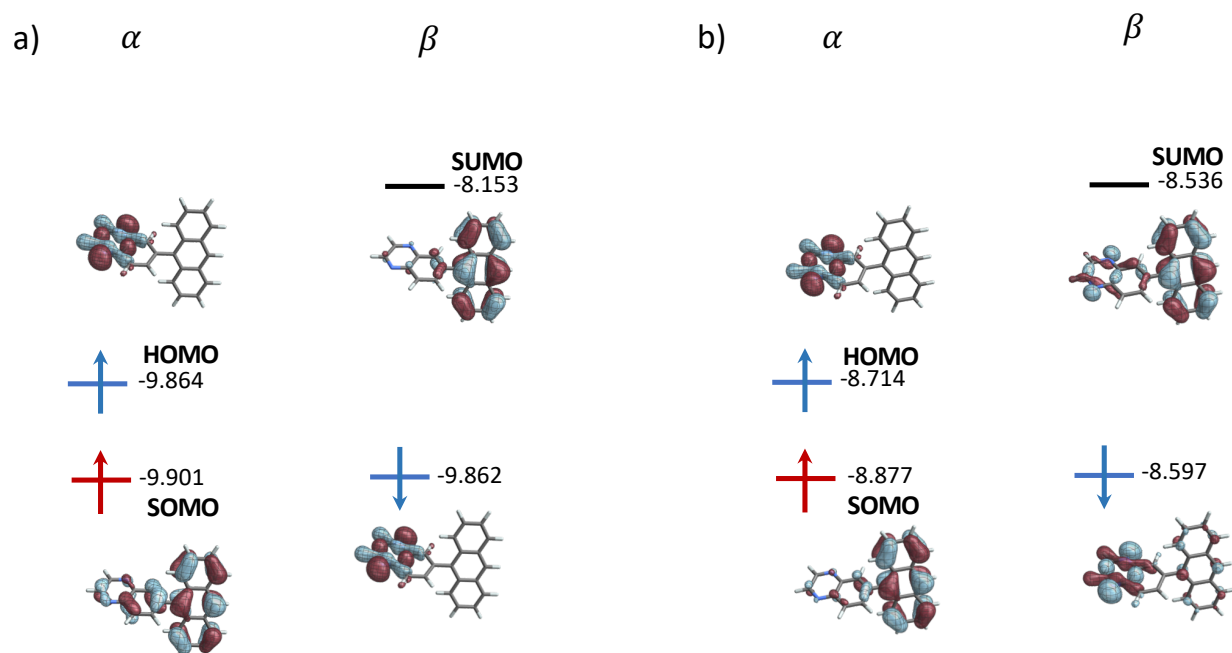


Figure S11: Isosurfaces ( $\pm 0.030$  au) of frontier molecular orbitals (MOs) of the radical cation system DAN-ANT $^{\bullet+}$  using a) PBE0 and b) PBE functionals.

Table S7: MO energy contributions (in eV) for the BCz system.<sup>(a)</sup> The numbers are for the  $\alpha$  spin orbitals. See also Figure S19.

HOMO $\rightarrow$ SOMO	CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$	41.18	0.00	41.18	0.51	41.69	-3.13	38.57
$V^{\text{nuc}}$	-1000 <sup>(b)</sup>	60.96	60.96	2.44	63.40	-0.70	62.70
$V^C$	+1000 <sup>(b)</sup>	-91.63	-96.01	-2.04	-98.05	3.36	-94.69
$V^{\text{XC}}$	-16.09	0.01	-16.08	-0.18	-16.26	0.58	-15.68
total $\epsilon$	-5.57	-4.37	-9.94	0.73	-9.21	0.11	-9.11
HOMO-1 $\rightarrow$ HOMO	CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$	40.41	0.00	40.41	-0.16	40.25	2.44	42.70
$V^{\text{nuc}}$	-1000 <sup>(b)</sup>	60.51	60.51	2.67	63.18	-6.69	56.48
$V^C$	+1000 <sup>(b)</sup>	-90.63	-95.01	-1.74	-96.75	5.43	-91.32
$V^{\text{XC}}$	-16.01	0.01	-15.99	-0.01	-16.01	-0.38	-16.39
total $\epsilon$	-5.71	-4.37	-10.08	0.75	-9.33	0.79	-8.54

<sup>(a)</sup> CS: Closed-shell system.  $\tilde{R}$ : Radical without SCF, using the MOs of the closed-shell system. R: Radical system. <sup>(b)</sup> The listed number was subtracted from  $V^{\text{nuc}} / V^C$  to avoid large values in the other Table columns. Add it to get the full value of  $V^{\text{nuc}} / V^C$ .

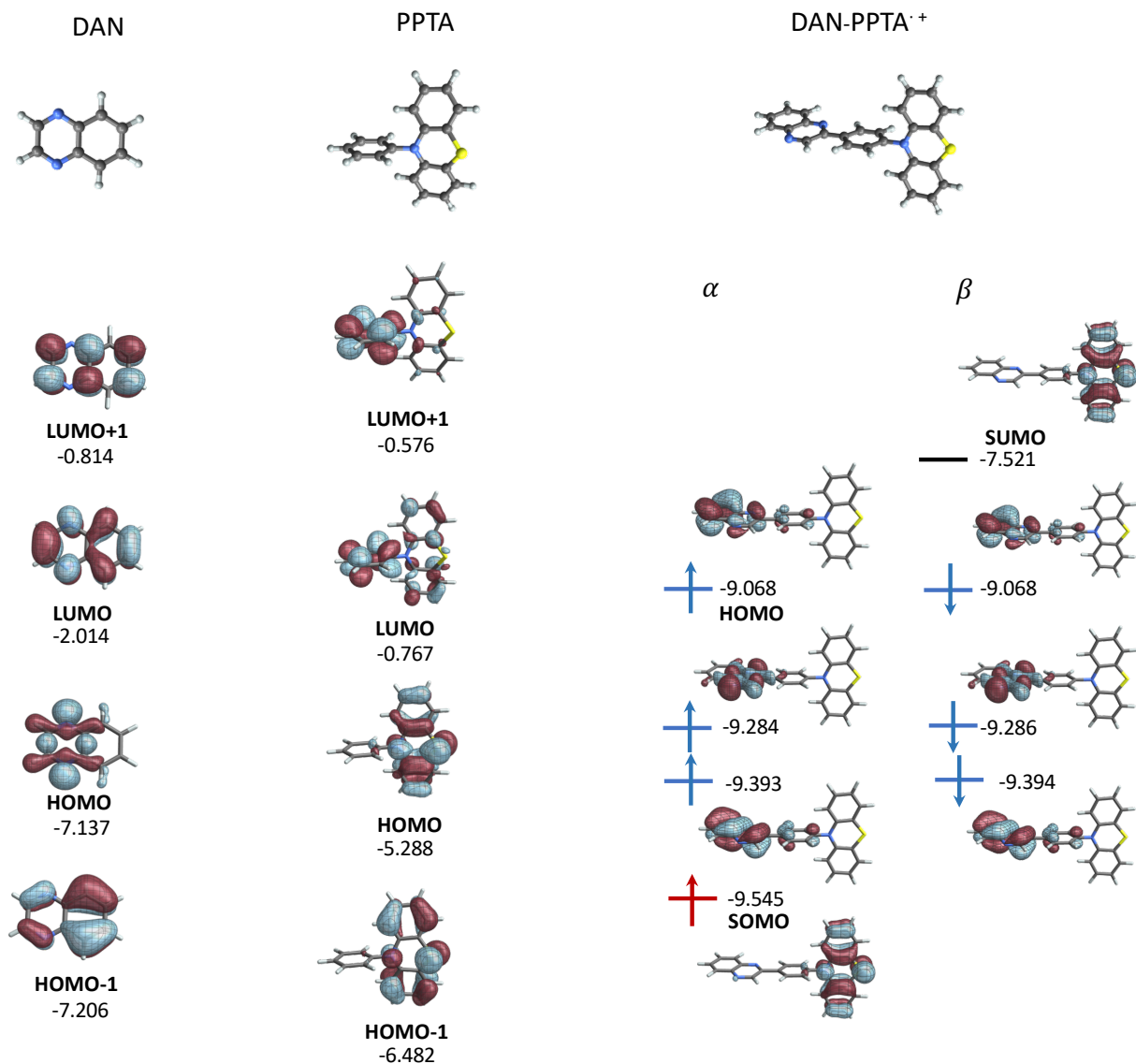


Figure S12: DAN, PPTA and the corresponding combined system DAN-PPTA<sup>•+</sup> in the radical cation form. The isosurfaces ( $\pm 0.03$  a.u.) of the frontier molecular orbitals (MOs) are also plotted with their corresponding orbital energy in eV.

Table S8: Selected Coulomb and exchange electron repulsion integrals (ERIs, in eV) for the closed-shell parent system of BCz<sup>•+</sup>.

ERI Type	BCz
self-Coulomb <sup>(a)</sup> HOMO-1	4.442
Coulomb HOMO-1 / HOMO	4.382
self-Coulomb <sup>(a)</sup> HOMO	4.380
exchange HOMO-1 / HOMO	1.630

<sup>(a)</sup> This corresponds to the Coulomb repulsion between the  $\alpha$  spin and the  $\beta$  spin component of the MO.

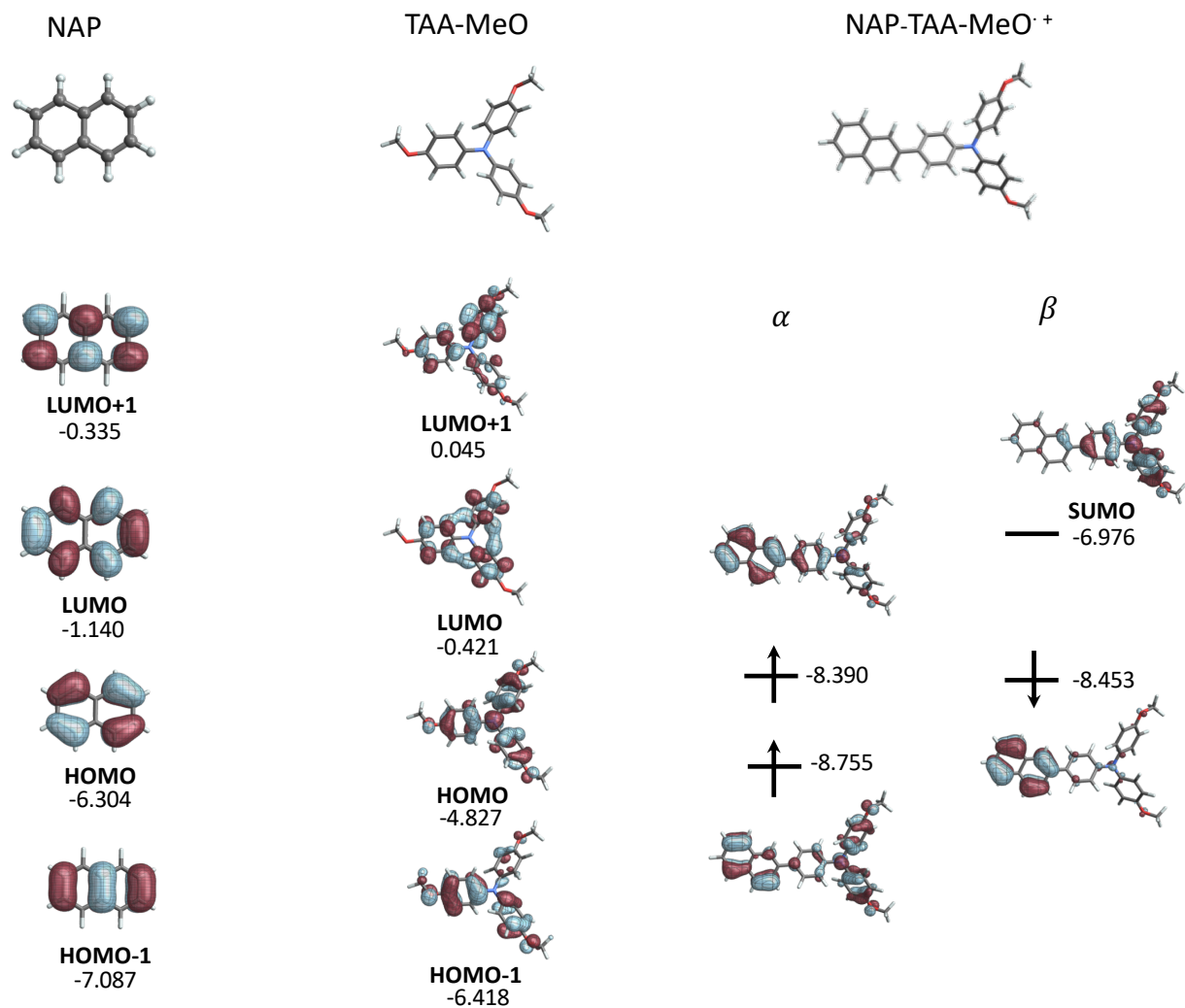


Figure S13: Naphtalene (NAP), TAA-MeO and the corresponding combined system NAP-TAA-MeO<sup>•+</sup> in the radical cation form. The isosurfaces ( $\pm 0.03$  a.u.) of the frontier molecular orbitals (MOs) are also plotted with their corresponding orbital energy in eV.

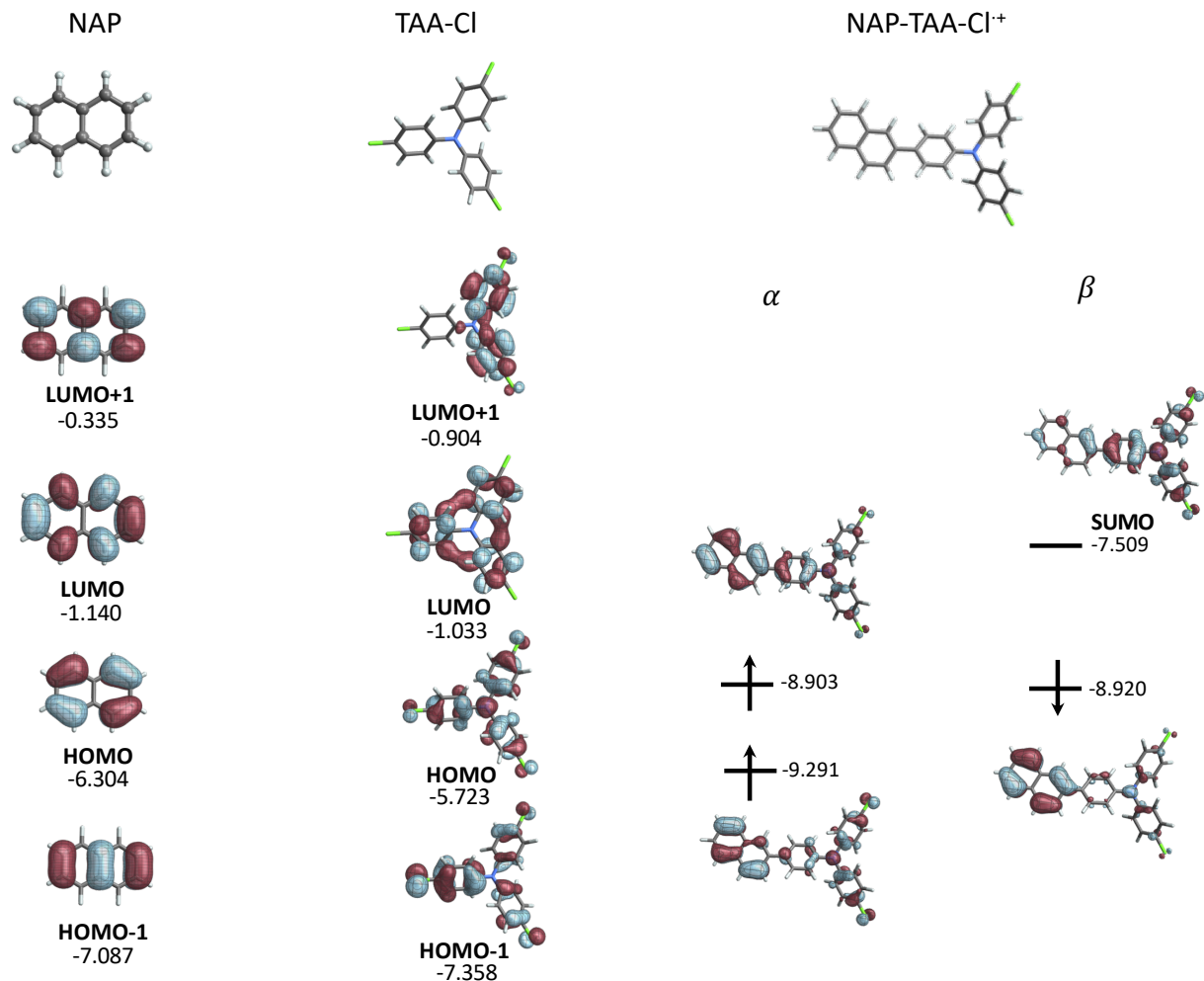


Figure S14: Naphtalene (NAP), TAA-Cl and the corresponding combined system NAP-TAA-Cl<sup>•+</sup> in the radical cation form. The isosurfaces ( $\pm 0.03$  a.u.) of the frontier molecular orbitals (MOs) are also plotted with their corresponding orbital energy in eV.

