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Probing the aromaticity of bis(diazolo)pyrazine radical anions

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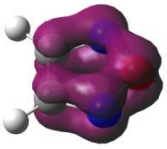
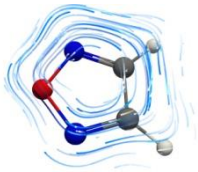
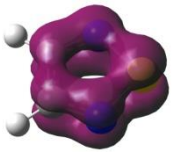
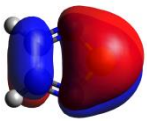
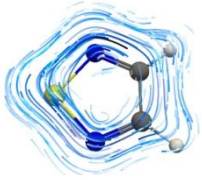
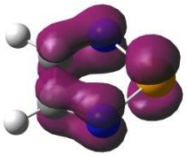
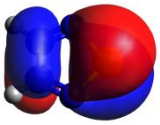
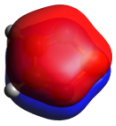
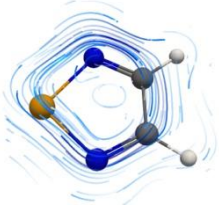
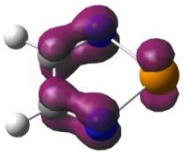
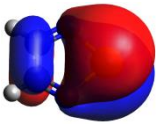
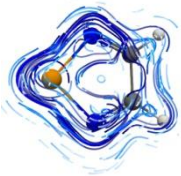
Computational details

The geometry optimization, magnetic shielding calculation using GIAO approach,[S1] sequent GIMIC analyses, and EDDB analysis were performed for structures **1**-**24** at the PBE0/aug-cc-pVTZ level[S2–S6] using the Gaussian.[S7] The aug-cc-pVTZ-pp[S8] basis set was utilized for the Te atom. The additional commands Pop(NBORead), Density=Current, NoSymm, and Int(NoBasisTransform) for Gaussian and also command set $NBO SKIPBO FILE=molecule_name DMNAO=W49 AONAO=W49 $END for built-in NBO v3.1 module were used. The EDDB analysis was performed using the RunEDDB script.[S9] The visualization of NODB orbitals for **1**-**10** (Figure S5) was done using the Avogadro program[S10] with default setting. For EDDB(**r**) isosurface plotting with a set of isovalues using the Paraview program (version 5.6),[S11] the RunEDDB FCHK output files were recalculated to the Cub-format using standard Cubgene utility[S7] and converted to the VTK-format using the MultiWFN program.[S12]

Since the magnetic current distribution depends on the direction of the external magnetic field, the latter is accepted to choose as normal to the ring plane (*Z* axis). The basis set and magnetic shielding matrix were extracted from FormCHK output file of Gaussian and converted using Gaussian2gimic.py script[S13] to format (MOL and XDENS files) suitable for the GIMIC calculation. The IC distribution were calculated with using the GIMIC 2.0 program.[S14] The IC distribution presented as streamline plots were obtained using Streamline modules implemented in the Paraview, parameters are adopted for the best view. It was noticed that the streamline extraction above 0.25 Å molecular plane possess a better clearness to view both the net IC and the circuit ICs for each ring. For calculation of IRCS value, integration grid with a 0.1 bohr step was chosen over a bond cross-section. It begins at the geometric ring center and extends up to 6 bohr in outward directions.

Table S1 EDDB and GMIC results for the monocyclic diazoles **21**-**24**

#	X	π-EDDB isosurface and π-EDDB$_H$(ē) value	View and occupation number (ē) for NODBs 1	2	3	IC stream line plot	IRCS (C–C), nA/T
21	O	 2.61	 0.941	 0.933	 0.742		11.8
22	S	 3.36	 1.188	 1.169	 1.007		13.4
23	Se	 2.63	 0.891	 0.877	 0.868		12.2
24	Te	 2.09	 0.790	 0.666	 0.639		10.6

The π-EDDB isosurfaces are presented at the standard isovalue 0.015 e.
The IC streamline plots are shown 0.25 Å above the ring plane.

Table S2 π-EDDB$_H$, π-EDDB$_F$, and IRCS values for **11**–**20**

#	X	Y	π-EDDB$_H$, ē	π-EDDB$_F$, ē			IRCS, nA/T			
				XN_2C_2	$C_2N_4H_2$	YN_2C_2	X–N	Y–N	C–N	C–C
11	O	O	6.82	2.70	2.96	2.70	6.5	6.5	-1.9	8.7, 8.8
12	O	S	7.14	2.71	3.59	3.17	6.2	7.4	-2.3	9.7
13	O	Se	6.87	2.72	3.37	2.57	6.5	6.7	-1.7	8.6, 8.4
14	O	Te	6.45	2.73	3.21	2.16	6.9	6.1	-1.2	8.5,6.9
15	S	S	8.02	3.17	2.78	3.17	6.8	6.8	-2.7	9.6
16	S	Se	7.48	3.19	3.65	2.59	7.4	6.3	-1.9	9.6, 8.2
17	S	Te	7.04	3.20	3.47	2.19	7.8	5.7	-1.3	9.1, 6.8
18	Se	Se	7.03	2.64	3.50	2.64	6.7	6.7	-1.4	8.0
19	Se	Te	6.63	2.67	3.35	2.24	7.1	6.1	-0.9	7.8, 6.6
20	Te	Te	6.29	2.28	3.23	2.28	6.3	6.3	-0.5	6.4

The IRCS values for X–N and Y–N bond describe ring current in the five-membered cycles, whereas the IRCS values for C–N bond corresponds to the six-membered cycle. It should be noted that hetereoatoms and the IRCS values being not additive for polycyclic molecules can prompt additional errors. The IRCS(C–C) being greater up to ~2 nA/T gives an insight into the reliability of the aromaticity estimation in the 5-membered rings. In the case of **11**-**20** the IRCS values for the X–N, Y–N and C–C bonds result in the same aromaticity degree series depending on heteroatom X/Y: Te < Se < O < S.

