# One-Electron Redox Processes in a Cyclic Selenide and a Selenoxide: A Pulse Radiolysis Study (Supporting Information-jp-2010-03727e)

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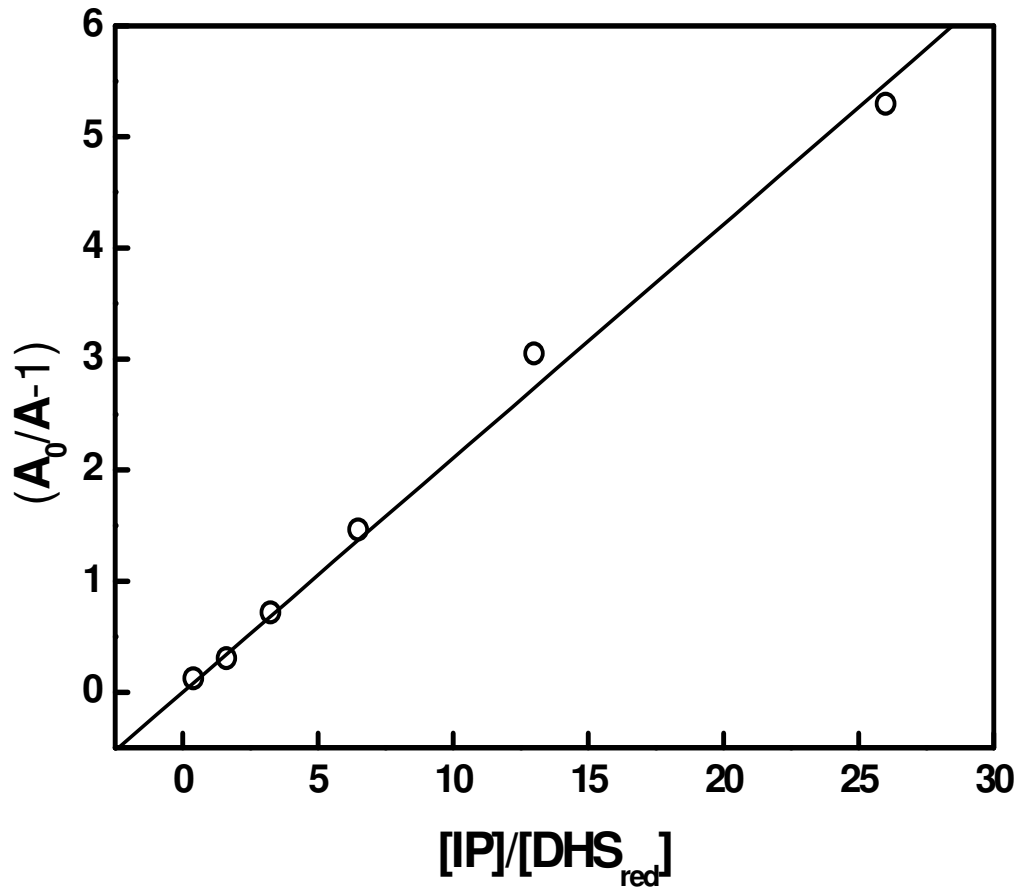


Supp. Fig. 1: Competition kinetic plot obtained in accordance to equation (5)

