Supporting Information for

On the influence of water molecules on the outer electronic shells of R–SeH, R–Se(–) and R–SeOH fragments in selenocysteine amino acid residue

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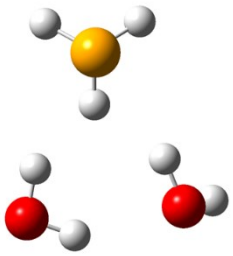

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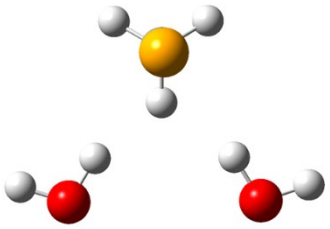

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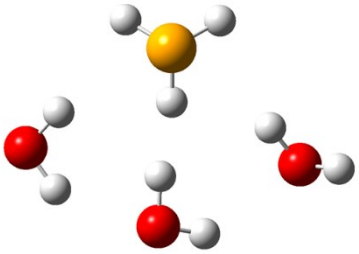

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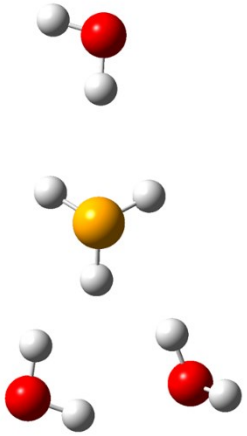

+0.6 kcal/mol

Figure S1. Structures of some conformers of $CH_3Se(–)\cdot nH_2O$, n = 2 and 3.

Table S1. Energies of OH···Se hydrogen bonds for $CH_3Se(-)\cdot nH_2O$ clusters that contains water molecules involved only in a single hydrogen bond.

***n* = 1**	**Δ*E*, kcal/mol**
1	–5.59
2	–5.85
3 (2 + 1)	–5.21
4 (3 + 1)	–5.13

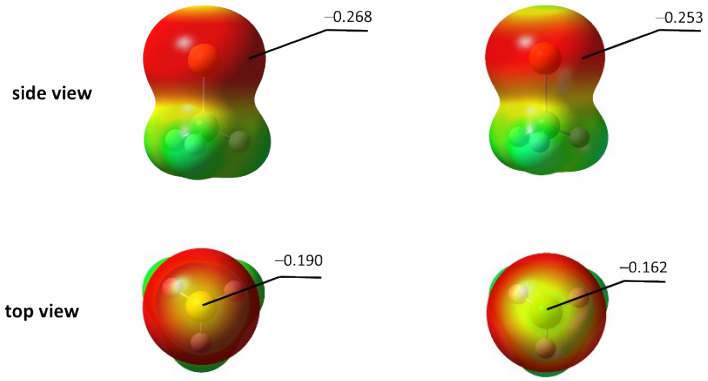

Figure S2. Isosurfaces of 0.01 a.u. electronic density mapped by molecular electrostatic potential for $CH_3S(-)$ (left) and for $CH_3Se(-)$ (right).

Coordinates of $CH_3Se(-)\cdot nH_2O$ (n = 0–6) complexes calculated at MP2/aug-cc-pVTZ level

$CH_3Se(-)$

Full electronic energy –2439.9557934

Sum of electronic and zero-point Energies -2439.919614

Sum of electronic and thermal Energies -2439.916486

Sum of electronic and thermal Enthalpies -2439.915542

Sum of electronic and thermal Free Energies -2439.944550

Coordinates (opt=tight freq mp2/aug-cc-pvtz)

Se	–0.43851300	0.00000000	0.00000000
C	1.52892600	0.00000000	0.00000000
H	1.91196400	–0.50361400	0.88839800
H	1.91196400	–0.51756900	–0.88034100
H	1.91196400	1.02118200	–0.00805700

$CH_3Se(-)\cdot H_2O$

Full electronic energy –2516.4033169

Coordinates (opt=tight mp2/aug-cc-pvtz scrf=(cpcm,solvent=water))

Se	0.53106500	–0.46589300	0.00480700
C	0.87188900	1.47067400	–0.00840600
H	–0.06966700	2.01338900	–0.05773000
H	1.39928900	1.76572900	0.89547900
H	1.47679100	1.74003100	–0.87084100
O	–2.68269800	0.14685200	–0.10358000
H	–2.91023600	0.39954400	0.79740600
H	–1.72213600	–0.07719900	–0.04867600