Table S3 The NODB occupancy numbers (ē) for **11**–**20**

Molecule			π-NODB							
#	X	Y	1	2	3	4	5	6	7	8
11	O	O	0.931	0.923	0.901	0.897	0.833	0.826	0.763	0.751
12	O	S	1.138	1.025	0.932	0.916	0.908	0.901	0.882	0.747
13	O	Se	0.945	0.939	0.927	0.903	0.857	0.783	0.774	0.751
14	O	Te	0.953	0.934	0.908	0.901	0.757	0.710	0.646	0.644
15	S	S	1.138	1.117	1.041	1.028	0.974	0.970	0.885	0.872
16	S	Se	1.138	1.047	0.991	0.989	0.894	0.859	0.794	0.769
17	S	Te	1.143	1.047	0.978	0.966	0.894	0.721	0.666	0.633
18	Se	Se	1.051	1.040	0.904	0.859	0.820	0.801	0.778	0.778
19	Se	Te	1.044	1.031	0.891	0.823	0.783	0.734	0.681	0.648
20	Te	Te	1.050	1.031	0.768	0.732	0.706	0.690	0.658	0.657

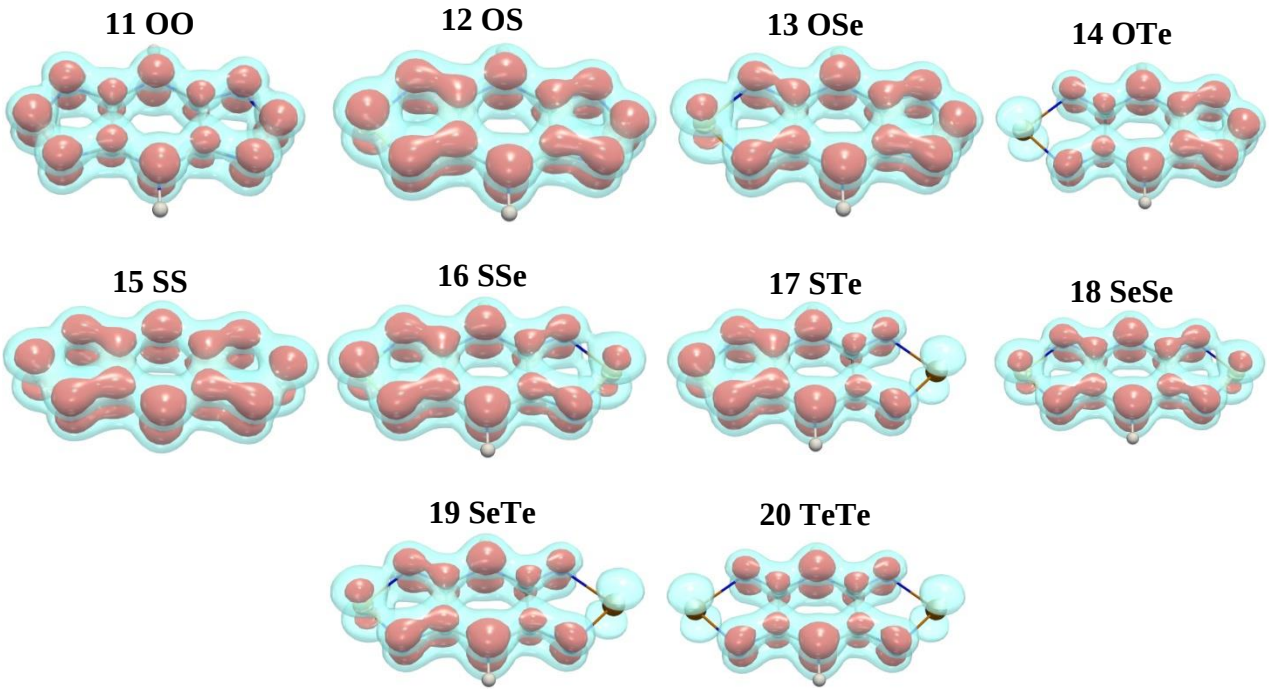


Figure S1 The isosurface plots of π-EDDB(**r**) function at the 0.01 ē (red) and 0.025 ē (cyan) isovalues for radicals **11**-**20**.