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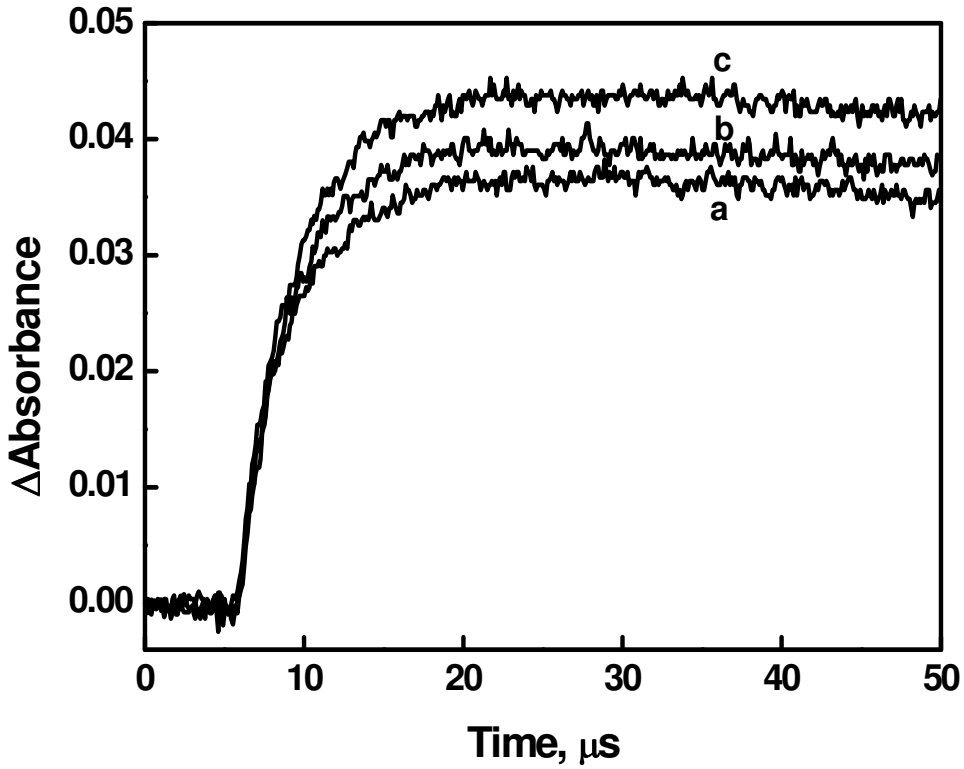
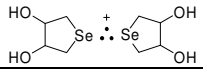
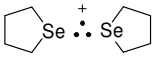
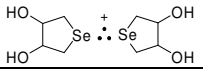
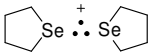


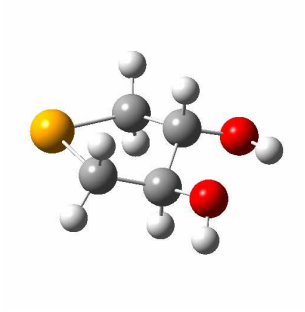

Supp. Fig. 2: Absorption-time plot at 645 nm obtained on pulse radiolysing $N_2O$ saturated aqueous solution containing 5 mM $DHS_{red}$ and 100 μM $ABTS^{2-}$ in (a) absence and presence of (b) 15 mM and (c) 50 mM phosphate ion.

**Table Supp.1. Summary of quantum chemical calculations obtained for the most stable conformer of $(DHS_{red})_2^{\bullet+}$ and dimer radical cation without –OH functional group**

| | In water | | In Vacuo | |
|---|---|---|---|---|
| | Conventional  | noOH  | Conventional  | noOH  |
| r(Se...Se) (Å) | 2.943 | 2.928 | 2.967 | 2.945 |
| Dipole moment (D) | 2.311 | 0.425 | 0.242 | 0.422 |
| Binding energy (kJ/mol) | 118.3 | 100.4 | 193.4 | 161.4 |
| Solvation energy (kJ/mol) | 260.6 | 183.7 | - | - |
| Bond order of Se...Se | 0.248 | 0.252 | 0.247 | 0.251 |
| Wiberg bond index on Se | 2.315 | 2.326 | 2.314 | 2.321 |
| Atomic spin population on Se | 0.497 | 0.501, 0.502 | 0.495 | 0.500 |
| $\lambda_{max}$ (nm) | 421.3 | 420.3 | 430.0 | 426.3 |
| HDOMO (eV) | -9.2321 | -9.4642 | -12.4561 | -13.0148 |
| LSOMO (eV) | -0.1233 | -0.3733 | -3.3873 | -3.9552 |

**Ab initio calculation**

**Structure of I optimized in vacuo at BHandHLYP/6-31G+(d,p) level.**



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E(RB+HF-LYP): -2706.86593464 a.u.

