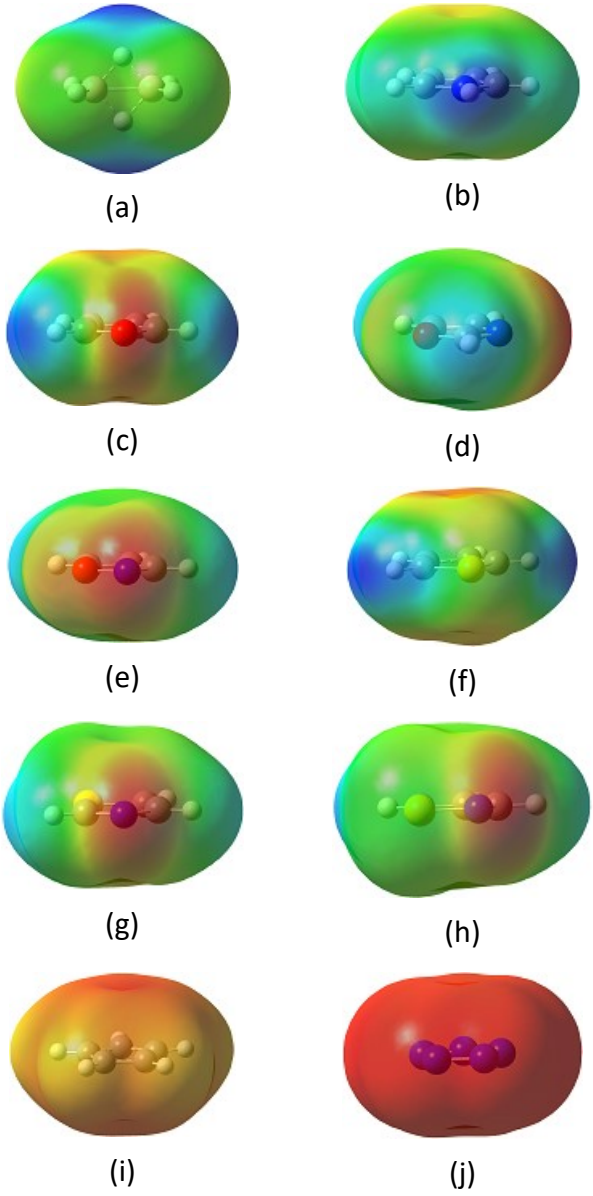
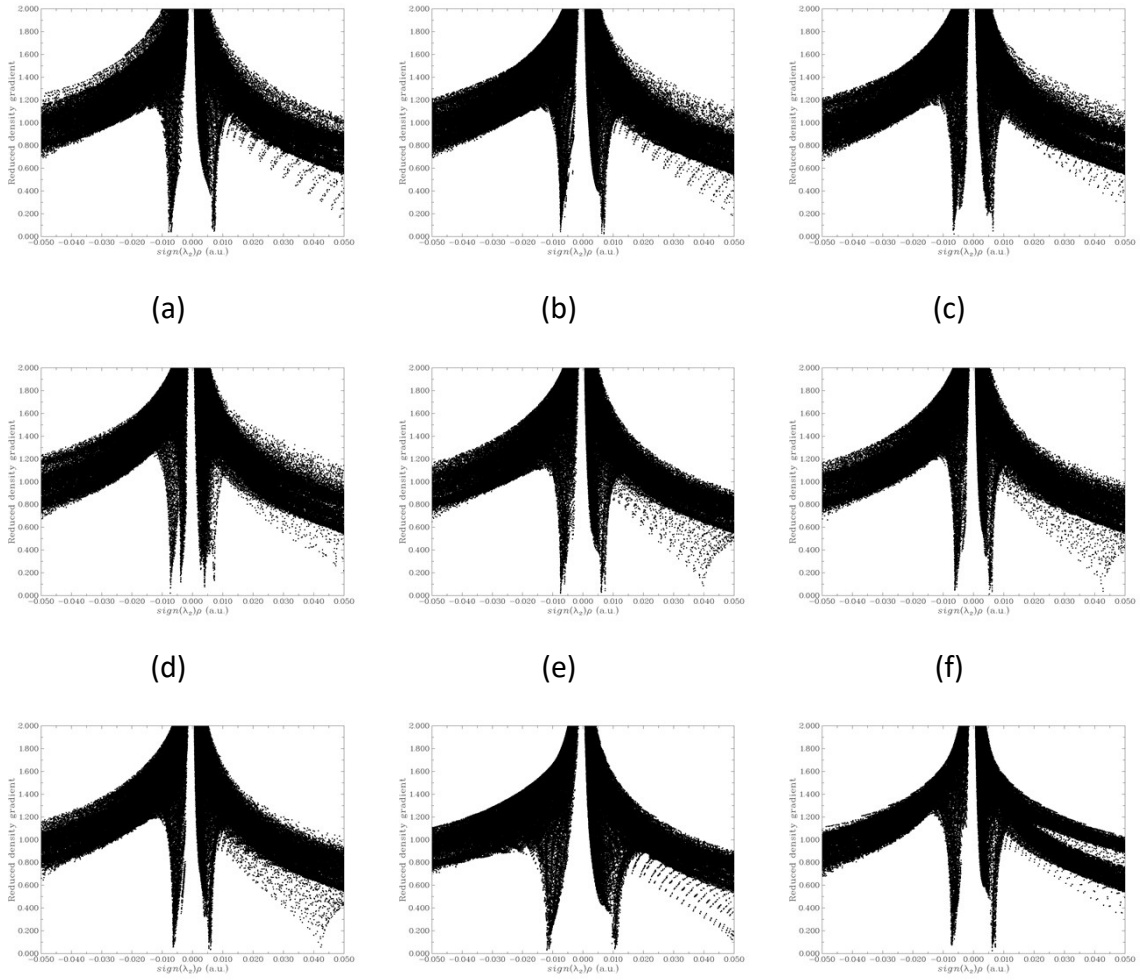
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information (ID: NJ-ART-04-2023-001797)