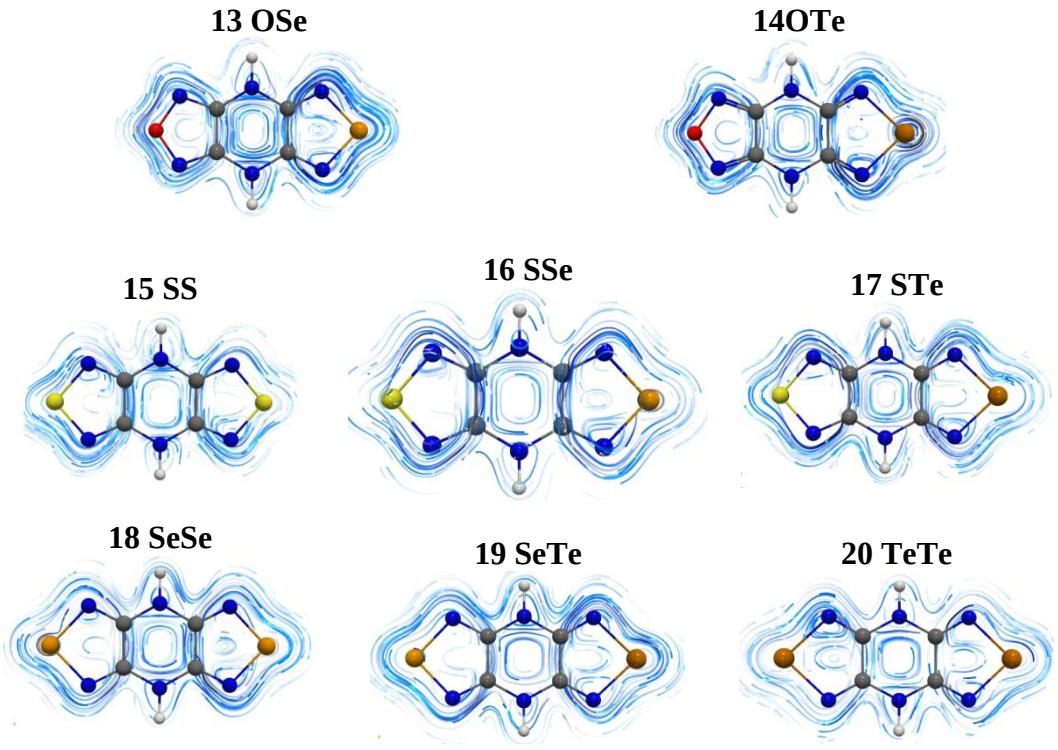


Figure S2. The streamline plots of IC density for **13**–**20**.

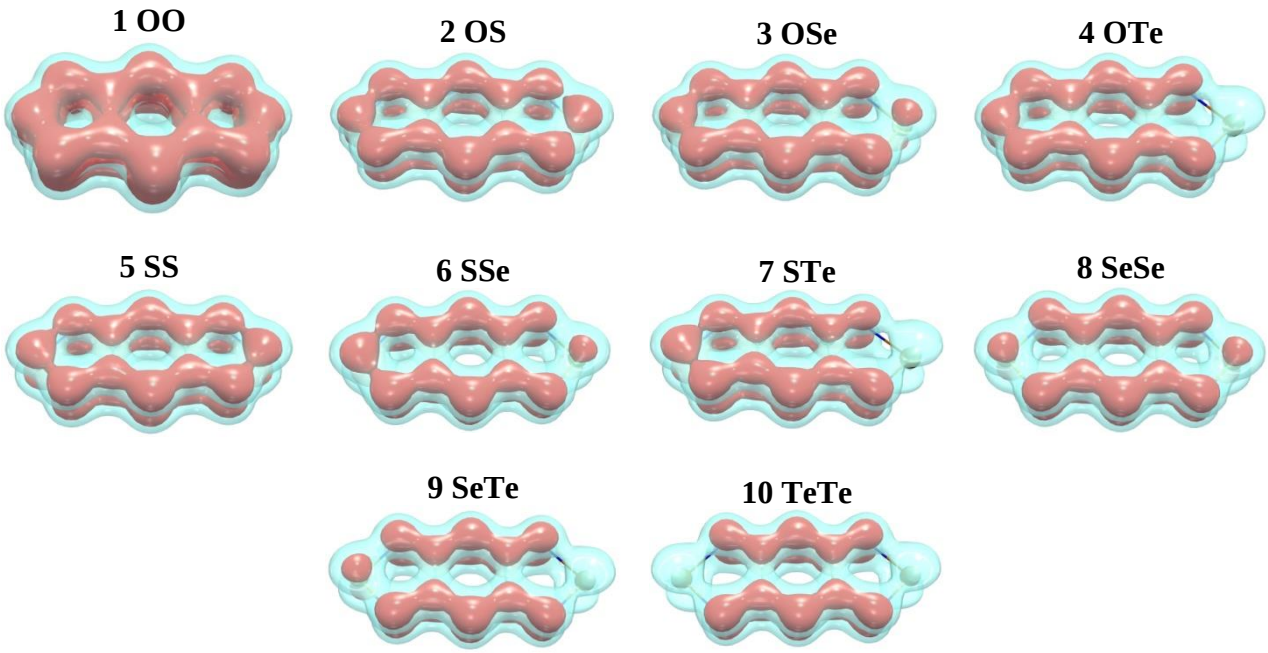


Figure S3. The isosurface plots of π-EDDB(**r**) function at the 0.01 ē (red) and 0.025 ē (cyan) isovalues for the radicals **1**-**10**.