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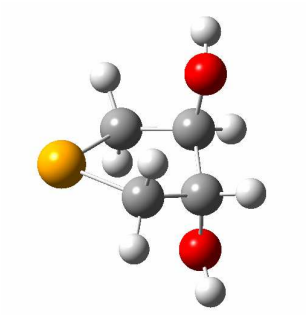
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.1007640 | 0.6755970 | -0.3160770 |
| 2 | C | 0.1713480 | 1.3844820 | 0.1092370 |
| 3 | C | 0.1934850 | -1.3906890 | -0.0750150 |
| 4 | C | -1.0945000 | -0.7047810 | 0.3236700 |
| 5 | H | -1.1164600 | 0.5459420 | -1.3991520 |
| 6 | H | 0.0814540 | 1.7429610 | 1.1283860 |
| 7 | H | 0.4260880 | 2.2127140 | -0.5420290 |
| 8 | H | 0.1144810 | -1.7841500 | -1.0816330 |

| | | | | |
|---|---|---|---|---|
| 9 | H | 0.4550130 | -2.1916890 | 0.6040540 |
| 10 | H | -1.1178230 | -0.5653210 | 1.4073300 |
| 11 | O | -2.1882070 | -1.4778910 | -0.0906260 |
| 12 | H | -2.9835470 | -0.9738960 | 0.0787470 |
| 13 | O | -2.2807530 | 1.3224000 | 0.1139220 |
| 14 | H | -2.4640350 | 2.0838700 | -0.4294510 |
| 15 | Se | 1.5687970 | 0.0113480 | -0.0059850 |

**Structure of I optimized in water at BHandHLYP/6-31G+(d,p) level with SCRF=(IEFPCM, solvent = water).**



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E(RB+HF-LYP): -2706.88990436 a.u.

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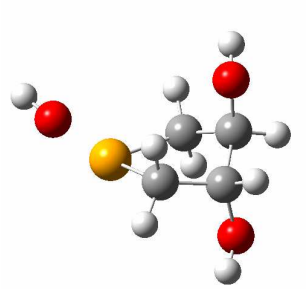
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 1.3298780 | 0.6941650 | -0.3120610 |
| 2 | C | 0.0303190 | 0.8514280 | -1.0889150 |
| 3 | C | 0.0306460 | -0.8510490 | 1.0890440 |
| 4 | C | 1.3300240 | -0.6937910 | 0.3117650 |
| 5 | H | 0.0899200 | 0.3498210 | -2.0475860 |
| 6 | H | -0.2172160 | 1.8962420 | -1.2438080 |
| 7 | H | 0.0902970 | -0.3490700 | 2.0475180 |
| 8 | H | -0.2164100 | -1.8959160 | 1.2442020 |
| 9 | Se | -1.3630310 | -0.0002010 | 0.0000250 |
| 10 | O | 1.4277530 | -1.6135660 | -0.7529280 |
| 11 | H | 1.5327300 | -2.5092420 | -0.3980890 |
| 12 | O | 1.4280770 | 1.6135040 | 0.7529640 |
| 13 | H | 1.5268750 | 2.5100710 | 0.3985200 |
| 14 | H | 2.1821980 | 0.7955300 | -0.9864560 |
| 15 | H | 2.1828270 | -0.7946110 | 0.9855790 |

**Structure of II optimized in vacuo at UBHandHLYP/6-31G+(d,p) level.**



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E(UB+HF-LYP): -2782.58541065 a.u.

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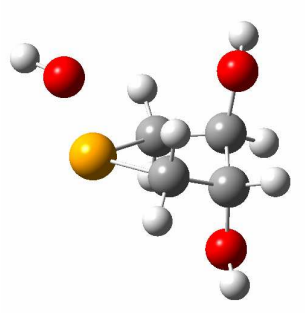
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Se | -1.0096430 | -0.2787010 | -0.4735620 |
| 2 | C | 0.0591220 | -0.5996360 | 1.1251250 |
| 3 | C | 1.5121200 | -0.4410520 | 0.7195140 |
| 4 | C | 1.6000400 | 0.7652240 | -0.2045240 |
| 5 | C | 0.5788820 | 0.5586130 | -1.3124030 |
| 6 | H | -0.1655150 | -1.5911520 | 1.5027100 |
| 7 | H | -0.2402620 | 0.1385060 | 1.8578820 |
| 8 | O | 1.9910190 | -1.5327250 | -0.0335720 |
| 9 | H | 1.8967590 | -2.3407100 | 0.4637000 |
| 10 | H | 2.1318720 | -0.2712830 | 1.5996120 |
| 11 | O | 1.3140620 | 1.8842940 | 0.5984920 |
| 12 | H | 1.2386900 | 2.6682160 | 0.0614540 |
| 13 | H | 2.6052830 | 0.8303980 | -0.6214020 |
| 14 | H | 0.2913670 | 1.4918040 | -1.7862990 |
| 15 | H | 0.9563760 | -0.1232260 | -2.0662680 |
| 16 | O | -2.5163640 | 0.4175910 | 1.0162870 |
| 17 | H | -3.1974080 | 0.8211370 | 0.4738000 |

**Structure of II optimized in water at UBHandHLYP/6-31G+(d,p) level with SCRF=(IEFPCM, solvent = water).**



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E(UB+HF-LYP): -2782.62077070 a.u.