$CH_3Se(-)\cdot 2H_2O$

Full electronic energy –2592.859928

Coordinates (opt=tight mp2/aug-cc-pvtz scrf=(cpcm,solvent=water))

Se	0.88070200	–0.05447100	–0.44658800
C	1.01884100	0.19671600	1.49814000
H	1.63955300	–0.58296300	1.93251600
H	1.46038700	1.16506300	1.72008200
H	0.02836600	0.14875000	1.94612100
O	–2.01088700	–1.53743400	0.20013800
H	–2.42518500	–0.66251400	0.22671200
H	–1.09158100	–1.28920300	–0.04107200
O	–2.05864300	1.38623900	–0.17549100
H	–1.13551000	1.06278200	–0.31450100
H	–1.97669900	2.03935700	0.52812600

$CH_3Se(-)\cdot 3H_2O$

Full electronic energy –2668.6900516

Coordinates (opt=tight mp2/aug-cc-pvtz scrf=(cpcm,solvent=water))

Se	–0.36349200	–0.03593800	–0.35911400
C	–0.30345400	–0.24294200	1.61453500
H	–0.68533800	–1.23231000	1.90505400
H	0.73323800	–0.14325500	1.96843800
H	–0.91800500	0.53196400	2.09519200
O	–3.71219100	0.02416300	–0.16952100
H	–3.92505100	0.91728800	0.13507400
H	–2.73184300	0.04164400	–0.26838700
O	2.74507200	–1.26447800	–0.30265900
H	2.77724300	–1.90810500	0.41933700
H	1.78585800	–1.04430700	–0.38147900
O	2.53711900	1.65779600	0.06060100
H	1.60893800	1.38839100	–0.11368800
H	2.97440200	0.78839100	0.05576000

$CH_3Se(-)\cdot 4H_2O$

Full electronic energy –2745.445213

Coordinates (opt=tight mp2/aug-cc-pvtz scrf=(cpcm,solvent=water))

Se	0.00182400	–0.59711800	–0.40543700
C	0.01758500	–0.74349600	1.55388200
H	0.10387300	–1.78696600	1.84517100
H	0.86146100	–0.18726000	1.95556800
H	–0.90492200	–0.33429400	1.95912800
O	–2.04014800	1.92808000	0.18692700
H	–2.00520800	2.62001400	–0.48292000
H	–1.34264100	1.29073900	–0.08891000
O	–3.34425500	–0.67573300	–0.13023900
H	–3.29676300	0.28342800	–0.00000400
H	–2.40328900	–0.87925100	–0.29937500
O	1.95266600	2.08365500	0.02509100
H	1.23031100	1.44965300	–0.16118700
H	2.70645100	1.47791900	0.08516600
O	3.30588400	–0.51429800	–0.16339800
H	3.54636400	–1.06803800	0.58759200
H	2.34365800	–0.67660300	–0.28570800

$CH_3Se(-)\cdot 5H_2O$

Full electronic energy –2821.7903872

Coordinates (opt=tight mp2/aug-cc-pvtz scrf=(cpcm,solvent=water))

Se	–0.01529500	0.01964100	–0.36972800
C	–0.02256800	–0.00359200	1.59574800
H	–0.07303100	1.01521500	1.97178100
H	–0.88510600	–0.56228800	1.95065000
H	0.88682800	–0.47617800	1.95880800
O	0.20299600	3.32342000	–0.15140900

H	0.99355900	3.46658000	0.37985700
H	0.16787800	2.34950600	–0.26159100
O	–3.24320100	0.61894900	0.12355000
H	–3.66527000	1.15409200	–0.55766600
H	–2.29724400	0.59815400	–0.13770300
O	2.33913600	–2.27648200	0.05069900
H	1.56287800	–1.73093500	–0.20060300
H	2.41395100	–2.92259800	–0.66024200
O	–2.52483300	–2.21047800	–0.11910300
H	–3.11122800	–1.44510400	–0.02038200
H	–1.67152000	–1.76324800	–0.27764300
O	3.30304400	0.48883800	–0.02588300
H	2.34774700	0.59336600	–0.19882900
H	3.36886900	–0.47679600	0.02699200

$CH_3Se(–)\cdot 6H_2O$

Full electronic energy –2898.1364044

Sum of electronic and zero-point Energies -2897.344845

Sum of electronic and thermal Energies -2897.322054

Sum of electronic and thermal Enthalpies -2897.321110

Sum of electronic and thermal Free Energies -2897.403199

Coordinates (opt=tight freq mp2/aug-cc-pvtz scrf=(cpcm,solvent=water))

