Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Unusual Chalcogen···Chalcogen Interactions in Like···Like and Unlike Y=C=Y···Y=C=Y Complexes (Y = O, S, and Se)

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Table S1. Topological parameters, including the electron density (ρ_b, au), Laplacian ($\nabla^2\rho_b$, au), and total energy density (H_b, au), at bond critical points (BCPs) for Y=C=Y···Y=C=Y complexes (where Y = O, S, and Se) in the fashion of type I, II, III, and IV chalcogen···chalcogen interactions at the most favorable parameters.

Complex	ρ_b (au)	$\nabla^2\rho_b$ (au)	H_b (au)	ρ_b (au)	$\nabla^2\rho_b$ (au)	H_b (au)
	Type I			**Type II**		
O=C=O···O=C=O	0.0057	0.0230	0.0012	0.0042	0.0186	0.0011
O=C=O···S=C=S	0.0054	0.0248	0.0016	0.0050	0.0199	0.0012
O=C=O···Se=C=Se	0.0061	0.0260	0.0015	0.0054	0.0198	0.0010
S=C=S···S=C=S	0.0069	0.0192	0.0009	0.0068	0.0224	0.0012
S=C=S···Se=C=Se	0.0072	0.0182	0.0007	0.0078	0.0234	0.0010
Se=C=Se···Se=C=Se	0.0080	0.0178	0.0042	0.0072	0.0202	0.0008
	Type III			**Type IV**		
O=C=O···O=C=O	0.0026	0.0127	0.0008	0.0060	0.0243	0.0013
O=C=O···S=C=S	0.0053	0.0246	0.0016	0.0046	0.0152	0.0008
O=C=O···Se=C=Se	0.0059	0.0255	0.0014	0.0045	0.0138	0.0006
S=C=S···S=C=S	0.0055	0.0219	0.0014	0.0066	0.0187	0.0009
S=C=S···Se=C=Se	0.0061	0.0225	0.0012	0.0072	0.0183	0.0007
Se=C=Se···Se=C=Se	0.0055	0.0194	0.0010	0.0071	0.0166	0.0005

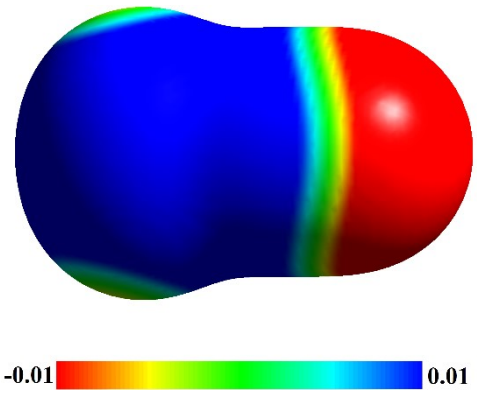

Figure S1. Molecular electrostatic potential (MEP) map of the SCN^- molecule mapped onto 0.002 au electron density contour. The electrostatic potential varies from −0.01 (red) to +0.01 (blue) au.