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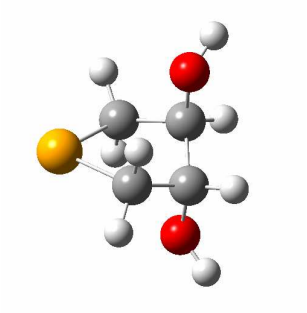
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Se | -0.9945030 | -0.4561680 | -0.3921130 |
| 2 | C | 0.1369570 | -0.5349170 | 1.1935960 |
| 3 | C | 1.5575360 | -0.2842360 | 0.7128980 |
| 4 | C | 1.5019180 | 0.8369050 | -0.3153890 |
| 5 | C | 0.4626470 | 0.4496340 | -1.3591890 |
| 6 | H | 0.0296540 | -1.5093300 | 1.6579810 |
| 7 | H | -0.2043260 | 0.2366380 | 1.8726150 |
| 8 | O | 2.0930930 | -1.4073180 | 0.0503290 |
| 9 | H | 2.2746140 | -2.1083420 | 0.6951490 |
| 10 | H | 2.1900610 | 0.0115040 | 1.5512960 |
| 11 | O | 1.1420010 | 2.0062320 | 0.3815560 |
| 12 | H | 1.2368930 | 2.7744220 | -0.2022680 |
| 13 | H | 2.4787640 | 0.9539700 | -0.7874990 |
| 14 | H | 0.0662920 | 1.3142880 | -1.8809000 |
| 15 | H | 0.8650780 | -0.2546630 | -2.0797810 |
| 16 | O | -2.4746780 | 0.7014150 | 0.9243100 |
| 17 | H | -3.1615870 | 0.8842600 | 0.2642080 |

**Structure of III optimized in vacuo at UBHandHLYP/6-31G+(d,p) level.**



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E(UB+HF-LYP): -2706.57909111 a.u.

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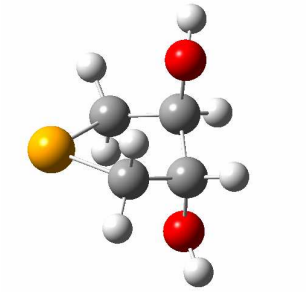
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | 1.3331080 | 0.6849620 | -0.3363300 |
| 2 | C | 0.0520700 | 0.7518340 | -1.1640160 |
| 3 | C | 0.0520690 | -0.7518330 | 1.1640170 |
| 4 | C | 1.3331070 | -0.6849630 | 0.3363300 |
| 5 | H | 0.0810170 | 0.1229430 | -2.0500750 |
| 6 | H | -0.2489050 | 1.7600670 | -1.4266130 |
| 7 | H | 0.0810180 | -0.1229410 | 2.0500750 |
| 8 | H | -0.2489050 | -1.7600650 | 1.4266140 |
| 9 | Se | -1.3198950 | 0.0000000 | 0.0000000 |
| 10 | O | 1.2860580 | -1.6409880 | -0.6856360 |
| 11 | H | 1.8071570 | -2.4155010 | -0.4859670 |
| 12 | O | 1.2860660 | 1.6409830 | 0.6856380 |
| 13 | H | 1.8071280 | 2.4155160 | 0.4859470 |
| 14 | H | 2.1993950 | 0.7919420 | -0.9832760 |
| 15 | H | 2.1993940 | -0.7919450 | 0.9832740 |

**Structure of III optimized in water at UBHandHLYP/6-31G+(d,p) level with SCRF=(IEFPCM, solvent = water).**



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E(UB+HF-LYP): -2706.68154878 a.u.

