Stability trends and tautomerization of chalcocyclopentadienes. The role of aromaticity

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Supporting Information

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Table S1. Calculated Gibbs free energies (hartrees)

		ΔG^a	ΔG^b
O	iso1	-269.26087	-268.578126
	iso2-2	-269.276363	-268.590375
	iso3-2	-269.277279	-268.591346
S	iso1	-592.240462	-591.19169
	iso2-1	-592.247604	-591.196924
	iso3-1	-592.247502	-591.196636
Se	iso1	-2593.46115	-2593.44468
	iso2-1	-2593.46706	-2593.44699
	iso3-1	-2593.46725	-2593.44665

[a] at B3LYP/6-31+G(d,p)
[b] CCSD/6-311+G(d,p)

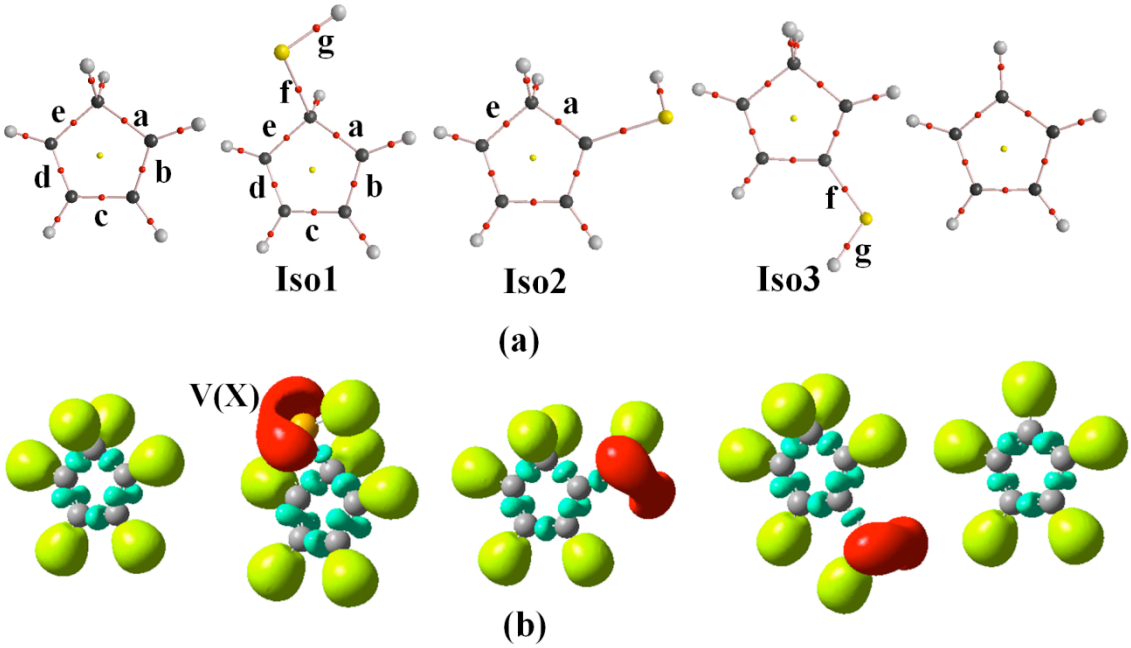

Table S2. Electron density (a.u.) at the BCP; ***basin population (e^-)***; *bond length (Å)* and `bond order`, evaluated at the C-C bonds of the ring (**a**, **b**, **c**, **d** and **e**), at the C-X bond (**f**) and at the X-H bond (**g**). **V(X)** is the electron-pair basin on the heteroatom.

	a	**b**	**c**	**d**	**e**	**f**	**g**	**V(X)**
Cyclopentadiene	0.256 ***1.97*** *1.507* `1.04`	0.337 ***3.44*** *1.352* `1.81`	0.273 ***2.20*** *1.469* `1.13`					

