

Supplementary Table 1.

Cartesian Coordinates of Global Minimum Conformers

				S	-1.886	-1.046	0.008
<i>GeS₂</i>				S	-1.881	1.054	-0.007
Ge	0.000	0.000	0.000	S	0.745	3.674	-0.023
S	0.000	0.000	2.000	S	0.730	-3.679	0.035
S	0.000	0.000	-2.000				
				<i>Ge₃S₄ (Edge)</i>			
<i>GeS₃</i>				Ge	0.298	-1.650	-0.056
Ge	0.088	-1.172	0.000	Ge	1.222	1.922	-0.474
S	-0.096	1.908	0.000	Ge	-1.446	0.766	1.044
S	-1.549	0.408	0.000	S	-1.810	-1.280	-0.147
S	1.525	0.593	0.000	S	-0.913	2.146	-0.830
				S	1.585	-3.067	-0.716
				S	0.974	0.126	1.180
<i>GeS₄</i>							
Ge	0.052	0.657	0.020	<i>Ge₃S₄ (Central)</i>			
S	0.469	2.630	0.073	Ge	-2.382	-0.199	-0.181
S	1.267	-1.178	-0.008	Ge	0.538	2.290	-0.111
S	-0.561	-2.253	-0.056	Ge	0.746	-0.918	0.093
S	-1.801	-0.530	-0.028	S	-1.198	-1.469	1.172
				S	1.564	0.889	1.241
<i>Ge₂S₂</i>				S	1.989	-2.349	-0.668
Ge	0.000	-1.543	0.000	S	-0.451	0.528	-1.404
Ge	0.000	1.543	0.000				
S	-1.681	0.000	0.000	<i>Ge₃S₅</i>			
S	1.681	0.000	0.000	Ge	-0.522	1.795	-0.044
				Ge	-0.513	-1.750	-0.037
<i>Ge₂S₃</i>				Ge	2.130	0.030	0.513
Ge	0.226	-2.057	0.000	S	1.434	1.865	-0.896
Ge	-0.163	0.955	0.000	S	1.441	-1.808	-0.895
S	0.024	-0.489	1.657	S	-2.269	2.801	-0.123
S	0.024	-0.489	-1.657	S	-2.251	-2.772	-0.105
S	-0.424	2.960	0.000	S	-0.211	0.025	1.421
<i>Ge₂S₄</i>				<i>Ge₄S₄</i>			
Ge	0.162	-0.000	-1.473	Ge	-1.768	-0.384	-1.004
Ge	0.162	-0.000	1.473	Ge	1.132	-1.731	0.088
S	0.166	1.664	0.000	Ge	-0.421	0.647	1.919
S	0.157	-1.665	0.000	Ge	1.060	1.466	-1.005
S	0.163	-0.000	3.489	S	-1.166	1.782	-0.092
S	0.163	-0.000	-3.489	S	1.824	0.395	1.033
				S	-1.091	-1.512	1.035
<i>Ge₂S₅</i>				S	0.437	-0.668	-1.979
Ge	0.207	-1.726	0.018				
Ge	0.215	1.724	-0.009				
S	1.584	-0.003	0.006				

Ge₄S₅ (Rhomboids)

Ge	0.146	-0.842	0.094
Ge	-1.420	1.848	0.898
Ge	0.705	-3.807	0.339
Ge	0.656	2.069	-1.174
S	-0.760	-2.399	1.386
S	0.976	0.951	1.117
S	-1.245	0.342	-1.175
S	1.594	-2.150	-0.960
S	-0.704	3.667	-0.280

Ge₄S₅ (cube)

Ge	1.247	0.622	1.736
Ge	1.214	0.868	-1.632
Ge	-1.602	1.466	0.131
Ge	-0.382	-1.623	-0.105
S	-1.014	-0.315	1.705
S	-1.048	-0.068	-1.694
S	-0.886	-3.594	-0.241
S	0.644	2.375	0.175
S	1.829	-0.919	-0.075

Ge₄S₆

Ge	0.967	0.326	2.110
Ge	2.016	-0.281	-1.044
Ge	-0.680	1.603	-0.494
Ge	-0.844	-1.589	0.067
S	-1.362	0.312	1.347
S	-0.307	-0.299	-1.822
S	-2.072	-3.207	-0.029
S	-1.744	3.204	-1.157
S	1.517	1.768	0.205
S	1.338	-1.723	0.819

Ge₄S₇

Ge	0.232	-0.084	-2.368
Ge	1.617	-0.793	0.594
Ge	-1.607	-1.036	0.260
Ge	-0.193	1.891	0.299
S	-1.700	0.832	-1.151
S	-0.213	0.074	1.813
S	-0.399	3.828	0.868
S	-3.258	-2.092	0.788
S	3.265	-1.599	1.463
S	0.219	-2.012	-0.838
S	1.718	1.091	-0.797

Supplementary Table 2.