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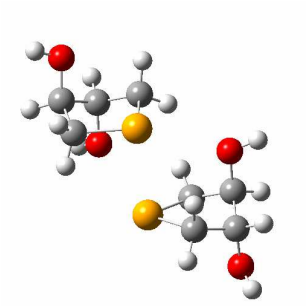
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -1.3329370 | 0.6906380 | 0.3193170 |

| | | | | |
|---|---|---|---|---|
| 2 | C | -0.0385390 | 0.8079830 | 1.1162110 |
| 3 | C | -0.0385420 | -0.8079840 | -1.1162100 |
| 4 | C | -1.3329400 | -0.6906330 | -0.3193170 |
| 5 | H | -0.0519920 | 0.2386420 | 2.0435420 |
| 6 | H | 0.2599410 | 1.8327930 | 1.3193770 |
| 7 | H | -0.0519910 | -0.2386460 | -2.0435420 |
| 8 | H | 0.2599340 | -1.8327960 | -1.3193720 |
| 9 | Se | 1.3322740 | -0.0000020 | 0.0000000 |
| 10 | O | -1.3591810 | -1.6209690 | 0.7295580 |
| 11 | H | -1.5667970 | -2.5065520 | 0.3871690 |
| 12 | O | -1.3591720 | 1.6209740 | -0.7295590 |
| 13 | H | -1.5667640 | 2.5065620 | -0.3871680 |
| 14 | H | -2.1875340 | 0.8007500 | 0.9877290 |
| 15 | H | -2.1875360 | -0.8007400 | -0.9877310 |

**Structure of IV optimized in vacuo at UBHandHLYP/6-31G+(d,p) level.**



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E(UB+HF-LYP): -5413.51724561 a.u.

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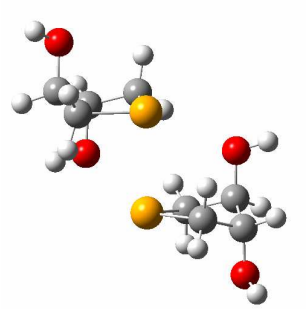
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Se | -1.0889080 | -1.0075940 | -0.5754730 |
| 2 | C | -1.7159910 | -0.6794900 | 1.2495250 |
| 3 | C | -2.4347290 | 0.6530930 | 1.2015080 |
| 4 | C | -3.2836420 | 0.6541040 | -0.0699050 |
| 5 | C | -2.3569860 | 0.3412450 | -1.2427110 |
| 6 | H | -0.8739430 | -0.6911200 | 1.9268170 |
| 7 | H | -2.3991460 | -1.4833370 | 1.4942070 |
| 8 | O | -1.4604420 | 1.6740850 | 1.1489250 |
| 9 | H | -1.8227010 | 2.4966750 | 1.4709730 |
| 10 | H | -3.0734860 | 0.7580770 | 2.0752400 |
| 11 | O | -4.2394190 | -0.3550810 | 0.1146130 |
| 12 | H | -4.9811920 | -0.2499560 | -0.4763760 |
| 13 | H | -3.7486470 | 1.6292770 | -0.2132160 |
| 14 | H | -2.8960830 | -0.0751060 | -2.0850830 |
| 15 | H | -1.7926680 | 1.2096680 | -1.5600720 |
| 16 | Se | 1.0887490 | 1.0071100 | -0.5760670 |
| 17 | C | 2.3569010 | -0.3420800 | -1.2425240 |
| 18 | C | 3.2836410 | -0.6541220 | -0.0695890 |
| 19 | C | 2.4348880 | -0.6521970 | 1.2019120 |
| 20 | C | 1.7162890 | 0.6805010 | 1.2490240 |

| | | | | |
|---|---|---|---|---|
| 21 | H | 2.8959640 | 0.0736600 | -2.0852010 |
| 22 | H | 1.7925270 | -1.2107890 | -1.5591280 |
| 23 | O | 4.2394760 | 0.3551900 | 0.1140880 |
| 24 | H | 4.9813710 | 0.2493820 | -0.4766260 |
| 25 | H | 3.7486130 | -1.6294170 | -0.2121760 |
| 26 | O | 1.4605930 | -1.6732050 | 1.1501230 |
| 27 | H | 1.8228930 | -2.4955960 | 1.4726430 |
| 28 | H | 3.0737510 | -0.7565610 | 2.0756420 |
| 29 | H | 0.8744910 | 0.6929770 | 1.9266040 |
| 30 | H | 2.3997620 | 1.4844010 | 1.4926840 |

**Structure of IV optimized in water at UBHandHLYP/6-31G+(d,p) level with SCRF=(IEFPCM, solvent = water).**



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E(UB+HF-LYP): -5413.61650194 a.u.