Se	0.00078700	–0.00038300	–0.32413900
C	0.00106700	0.00092300	1.64051300
H	–0.72809600	–0.71918700	2.00329300
H	0.98953400	–0.26998300	2.00295400
H	–0.25823500	0.99277000	2.00220600
O	–3.05004000	–1.49338900	–0.12269900
H	–2.57187400	–2.32992000	–0.01624300
H	–2.30713400	–0.87934100	–0.26736400
O	–0.72993200	–3.25448900	–0.11005900

H	–0.29915700	–3.58151100	0.68769300
H	–0.38894400	–2.34060500	–0.21116200
O	–2.45555600	2.25612800	–0.10400800
H	–1.83401500	1.50475400	–0.20778300
H	–2.95267200	2.04433600	0.69409900
O	2.82038200	–1.89308600	–0.10715300
H	3.30466400	–1.05942000	–0.00602100
H	1.91700500	–1.55908200	–0.25609800
O	0.22826700	3.38860300	–0.11614200
H	0.38974900	2.43876500	–0.26322800
H	–0.73524600	3.39150800	–0.00953500
O	3.18310800	0.99611800	–0.11855700
H	3.25024300	1.54162900	0.67315600
H	2.22119700	0.83368700	–0.21937800

Coordinates of $CH_3SeH \cdot nH_2O$ (n = 0–2) complexes calculated at MP2/aug-cc-pVTZ level

CH_3SeH

Full electronic energy –2440.5172992

Sum of electronic and zero-point Energies -2440.471973

Sum of electronic and thermal Energies -2440.468232

Sum of electronic and thermal Enthalpies -2440.467288

Sum of electronic and thermal Free Energies -2440.497620

Coordinates (opt=tight freq mp2/aug-cc-pvtz)

H	0.58965200	1.39752300	0.00000100
Se	0.41707800	-0.04421500	0.00000000
C	-1.52335900	0.01675100	0.00000000
H	-1.85449000	-1.01793000	0.00000000
H	-1.88783600	0.51161100	0.89356500
H	-1.88783600	0.51161200	-0.89356300

$CH_3SeH \cdot 1H_2O$

Full electronic energy –2516.5868779

Coordinates (opt=tight mp2/aug-cc-pvtz scrf=(cpcm,solvent=water))

H	-0.80965600	-0.28831600	-0.01191600
Se	0.64906400	-0.45949600	0.00134200
C	1.05232800	1.46148900	-0.00425100
H	2.14719700	1.54824900	0.00483300
H	0.65410800	1.92997000	-0.91260100
H	0.63849600	1.93853100	0.89259200
O	-2.99078500	0.21766900	-0.01036000
H	-3.59244300	-0.07212500	-0.71082900
H	-3.49356600	0.05628500	0.80068800

$CH_3SeH \cdot 2H_2O$

Full electronic energy –2592.8626986

Sum of electronic and zero-point Energies	-2592.771538
Sum of electronic and thermal Energies	-2592.759885
Sum of electronic and thermal Enthalpies	-2592.758940
Sum of electronic and thermal Free Energies	-2592.813691

Coordinates (opt=tight freq mp2/aug-cc-pvtz scrf=(cpcm,solvent= water))

H	0.00000100	-0.15062600	1.60278900
Se	0.00000000	-0.20384400	0.15105800
C	0.00000200	1.72074200	-0.10892400
H	0.00000100	1.87552000	-1.18370000
H	-0.89398300	2.15065700	0.32829600
H	0.89398800	2.15065500	0.32829500
O	3.41367600	-0.55634500	-0.34087400
H	3.81718000	0.19442800	0.10752500
H	2.46580800	-0.45365600	-0.15958300
O	-3.41367700	-0.55634600	-0.34087200
H	-2.46580900	-0.45365600	-0.15958200
H	-3.81717900	0.19443900	0.10750900

Coordinates of $CH_3SeOH \cdot nH_2O$ (n = 0–3) complexes calculated at MP2/aug-cc-pVTZ level

CH_3SeOH

Full electronic energy –2515.6362341

Sum of electronic and zero-point Energies -2515.584914

Sum of electronic and thermal Energies -2515.580175

Sum of electronic and thermal Enthalpies -2515.579231

Sum of electronic and thermal Free Energies -2515.612865

Coordinates (opt=tight freq mp2/aug-cc-pvtz)