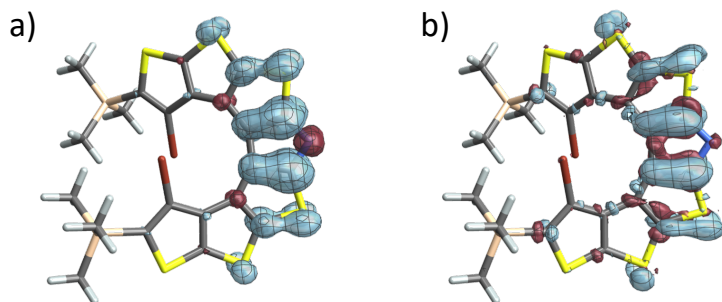


Figure S15: a) Isosurface ( $\pm 0.002$  a.u.) of the spin density of ATH<sup>•0</sup> b) Isosurface ( $\pm 0.002$  a.u.) of the density difference between the closed-shell parent and the radical (using the radical geometry) of ATH<sup>•0</sup>.

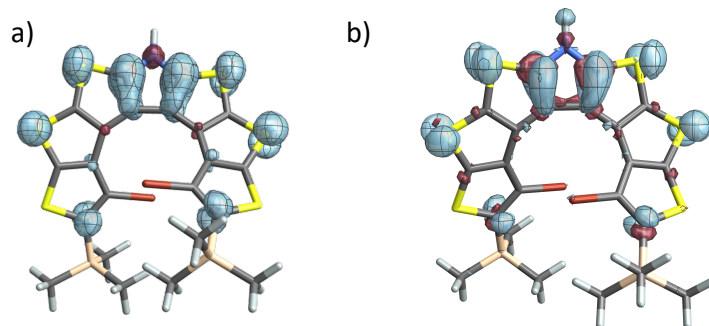


Figure S16: a) Isosurface ( $\pm 0.002$  a.u.) of the spin density and b) Isosurface ( $\pm 0.002$  a.u.) of the density difference between the closed-shell parent and the radical cation (using the radical geometry) of the N-protonated form of ATH.

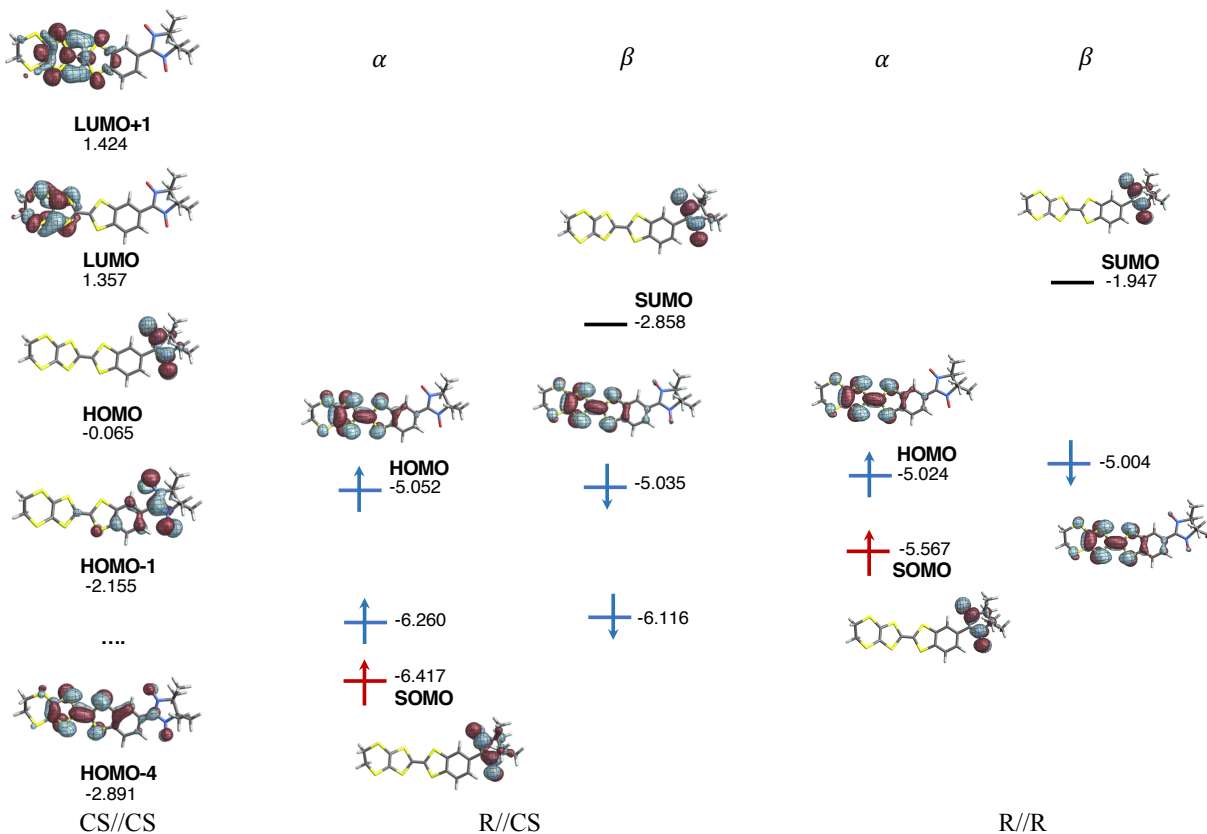


Figure S17: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of selected MOs of the ETBN system. See Section 3.1 for a description of the labeling.

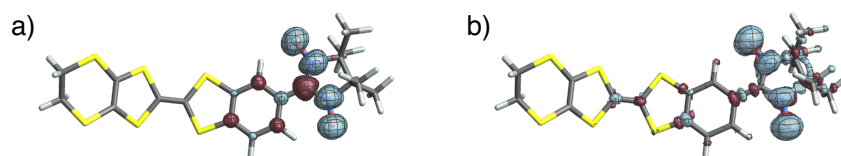


Figure S18: a) Isosurface ( $\pm 0.003$  a.u.) of the spin density of  $\text{ETBN}^{\bullet 0}$ . b) Isosurface ( $\pm 0.003$  a.u.) of the density difference between the closed-shell parent and the radical (using the radical geometry) of  $\text{ETBN}^{\bullet 0}$ .

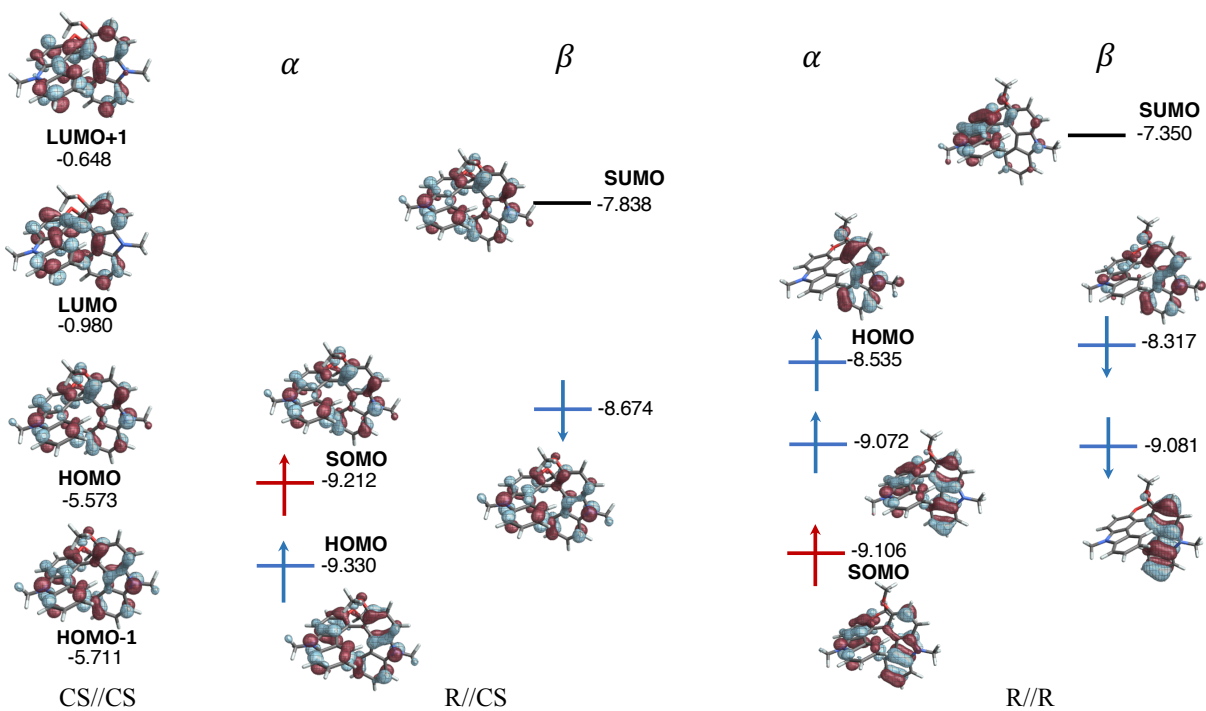


Figure S19: Orbital energies (in eV) and isosurfaces ( $\pm 0.035$  a.u.) of selected MOs of the BCz system. See Section 3.1 for a description of the labeling.

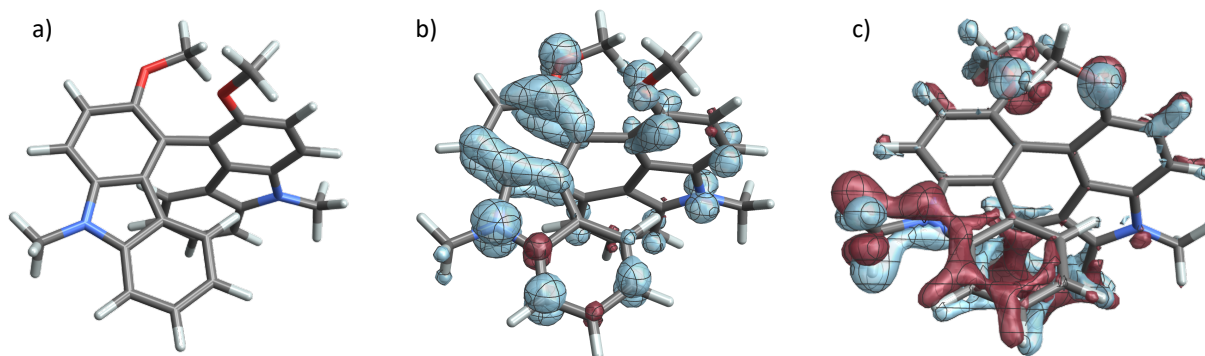


Figure S20: a) DFT-optimized structure of BCz<sup>•+</sup>. b) Isosurface ( $\pm 0.002$  a.u.) of the spin density and c) Isosurface ( $\pm 0.035$  a.u.) of the density difference between the neutral and the radical cation (using the radical geometry) of BCz system.

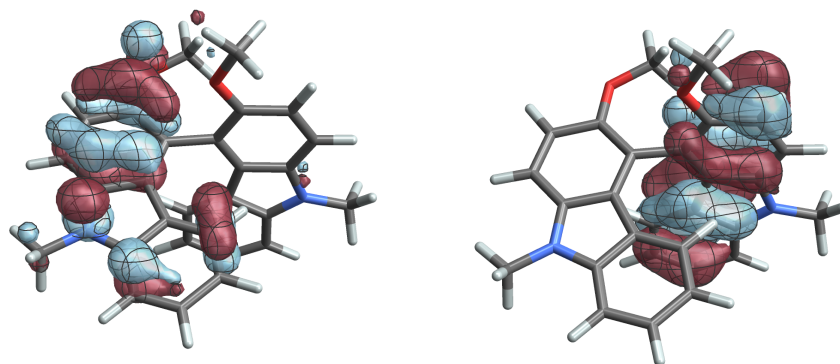


Figure S21: Isosurfaces ( $\pm 0.035$  a.u.) of normalized  $\pm$  linear combinations of the second and third highest occupied  $\alpha$  spin molecular orbital of the radical cation BCz<sup>•+</sup>. The orbital on the left closely matches the appearance of the SUMO and therefore constitutes the SOMO.



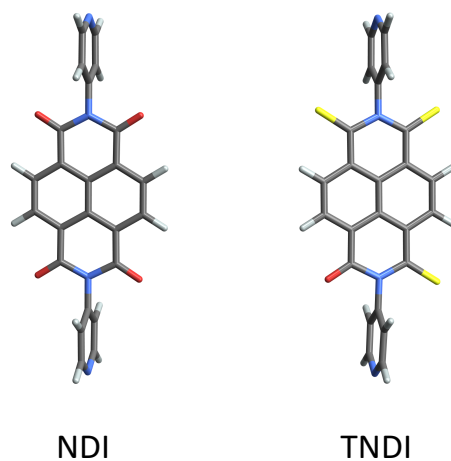


Figure S22: Optimized geometries of the selected naphthalene diimide (NDI) and thionated NDI (TNDI) derivatives used in this work.

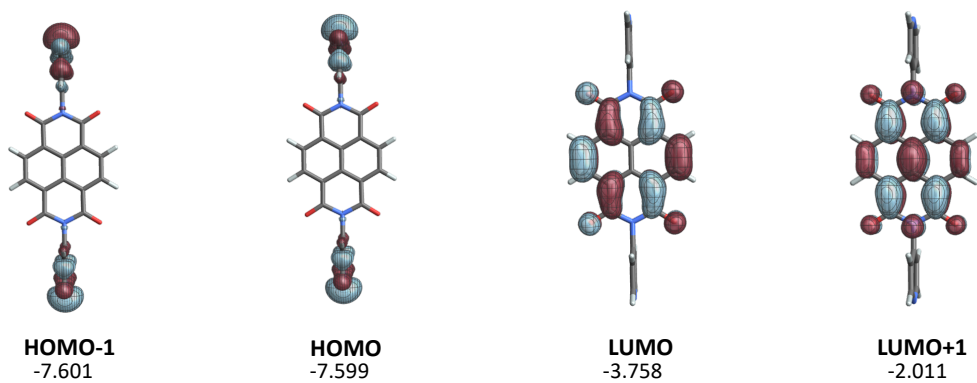


Figure S23: Isosurfaces ( $\pm 0.03$  a.u.) of the frontier molecular orbitals (MOs) of a selected axially substituted naphthalene diimide (NDI) derivative.

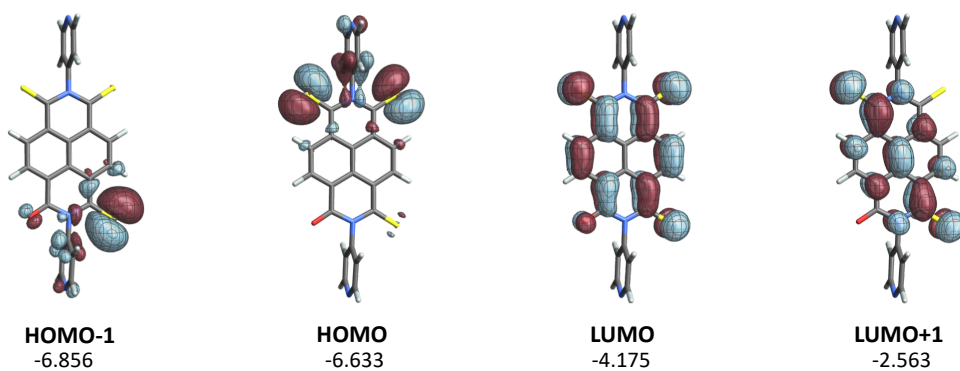


Figure S24: Isosurfaces ( $\pm 0.03$  a.u.) of the frontier molecular orbitals (MOs) of a selected axially substituted thionated naphthalene diimide (TNDI) derivative.

