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

The One-Electron Reduction of Dithiolate and Diselenolate Ligands.

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Supplementary Information

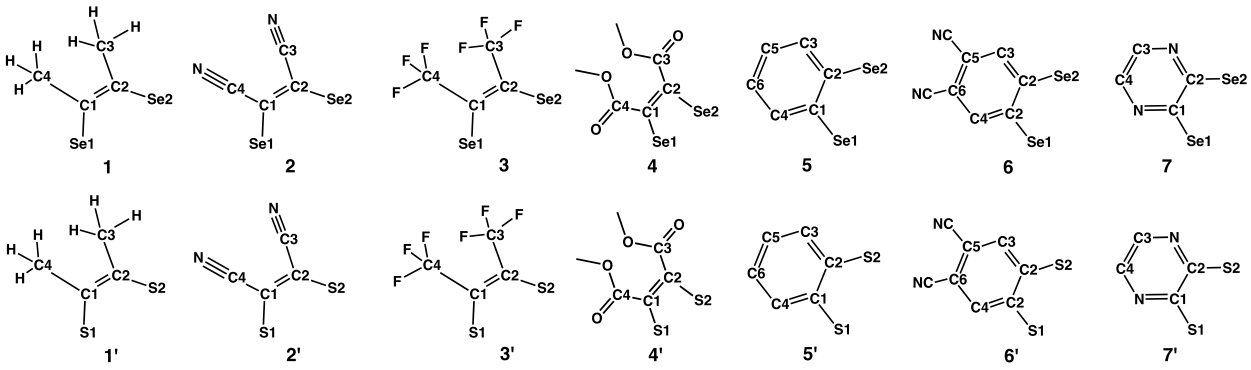
(**Tables S1 and S2, 3 pages in total**)

Table S1. The absolute C=C, C–S and C-Se bond lengths for all oxidized and reduced species.

Selenium	Ox		Red			
	C=C	C-Se	C=C	C-Se	Δ*r*(C=C)	Δ*r*(C-Se)
H	1.343	1.897	1.351	1.918	0.009	0.020
1	1.406	1.856	1.367	1.929	-0.039	0.073
2	1.421	1.841	1.400	1.895	-0.022	0.054
3	1.363	1.891	1.392	1.907	0.029	0.016
4	1.370	1.886	1.390	1.898	0.021	0.012
5	1.411	1.901	1.441	1.918	0.030	0.017
6	1.419	1.883	1.452	1.887	0.033	0.004
7	1.434	1.889	1.476	1.899	0.042	0.010

Sulphur	Ox		Red			
	C=C	C-S	C=C	C-S	Δ*r*(C=C)	Δ*r*(C-S)
H	1.404	1.685	1.360	1.768	-0.044	0.083
1'	1.423	1.696	1.374	1.770	-0.049	0.074
2'	1.437	1.681	1.406	1.737	-0.031	0.056
3'	1.438	1.680	1.400	1.745	-0.038	0.065
4'	1.374	1.737	1.401	1.738	0.027	0.001
5'	1.464	1.705	1.454	1.753	-0.010	0.048
6'	1.423	1.731	1.465	1.725	0.042	-0.006
7'	1.437	1.735	1.489	1.734	0.052	-0.001

Table S2. The calculated SDs for the carbon, sulphur and selenium atoms for all oxidized species.



	1	2	3	4	5	6	7
C1	0.07	0.01	-0.15	-0.24	-0.36	-0.48	-0.05
Se1	0.43	0.47	0.55	0.56	0.55	0.57	0.55
C2	0.07	0.01	-0.15	-0.24	-0.36	-0.48	-0.05
Se2	0.43	0.47	0.55	0.56	0.55	0.57	0.55
C3			0.10	0.18	0.28	0.30	
C4			0.10	0.18	0.28	0.30	
C5						0.10	
C6						0.10	
	1'	2'	3'	4'	5'	6'	7'
C1	0.11	0.05	0.09	-0.23	0.05	-0.43	-0.07
S1	0.40	0.43	0.44	0.62	0.42	0.64	0.60
C2	0.11	0.05	0.09	-0.23	0.05	-0.43	-0.07
S2	0.40	0.43	0.44	0.62	0.42	0.64	0.60
C3				0.11		0.20	
C4				0.11		0.20	
C5						0.08	
C6						0.08	