Cyclopentadienyl anion	0.295 ***2.96*** *1.418* 1.40							
O-ISO1	0.256 ***2.04*** *1.519* 1.00	0.339 ***3.43*** *1.347* 1.84	0.269 ***2.160*** *1.479* 1.10	0.340 ***3.46*** *1.346* 1.84	0.260 ***2.04*** *1.511* 1.01	0.254 ***1.26*** *1.427* 0.93	0.365 ***1.71*** *0.966* 0.77	***4.72***
O-ISO2	0.262 ***2.06*** *1.504* 1.02	0.335 ***3.68*** *1.355* 1.70	0.271 ***2.18*** *1.470* 1.12	0.337 ***3.50*** *1.352* 1.82	0.254 ***1.97*** *1.510* 1.03	0.286 ***1.47*** *1.362* 1.03	0.363 ***1.73*** *0.967* 0.75	***4.48***
O-ISO3	0.253 ***1.95*** *1.508* 1.03	0.335 ***3.70*** *1.354* 1.70	0.279 ***2.28*** *1.466* 1.10	0.339 ***3.42*** *1.349* 1.82	0.256 ***1.95*** *1.509* 1.04	0.285 ***1.44*** *1.365* 1.02	0.364 ***1.75*** *0.966* 0.76	***4.53***
S-ISO1	0.258 ***2.00*** *1.507* 1.03	0.338 ***3.43*** *1.350* 1.81	0.272 ***2.180*** *1.472* 1.12	0.339 ***3.43*** *1.50* 1.81	0.256 ***2.02*** *1.509* 1.03	0.164 ***1.48*** *1.859* 0.97	0.212 ***1.87*** *1.350* 0.97	***4.54***
S-ISO2	0.253 ***2.00*** *1.513* 1.02	0.334 ***3.53*** *1.356* 1.73	0.274 ***2.20*** *1.466* 1.13	0.337 ***3.43*** *1.352* 1.81	0.256 ***1.95*** *1.508* 1.04	0.194 ***1.82*** *1.771* 1.09	0.212 ***1.85*** *1.351* 0.96	***4.39***
S-ISO3	0.256 ***1.95*** *1.506* 1.04	0.335 ***3.54*** *1.354* 1.73	0.270 ***2.20*** *1.474* 1.10	0.339 ***3.43*** *1.349* 1.82	0.256 ***1.97*** *1.506* 1.04	0.192 ***1.78*** *1.778* 1.07	0.212 ***1.86*** *1.349* 0.96	***4.36***
Se-ISO1	0.262 ***2.01*** *1.498* 1.05	0.337 ***3.42*** *1.352* 1.79	0.271 ***2.180*** *1.468* 1.13	0.337 ***3.4*** *1.352* 1.80	0.259 ***2.04*** *1.503* 1.04	0.135 ***1.39*** *1.989* 0.92	0.170 ***1.86*** *1.468* 0.98	***4.91***
Se-ISO2	0.254 ***1.99*** *1.510* 1.03	0.334 ***3.49*** *1.355* 1.74	0.274 ***2.22*** *1.466* 1.12	0.337 ***3.42*** *1.352* 1.81	0.256 ***1.98*** *1.507* 1.03	0.160 ***1.79*** *1.890* 1.06	0.171 ***1.85*** *1.468* 0.97	***4.78***
Se-ISO3	0.255 ***1.94*** *1.506* 1.03	0.334 ***3.55*** *1.353* 1.73	0.271 ***2.21*** *1.471* 1.11	0.339 ***3.46*** *1.349* 1.81	0.257 ***1.97*** *1.505* 1.04	0.160 ***1.77*** *1.894* 1.05	0.172 ***1.86*** *1.463* 0.98	***4.72***
Te-ISO1	0.264 ***2.04*** *1.492* 1.07	0.334 ***3.41*** *1.356* 1.76	0.275 ***2.22*** *1.465* 1.14	0.335 ***3.38*** *1.356* 1.77	0.260 ***2.05*** *1.497* 1.06	0.093 ***1.34*** *2.237* 0.86	0.125 ***1.86*** *1.679* 0.98	***5.29***
Te-ISO2	0.253 ***1.94*** *1.512* 1.03	0.334 ***3.38*** *1.356* 1.77	0.274 ***2.19*** *1.468* 1.12	0.337 ***3.41*** *1.353* 1.81	0.256 ***1.97*** *1.506* 1.03	0.111 ***1.95*** *2.128* 0.98	0.123 ***1.93*** *1.680* 0.97	***5.18***
Te-ISO3	0.256 ***1.94*** *1.507* 1.03	0.335 ***3.43*** *1.354* 1.78	0.269 ***2.16*** *1.474* 1.12	0.338 ***3.44*** *1.351* 1.82	0.256 ***1.96*** *1.506* 1.04	0.110 ***1.86*** *2.134* 0.97	0.124 ***1.84*** *1.677* 0.98	***5.36***