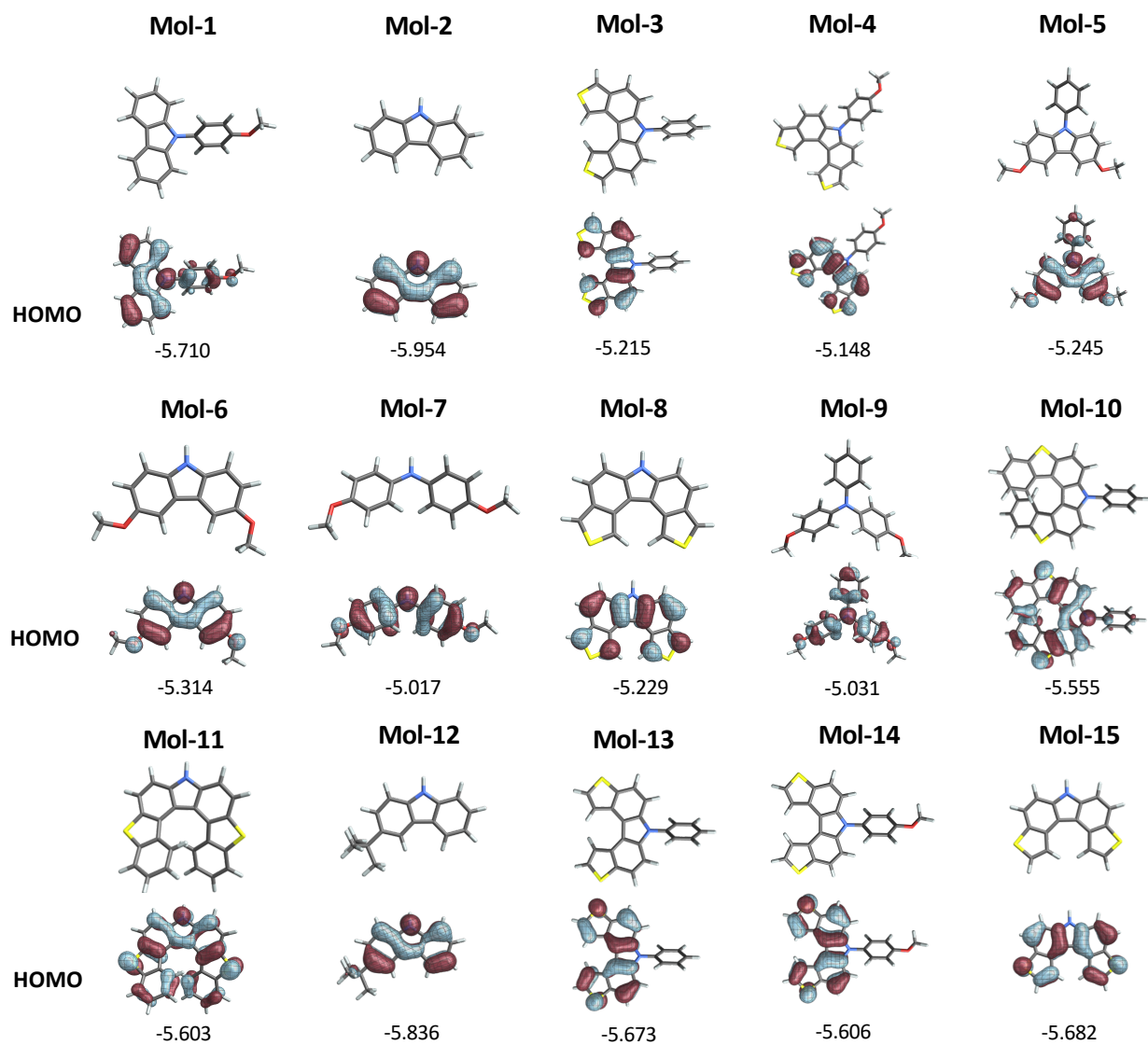


Figure S25: Organic molecules acting as electron-rich group. Mol-X (X=1-15) is the label for each molecule. The isosurface ( $\pm 0.03$  a.u.) of the HOMO and the corresponding orbital energy (in eV) are shown below each molecule.

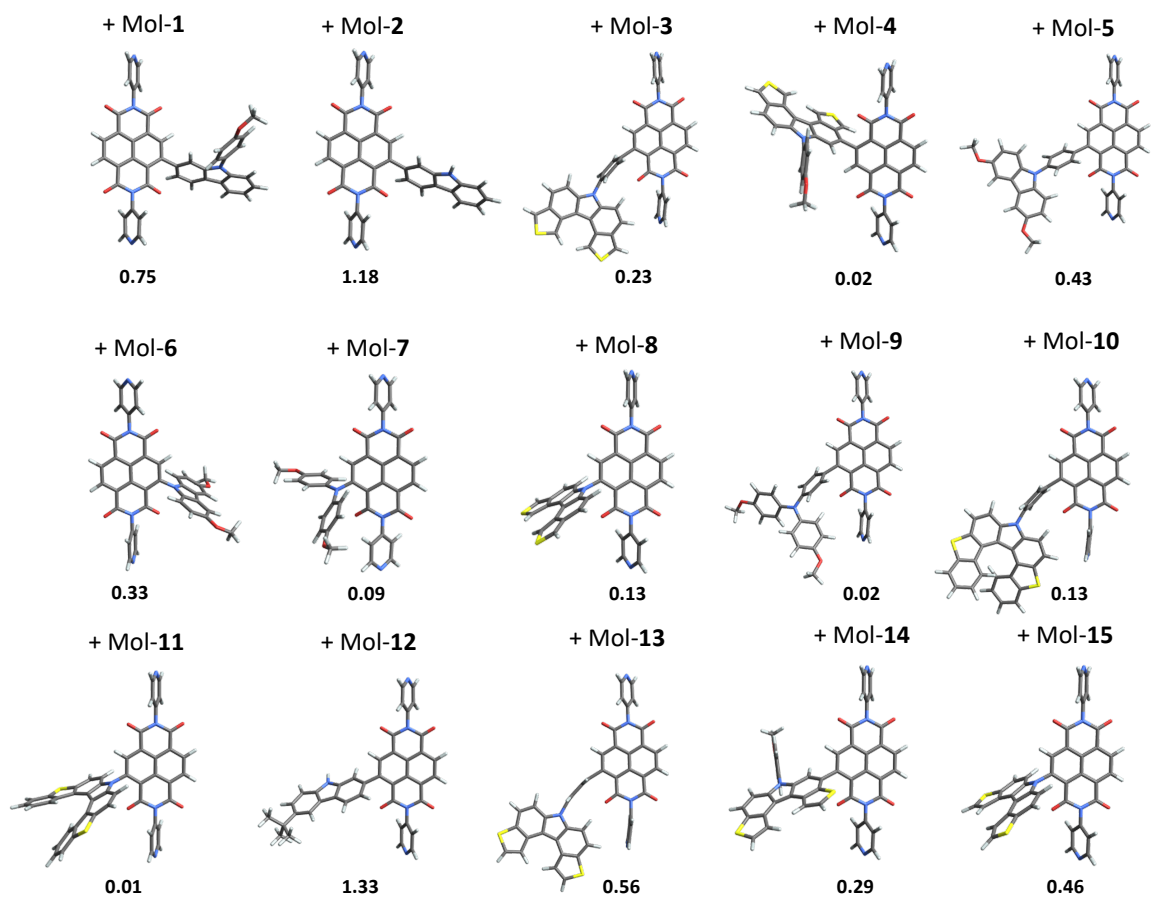


Figure S26: Combined systems between the NDI and the Mol-X (X=1-15) in the radical cation form (NDI-Mol-X<sup>•+</sup>). All the systems show SOMO/HOMO inversion (SHI). The energy difference (in eV) between the SOMO and the HOMO is indicated for each system. The numbers are for the  $\alpha$  spin orbitals.

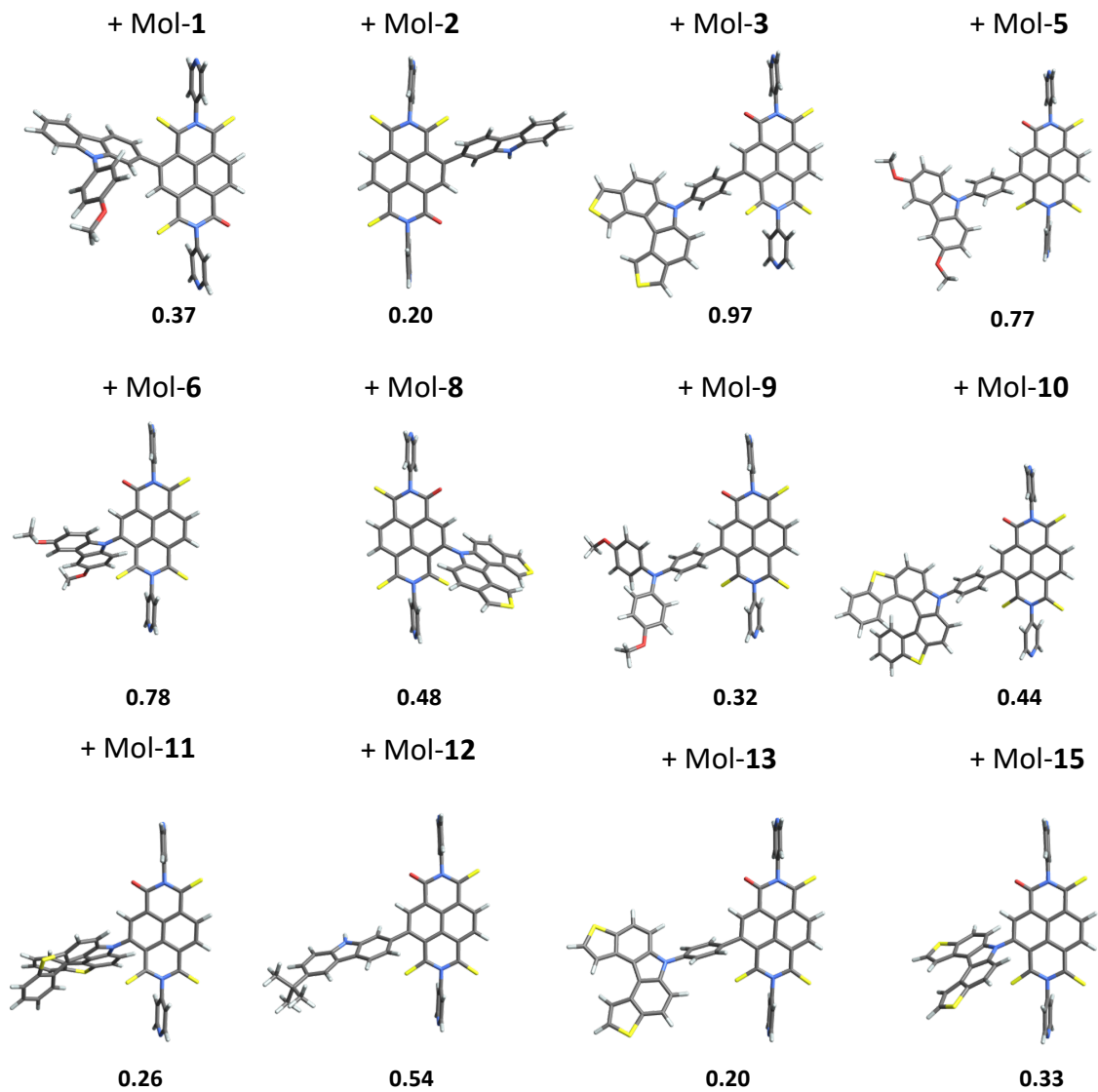


Figure S27: Combined systems between the TNDI and the Mol-X (X=1-15) in the radical cation form (TNDI-Mol-X<sup>•+</sup>). All the systems show SOMO/HOMO inversion (SHI). The energy difference (in eV) between the SOMO and the HOMO is indicated for each system. The numbers are for the  $\alpha$  spin orbitals.

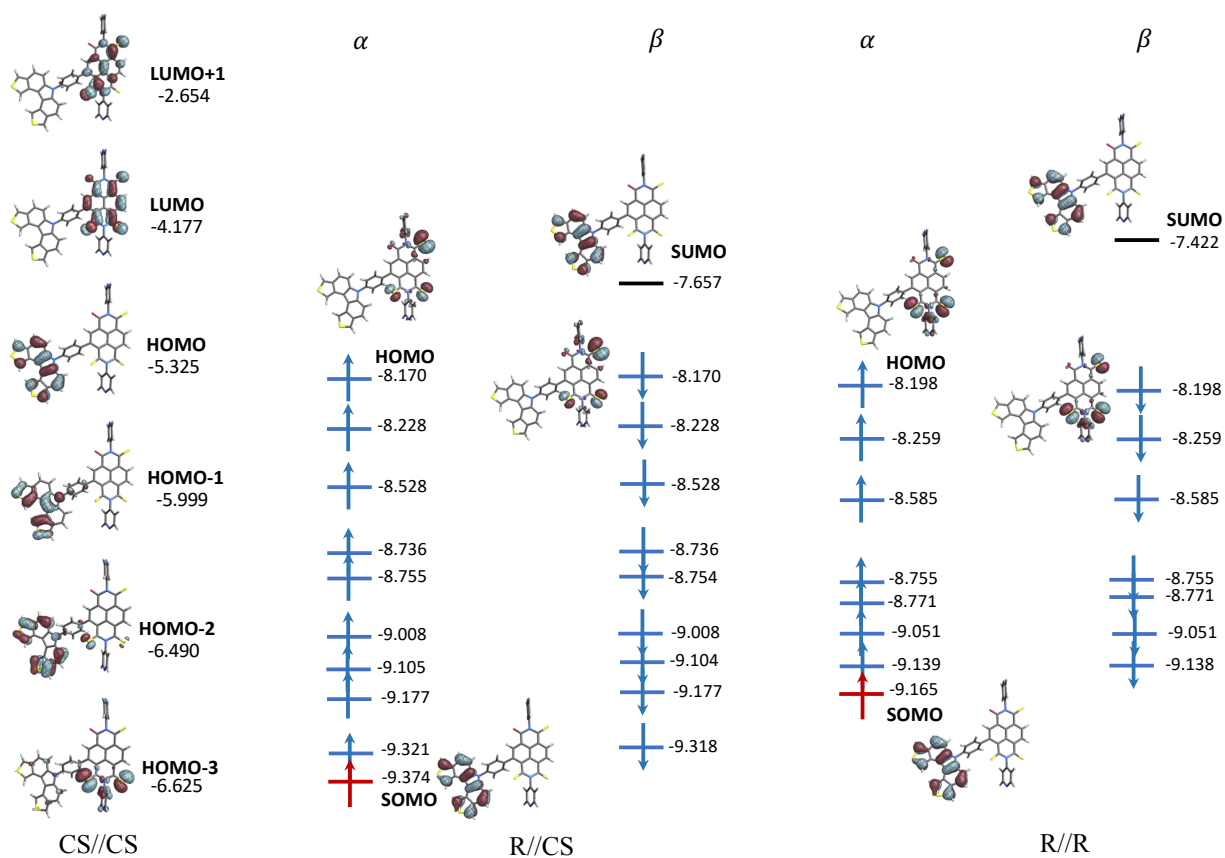


Figure S28: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of selected MOs of the TNDI-Mol-3 system. See Section 3.1 for a description of the labeling.

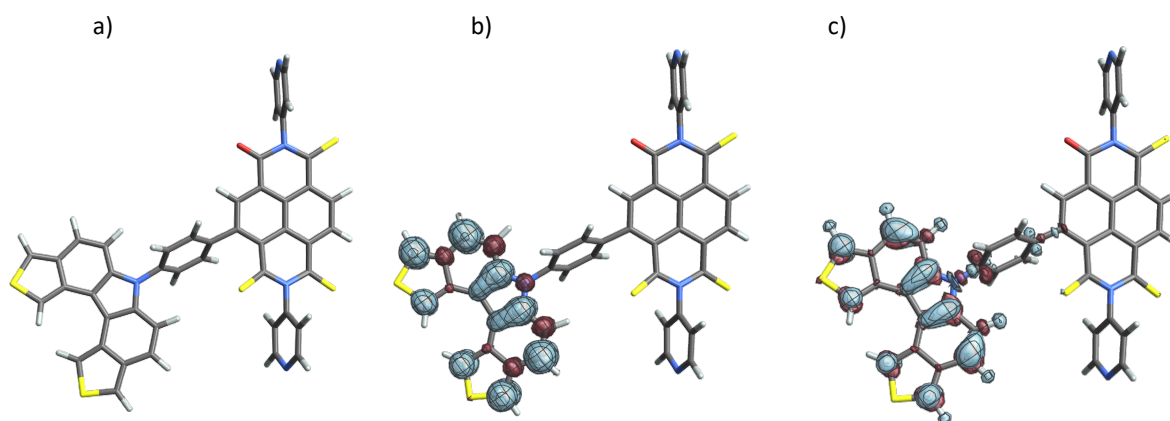


Figure S29: a) DFT-optimized structure of TNDI-Mol-3<sup>•+</sup>. b) Isosurface ( $\pm 0.002$  a.u.) of the spin density and c) Isosurface ( $\pm 0.002$  a.u.) of the density difference between the neutral and radical cation (using the radical geometry) of TNDI-Mol-3 system.