Cartesian Coordinates of Global Minimum Cationic Conformers

<i>GeS⁺</i>				<i>Ge₂S₅⁺</i>			
Ge	0.000	0.000	-0.673	Ge	0.031	-2.524	0.020
S	0.000	0.000	1.346	Ge	1.057	2.897	-0.093
<i>GeS₂⁺</i>				S	0.510	0.519	-0.080
Ge	-0.119	-1.058	0.000	S	-1.478	1.045	-0.116
S	-0.913	1.111	0.000	S	-1.941	-2.052	-0.005
S	1.106	0.900	0.000	S	-1.264	3.076	0.204
<i>GeS₃⁺</i>				S	1.902	-3.178	0.057
Ge	0.005	1.344	0.000	<i>Ge₃S₄⁺</i>			
S	-0.006	-1.700	0.000	Ge	-1.412	-1.940	-0.064
S	1.579	-0.439	0.000	Ge	-1.419	1.933	-0.060
S	-1.582	-0.427	0.000	Ge	1.097	0.001	0.079
<i>GeS₄⁺</i>				S	-0.714	0.000	-1.364
Ge	0.000	0.000	-0.694	S	0.470	-1.826	1.167
S	0.000	0.000	2.238	S	0.464	1.827	1.167
S	0.000	-1.570	0.913	S	3.081	0.006	-0.829
S	0.000	1.570	0.913	<i>Ge₃S₅⁺</i>			
S	0.000	0.000	-2.696	Ge	-0.508	1.761	-0.077
<i>Ge₂S₂⁺</i>				Ge	-0.501	-1.768	-0.081
Ge	0.000	-1.452	0.000	Ge	2.106	0.006	0.498
Ge	0.000	1.452	0.000	S	-0.321	0.000	1.373
S	1.717	0.000	0.000	S	1.399	1.845	-0.960
S	-1.717	0.000	0.000	S	1.413	-1.836	-0.956
<i>Ge₂S₃⁺</i>				S	-2.304	2.781	-0.071
Ge	0.000	0.000	-2.055	S	-2.292	-2.789	-0.074
Ge	0.000	0.000	0.888	<i>Ge₄S₄⁺</i>			
S	0.000	1.701	-0.406	Ge	1.772	-0.985	-0.559
S	0.000	-1.701	-0.406	Ge	-1.374	-1.411	0.737
S	0.000	0.000	3.027	Ge	-0.823	0.957	-1.682
<i>Ge₂S₄⁺</i>				Ge	0.369	1.250	1.307
Ge	-0.975	-1.519	0.234	S	-0.418	-1.414	-1.479
Ge	0.975	1.519	-0.234	S	0.851	-0.930	1.762
S	-1.135	1.810	0.668	S	1.414	1.483	-0.703
S	1.173	-0.668	1.052	S	-1.792	1.049	0.618
S	-1.173	0.668	-1.052	<i>Ge₄S₆⁺</i>			
S	1.173	-1.810	-0.668	Ge	0.000	-1.719	-1.585
				Ge	0.000	1.719	-1.585
				Ge	1.567	0.000	0.772
				Ge	-1.567	0.000	0.772

S	1.782	0.000	-1.487
S	-1.782	0.000	-1.487
S	0.000	-1.706	0.928
S	0.000	1.706	0.927
S	-3.164	0.000	2.098
S	3.164	0.000	2.098

Ge₄S₇⁺

Ge	0.000	0.000	2.369
Ge	-0.602	1.779	-0.401
Ge	-1.239	-1.411	-0.401
Ge	1.842	-0.367	-0.401
S	-1.952	0.389	0.920
S	1.313	1.495	0.920
S	0.639	-1.884	0.920
S	0.000	0.000	-1.839
S	3.724	-0.744	-1.058
S	-2.506	-2.853	-1.058
S	-1.218	3.597	-1.058