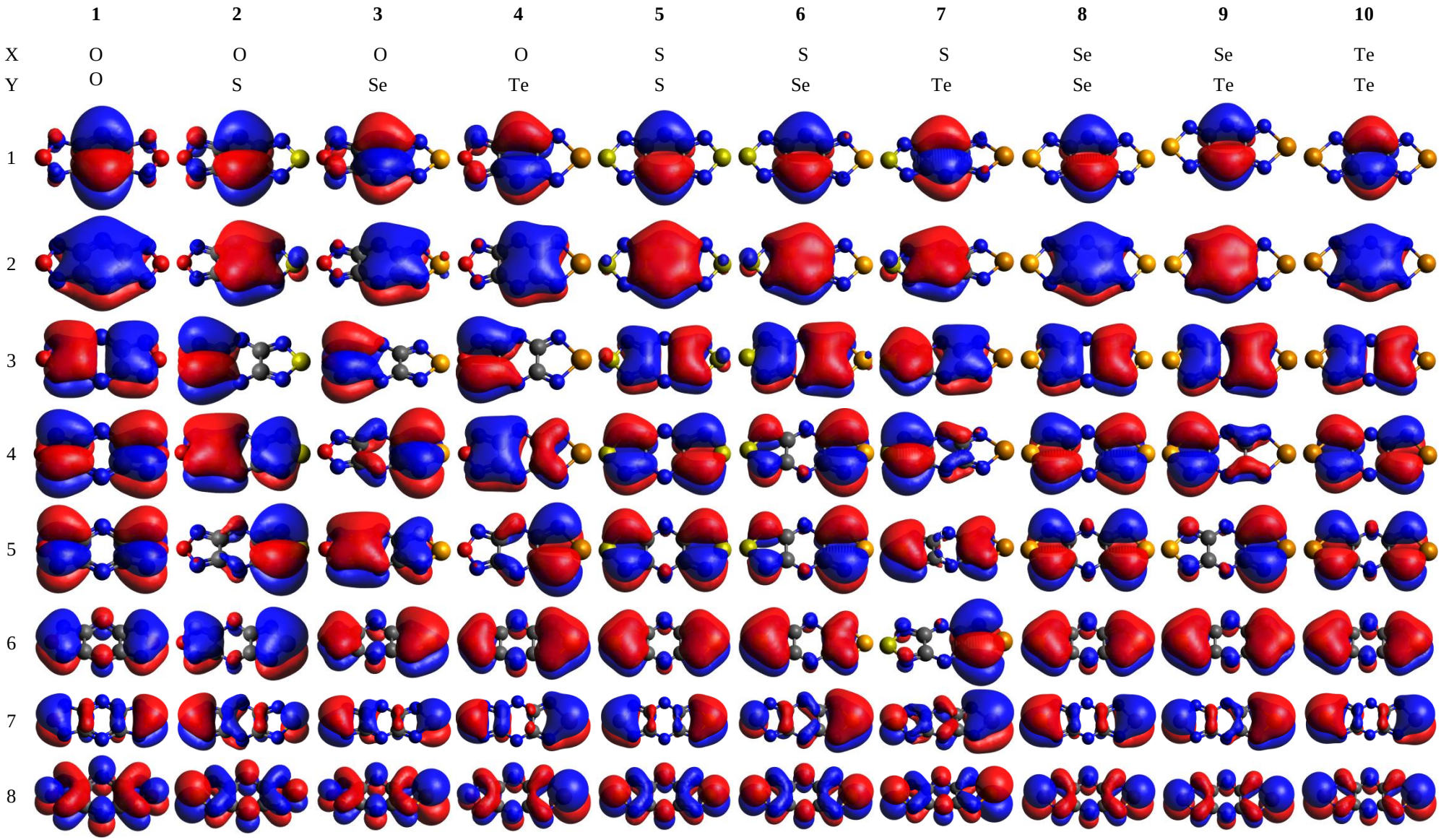


Figure S4. The NODB plots for **1**–**10**.