Table S9: MO energy contributions (in eV) for the TNDI-Mol-3 system.<sup>(a)</sup> The numbers are for the  $\alpha$  spin orbitals. See also Figure S28.

HOMO $\rightarrow$ SOMO		CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$		34.65	0.00	34.65	0.77	35.42	0.09	35.51
$V^{\text{nuc}}$	-1150 <sup>(b)</sup>	21.92	0.00	21.92	9.65	31.58	-2.26	29.32
$V^C$	+1150 <sup>(b)</sup>	-47.21	-5.11	-52.32	-9.13	-61.44	2.33	-59.12
$V^{\text{XC}}$		-14.69	0.02	-14.67	-0.26	-14.93	0.05	-14.87
total $\epsilon$		-5.32	-5.09	-10.42	1.04	-9.37	0.21	-9.17

HOMO-3 $\rightarrow$ HOMO		CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$		50.32	0.00	50.32	1.60	51.92	0.19	52.12
$V^{\text{nuc}}$	-1200 <sup>(c)</sup>	-53.44	0.00	-53.44	88.15	34.71	-60.23	-25.52
$V^C$	+1200 <sup>(c)</sup>	12.51	-1.98	10.53	-89.18	-78.65	60.02	-18.63
$V^{\text{XC}}$		-16.01	0.00	-16.01	-0.14	-16.15	-0.01	-16.16
total $\epsilon$		-6.63	-1.97	-8.60	0.43	-8.17	-0.03	-8.20

<sup>(a)</sup> CS: Closed-shell system.  $\tilde{R}$ : Radical without SCF, using the MOs of the closed-shell system. R: Radical system. <sup>(b),(c)</sup> The listed number was subtracted from  $V^{\text{nuc}} / V^C$  to avoid large values in the other Table columns. Add it to get the full value of  $V^{\text{nuc}} / V^C$ .

Table S10: Selected Coulomb and exchange electron repulsion integrals (ERIs, in eV) for the closed-shell parent systems of NDI-Mol-2 $\cdot^+$  and NDI-Mol-12 $\cdot^+$

ERI Type	NDI-Mol-2	NDI-Mol-12
self-Coulomb <sup>(a)</sup> HOMO-4	-	4.928
self-Coulomb <sup>(a)</sup> HOMO-3	12.949	-
self-Coulomb <sup>(a)</sup> HOMO-1	5.725	5.701
Coulomb HOMO-4 / HOMO	-	1.641
Coulomb HOMO-3 / HOMO	1.235	-
Coulomb HOMO-1 / HOMO	5.274	5.200
self-Coulomb <sup>(a)</sup> HOMO	6.222	6.154
exchange HOMO-1 / HOMO	0.305	0.300

<sup>(a)</sup> This corresponds to the Coulomb repulsion between the  $\alpha$  spin and the  $\beta$  spin component of the MO.

NDI-Mol-2 vs. NDI-Mol-12

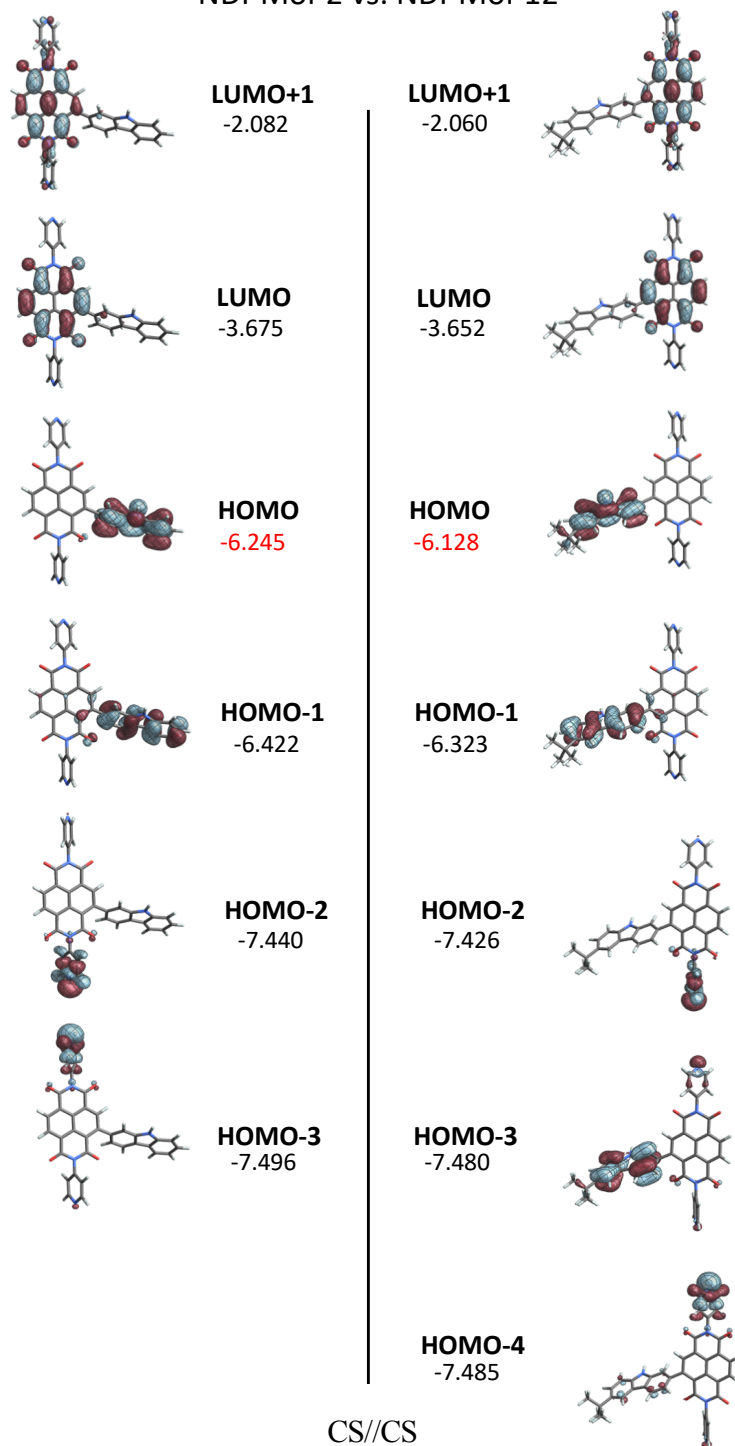


Figure S30: Isosurfaces ( $\pm 0.03$  a.u.) and orbital energies (in eV) of selected molecular orbitals (MOs) of the NDI-Mol2 and NDI-Mol-12 systems in their closed-shell configuration.

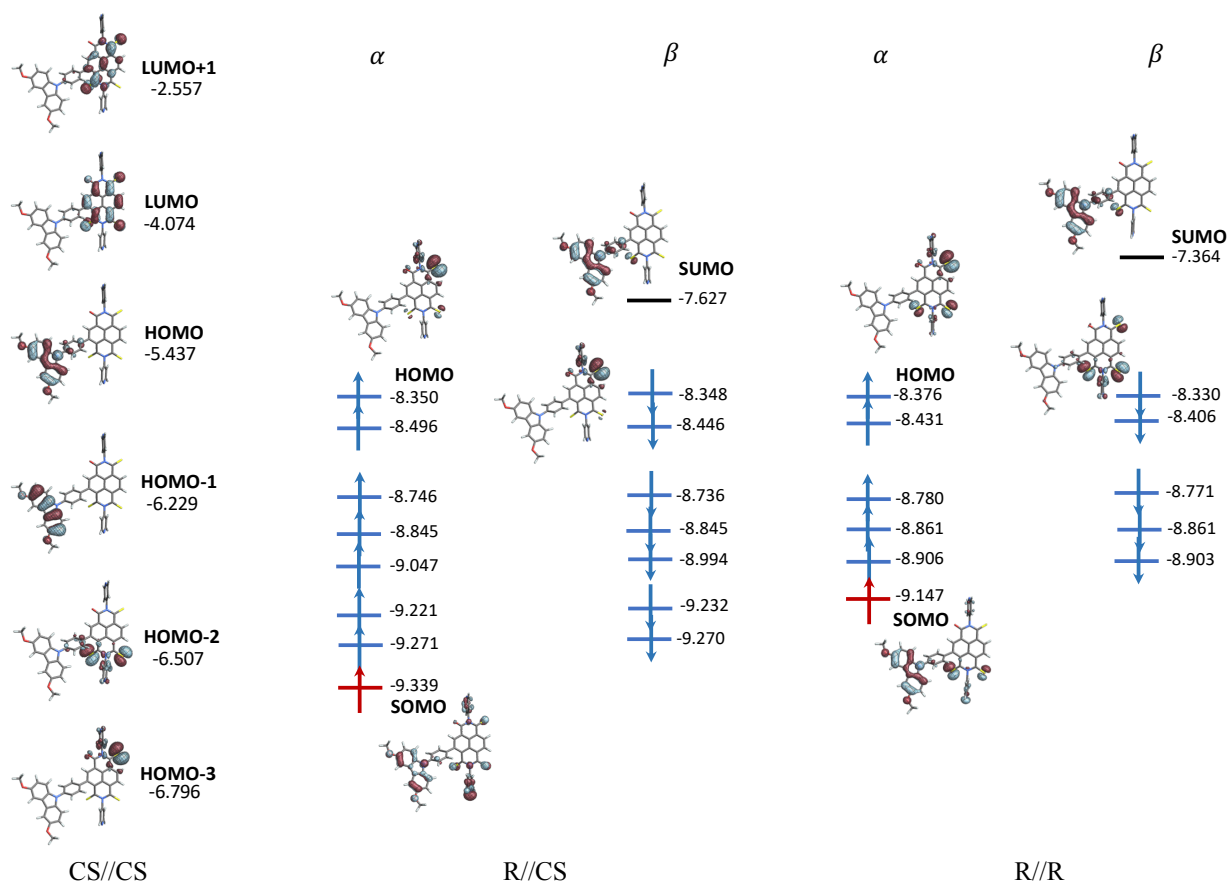
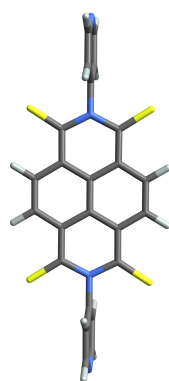


Figure S31: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of selected MOs of the TNDI-Mol-5 system. See Section 3.1 for a description of the labeling.



TNDI-S<sub>4</sub>

Figure S32: Optimized geometry of the selected thionated naphthalene diimide (TDNI-S<sub>4</sub>) derivative used in this work.



Table S11: MO energy contributions (in eV) for the TNDI-Mol-5 system.<sup>(a)</sup> The numbers are for the  $\alpha$  spin orbitals. See also Figure S31.

HOMO $\rightarrow$ SOMO		CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$		45.27	0.00	45.27	2.65	47.92	-0.32	47.59
$V^{\text{nuc}}$	-1150 <sup>(b)</sup>	24.94	0.00	24.94	26.97	51.91	-40.67	11.24
$V^C$	+1150 <sup>(b)</sup>	-58.98	-5.24	-64.21	-27.64	-91.85	40.64	-51.21
$V^{\text{XC}}$		-16.67	0.02	-16.65	-0.66	-17.31	0.54	-16.77
total $\epsilon$		-5.44	-5.22	-10.66	1.32	-9.34	0.19	-9.15

HOMO-2 $\rightarrow$ HOMO		CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$		51.52	0.00	51.52	0.23	51.75	0.32	52.07
$V^{\text{nuc}}$	-1150 <sup>(b)</sup>	-97.49	0.00	-97.49	134.08	36.58	-35.99	0.59
$V^C$	+1150 <sup>(b)</sup>	55.59	-2.05	53.54	-134.08	-80.54	35.69	-44.85
$V^{\text{XC}}$		-16.11	0.00	-16.11	-0.03	-16.14	-0.04	-16.19
total $\epsilon$		-6.51	-2.05	-8.55	0.20	-8.35	-0.03	-8.38

<sup>(a)</sup> CS: Closed-shell system.  $\tilde{R}$ : Radical without SCF, using the MOs of the closed-shell system. R: Radical system. <sup>(b)</sup> The listed number was subtracted from  $V^{\text{nuc}} / V^C$  to avoid large values in the other Table columns. Add it to get the full value of  $V^{\text{nuc}} / V^C$ .

Table S12: Selected Coulomb and exchange electron repulsion integrals (ERIs, in eV) for the closed-shell parent system of the TNDI-Mol-5<sup>•+</sup>.

ERI Type	TNDI-Mol-5
self-Coulomb <sup>(a)</sup> HOMO-2	6.621
self-Coulomb <sup>(a)</sup> HOMO-1	5.906
Coulomb HOMO-2 / HOMO	2.047
Coulomb HOMO-1 / HOMO	4.955
self-Coulomb <sup>(a)</sup> HOMO	5.237
exchange HOMO-1 / HOMO	0.775

<sup>(a)</sup> This corresponds to the Coulomb repulsion between the  $\alpha$  spin and the  $\beta$  spin component of the MO.

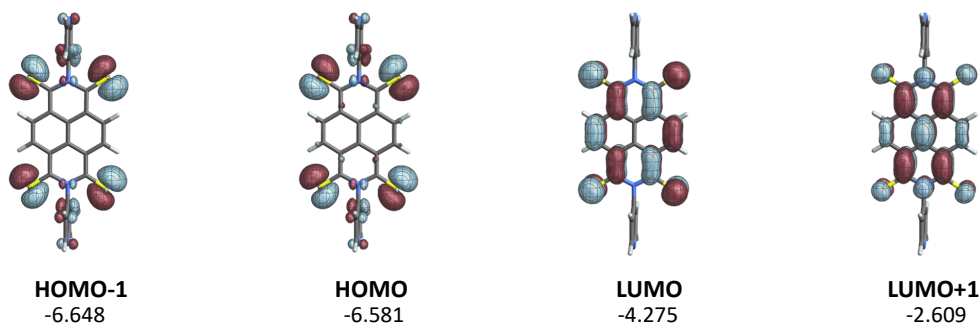


Figure S33: Isosurfaces ( $\pm 0.03$  a.u.) of the frontier molecular orbitals (MOs) of a selected axially substituted thionated naphthalene diimide (TDNI-S<sub>4</sub>) derivative.

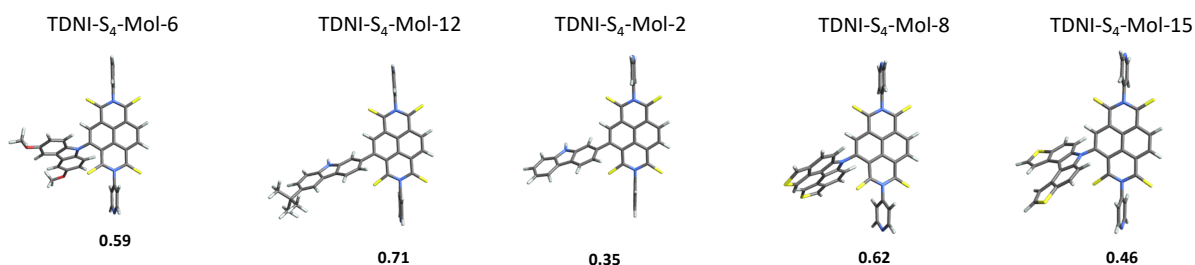


Figure S34: Selected combined systems between the TDNI-S<sub>4</sub> and selected Mol-X fragments (X=2, 6, 8, 12, 15) in the radical cation form (TDNI-S<sub>4</sub>-Mol-X<sup>•+</sup>). All the systems show SOMO/HOMO inversion (SHI). The energy difference (in eV) between the SOMO and the HOMO is indicated for each system. The numbers are for the  $\alpha$  spin orbitals.