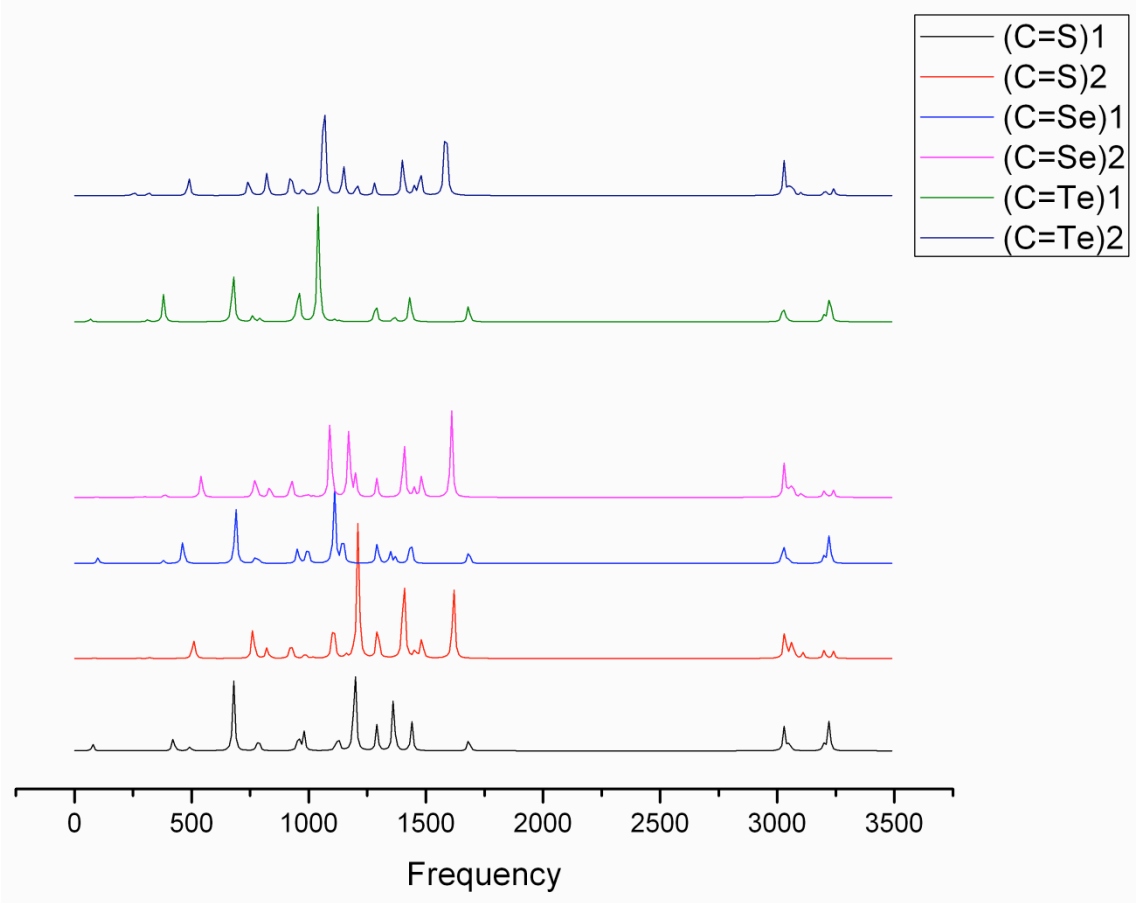

Figure S1. IR spectrum for the keto forms of S, Se and Te containing derivatives. Frequencies in cm^{-1}.