Se	-0.07429400	-0.43513500	0.00393900
O	-1.29335100	0.89431700	-0.11638100
H	-1.54834700	1.10639200	0.79054800
C	1.50221500	0.66586000	0.00277000
H	2.34933000	-0.01946600	-0.02708600
H	1.50557300	1.28853600	-0.88686300
H	1.55297600	1.26943600	0.90389300

$CH_3SeOH \cdot 1H_2O$

Full electronic energy –2591.6380861

Coordinates (opt=tight mp2/aug-cc-pvtz scrf=(cpcm,solvent=water))

Se	0.53837600	-0.01188500	-0.44731100
O	1.22333400	-0.98278600	0.96032500
H	2.14908900	-0.70071300	1.04781400
C	-0.19525500	1.46499800	0.57990600
H	-0.76283100	2.07913400	-0.13844700
H	-0.88298700	1.07259100	1.34008400
H	0.60912700	2.06235600	1.02821000
O	-2.83700400	-0.39634100	0.11579600
H	-3.38436700	-1.18446000	0.00761200
H	-1.95193600	-0.68178000	-0.16512100

$CH_3SeOH \cdot 2H_2O$

Full electronic energy –2667.9110655

Coordinates (opt=tight mp2/aug-cc-pvtz scrf=(cpcm,solvent=water))

Se	-0.03549900	-0.16971100	-0.48708900
O	0.71878700	-1.02768500	0.94243100
H	1.65687900	-0.74216300	0.92460500
C	-0.48861200	1.50014800	0.40079600
H	-1.03187500	2.10824000	-0.34080800
H	-1.14885200	1.28888300	1.25186300
H	0.42538100	2.01890600	0.71843300
O	3.16334200	0.25782900	0.22932800
H	4.04010300	-0.10029500	0.03800100
H	2.75118000	0.38364000	-0.63955600
O	-3.38443400	-0.08734200	0.30022200
H	-3.99212800	-0.83248100	0.38920600
H	-2.54361800	-0.49786600	0.03864400

$CH_3SeOH \cdot 3H_2O$

Full electronic energy –2744.6613968

Coordinates (opt=tight freq mp2/aug-cc-pvtz scrf=(cpcm,solvent= water))

Se	0.38513000	-0.22935500	-0.36049400
O	-0.16686700	1.46707200	-0.39131700
H	-1.11025400	1.45362600	-0.10676200
C	0.82781500	-0.35910300	1.50979200
H	1.24913100	-1.35284700	1.66054200
H	1.57693900	0.39111400	1.74426300
H	-0.06744400	-0.23090700	2.11090800
O	-2.76000400	1.23754500	0.45487100
H	-3.43358300	1.78546200	0.04203900
H	-3.00145700	0.31608200	0.23996500

O	3.73932400	0.03378600	0.02519000
H	4.36324400	0.46561700	-0.56519100
H	2.88892600	0.10332100	-0.43172000
O	-2.78331400	-1.41823300	-0.26868300
H	-1.81356900	-1.35011400	-0.33819700
H	-2.94637200	-2.19002900	0.28169700

Table S1. NMR data for $CH_3Se(–)\cdot nH_2O$ (n= 1–6), $CH_3SeH\cdot kH_2O$ (k = 0, 2), $CH_3SeOH\cdot mH_2O$ (m = 0, 3): shielding constants σ_{Se} and chemical shifts $\delta_{Se} = \sigma_{Se,ref} - \sigma_{Se,complex}$, where $\sigma_{Se,ref}$ shielding constant of neat $(CH_3)_2Se$, $\sigma_{Se,ref}$.= 1994.23 ppm.

	σ_{Se}, ppm	δ_{Se}, ppm
$CH_3Se(–)$	2215.29	–221.06
$CH_3Se(–)\cdot H_2O$	2252.11	–257.88
$CH_3Se(–)\cdot 2H_2O$	2360.33	–366.10
$CH_3Se(–)\cdot 3H_2O$	2368.34	–374.11
$CH_3Se(–)\cdot 4H_2O$	2335.19	–340.96
$CH_3Se(–)\cdot 5H_2O$	2325.92	–331.69
$CH_3Se(–)\cdot 6H_2O$	2319.15	–324.93
CH_3SeH	2165.99	–171.77
$CH_3SeH\cdot 2H_2O$	2215.70	–221.47
CH_3SeOH	924.68	1069.54
$CH_3SeOH\cdot 3H_2O$	1113.50	880.73