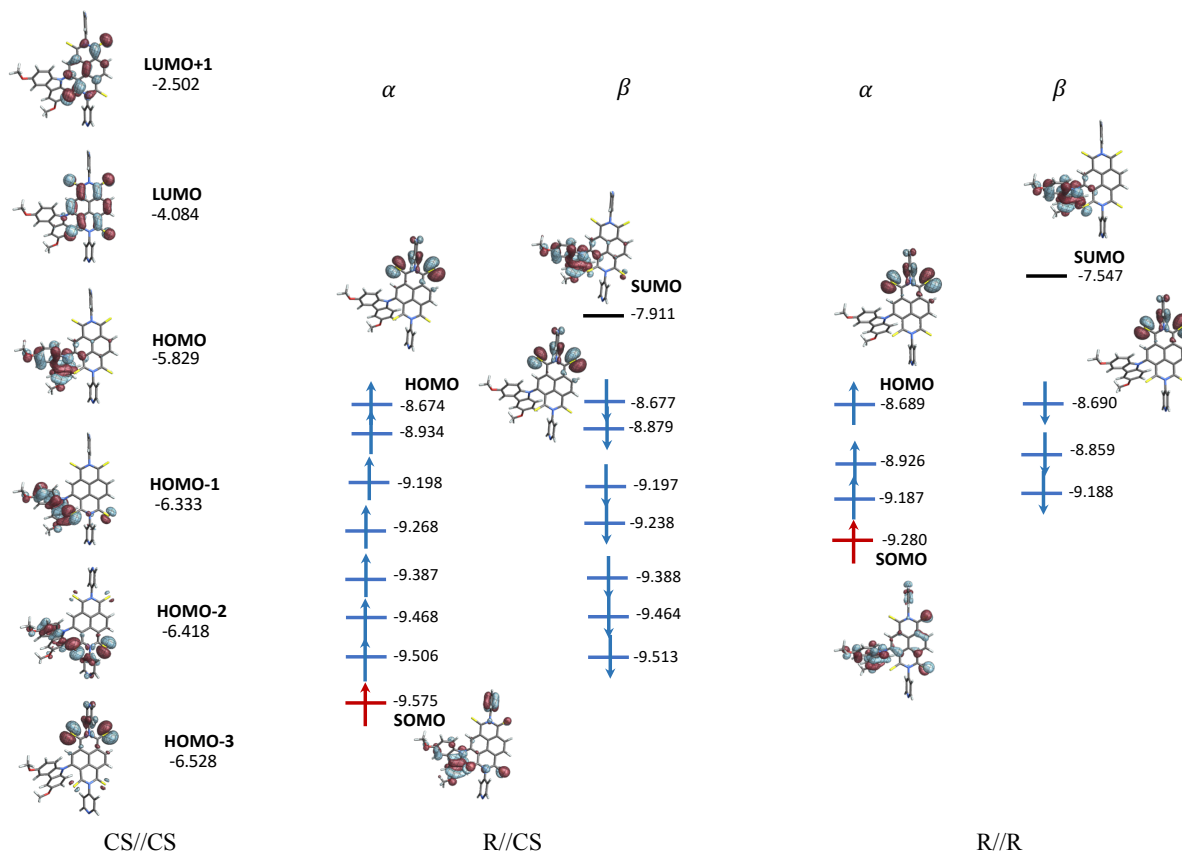


Figure S35: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of selected MOs of TDNI-S<sub>4</sub>-Mol-6. See Section 3.1 for a description of the labeling.

Table S13: MO energy contributions (in eV) for the TDNI-S<sub>4</sub>-Mol-6 system.<sup>(a)</sup> The numbers are for the  $\alpha$  spin orbitals. See also Figure S35.

HOMO $\rightarrow$ SOMO	CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$	45.15	0.00	45.15	-0.94	44.21	1.19	45.41
$V^{\text{nuc}}$	-1200 <sup>(b)</sup>	-0.27	-0.27	38.07	37.79	-10.68	27.12
$V^C$	+1200 <sup>(b)</sup>	-34.13	-5.12	-39.25	-36.14	-75.38	9.89
$V^{\text{XC}}$		-16.58	0.02	-16.57	0.37	-16.20	-0.11
total $\epsilon$		-5.83	-5.10	-10.93	1.36	-9.57	-9.28

HOMO-3 $\rightarrow$ HOMO	CS // CS	$\xrightarrow{\Delta}$	$\tilde{R}$ // CS	$\xrightarrow{\Delta}$	R // CS	$\xrightarrow{\Delta}$	R // R
$T$	51.93	0.00	51.93	0.04	51.98	0.08	52.05
$V^{\text{nuc}}$	-1060 <sup>(c)</sup>	-94.65	0.00	-94.65	13.28	-81.38	-4.27
$V^C$	+1060 <sup>(c)</sup>	52.29	-1.94	50.35	-13.49	36.86	4.19
$V^{\text{XC}}$		-16.10	0.00	-16.10	-0.03	-16.14	-0.01
total $\epsilon$		-6.53	-1.94	-8.47	-0.20	-8.67	-8.69

<sup>(a)</sup> CS: Closed-shell system.  $\tilde{R}$ : Radical without SCF, using the MOs of the closed-shell system. R: Radical system. <sup>(b),(c)</sup> The listed number was subtracted from  $V^{\text{nuc}} / V^C$  to avoid large values in the other Table columns. Add it to get the full value of  $V^{\text{nuc}} / V^C$ .

Table S14: Selected Coulomb and exchange electron repulsion integrals (ERIs, in eV) for the closed-shell parent system of TDNI-S<sub>4</sub>-Mol-6<sup>•+</sup>.

ERI Type	TDNI-S <sub>4</sub> -Mol-6
self-Coulomb <sup>(a)</sup> HOMO-3	6.454
self-Coulomb <sup>(a)</sup> HOMO-1	4.802
Coulomb HOMO-3 / HOMO	1.941
Coulomb HOMO-1 / HOMO	4.402
self-Coulomb <sup>(a)</sup> HOMO	5.120
exchange HOMO-1 / HOMO	0.608

<sup>(a)</sup> This corresponds to the Coulomb repulsion between the  $\alpha$  spin and the  $\beta$  spin component of the MO.

Table S15: Orbital energies (in eV) for the SOMO,  $\alpha$  HOMO,  $\beta$  HOMO and SUMO of DAN-PPTA<sup>•+</sup> system using different functionals. Energy difference between the SOMO and  $\alpha$  HOMO (SH gap) is also given.

Functional	SOMO	$\alpha$ HOMO	$\beta$ HOMO	SUMO	SH gap
PBE0	-9.545	-9.068	-9.068	-7.521	0.478
PBE	-8.287	-8.039	-7.979	-7.892	0.248
B3LYP	-9.269	-8.776	-8.776	-7.596	0.494
CAMB3LYP	-10.670	-10.113	-10.114	-6.591	0.557
M06	-9.516	-9.067	-9.067	-7.595	0.449
HF	-11.731	-10.727	-10.712	-4.539	1.004

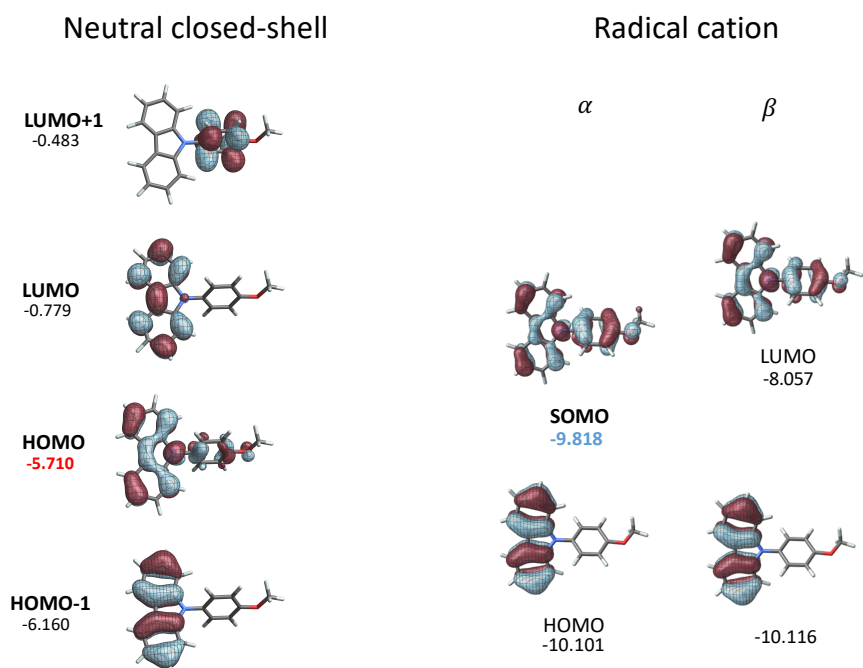


Figure S36: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of frontier MOs of the Mol-1 system.

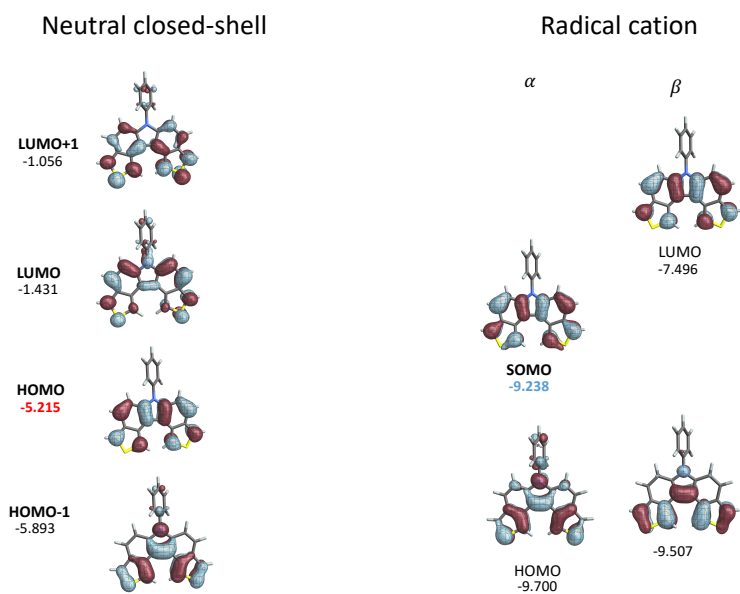


Figure S37: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of frontier MOs of the Mol-3 system.

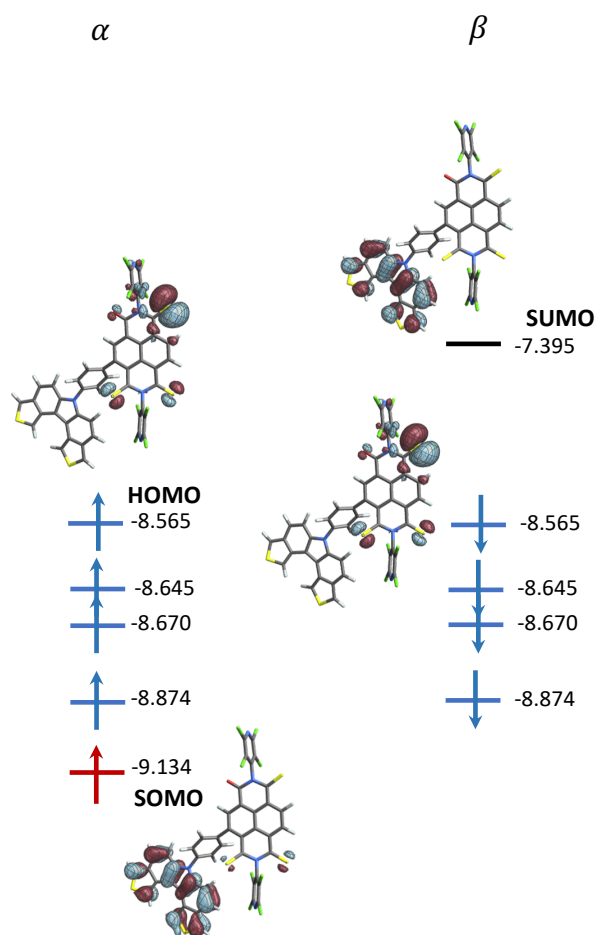


Figure S38: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  au) of selected molecular orbitals (MOs) of a chlorinated derived system of TNDI-Mol-3 $^{*+}$ .

Table S16: Orbital energies (in eV) for the SOMO,  $\alpha$  HOMO,  $\beta$  HOMO and SUMO of BCz $^{*+}$  system using different functionals. Energy difference between the SOMO and  $\alpha$  HOMO (SH gap) is also given.

Functional	SOMO	$\alpha$ HOMO	$\beta$ HOMO	SUMO	SH gap
PBE0	-9.106	-8.535	-8.317	-7.350	0.571
PBE	-7.881	-7.732	-7.690	-7.531	0.149
B3LYP	-8.729	-8.371	-8.135	-7.355	0.358
CAMB3LYP	-10.472	-9.241	-9.237	-6.443	1.231
M06	-9.159	-8.608	-8.409	-7.414	0.551
HF	-13.273	-9.598	-9.809	-3.723	3.675

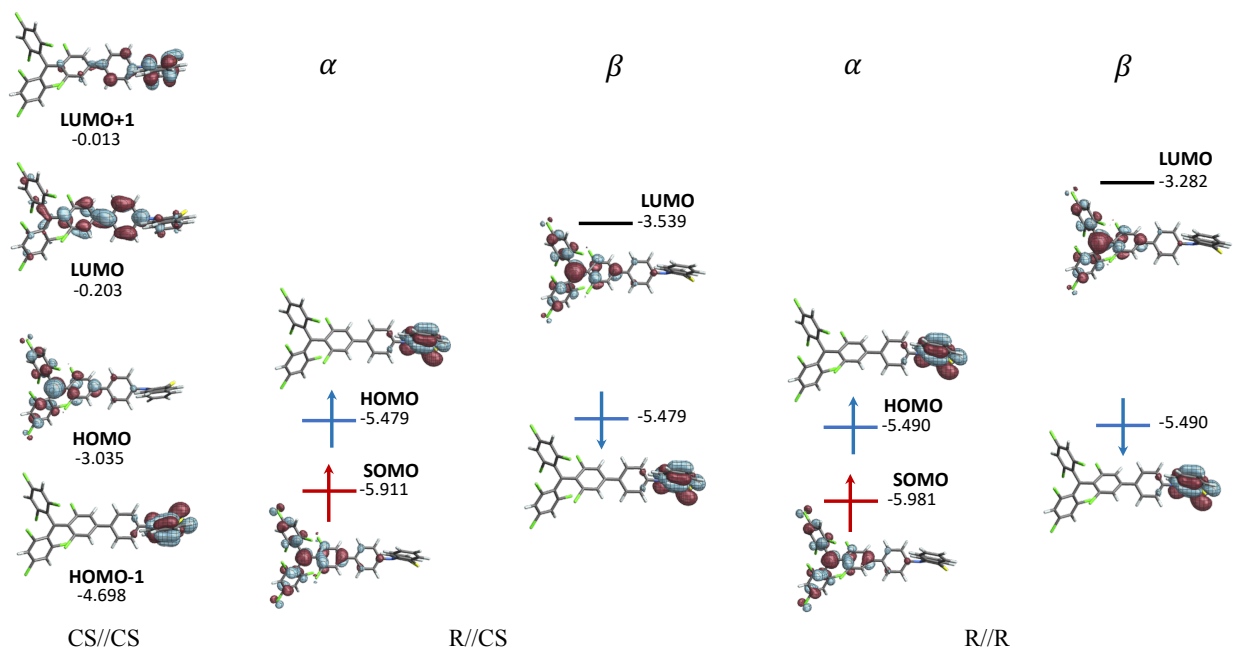


Figure S39: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of selected MOs of the TTM-PPTA system in solution. See Section 3.1 for a description of the labeling.