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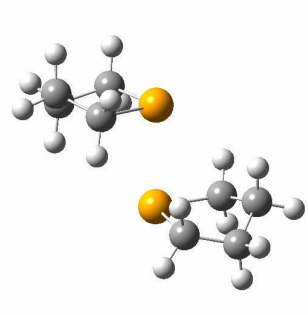
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Se | 1.0532530 | 1.0256180 | -0.5478640 |
| 2 | C | 1.7005260 | 0.6673480 | 1.2633840 |
| 3 | C | 2.4340620 | -0.6555890 | 1.1853930 |
| 4 | C | 3.2676190 | -0.6359440 | -0.0944720 |
| 5 | C | 2.3376900 | -0.2865500 | -1.2524540 |
| 6 | H | 0.8677610 | 0.6586820 | 1.9532420 |
| 7 | H | 2.3741230 | 1.4763760 | 1.5217190 |
| 8 | O | 1.4706830 | -1.6820320 | 1.1382590 |
| 9 | H | 1.9131480 | -2.5454830 | 1.1957410 |
| 10 | H | 3.0854700 | -0.7679110 | 2.0533450 |
| 11 | O | 4.2588270 | 0.3462830 | 0.0887320 |
| 12 | H | 4.9302570 | 0.2593040 | -0.6044110 |
| 13 | H | 3.7156790 | -1.6175980 | -0.2637780 |
| 14 | H | 2.8749640 | 0.1608510 | -2.0813830 |
| 15 | H | 1.7778220 | -1.1468700 | -1.6012270 |
| 16 | Se | -1.0543540 | -1.0287450 | -0.5445140 |
| 17 | C | -2.3377870 | 0.2822950 | -1.2536840 |
| 18 | C | -3.2669350 | 0.6368180 | -0.0965430 |
| 19 | C | -2.4325600 | 0.6609870 | 1.1827140 |
| 20 | C | -1.7007750 | -0.6625410 | 1.2651920 |
| 21 | H | -2.8756640 | -0.1676690 | -2.0808150 |
| 22 | H | -1.7770310 | 1.1407900 | -1.6055790 |

| | | | | |
|---|---|---|---|---|
| 23 | O | -4.2583080 | -0.3445150 | 0.0918150 |
| 24 | H | -4.9310510 | -0.2598320 | -0.6003380 |
| 25 | H | -3.7147810 | 1.6179060 | -0.2694710 |
| 26 | O | -1.4683890 | 1.6866700 | 1.1316610 |
| 27 | H | -1.9098880 | 2.5504730 | 1.1913330 |
| 28 | H | -3.0838070 | 0.7773820 | 2.0501920 |
| 29 | H | -0.8676960 | -0.6525600 | 1.9546730 |
| 30 | H | -2.3753900 | -1.4697020 | 1.5266690 |

**Structure of IV(noOH) optimized in vacuo at UBHandHLYP/6-31G+(d,p) level.**



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E(UB+HF-LYP): -5112.75431881 a.u.