Supplementary Fig. 1: MESP surface for (a) DB, (b) Pyr, (c) Fur, (d) Oxa, (e) iOxa, (f) Thio, (g) Thia, (h) iThia, (i) Cp^- and (j) Pnz^- obtained at B3LYP-D3/6-311++G(d,p) level of theory



Supplementary Fig. 2 RDG vs sign(λ_2) ρ plot for (a) DB···Pyr, (b) DB···Fur, (c) DB···Oxa, (d) DB···iOxa, (e) DB···Thio, (f) DB···Thia, (g) DB···iThia, (h) DB···Cp^- and (i) DB···Pnz^- complexes

Supplementary Table 1: Electron density (ρ), laplacian of electron density ($\nabla^2\rho$), local electronic energy density (H(r)) and electron localization function (ELF) values (in a.u.) for the complexes at the bond critical point obtained at B3LYP-D3/6-311++G(d,p) level of theory

Complexes	**CPs**	**ρ**	**$\nabla^2\rho$**	**H(r)**	**ELF**
DB···Pyr	25	0.0078	0.0265	0.0009	0.0237
DB···Fur	24	0.0075	0.0232	0.0010	0.0286
	33	0.0075	0.0233	0.0010	0.0286
DB···Oxa	22	0.0065	0.0207	0.0008	0.0212
	28	0.0067	0.0204	0.0009	0.0256
DB···iOxa	25	0.0073	0.0254	0.0008	0.0199
	32	0.0073	0.0244	00010	0.0223
DB···Thio	35	0.0074	0.0229	0.0010	0.0286
	41	0.0074	0.0227	0.0009	0.0279
DB···Thia	21	0.0056	0.0197	0.0009	0.0159
	30	0.0062	0.0192	0.0008	0.0192
DB···iThia	21	0.0065	0.0217	0.0010	0.0202
	31	0.0064	0.0207	0.0009	0.0213
DB···Cp^-	36	0.0119	0.0359	0.0015	0.0533
	43	0.0112	0.0361	0.0016	0.0451
DB···Pnz^-	21	0.0073	0.0257	0.0009	0.0206