Table S4. The IRCS values (nA/T) for **1**–**10**

#	X	Y	Bond	Contribution			
				alpha	beta	spin	total
1	O	O	O–N	2.3	7.7	5.4	9.9
			C–N	-0.9	6.9	7.8	6.1
			C–C	3.2	0.9	2.3	4.1
2	O	S	O–N	2.4	7.9	5.5	10.3
			C–N	-0.5	6.6	7.1	6.0
			S–N	2.4	6.8	4.4	9.2
			$C–C_O$	43.0	1.5	1.5	4.5
			$C–C_S$	3.0	0.3	2.7	3.3
3	O	Se	O–N	2.8	7.8	4.9	10.6
			C–N	-0.1	6.6	6.7	6.5
			Se–N	2.1	7.3	5.2	9.4
			$C–C_O$	2.9	1.4	1.5	4.4
			$C–C_{Se}$	2.2	0.7	1.4	2.9
4	O	Te	O–N	3.1	7.5	4.4	**10.7**
			C–N	0.2	6.3	6.1	6.5
			Te–N	1.9	7.2	5.4	***9.1***
			$C–C_O$	2.9	1.4	1.5	4.3
			$C–C_{Te}$	1.6	0.9	0.6	2.5
5	S	S	S–N	2.4	7.6	5.2	10.0
			C–N	-0.5	7.2	7.7	5.7
			C–C	3.0	0.6	2.4	3.5
6	S	Se	S–N	2.9	7.1	4.2	10.0
			C–N	0.0	6.8	6.8	6.8
			Se–N	2.1	7.8	5.8	9.9
			$C–C_S$	2.9	0.3	2.5	3.2
			$C–C_{Se}$	2.1	1.1	1.0	3.3
7	S	Te	S–N	3.3	6.7	3.4	10.0
			C–N	0.4	6.3	5.9	6.7
			Te–N	1.8	7.6	5.8	9.5
			$C–C_S$	2.9	0.3	2.5	3.2
			$C–C_{Te}$	1.4	1.2	0.2	2.6
8	Se	Se	Se–N	2.5	7.5	5.0	10.0
			C–N	0.3	6.6	6.3	7.0
			C–C	2.1	0.9	1.3	3.0
9	Se	Te	Se–N	2.8	7.1	4.3	10.0
			C–N	0.5	6.3	5.7	6.8
			Te–N	2.1	7.3	5.2	9.5
			$C–C_{Se}$	2.2	0.8	1.2	3.0
			$C–C_{Te}$	1.5	1.0	0.5	2.5
10	Te	Te	Te–N	2.6	7.3	4.7	9.9
			C–N	0.7	6.1	5.3	6.8
			C–C	1.7	0.9	0.7	2.6

Table S5. The NODB occupancy numbers for **1**–**10**

Molecule			Contribution	π-NODB occupancy, ē								π-EDDB$_H$,
#	X	Y		1	2	3	4	5	6	7	8	ē
			alpha	0.688	0.674	0.537	0.523	0.512	0.507	0.289	0.273	**4.00**
1	O	O	beta	0.888	0.884	0.862	0.853	0.848	0.771	0.748	0.126	**5.98**
			total	1.535	1.467	1.396	1.396	1.394	1.134	1.036	0.490	**9.85**
			alpha	0.645	0.638	0.560	0.535	0.469	0.462	0.308	0.261	**3.88**
2	O	S	beta	0.838	0.827	0.789	0.776	0.767	0.705	0.684	0.128	**5.51**
			total	1.437	1.405	1.296	1.266	1.239	1.197	0.977	0.441	**9.26**
			alpha	0.611	0.606	0.534	0.518	0.474	0.472	0.278	0.231	**3.72**
3	O	Se	beta	0.862	0.852	0.824	0.798	0.791	0.776	0.704	0.127	**5.73**
			total	1.440	1.433	1.326	1.295	1.290	1.149	0.991	0.402	**9.33**
			alpha	0.601	0.600	0.512	0.491	0.483	0.480	0.293	0.179	**3.64**
4	O	Te	beta	0.871	0.853	0.837	0.809	0.774	0.750	0.700	0.128	**5.72**
			total	1.444	1.433	1.347	1.303	1.264	1.098	0.973	0.366	**9.23**
			alpha	0.698	0.683	0.588	0.552	0.545	0.534	0.351	0.323	**4.27**
5	S	S	beta	0.882	0.870	0.864	0.817	0.810	0.770	0.755	0.132	**5.90**
			total	1.579	1.522	1.408	1.315	1.289	1.259	1.201	0.463	**10.04**
			alpha	0.656	0.646	0.579	0.551	0.522	0.509	0.358	0.246	**4.07**
6	S	Se	beta	0.849	0.834	0.812	0.786	0.758	0.739	0.734	0.131	**5.64**
			total	1.488	1.455	1.344	1.291	1.261	1.246	1.061	0.424	**9.57**
			alpha	0.639	0.635	0.588	0.570	0.504	0.486	0.371	0.196	**3.99**
7	S	Te	beta	0.834	0.804	0.787	0.749	0.737	0.719	0.714	0.132	**5.48**
			total	1.443	1.430	1.302	1.291	1.239	1.221	1.005	0.397	**9.33**
			alpha	0.627	0.614	0.540	0.518	0.518	0.512	0.278	0.251	**3.86**
8	Se	Se	beta	0.866	0.854	0.822	0.775	0.765	0.764	0.760	0.131	**5.74**
			total	1.492	1.444	1.354	1.293	1.272	1.163	1.046	0.393	**9.46**
			alpha	0.609	0.597	0.534	0.517	0.498	0.484	0.280	0.206	**3.73**
9	Se	Te	beta	0.848	0.846	0.795	0.769	0.760	0.746	0.724	0.132	**5.62**
			total	1.455	1.420	1.324	1.286	1.230	1.140	0.988	0.365	**9.21**
			alpha	0.608	0.597	0.527	0.502	0.499	0.493	0.236	0.211	**3.67**
10	Te	Te	beta	0.848	0.837	0.803	0.762	0.745	0.726	0.712	0.132	**5.57**
			total	1.456	1.416	1.326	1.263	1.237	1.107	0.948	0.346	**9.10**