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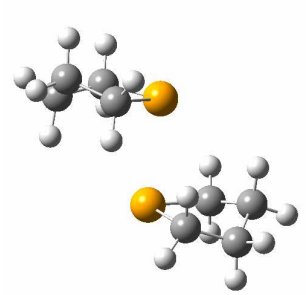
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 2 | C | -2.1356950 | -0.1176030 | -1.3254950 |
| 3 | C | -2.7720090 | -1.1563110 | -0.4123060 |
| 4 | C | -3.1774070 | -0.4686910 | 0.8859580 |
| 5 | C | -1.9655050 | 0.2765420 | 1.4347980 |
| 6 | H | -1.4960600 | -0.5397940 | -2.0919390 |
| 7 | H | -2.8670780 | 0.5306850 | -1.7954600 |
| 8 | H | -2.0595060 | -1.9521880 | -0.2075420 |
| 9 | H | -3.6282760 | -1.6062120 | -0.9074350 |
| 10 | H | -3.9884280 | 0.2315370 | 0.7008800 |
| 11 | H | -3.5290950 | -1.1877330 | 1.6207330 |
| 12 | H | -2.2163070 | 1.0973400 | 2.0949850 |
| 13 | H | -1.2704850 | -0.3866570 | 1.9391950 |
| 14 | Se | 1.0557200 | -1.0256350 | -0.1446740 |
| 15 | C | 1.9666730 | -0.2819280 | 1.4337120 |
| 16 | C | 3.1780620 | 0.4656460 | 0.8868220 |
| 17 | C | 2.7719270 | 1.1574660 | -0.4089680 |
| 18 | C | 2.1355990 | 0.1215070 | -1.3252360 |
| 19 | H | 2.2182440 | -1.1054100 | 2.0902550 |
| 20 | H | 1.2721120 | 0.3790790 | 1.9415280 |
| 21 | H | 3.9892370 | -0.2336650 | 0.6990320 |
| 22 | H | 3.5298170 | 1.1823130 | 1.6238750 |
| 23 | H | 2.0592420 | 1.9524210 | -0.2013000 |
| 24 | H | 3.6278610 | 1.6092730 | -0.9029400 |
| 25 | H | 1.4961390 | 0.5459020 | -2.0906100 |
| 26 | H | 2.8670010 | -0.5255530 | -1.7968670 |

**Structure of IV(noOH) optimized in water at UBHandHLYP/6-31G+(d,p) level with SCRF=(IEFPCM, solvent = water).**



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E(UB+HF-LYP): -5112.82430054 a.u.

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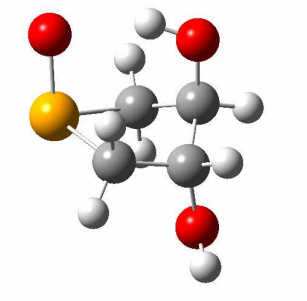
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Se | 1.0438210 | -1.0269080 | -0.1695110 |
| 2 | C | 2.1259100 | 0.1571420 | -1.3075990 |
| 3 | C | 2.7444170 | 1.1726800 | -0.3575830 |
| 4 | C | 3.1425680 | 0.4474770 | 0.9223180 |
| 5 | C | 1.9268070 | -0.3147320 | 1.4350590 |
| 6 | H | 1.4866870 | 0.5963930 | -2.0662520 |
| 7 | H | 2.8688120 | -0.4726420 | -1.7869990 |
| 8 | H | 2.0193380 | 1.9524660 | -0.1320620 |
| 9 | H | 3.6020360 | 1.6448930 | -0.8316500 |
| 10 | H | 3.9557300 | -0.2468580 | 0.7192670 |
| 11 | H | 3.4833600 | 1.1466670 | 1.6826140 |
| 12 | H | 2.1693900 | -1.1531270 | 2.0775510 |
| 13 | H | 1.2255580 | 0.3371750 | 1.9464930 |
| 14 | Se | -1.0435200 | 1.0266270 | -0.1695640 |
| 15 | C | -1.9255630 | 0.3137210 | 1.4351160 |
| 16 | C | -3.1431300 | -0.4457260 | 0.9227360 |
| 17 | C | -2.7468850 | -1.1715480 | -0.3574610 |
| 18 | C | -2.1254960 | -0.1576380 | -1.3075600 |
| 19 | H | -2.1659060 | 1.1515000 | 2.0792560 |
| 20 | H | -1.2246880 | -0.3402540 | 1.9444610 |
| 21 | H | -3.9548280 | 0.2504310 | 0.7200250 |
| 22 | H | -3.4852640 | -1.1442960 | 1.6830120 |
| 23 | H | -2.0244250 | -1.9538030 | -0.1322110 |
| 24 | H | -3.6058580 | -1.6411720 | -0.8316400 |
| 25 | H | -1.4851690 | -0.5985680 | -2.0644540 |
| 26 | H | -2.8667720 | 0.4724760 | -1.7890190 |

**Structure of V optimized in vacuo at BHandHLYP/6-31G+(d,p) level.**



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E(RB+HF-LYP): -2782.00919619 a.u.