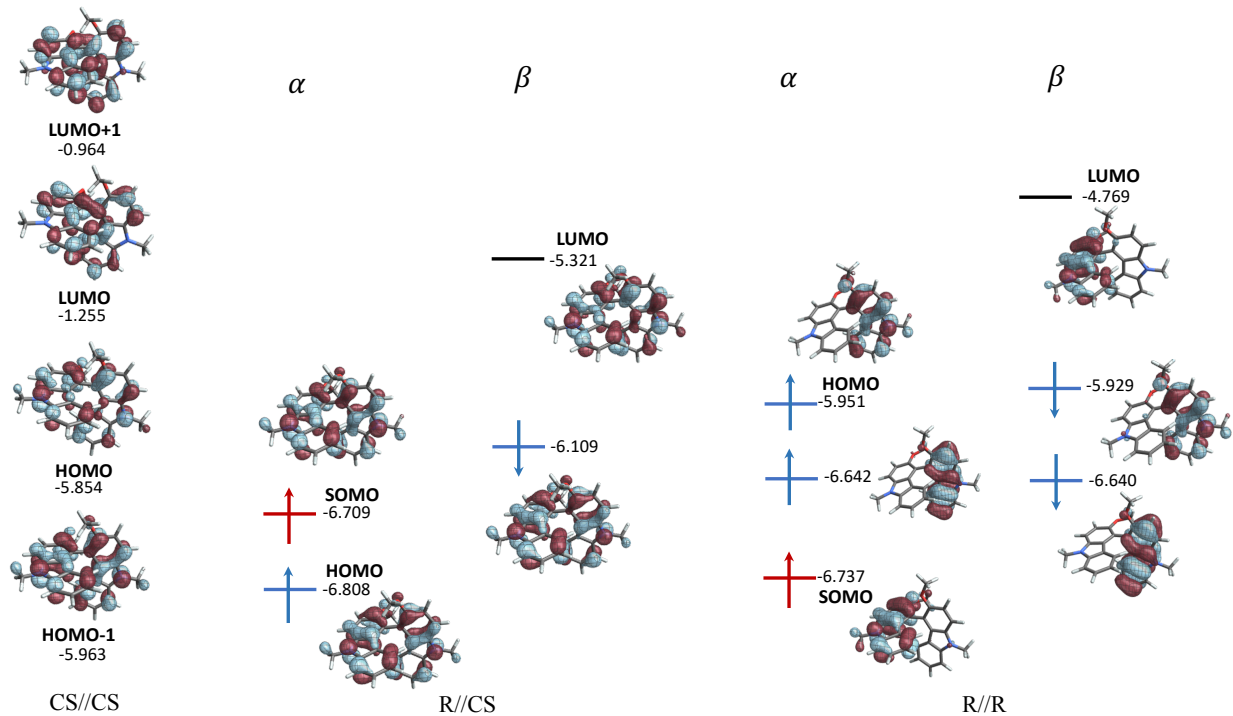


Figure S40: Orbital energies (in eV) and isosurfaces ( $\pm 0.030$  a.u.) of selected MOs of the BCz system in solution. See Section 3.1 for a description of the labeling.

Table S17: Orbital energies (in eV) for the SOMO,  $\alpha$  HOMO,  $\beta$  HOMO and SUMO of NDI-Mol-2<sup>•+</sup> system using different functionals. Energy difference between the SOMO and  $\alpha$  HOMO (SH gap) is also given.

Functional	SOMO	$\alpha$ HOMO	$\beta$ HOMO	SUMO	SH gap
PBE0	-10.243	-9.065	-9.064	-8.346	1.178
B3LYP	-10.112	-8.750	-8.744	-8.381	1.361
CAMB3LYP	-11.476	-10.405	-10.405	-7.449	1.071
M06	-10.287	-9.101	-9.101	-8.332	1.187
HF	-14.533	-11.269	-11.269	-4.840	3.264

xyz coordinates

a) TTM

a.1) CS//CS

C	0.000085	0.000106	-0.000155
C	1.364653	0.488432	-0.000074
C	1.812974	1.570013	-0.810996
C	2.397317	-0.063162	0.810947
C	3.113801	2.060588	-0.810010
C	3.714038	0.382977	0.810148
C	4.068798	1.456136	0.000113
H	3.382138	2.889079	-1.466976
H	4.447014	-0.087164	1.467200
C	-1.105155	0.937643	-0.000142
C	-1.144056	2.107737	0.810887
C	-2.265916	0.784820	-0.811078
C	-2.188969	3.024782	0.809986
C	-3.341346	1.665872	-0.810215
C	-3.295628	2.795190	-0.000132
H	-2.148536	3.894636	1.467040
H	-4.192957	1.483791	-1.467184
C	-0.259335	-1.425787	-0.000161
C	-1.253535	-2.044249	0.810671
C	0.453328	-2.354866	-0.810915
C	-1.525493	-3.407646	0.809924
C	0.227807	-3.726707	-0.809871
C	-0.773293	-4.251501	0.000111
H	-2.299264	-3.807314	1.466845
H	0.811296	-4.373377	-1.466655
C1	-2.370408	-0.525979	-1.950540
C1	0.131781	2.424851	1.950706
C1	2.033731	-1.326638	1.950654
C1	0.730378	2.316118	-1.950663
C1	5.709660	2.043278	0.000196



C1	-2.166262	-1.097482	1.950017
C1	1.641039	-1.790424	-1.950321
C1	-1.085090	-5.966129	0.000349
C1	-4.624836	3.922293	-0.000075

a.2) R//R

C	3.468064	-0.011084	-0.003100
C	4.192881	1.251922	0.154901
C	3.878536	2.400314	-0.607663
C	5.251786	1.401214	1.079867
C	4.557111	3.605279	-0.464835
C	5.948763	2.593808	1.237140
C	5.593538	3.693217	0.460463
H	4.290014	4.460599	-1.086394
H	6.748527	2.666873	1.974894
C	2.003324	-0.019602	-0.004599
C	1.245880	0.648529	0.984845
C	1.255878	-0.696507	-0.995680
C	-0.144340	0.650009	0.992470
C	-0.134205	-0.714053	-1.006473
C	-0.827770	-0.035981	-0.007795
H	-0.686593	1.166331	1.785318
H	-0.668649	-1.236613	-1.800533
C	4.207699	-1.265643	-0.159666
C	3.904770	-2.417714	0.601944
C	5.270159	-1.402695	-1.082447
C	4.597235	-3.614886	0.460251
C	5.980967	-2.587262	-1.238497
C	5.636576	-3.690827	-0.462838
H	4.338438	-4.473372	1.080949
H	6.783029	-2.651079	-1.974609
C1	2.054562	-1.474974	-2.317534
C1	2.032469	1.436103	2.308559
C1	5.677315	0.104822	2.142599
C1	2.668891	2.329820	-1.841725
C1	6.447433	5.181393	0.646730

C1	2.691533	-2.361305	1.833195
C1	5.683087	-0.101436	-2.144205
C1	6.507502	-5.169269	-0.647793
C1	-2.553541	-0.045940	-0.009759

b) PTM

b.1) CS//CS

C	0.000119	-0.000174	0.000185
C	1.357128	-0.509167	0.000093
C	1.770406	-1.581611	0.838621
C	2.373658	0.027022	-0.838490
C	3.071392	-2.092085	0.824555
C	3.689415	-0.444070	-0.824661
C	4.048899	-1.518843	-0.000125
C1	3.511975	-3.399180	1.863387
C1	4.880806	0.250827	-1.863637
C	-1.119308	-0.920691	0.000239
C	-1.163661	-2.069028	-0.838447
C	-2.254604	-0.742086	0.838868
C	-2.229759	-2.972654	-0.824576
C	-3.347471	-1.613158	0.824772
C	-3.340179	-2.746276	0.000019
C1	-2.224035	-4.351883	-1.863554
C1	-4.699600	-1.340843	1.863691
C	-0.237518	1.429530	0.000080
C	-1.210186	2.041726	-0.838446
C	0.484772	2.323628	0.838451
C	-1.460122	3.416742	-0.824590
C	0.276389	3.705540	0.824384
C	-0.708960	4.265442	-0.000139
C1	-2.657837	4.101010	-1.863350
C1	1.188279	4.740693	1.862979
C1	-4.672922	-3.841798	-0.000155
C1	-2.267788	0.542229	1.994811
C1	0.094064	-2.330502	-1.994101

C1	1.970926	1.246871	-1.994153
C1	0.664822	-2.235787	1.994274
C1	5.664186	-2.124835	-0.000319
C1	-2.065487	1.082794	-1.993742
C1	1.604372	1.693187	1.993785
C1	-0.991904	5.967291	-0.000197

b.2) R//R

C	-0.000227	-0.000145	-0.000192
C	0.938740	-1.129651	-0.000306
C	0.806039	-2.191343	0.919781
C	2.006876	-1.192783	-0.920348
C	1.693701	-3.274149	0.921078
C	2.909951	-2.262761	-0.921285
C	2.751874	-3.309428	0.000023
C1	1.514135	-4.544173	2.059267
C1	4.191560	-2.317716	-2.059319
C	-1.447895	-0.248427	-0.000103
C	-2.036937	-1.141636	-0.920196
C	-2.300760	0.397486	0.920103
C	-3.415187	-1.388268	-0.921149
C	-3.682409	0.170668	0.921354
C	-4.242365	-0.727786	0.000185
C1	-4.103946	-2.470404	-2.059251
C1	-4.692235	0.961454	2.059585
C	0.508621	1.377732	-0.000034
C	0.029572	2.334484	-0.920081
C	1.494483	1.793334	0.920132
C	0.505211	3.651360	-0.921107
C	1.988969	3.103257	0.921317
C	1.490892	4.037423	0.000142
C1	-0.087562	4.788908	-2.059211
C1	3.178790	3.582372	2.059493
C1	-5.929884	-1.017261	0.000375
C1	-1.640515	1.414272	2.141172
C1	-1.075832	-1.880197	-2.141505

Cl	2.165630	0.008939	-2.141592
Cl	-0.404849	-2.128531	2.140678
Cl	3.846858	-4.625677	0.000301
Cl	-1.090771	1.871476	-2.141232
Cl	2.044865	0.713204	2.141268
Cl	2.084054	5.643556	0.000212

c) TTM-PPTA

c.1) CS//CS

C	3.441609	-0.009390	-0.002910
C	4.169962	1.238969	0.165655
C	3.841049	2.432860	-0.533034
C	5.292029	1.379184	1.025840
C	4.531049	3.631643	-0.390149
C	6.021089	2.554969	1.168489
C	5.630369	3.685398	0.459519
H	4.225973	4.506905	-0.965112
H	6.867757	2.590774	1.855253
C	2.006365	-0.024184	-0.004859
C	1.198726	0.788470	0.851426
C	1.217542	-0.852808	-0.863499
C	-0.184442	0.791529	0.842160
C	-0.165368	-0.882174	-0.859606
C	-0.915848	-0.052126	-0.010335
H	-0.695460	1.422578	1.572575
H	-0.661876	-1.522872	-1.591614
C	4.196420	-1.242264	-0.169304
C	3.890792	-2.442615	0.528840
C	5.323528	-1.358898	-1.026362
C	4.606441	-3.626551	0.388312
C	6.077722	-2.519021	-1.166565
C	5.709058	-3.657221	-0.458224
H	4.318301	-4.507942	0.962642
H	6.926883	-2.537124	-1.850937

C	-2.381880	-0.064853	-0.014113
C	-3.129833	1.066364	0.376702
C	-3.110825	-1.205412	-0.408626
C	-4.518820	1.056243	0.377229
H	-2.607001	1.983781	0.659462
C	-4.501258	-1.215832	-0.417936
H	-2.573252	-2.115142	-0.688433
C	-5.219277	-0.086637	-0.023111
H	-5.077428	1.948260	0.677460
H	-5.049718	-2.112169	-0.721122
C	-7.306382	0.432229	-1.151043
C	-7.313687	-0.365376	1.176232
C	-6.600984	1.156912	-2.125257
C	-8.694847	0.271283	-1.335128
C	-8.703088	-0.601948	1.214620
C	-6.615521	-0.394126	2.394257
C	-7.252363	1.710842	-3.225935
H	-5.521370	1.277314	-2.022767
C	-9.345203	0.862523	-2.417657
C	-9.361194	-0.797528	2.428293
H	-5.535333	-0.240166	2.393668
C	-7.274749	-0.630427	3.599346
C	-8.629938	1.579725	-3.375782
H	-6.664198	2.259037	-3.968054
H	-10.427732	0.732782	-2.514485
C	-8.653149	-0.821331	3.629165
H	-10.444124	-0.956427	2.418662
H	-6.692004	-0.655484	4.525081
H	-9.147312	2.022773	-4.231455
H	-9.176645	-0.995072	4.573573
N	-6.649505	-0.114115	-0.035845
S	-9.616680	-0.804543	-0.282160
C1	1.986791	-1.828653	-2.086917
C1	1.944400	1.778309	2.078366
C1	5.783765	0.058256	2.044173
C1	2.552667	2.436407	-1.698370

C1	6.519022	5.172163	0.637130
C1	2.599440	-2.473037	1.690393
C1	5.790034	-0.028110	-2.043760
C1	6.629609	-5.124796	-0.632709

c.2) R//R

C	3.447059	-0.011380	-0.003337
C	4.172885	1.250936	0.157381
C	3.860310	2.399772	-0.605133
C	5.231068	1.398695	1.083116
C	4.540299	3.603860	-0.461635
C	5.929253	2.590503	1.241437
C	5.575945	3.690389	0.464666
H	4.274865	4.459619	-1.083289
H	6.728471	2.662473	1.979886
C	1.984287	-0.019784	-0.004767
C	1.223094	0.659914	0.974033
C	1.232741	-0.708114	-0.985097
C	-0.165216	0.657339	0.975699
C	-0.155525	-0.721461	-0.989494
C	-0.881114	-0.036193	-0.007560
H	-0.686792	1.168871	1.786804
H	-0.669889	-1.238875	-1.801475
C	4.187769	-1.265187	-0.162573
C	3.886850	-2.417643	0.599200
C	5.249593	-1.400565	-1.086022
C	4.581033	-3.613761	0.457017
C	5.961860	-2.584176	-1.242954
C	5.619618	-3.688177	-0.467046
H	4.324094	-4.472645	1.077932
H	6.763424	-2.646831	-1.979706
C	-2.358963	-0.044387	-0.009102
C	-3.085681	1.093636	0.376819
C	-3.073180	-1.188278	-0.396180
C	-4.476208	1.088053	0.374660
H	-2.553859	2.007354	0.657197

C	-4.464948	-1.196739	-0.397474
H	-2.531945	-2.096652	-0.675707
C	-5.175269	-0.059678	-0.012620
H	-5.035266	1.981631	0.666248
H	-5.020258	-2.091418	-0.690141
C	-7.259560	0.437664	-1.153111
C	-7.268284	-0.319620	1.193428
C	-6.573796	1.194147	-2.114807
C	-8.635768	0.212501	-1.350708
C	-8.645848	-0.613013	1.211845
C	-6.591284	-0.273574	2.420988
C	-7.234986	1.714737	-3.226730
H	-5.502768	1.369651	-2.001046
C	-9.297827	0.770409	-2.443738
C	-9.317711	-0.797069	2.419734
H	-5.519165	-0.071221	2.439637
C	-7.262422	-0.499164	3.622361
C	-8.602046	1.516778	-3.393799
H	-6.665216	2.289979	-3.962415
H	-10.371836	0.593010	-2.555258
C	-8.630851	-0.750483	3.632096
H	-10.392395	-1.002007	2.398296
H	-6.699137	-0.466848	4.559616
H	-9.127656	1.933039	-4.257519
H	-9.164210	-0.915784	4.572173
N	-6.600102	-0.089551	-0.025251
S	-9.517420	-0.894900	-0.296723
C1	2.028309	-1.493829	-2.307297
C1	2.006979	1.454968	2.297757
C1	5.654348	0.101366	2.145579
C1	2.650568	2.331006	-1.839328
C1	6.431298	5.177803	0.651988
C1	2.673774	-2.363057	1.830767
C1	5.660138	-0.098254	-2.147433
C1	6.492580	-5.165501	-0.652650

d) TTM-3CNz

d.1) CS//CS

C	-3.663189	0.076459	0.107633
C	-4.403114	-1.088851	0.556523
C	-5.603923	-1.540944	-0.058363
C	-4.006186	-1.889444	1.664469
C	-6.337925	-2.638780	0.376863
C	-4.700503	-3.010765	2.104341
C	-5.876275	-3.378965	1.459661
H	-7.246522	-2.929564	-0.152110
H	-4.337498	-3.570776	2.967185
C	-2.224117	0.029892	0.001331
C	-1.363675	1.095543	0.399182
C	-1.501112	-1.086418	-0.513872
C	0.017594	1.064099	0.287573
C	-0.119584	-1.141138	-0.610949
C	0.683725	-0.061088	-0.218361
H	0.576620	1.946328	0.607028
H	0.330828	-2.054404	-1.005964
C	-4.383177	1.289625	-0.234687
C	-5.449532	1.816523	0.546046
C	-4.100424	2.067258	-1.392871
C	-6.165740	2.961972	0.216654
C	-4.776541	3.233610	-1.732687
C	-5.819196	3.675163	-0.925574
H	-6.966762	3.309160	0.870665
H	-4.507329	3.772361	-2.642162
C	2.152061	-0.107502	-0.336936
C	2.977776	0.587034	0.580869
C	2.777337	-0.834685	-1.359095
C	4.365488	0.567239	0.512986
H	2.504514	1.145669	1.392968
C	4.170103	-0.875804	-1.444894
H	2.172371	-1.348486	-2.111170
C	4.961557	-0.182401	-0.502943