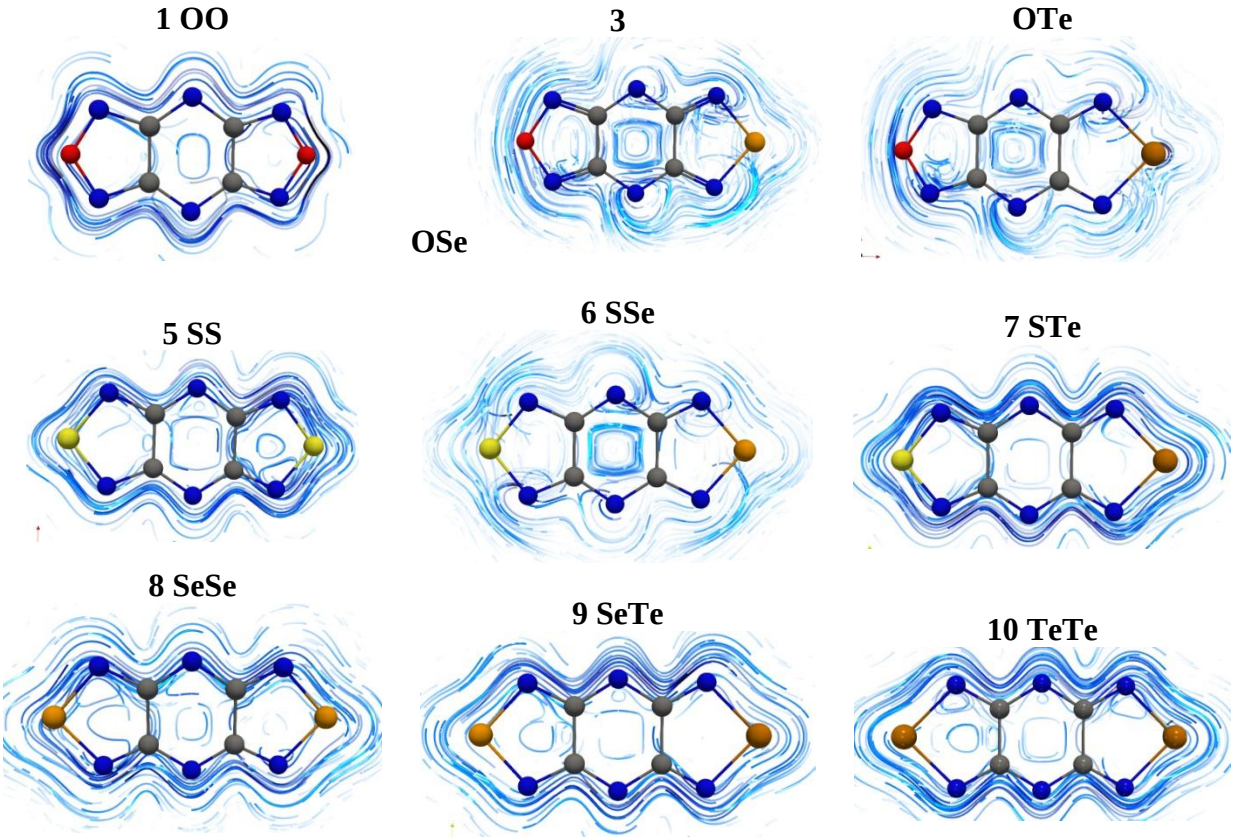


Figure S5. The IC streamline plots for **1**,**3-10** above 0.25 Å molecular plane.