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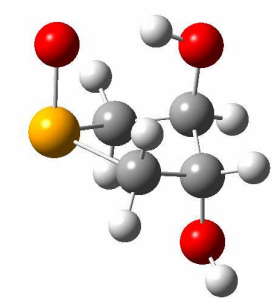
Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Se | 1.0724890 | -0.5294410 | 0.1702330 |
| 2 | C | -0.3951840 | -0.7916070 | -1.1193670 |
| 3 | C | -1.6403040 | -0.1394580 | -0.5239900 |
| 4 | C | -1.1770390 | 1.0303370 | 0.3467460 |
| 5 | C | -0.1679590 | 0.4447060 | 1.3251430 |
| 6 | H | -0.5358160 | -1.8476450 | -1.3215190 |
| 7 | H | -0.0360990 | -0.2844690 | -2.0083810 |
| 8 | O | -2.3250280 | -1.0337680 | 0.3290570 |
| 9 | H | -2.8541730 | -1.6417500 | -0.1798050 |
| 10 | H | -2.2926340 | 0.2333710 | -1.3110190 |
| 11 | O | -0.6201290 | 2.0388780 | -0.4447400 |
| 12 | H | 0.3153780 | 1.8523460 | -0.6190060 |
| 13 | H | -2.0305260 | 1.4465290 | 0.8751650 |
| 14 | H | 0.4157850 | 1.2019210 | 1.8353680 |
| 15 | H | -0.6259130 | -0.2388620 | 2.0300350 |
| 16 | O | 1.8779430 | 0.7468490 | -0.5418120 |

**Structure of V optimized in water at BHandHLYP/6-31G+(d,p) level with SCRF=(IEFPCM, solvent = water).**



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E(RB+HF-LYP): -2782.03931253 a.u.

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Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Se | 1.0733260 | -0.5326430 | 0.1750600 |

| | | | | |
|---|---|---|---|---|
| 2 | C | -0.3927190 | -0.8116220 | -1.1015110 |
| 3 | C | -1.6381780 | -0.1412960 | -0.5202700 |
| 4 | C | -1.1767390 | 1.0282080 | 0.3492570 |
| 5 | C | -0.1546660 | 0.4582570 | 1.3208770 |
| 6 | H | -0.5366850 | -1.8742260 | -1.2651880 |
| 7 | H | -0.0395280 | -0.3400430 | -2.0134630 |
| 8 | O | -2.3450600 | -1.0211550 | 0.3228380 |
| 9 | H | -2.8518520 | -1.6510800 | -0.2133280 |
| 10 | H | -2.2744300 | 0.2260630 | -1.3254800 |
| 11 | O | -0.6196360 | 2.0503890 | -0.4450960 |
| 12 | H | 0.3021820 | 1.8347740 | -0.6532920 |
| 13 | H | -2.0268000 | 1.4479840 | 0.8834320 |
| 14 | H | 0.4274300 | 1.2152370 | 1.8358900 |
| 15 | H | -0.5997370 | -0.2310670 | 2.0302640 |
| 16 | O | 1.8747150 | 0.7558840 | -0.5678660 |

**Structure of OH· optimized in vacuo at UBHandHLYP/6-31G+(d,p) level.**

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E(UB+HF-LYP): -75.70705134 a.u.

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Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | O | 0.0000000 | 0.0000000 | 0.1073600 |
| 2 | H | 0.0000000 | 0.0000000 | -0.8588810 |

**Structure of OH· optimized in water at UBHandHLYP/6-31G+(d,p) level with SCRF=(IEFPCM, solvent = water).**

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E(UB+HF-LYP): -75.71945769 a.u.

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Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | O | 0.0000000 | 0.0000000 | 0.1096300 |
| 2 | H | 0.0000000 | 0.0000000 | -0.8770390 |

**Structure of $O_2^{-}$· optimized in vacuo at UBHandHLYP/6-31G+(d,p) level.**

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E(UB+HF-LYP): -150.26272342 a.u.

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Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | O | 0.0000000 | 0.0000000 | 0.6600420 |
| 2 | O | 0.0000000 | 0.0000000 | -0.6600420 |

**Structure of $O_2^{-}\cdot$ optimized in water at UBHandHLYP/6-31G+(d,p) level with SCRF=(IEFPCM, solvent = water).**

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E(UB+HF-LYP): -150.38474115 a.u.

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Cartesian coordinates:

| No. | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | O | 0.0000000 | 0.0000000 | 0.6585280 |
| 2 | O | 0.0000000 | 0.0000000 | -0.6585280 |