H	4.964393	1.121780	1.239357
C	7.399217	0.180576	-0.114955
C	6.395280	-1.155493	-1.956202
C	7.497422	0.027355	1.254015
C	8.399755	0.908973	-0.814087
C	7.523140	-1.644144	-2.621014
C	5.085482	-1.497273	-2.376417
C	8.577154	0.592761	1.975864
H	6.734939	-0.545702	1.788381
C	9.466890	1.448485	-0.138894
C	7.321137	-2.455399	-3.735386
C	4.909629	-2.313906	-3.496698
C	9.590597	1.312188	1.268803
H	10.230572	2.012004	-0.684563
C	6.029556	-2.784644	-4.176257
H	8.190691	-2.847205	-4.272572
H	3.901654	-2.581315	-3.827586
H	5.904459	-3.423656	-5.055443
N	6.310931	-0.355343	-0.822516
C1	-2.356048	-2.469570	-1.142952
C1	-2.026677	2.524928	1.145818
C1	-2.615561	-1.446250	2.609316
C1	-6.200308	-0.759144	-1.493519
C1	-6.771364	-4.769284	2.008615
C1	-5.880798	1.068586	2.056404
C1	-2.894824	1.538218	-2.528379
C1	-6.691848	5.123528	-1.345442
C	8.693862	0.453184	3.384381
C	10.675373	1.866491	1.994840
H	8.293457	1.047031	-1.893023
H	7.917836	-0.098485	3.924410
H	8.532390	-1.409007	-2.274484
C	9.759963	1.000808	4.060821
C	10.760602	1.715710	3.360691
H	11.602172	2.149161	3.909671
H	9.835536	0.886068	5.146512

H	11.446517	2.419396	1.448431
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d.2) R//R

C	3.657180	-0.005662	-0.135888
C	4.374702	-1.281908	-0.082037
C	5.501520	-1.478762	0.748560
C	3.984689	-2.396947	-0.859059
C	6.192137	-2.684140	0.805532
C	4.655215	-3.614159	-0.815542
C	5.760433	-3.748982	0.019874
H	7.046934	-2.793984	1.473712
H	4.326907	-4.442193	-1.444643
C	2.200019	0.021626	-0.017708
C	1.380573	0.756562	-0.905446
C	1.507452	-0.685102	0.992581
C	-0.002677	0.788203	-0.796323
C	0.124517	-0.664815	1.107360
C	-0.661243	0.075863	0.214568
H	-0.567568	1.389521	-1.510899
H	-0.341122	-1.247120	1.904579
C	4.403687	1.243131	-0.307997
C	5.389749	1.400129	-1.308721
C	4.184840	2.369807	0.517858
C	6.106979	2.578954	-1.479149
C	4.884879	3.561171	0.363844
C	5.846611	3.656934	-0.637901
H	6.847441	2.658657	-2.275746
H	4.692543	4.399091	1.034737
C	-2.132737	0.105463	0.338111
C	-2.948463	0.157988	-0.815362
C	-2.743478	0.087032	1.597274
C	-4.334885	0.179823	-0.743277
H	-2.475916	0.153817	-1.801652
C	-4.134063	0.114692	1.697099
H	-2.133839	0.084301	2.505359
C	-4.925063	0.150142	0.522678

H	-4.941854	0.216002	-1.650664
C	-7.354563	0.240034	-0.016265
C	-6.355016	0.177782	2.266267
C	-7.498652	-0.715551	-0.999997
C	-8.295996	1.296653	0.093235
C	-7.490619	0.169135	3.079724
C	-5.050340	0.135725	2.814365
C	-8.573720	-0.653211	-1.921137
H	-6.778902	-1.536282	-1.067068
C	-9.357677	1.366785	-0.775618
C	-7.297062	0.141429	4.457843
C	-4.882494	0.106878	4.202271
C	-9.528626	0.404662	-1.805471
H	-10.080827	2.183894	-0.690274
C	-6.008851	0.115048	5.017919
H	-8.170094	0.135409	5.117499
H	-3.879093	0.074792	4.637123
H	-5.893809	0.094215	6.105356
N	-6.264277	0.187418	0.878418
C1	2.380809	-1.565184	2.203737
C1	2.079857	1.606569	-2.244355
C1	2.681029	-2.266925	-1.987999
C1	6.029264	-0.228587	1.821406
C1	6.605267	-5.253692	0.082135
C1	5.692085	0.134219	-2.448297
C1	3.074422	2.285734	1.840987
C1	6.726378	5.129079	-0.839180
C	-8.739990	-1.619505	-2.947768
C	-10.609351	0.458722	-2.722635
H	-8.154027	2.054419	0.868145
H	-8.009803	-2.430502	-3.032627
H	-8.495264	0.176122	2.650347
C	-9.800064	-1.540642	-3.821563
C	-10.743120	-0.491549	-3.709306
H	-11.580828	-0.439156	-4.411086
H	-9.917156	-2.291473	-4.608747

H	-11.337274	1.271269	-2.632548
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e) ETBN

e.1) CS//CS

S	-6.227680	2.186576	0.757637
C	-7.930956	1.490821	0.729777
C	-8.057381	0.106504	0.129463
S	-6.953988	-1.111021	0.921095
C	-5.464949	-0.452810	0.281664
C	-5.230136	0.877046	0.168760
H	-8.550727	2.204980	0.157857
H	-9.087674	-0.262987	0.273510
S	-3.794083	1.348277	-0.749268
S	-4.310959	-1.532614	-0.509768
C	-3.083155	-0.266823	-0.630304
H	-8.282434	1.480898	1.773880
H	-7.833927	0.109313	-0.950258
C	-1.748363	-0.502707	-0.630622
S	-0.556324	0.776306	-0.784273
C	0.841531	-0.244284	-0.430059
C	0.585766	-1.616678	-0.312583
S	-1.085473	-2.127415	-0.533798
C	1.640093	-2.496669	-0.062090
C	2.933886	-2.005191	0.070475
C	3.193773	-0.623509	-0.053823
C	2.128267	0.263370	-0.309144
C	4.545563	-0.109064	0.081137
N	4.865860	1.206006	-0.001061
C	6.341623	1.306632	-0.094032
C	6.765717	0.015608	0.643001
N	5.634138	-0.882199	0.305245
O	4.156300	2.166896	-0.551272
O	5.667933	-2.106058	0.775571
C	6.804665	2.619538	0.513713
H	6.273273	3.432054	-0.008504

H	6.550106	2.687449	1.583050
H	7.895168	2.751024	0.393886
C	6.676645	1.281108	-1.590977
H	6.059046	2.060175	-2.069046
H	7.746637	1.476853	-1.780630
H	6.408213	0.305510	-2.031316
C	8.072825	-0.620706	0.202873
H	8.937264	-0.002927	0.506016
H	8.137865	-1.611158	0.682425
H	8.106401	-0.774587	-0.887150
C	6.747606	0.161613	2.169961
H	3.794393	-2.648628	0.283700
H	5.833215	0.685123	2.497828
H	6.733758	-0.859251	2.587932
H	1.448300	-3.569740	0.037168
H	2.386686	1.326450	-0.408075
H	7.628570	0.711562	2.544921

e.2) R//R

S	-6.219959	2.245084	0.664795
C	-7.920124	1.544310	0.714298
C	-8.061008	0.137310	0.173927
S	-6.959711	-1.054199	1.007150
C	-5.470831	-0.424357	0.342688
C	-5.229550	0.896057	0.163285
H	-8.551597	2.236013	0.128703
H	-9.090410	-0.219862	0.349039
S	-3.779261	1.316739	-0.755222
S	-4.310561	-1.551758	-0.366874
C	-3.090341	-0.301367	-0.604639
H	-8.244101	1.579668	1.766288
H	-7.854441	0.090733	-0.908008
C	-1.764820	-0.553317	-0.692226
S	-0.569261	0.707665	-0.981152
C	0.808777	-0.287183	-0.522961
C	0.551833	-1.654420	-0.335160

S	-1.101806	-2.183116	-0.575022
C	1.602437	-2.512236	-0.010553
C	2.892913	-2.014777	0.122920
C	3.159815	-0.641842	-0.064268
C	2.093375	0.222463	-0.389399
C	4.510867	-0.118996	0.079798
N	4.886290	1.176936	-0.095669
C	6.374039	1.317417	-0.090029
C	6.781958	0.048183	0.693450
N	5.614633	-0.842158	0.412951
O	4.168443	2.158699	-0.395299
O	5.698007	-2.070355	0.641780
C	6.759026	2.635866	0.558195
H	6.371935	3.467647	-0.049829
H	6.342327	2.739302	1.571040
H	7.857631	2.717782	0.613987
C	6.803220	1.305522	-1.558369
H	6.280109	2.122999	-2.080969
H	7.890003	1.462107	-1.653435
H	6.537422	0.354877	-2.050184
C	8.060297	-0.624710	0.224715
H	8.917159	0.052408	0.379826
H	8.223949	-1.543053	0.808870
H	8.017203	-0.906784	-0.837743
C	6.811085	0.238027	2.211164
H	3.712877	-2.685377	0.375659
H	5.893202	0.728818	2.575659
H	6.883727	-0.754487	2.685170
H	1.414423	-3.578418	0.143516
H	2.290573	1.285533	-0.527168
H	7.681071	0.841563	2.516962

f) ATH

f.1) CS//CS

C	0.171139	2.118180	-0.513315
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C	-0.690890	2.289966	0.616096
C	-1.458674	3.442910	0.436347
C	0.000000	3.023695	-1.536816
C	-0.863474	1.713220	1.928453
C	-1.633651	2.579664	2.710453
S	-1.609480	2.248862	4.414672
C	-0.566629	0.864249	4.097913
C	-0.354364	0.622442	2.712393
C	0.354364	-0.622442	2.712393
C	0.566629	-0.864249	4.097913
S	1.609480	-2.248862	4.414672
C	1.633651	-2.579664	2.710453
C	0.863474	-1.713220	1.928453
S	-2.295028	3.952506	1.860591
C	0.690890	-2.289966	0.616096
C	-0.171139	-2.118180	-0.513315
C	-0.000000	-3.023695	-1.536816
S	1.232086	-4.183016	-1.098809
C	1.458674	-3.442910	0.436347
S	2.295028	-3.952506	1.860591
S	-1.232086	4.183016	-1.098809
Br	-1.570309	-0.859801	-0.518844
Br	1.570309	0.859801	-0.518844
Si	-0.936170	-3.227855	-3.149694
Si	0.936170	3.227855	-3.149694
C	0.893958	1.637856	-4.156047
H	1.324402	0.802534	-3.577644
H	-0.143623	1.363355	-4.413701
H	1.468525	1.747745	-5.094423
C	0.086873	4.609124	-4.122401
H	0.100901	5.563909	-3.566406
H	0.603109	4.771505	-5.086399
H	-0.966982	4.358141	-4.339505
C	2.718509	3.726691	-2.788369
H	2.748980	4.680108	-2.231493
H	3.213280	2.958160	-2.169280

H	3.297426	3.849305	-3.722482
C	-0.086873	-4.609124	-4.122401
H	-0.100901	-5.563909	-3.566406
H	-0.603109	-4.771505	-5.086399
H	0.966982	-4.358141	-4.339505
C	-2.718509	-3.726691	-2.788369
H	-2.748980	-4.680108	-2.231493
H	-3.213280	-2.958160	-2.169280
H	-3.297426	-3.849305	-3.722482
C	-0.893958	-1.637856	-4.156047
H	-1.324402	-0.802534	-3.577644
H	0.143623	-1.363355	-4.413701
H	-1.468525	-1.747745	-5.094423
N	-0.000000	-0.000000	4.950023

f.2) R//R

C	0.168385	2.119289	-0.524561
C	-0.684874	2.277981	0.612575
C	-1.480849	3.411422	0.451822
C	-0.033480	3.033720	-1.531966
C	-0.845715	1.702759	1.921928
C	-1.636695	2.529845	2.709878
S	-1.652620	2.177720	4.435745
C	-0.568398	0.857590	4.131294
C	-0.324376	0.613604	2.706597
C	0.324387	-0.613610	2.706598
C	0.568409	-0.857593	4.131296
S	1.652626	-2.177727	4.435749
C	1.636695	-2.529859	2.709883
C	0.845722	-1.702769	1.921932
S	-2.330451	3.880761	1.886019
C	0.684876	-2.277992	0.612580
C	-0.168377	-2.119289	-0.524558
C	0.033475	-3.033727	-1.531960
S	1.278160	-4.166511	-1.076088
C	1.480837	-3.411443	0.451831



S	2.330436	-3.880785	1.886029
S	-1.278184	4.166485	-1.076101
Br	-1.574617	-0.872667	-0.547801
Br	1.574651	0.872697	-0.547795
Si	-0.874153	-3.272581	-3.176819
Si	0.874150	3.272585	-3.176823
C	0.812014	1.677980	-4.168068
H	1.277838	0.847331	-3.611210
H	-0.230063	1.391046	-4.391320
H	1.349322	1.796624	-5.126729
C	-0.021863	4.649939	-4.099696
H	-0.005270	5.600966	-3.537581
H	0.469552	4.831000	-5.072951
H	-1.076096	4.388190	-4.301076
C	2.647568	3.780941	-2.810549
H	2.673619	4.724102	-2.236710
H	3.165508	3.007364	-2.217655
H	3.212406	3.932742	-3.748454
C	0.021842	-4.649951	-4.099687
H	0.005231	-5.600977	-3.537569
H	-0.469573	-4.831006	-5.072943
H	1.076079	-4.388220	-4.301063
C	-2.647580	-3.780907	-2.810551
H	-2.673648	-4.724067	-2.236710
H	-3.165510	-3.007321	-2.217661
H	-3.212418	-3.932701	-3.748458
C	-0.811987	-1.677979	-4.168068
H	-1.277799	-0.847321	-3.611214
H	0.230096	-1.391063	-4.391317
H	-1.349293	-1.796616	-5.126731
N	0.000006	-0.000001	4.979290

g) BCz

g.1) CS//CS

C	-3.080707	1.219358	-1.858649
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H	-4.017168	1.253869	-2.420701
C	4.977569	-1.051900	0.956016
H	5.481466	-0.126788	1.280017
H	5.604363	-1.517267	0.179019
H	4.915990	-1.741598	1.819889
N	3.686727	-0.740034	0.415776
C	3.041119	-1.434172	-0.588030
C	3.479679	-2.539643	-1.323090
H	4.451326	-3.003347	-1.134808
C	2.633155	-3.043135	-2.306365
H	2.955170	-3.908286	-2.894287
C	1.376189	-2.468172	-2.553982
H	0.733730	-2.889893	-3.332264
C	0.936024	-1.375688	-1.814243
H	-0.045598	-0.934605	-2.001736
C	1.767398	-0.848943	-0.817826
C	1.646730	0.244162	0.121497
C	0.636988	1.187072	0.377383
C	0.867018	2.138781	1.377958
C	2.065186	2.143009	2.110982
H	2.186260	2.909825	2.880715
C	3.070896	1.213458	1.870325
H	3.994356	1.231189	2.454243
C	2.853401	0.267475	0.866095
O	-0.071360	3.088598	1.652408
C	-0.926121	-1.383665	1.803917
H	0.054623	-0.940323	1.990859
C	-1.756466	-0.862930	0.803522
C	-1.640453	0.233282	-0.132687
C	-0.637843	1.185803	-0.380493
C	-2.845708	0.251468	-0.879587
C	-4.978985	-1.054098	-0.948489
H	-5.207039	-2.125703	-0.835241
H	-5.035445	-0.813656	-2.022546
H	-5.753156	-0.469610	-0.414722
C	-1.085376	2.681770	2.538867