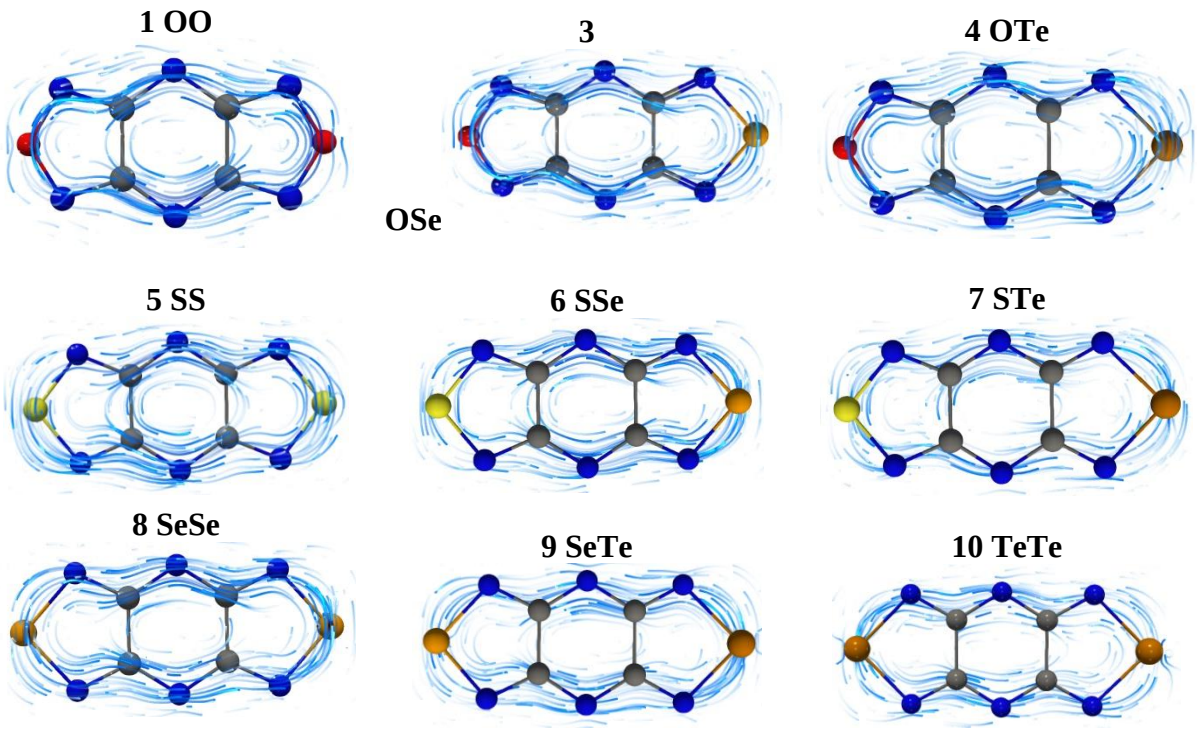


Figure S6. The streamline plots of IC spin density for **1**, **3-10**.

It should be noted that the direction of IC situated outside the cycles is anticlockwise. This fact points out that the aromatic net current (Figure S5) is determined by β-electrons.

Comparison aromaticity degree for 1–24 with classical aromatic heterocycles and arenes

To compare the aromaticity of **1**–**24** and simple heterocycles and some arenes, the IRCS, π-EDDB, and stabilization energies are presented in Table S6. As a result of the analysis of the data obtained, several features should be noted. The degree of aromaticity in monocyclic **21-24** is expected to be greater than in the five-membered cycle of tricyclic molecules **1-20**, moreover, it was comparable to that in furan **25**, thiophene **26**, selenophene **27** and tellurophene **28** or even a little more. The IRCS and EDDB aromatic dependences upon heteroatom changing are the same for monocyclic molecules **21-28**, the aromaticity degree increases in the series Te < Se < O < S. As commonly accepted, the molecules **21** and **25** (X=O) occupy intermediate position, due to the difference in the electronegativity of atoms. When comparing the fully aromatic tricyclic radicals **1-10** with anthracene **29** and phenanthrene **30**, it can be observed that the IRCS values for **29** and **30** are significantly higher (by 2 nA/T and more), while all π-EDDB values range in 9–10 ē, whereas molecules **1** and **5** exhibit a slightly stronger delocalization (π-EDDB values) than anthracene **29**. These inconsistencies are caused by the presence of heteroatoms, as well as the well-known fact that the induced currents of adjacent cycles interact, this generates a global, local, and semi-local currents,[S15] for the same reason the IRCS values are not additive. In general, aromaticity in radicals **1-10** appears strength, they have a high degree of delocalization and a rather strong (~10 nA/T) diamagnetic current.

Tables S6. The IRCS, π-EDDB, ASE and ISE values for simple aromatic molecules.

Molecule	IRCS, nA/T	π-EDDB, ē	– ASE, kcal mol^{-1}	– ISE, kcal mol^{-1}
Benzene	11.8* [S15]	5.5 [S21], 5.3 [S22]	34 *[S16]	33.2 *[S16]
Cyclopentadienyl anion	12.9* [S15]	5.73*		26.0 [S17]
Pyridine	11.6* [S15]	5.25 [S22]	31.0* [S16]	33.5* [S15]
Pyrrole	11.6* [S15], 11.8 [S18]	2.86 [S22]	20.6 [S19]	22.5*[S23]
Furan **25**	10.3* [S15]	2.54*	14.7 [S19]	18.8*
Thiophene **26**	11.6* [S15]	2.93*	18.6 [S19]	19.6*
Selenophene **27**	11.0*	2.59*		15.2*
Tellurophene **28**	10.1*	2.28*		12.0*
Naphthalene	12.9*	6.97 [S21]	39.4 [S20]	52* [S15]
Anthracene **29**	12.4, 15.9*	9.63 [S21]	42.0 [S20]	
Phenanthrene **30**	13.1, 10.7*	10.10 [S21]	51.4 [S20]	

* Calculated at the B3LYP level
ASE – aromatic stabilization energy [S16]
ISE – isomerisation stabilization energy [S16]

References

S1. T. Helgaker, M. Jaszuński, and K. Ruud, *Chem. Rev.*, 1999, **99**, 293.

S2. C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158 .

S3. T.H.Dunning, *J. Chem. Phys.*, 1989, **90**, 1007.

S4. R. A.Kendall, T. H. Dunning, and R.J. Harrison, *Chem. Phys.*, 1992, **96**, 6796.

S5. A. K. Wilson, D. E.Woon, K. A. Peterson, and T. H. Dunning, *J. Chem. Phys.*, 1999, **110**, 7667.

S6. D. E. Woon and T.H. Dunning, *J. Chem. Phys.*, 1993, **98**, 1358.

S8. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09 Revision D.01, Gaussian, Inc., Wallingford CT, 2013.

S8. K. A. Peterson, D. Figgen, E. Goll, H. Stoll, and M. Dolg, *J. Chem. Phys.*, 2003, **119**, 11113.

S9. *RunEDDB script*, http://www.eddb.pl/runeddb.

