

Supplementary Material
Complexation of Ca²⁺ with selenocysteine
and effects on its intrinsic acidity

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This paper is dedicated to Prof. Rosa Claramunt on the occasion of her 65th birthday

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Table S1. Total energies (**E**, hartrees), zero point energy corrections (**ZPE**, hartrees), thermal corrections to the free energies and to the enthalpies evaluated at 298.2 K (**Gcorr**, **Hcorr**, respectively in hartrees), entropy values (**S** in cal mol⁻¹ K⁻¹). Values calculated at the B3LYP/6-311+G(3df,2p)// B3LYP/6-311+g(d,p) level

[Selenocysteine–Ca] ²⁺	E	ZPE	Gcorr	Hcorr	S
<i>a</i>	-3402.549264	0.109485	0.07416	0.119618	95.674
<i>b(z)</i>	-3402.546584	0.108935	0.071835	0.119637	100.607
<i>c</i>	-3402.548834	0.109619	0.074244	0.11974	95.754
<i>d(z)</i>	-3402.545132	0.108806	0.071429	0.119646	101.482
<i>e(z)</i>	-3402.545175	0.109014	0.071982	0.119584	100.188
<i>f(z)</i>	-3402.542958	0.109664	0.073453	0.120291	98.579
<i>g</i>	-3402.54056	0.109244	0.073873	0.119422	95.865
<i>h</i>	-3402.539942	0.10932	0.073866	0.119513	96.072
<i>i(z)</i>	-3402.535127	0.108778	0.070905	0.119878	103.071
<i>j(z)</i>	-3402.534397	0.109235	0.072467	0.119933	99.901
<i>k(z)</i>	-3402.53304	0.10908	0.072022	0.119849	100.66
<i>l(z)</i>	-3402.529013	0.108896	0.070522	0.119815	103.747
<i>m(z)</i>	-3402.529273	0.10938	0.072724	0.120077	99.661
<i>n</i>	-3402.526732	0.107971	0.071444	0.118572	99.19
<i>o</i>	-3402.520988	0.10845	0.071657	0.118961	99.56
<i>p</i>	-3402.521296	0.108564	0.072882	0.118908	96.869
<i>q</i>	-3402.519094	0.10786	0.071191	0.11849	99.551
<i>r</i>	-3402.52056	0.108709	0.072925	0.119059	97.099
<i>s(z)</i>	-3402.510792	0.112938	0.073733	0.124159	106.131
<i>t</i>	-3402.501473	0.108507	0.071381	0.119194	100.631
<i>u</i>	-3402.501024	0.108562	0.071524	0.119226	100.397
<i>v</i>	-3402.493315	0.107479	0.070742	0.117993	99.45
<i>w</i>	-3402.490803	0.107368	0.070427	0.118006	100.137
<i>x</i>	-3402.485149	0.107897	0.070931	0.118659	100.451
<i>y</i>	-3402.47187	0.105652	0.067375	0.117051	104.551
<i>z</i>	-3402.47074	0.10566	0.067893	0.116913	103.171
<i>aa</i>	-3402.467675	0.107369	0.069241	0.118521	103.719

Table S2. Structures of [Selenocysteine–Ca]²⁺ optimized at the B3LYP/6-311+G(d,p) level**ESTRUCTURE OF COMPLEXES AT B3LYP/6-311+G(d,p)**