H	-1.644577	1.809472	2.149467
H	-1.776759	3.532148	2.648002
H	-0.670457	2.421626	3.533562
N	-3.659028	-0.784528	-0.458090
C	-3.026623	-1.454465	0.570291
C	-3.474593	-2.542559	1.325290
H	-4.457970	-2.989263	1.158010
C	-2.629225	-3.040073	2.312628
H	-2.958570	-3.891648	2.916105
C	-1.368557	-2.469653	2.551853
H	-0.728391	-2.884763	3.335567
C	-2.081935	2.158389	-2.091599
H	-2.216338	2.942162	-2.841776
C	-0.877984	2.148394	-1.368182
O	0.052455	3.108792	-1.632749
C	1.067810	2.719677	-2.525553
H	1.633038	1.846031	-2.147926
H	1.753774	3.575650	-2.624681
H	0.653197	2.469577	-3.522950

g.2) R//R

C	-3.193336	0.774772	-1.947206
H	-4.140527	0.637038	-2.472439
C	4.748894	-1.417675	0.878880
H	4.898722	-0.962662	1.868946
H	5.568245	-1.096299	0.210181
H	4.797407	-2.511446	1.000811
N	3.460751	-1.041505	0.358446
C	2.780285	-1.718676	-0.633264
C	3.142238	-2.894364	-1.299133
H	4.076499	-3.414814	-1.076328
C	2.273387	-3.379333	-2.270315
H	2.531943	-4.296380	-2.807374
C	1.076696	-2.711642	-2.580537
H	0.420391	-3.117938	-3.354898
C	0.720644	-1.539451	-1.919988

H	-0.209413	-1.026055	-2.173582
C	1.575574	-1.030981	-0.935157
C	1.552173	0.130586	-0.075976
C	0.642688	1.180246	0.096990
C	0.935370	2.173483	1.055831
C	2.118719	2.113561	1.814416
H	2.340297	2.888359	2.549745
C	3.025008	1.071577	1.644799
H	3.937588	1.047870	2.244585
C	2.741159	0.081168	0.700843
O	0.016060	3.147824	1.171381
C	-0.741337	-0.952048	2.060851
H	0.222940	-0.446791	2.133950
C	-1.627378	-0.668376	1.020405
C	-1.617998	0.235902	-0.118301
C	-0.673167	1.151634	-0.583462
C	-2.866286	0.043769	-0.786097
C	-4.913352	-1.369672	-0.459892
H	-4.889924	-2.457096	-0.644844
H	-5.277980	-0.865634	-1.364509
H	-5.612598	-1.162236	0.368027
C	0.162540	4.140775	2.159744
H	0.194166	3.694464	3.170541
H	-0.722640	4.787387	2.077460
H	1.071944	4.747663	1.994989
N	-3.593520	-0.895246	-0.126357
C	-2.868221	-1.346323	0.972695
C	-3.243272	-2.296200	1.918368
H	-4.205617	-2.810767	1.867279
C	-2.338412	-2.567224	2.946700
H	-2.598667	-3.308393	3.707323
C	-1.109919	-1.902422	3.018443
H	-0.422784	-2.131335	3.837448
C	-2.274153	1.683626	-2.402598
H	-2.467047	2.285401	-3.293364
C	-1.022131	1.897504	-1.748829

O	-0.271833	2.778048	-2.386122
C	0.945038	3.323262	-1.913730
H	0.776003	3.866487	-0.970756
H	1.272960	4.020445	-2.697290
H	1.704948	2.538153	-1.769484

h) NDI-Mol-2

h.1) CS//CS

C	-3.603374	1.366547	0.054024
C	-3.773072	2.740315	0.079356
C	-2.650342	3.582593	0.085703
C	-1.370092	3.053521	0.055139
C	0.307809	-0.297051	0.057281
C	-0.851256	-1.115653	0.041072
C	-2.123742	-0.588796	0.021595
C	-2.306490	0.810184	0.036267
C	-1.165660	1.653341	0.029961
C	0.140828	1.093914	0.006710
H	-4.788246	3.144323	0.095623
H	-2.757990	4.669795	0.115265
C	-0.218769	3.985807	0.067597
H	4.311278	-1.156718	2.285790
H	-0.740940	-2.202602	0.071837
C	-3.290552	-1.507011	0.012498
C	1.301322	2.010373	-0.184233
C	-4.799710	0.487202	0.044776
N	-4.558822	-0.899577	0.024145
N	1.043745	3.393916	-0.064176
O	-0.350328	5.183340	0.162353
O	2.414642	1.627734	-0.445018
O	-3.169768	-2.708412	-0.007523
O	-5.924491	0.926286	0.055256
H	2.725860	3.723552	-2.157996
H	-5.211197	-2.740327	1.886508
C	-5.700750	-1.764103	0.014860

C	-6.617236	-1.714597	-1.031592
C	-7.711440	-2.577655	-0.985073
N	-7.923014	-3.449363	-0.003723
C	-7.037204	-3.488468	0.986999
C	-5.911567	-2.668109	1.052052
H	-6.489228	-1.013755	-1.858917
H	-8.455084	-2.558460	-1.791622
H	-7.228004	-4.215908	1.785932
C	2.170477	4.275679	-0.138067
C	2.499995	5.081644	0.947836
C	3.601068	5.928349	0.825414
N	4.357064	6.002062	-0.265741
C	4.032395	5.223935	-1.293870
C	2.949151	4.345756	-1.289538
H	1.906557	5.059020	1.864188
H	3.882655	6.581006	1.661317
H	4.670234	5.297357	-2.183624
C	1.607089	-0.997281	0.186640
C	5.106192	-3.332877	0.440045
C	4.852636	-4.142088	-0.697670
N	3.651556	-3.755749	-1.252430
C	2.476189	-0.694365	1.257006
C	3.653172	-1.399993	1.446922
C	3.990921	-2.423643	0.553846
C	3.111774	-2.724674	-0.517292
C	1.915541	-2.032329	-0.700257
C	5.742911	-5.139821	-1.101076
H	5.540874	-5.759784	-1.978982
H	7.612934	-6.092083	-0.640053
C	6.276638	-3.532830	1.181184
C	7.165722	-4.524501	0.783591
C	6.897890	-5.317613	-0.346244
H	6.486669	-2.915776	2.059807
H	8.084421	-4.692008	1.352845
H	1.245271	-2.273802	-1.530172
H	2.207108	0.108343	1.948290

H	3.231897	-4.166973	-2.073858
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h.2) R//R

C	3.618440	1.415355	0.013887
C	3.739675	2.792100	0.064699
C	2.588755	3.603297	0.073978
C	1.326421	3.036930	0.031389
C	-0.221824	-0.362878	-0.146758
C	0.948593	-1.156003	-0.127275
C	2.202499	-0.582274	-0.077529
C	2.339312	0.819418	-0.037202
C	1.176034	1.631202	-0.033491
C	-0.104013	1.031292	-0.084551
H	4.740494	3.230233	0.102528
H	2.669243	4.692740	0.118317
C	0.137073	3.918739	0.056390
H	-4.297811	-1.131304	-2.326125
H	0.882117	-2.246101	-0.179225
C	3.403143	-1.466614	-0.071711
C	-1.311081	1.891498	0.009152
C	4.843450	0.568684	0.018629
N	4.643909	-0.824354	-0.025667
N	-1.116635	3.262938	0.057549
O	0.204529	5.119423	0.084396
O	-2.436789	1.423852	0.041380
O	3.301036	-2.668856	-0.101644
O	5.948700	1.044815	0.058808
H	-2.854372	3.450927	2.115301
H	5.489900	-2.440746	-2.014566
C	5.815966	-1.655386	-0.020022
C	6.651578	-1.683873	1.091427
C	7.776052	-2.508054	1.038210
N	8.082158	-3.266958	-0.008870
C	7.273024	-3.230118	-1.062347
C	6.125927	-2.438758	-1.126644
H	6.441754	-1.074761	1.973384

H	8.461843	-2.552371	1.893160
H	7.547397	-3.865066	-1.913739
C	-2.288347	4.093660	0.123443
C	-2.622113	4.917955	-0.945386
C	-3.770366	5.702122	-0.825810
N	-4.555539	5.695932	0.246301
C	-4.220915	4.905472	1.260574
C	-3.093765	4.083122	1.257260
H	-2.002420	4.959670	-1.843917
H	-4.064709	6.368880	-1.645514
H	-4.882782	4.923237	2.135185
C	-1.522966	-1.061273	-0.243854
C	-5.145185	-3.236436	-0.409797
C	-4.891624	-4.033830	0.729301
N	-3.637686	-3.678254	1.239702
C	-2.423093	-0.748807	-1.327052
C	-3.643234	-1.394309	-1.492151
C	-4.000147	-2.376867	-0.576365
C	-3.082937	-2.706729	0.495628
C	-1.843163	-2.058149	0.654148
C	-5.789453	-4.980270	1.188436
H	-5.585952	-5.592659	2.070467
H	-7.721860	-5.865346	0.804737
C	-6.342219	-3.394977	-1.110252
C	-7.262558	-4.349971	-0.657859
C	-6.989876	-5.125879	0.468356
H	-6.560439	-2.788375	-1.993346
H	-8.204996	-4.487978	-1.193763
H	-1.175013	-2.312751	1.480350
H	-2.109408	-0.003734	-2.060606
H	-3.208616	-4.099840	2.057648

i) TNDI-Mol-3

i.1) CS//CS

C	-5.998240	0.146308	-0.181329
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C	-6.565825	1.403309	-0.358752
C	-5.770906	2.550315	-0.409515
C	-4.391664	2.485265	-0.237773
C	-1.768808	-0.143320	0.209635
C	-2.588331	-1.289792	0.178535
C	-3.963745	-1.201479	0.101701
C	-4.591297	0.054027	-0.025433
C	-3.782433	1.224728	-0.007684
C	-2.378677	1.123378	0.209220
H	-7.650037	1.472412	-0.477990
H	-6.221546	3.527777	-0.599092
C	-3.555425	3.687690	-0.364301
H	-0.046388	0.859537	-1.612299
H	-2.132848	-2.283276	0.200620
C	-4.763664	-2.441924	0.103290
C	-1.659799	2.372289	0.528253
C	-6.830290	-1.073653	-0.159909
N	-6.156178	-2.277512	-0.019768
N	-2.241798	3.552110	0.061522
S	-4.122405	5.116940	-0.957845
S	-0.310581	2.424885	1.467398
O	-4.279555	-3.544025	0.205271
S	-8.472441	-1.033199	-0.290640
H	-0.451183	4.325509	-1.776496
H	-7.170361	-3.505625	2.151361
C	-6.913250	-3.499533	0.002304
C	-7.172815	-4.184324	-1.178831
C	-7.893075	-5.375352	-1.093764
N	-8.337489	-5.886858	0.050172
C	-8.074739	-5.221626	1.170904
C	-7.364195	-4.022299	1.208421
H	-6.826024	-3.797059	-2.139763
H	-8.119174	-5.943871	-2.004508
H	-8.448792	-5.664953	2.102219
C	-1.430626	4.741287	0.108146
C	-1.523470	5.626058	1.176456

C	-0.700895	6.750425	1.156984
N	0.159307	7.018970	0.177861
C	0.232097	6.163093	-0.835825
C	-0.539761	5.004471	-0.924861
H	-2.215117	5.440591	2.001073
H	-0.740812	7.470719	1.983505
H	0.945550	6.407113	-1.632976
C	-0.304947	-0.352889	0.159156
C	0.338392	-1.183328	1.083316
C	1.717274	-1.361036	1.036249
C	2.468209	-0.739305	0.035100
C	1.823367	0.042486	-0.931095
C	0.452067	0.237751	-0.862488
H	-0.239483	-1.651360	1.885563
H	2.226393	-1.965770	1.791014
N	3.869645	-0.888350	-0.004095
H	2.412440	0.492858	-1.734022
C	4.781596	0.148419	0.025764
C	4.559863	-2.081520	-0.079632
C	5.940070	-1.812468	-0.081753
C	6.080924	-0.382419	-0.054834
C	4.487175	1.531698	0.188926
C	5.519340	2.424860	0.212159
C	6.866333	1.970549	0.035248
C	7.172050	0.556250	-0.114613
C	3.995526	-3.381611	-0.207523
C	4.831976	-4.457951	-0.284106
C	6.249634	-4.272756	-0.197230
C	6.830923	-2.944412	-0.080496
C	8.524394	0.364339	-0.346028
S	9.390366	1.834726	-0.351846
C	7.998569	2.764473	-0.057964
C	8.206736	-3.017680	0.064731
S	8.771615	-4.627463	0.031409
C	7.211206	-5.270558	-0.166505
H	9.047855	-0.558155	-0.579881

H	5.327813	3.492694	0.348432
H	8.055478	3.850410	0.021238
H	8.911795	-2.213987	0.256179
H	7.052752	-6.346943	-0.237486
H	4.429997	-5.468965	-0.392515
H	3.452695	1.861623	0.313107
H	2.911079	-3.505219	-0.258464

i.2) R//R

C	6.012235	0.208483	0.109707
C	6.554316	1.478062	0.268589
C	5.733249	2.605172	0.355620
C	4.349795	2.508353	0.243523
C	1.787715	-0.189996	-0.133985
C	2.632647	-1.314749	-0.137501
C	4.006769	-1.187230	-0.100292
C	4.601667	0.083667	0.011075
C	3.762077	1.233822	0.035361
C	2.353386	1.096614	-0.122029
H	7.640431	1.575836	0.343093
H	6.170028	3.592486	0.526273
C	3.494402	3.690603	0.404689
H	0.100935	0.478122	1.866523
H	2.207627	-2.321592	-0.162185
C	4.837971	-2.410194	-0.138230
C	1.571646	2.327381	-0.354289
C	6.873540	-0.991930	0.049020
N	6.224790	-2.214347	-0.068762
N	2.155594	3.517538	0.057399
S	4.051118	5.140928	0.944675
S	0.120292	2.345988	-1.143144
O	4.365371	-3.518656	-0.225984
S	8.514719	-0.906660	0.113933
H	0.535261	4.316842	2.038481
H	7.185221	-3.412371	-2.282813
C	7.012570	-3.417573	-0.124118

C	7.337384	-4.094519	1.045147
C	8.084820	-5.266438	0.928531
N	8.494371	-5.764189	-0.233906
C	8.171134	-5.105694	-1.342329
C	7.428308	-3.925017	-1.349065
H	7.021593	-3.717043	2.020626
H	8.363825	-5.829463	1.827795
H	8.520386	-5.537995	-2.288181
C	1.319117	4.691728	0.055703
C	1.295901	5.546575	-1.039936
C	0.448593	6.651693	-0.977617
N	-0.327899	6.927355	0.067060
C	-0.282486	6.104976	1.109755
C	0.522930	4.967350	1.160503
H	1.916144	5.354108	-1.918141
H	0.396656	7.348690	-1.823056
H	-0.921478	6.361676	1.964181
C	0.328082	-0.450025	-0.072910
C	-0.316713	-1.158714	-1.092608
C	-1.693060	-1.354826	-1.051871
C	-2.420858	-0.874265	0.036756
C	-1.777979	-0.246055	1.105580
C	-0.407206	-0.037414	1.046925
H	0.255299	-1.501340	-1.959113
H	-2.209727	-1.851411	-1.877832
N	-3.841810	-0.986507	0.046060
H	-2.358728	0.091357	1.968451
C	-4.707898	0.061533	-0.129173
C	-4.572193	-2.132449	0.211539
C	-5.972914	-1.817820	0.124887
C	-6.059121	-0.422800	-0.048885
C	-4.350570	1.394456	-0.385298
C	-5.361175	2.322142	-0.537586
C	-6.724800	1.935491	-0.402085
C	-7.106836	0.561537	-0.140024
C	-4.057457	-3.414588	0.459385

C	-4.946780	-4.459885	0.600196
C	-6.347262	-4.241902	0.462463
C	-6.892828	-2.923101	0.207037
C	-8.475927	0.455720	0.020585
S	-9.276250	1.959037	-0.161700
C	-7.821073	2.786030	-0.452289
C	-8.264168	-2.983653	0.042047
S	-8.875591	-4.574190	0.212209
C	-7.331715	-5.219965	0.503220
H	-9.065439	-0.416525	0.289362
H	-5.117394	3.367553	-0.746035
H	-7.815759	3.861329	-0.639069
H	-8.954774	-2.187917	-0.223114
H	-7.196443	-6.287871	0.683102
H	-4.578953	-5.469911	0.800699
H	-3.298016	1.676963	-0.467654
H	-2.978985	-3.566379	0.541618