S10. M. D. Hanwell, D. E. Curtis, D. C. Lonie, T. Vandermeersch, E. Zurek, and G. R. Hutchison, *J. Cheminform.* 2012, **4**, 17.

S11. *Paraview*, https://www.paraview.org.

S12. *Multiwfn program*, http://sobereva.com/multiwfn.

S13. M. Rauhalahti, S. Taubert, D. Sundholm and V. Liégeois, *Phys. Chem. Chem. Phys.*, 2017, **19**, 7124.

S14. D. Sundholm, H. Fliegl, and R. J. F. Berger, *WIREs Comput. Mol. Sci.*, 2016, **6**, 639.

S15. R. R. Aysin and S. S. Bukalov, *INEOS OPEN*, 2021, **4**, 154.

S16. P. v. R. Schleyer and F. Pühlhofer, *Org. Lett*., 2002, **4**, 17, 2873

S17. R. R. Aysin and S. S. Bukalov, *Organometallics*, 2021, **40**, 7, 938.

S18. M. P. Johansson and J. Jusélius, *Lett. Org. Chem.*, 2005, **2**, 469.

S19. M. K. Cyrañski, T. M. Krygowski, A. R. Katritzky, and P. von R. Schleyer, *J. Org. Chem.*, 2002, **67**, 1333.

S20. A. Ciesielski, D. K. Stepien, M. A. Dobrowolski, Ł. Dobrzycki, and M. K. Cyrañski, *Chem. Commun.*, 2012, **48**, 10129.

S21. D. W. Szczepanik, M. Andrzejak, K. Dyduch, E. Zak, M. Makowski, G. Mazur, and J. Mrozek, *Phys. Chem. Chem. Phys.*, 2014, **16**, 20514.

S22. D. W. Szczepanik, M. Andrzejak, J. Dominikowska, B. Pawełek, T. M. Krygowski, H. Szatylowicze, and M. Sola, *Phys. Chem. Chem. Phys.*, 2017, **19**, 28970.

Optimized Cartesian xyz-coordinates

1

C	-1.0811720767	-0.7251900515	-0.0000010000
C	1.0811710767	-0.7251900515	0.0000000000
C	1.0811700767	0.7251890515	0.0000000000
C	-1.0811720767	0.7251890515	0.0000000000
N	0.0000010000	-1.4923721059	0.0000020000
N	0.0000000000	1.4923711059	0.0000020000
N	2.3496771668	-1.1315340803	0.0000000000
N	-2.3496761668	-1.1315340803	0.0000000000
N	-2.3496761668	1.1315350803	0.0000030000
N	2.3496761668	1.1315350803	-0.0000040000
O	-3.0484922164	0.0000000000	-0.0000040000
O	3.0484902164	0.0000000000	0.0000010000

2

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C	1.0835723063	-0.7425589426	0.0000003970
C	-1.1226385831	-0.7237770636	0.0000002139
C	-1.1226387810	0.7237772905	-0.0000017524
O	-3.1190921238	-0.0000002712	0.0000018499
S	3.3364723630	-0.0000001584	0.0000048776
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N	-2.3692612738	-1.1404503288	0.0000028565
N	-0.0190306430	-1.4871570433	-0.0000012076
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3

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C	-1.1320231383	0.7226762181	-0.0000015883
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N	-2.3805427142	-1.1401944434	-0.0000106364
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C	-1.1457374580	-0.7212966900	-0.0000105011
C	-1.1457375537	0.7212964495	-0.0000071068
O	-3.1409463282	-0.0000002779	-0.0000294782
Te	3.6360221546	-0.0000009897	-0.0000452727

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5

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S	-0.0000005080	3.3652554979	-0.0002882048
S	-0.0000004566	-3.3652555260	0.0000153066
N	-1.2534844348	-2.3414023825	-0.0000280204
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7

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9

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C	-1.1384164450	0.7433037978	-0.0000051859
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10

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N	-2.3810461690	-1.1321700822	0.0000020000
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12

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13

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N	2.3089301635	1.3072690922	-0.0000020000
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N	-2.4215401720	-1.1334600788	-0.0000020000
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N	-0.0368530026	1.4253830998	-0.0000020000
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14

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H	-0.0474590033	2.4237741732	0.0000560000

H	-0.0474590033	-2.4237741732	0.0000560000

15

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16

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17

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18

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19

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20

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21

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22

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H	-2.0402966036	-1.3450348425	-0.0001245761

23

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C	1.1282910807	-0.7154510531	0.0000010000
Se	3.5195602503	0.0000000000	-0.0000010000
N	2.2905221614	-1.3026350923	-0.0000010000
N	2.2905221614	1.3026350923	0.0000000000
H	0.2266600159	1.3193170929	0.0000000000
H	0.2266600159	-1.3193160927	0.0000010000

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C	1.1237490783	0.7235000508	-0.0000700000
C	1.1237470780	-0.7234980505	-0.0001150000
Te	3.6931242600	-0.0000020000	-0.0001580000
N	2.2444701568	-1.3698990981	0.0002100000
N	2.2444731572	1.3698990981	0.0002040000
H	0.1924870139	-1.2879780891	-0.0000060000
H	0.1924900138	1.2879830898	0.0000250000