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# Supporting Information

## Structures and Charge Transport Properties of "Selenosulflower" and its Selenium Analogue "Selflower": Computer-Aided Design of High-Performance Ambipolar Organic Semiconductors

Jun Yin, Kadali Chaitanya, Xue-Hai Ju

Table S1. Optimized bond lengths of ground, anionic and cationic states for the $C_{16}S_4Se_4$ molecule at the B3P86/6-31G (d,p) level

| Index | Bond length | Ground state | Anion state | Cation state | Δ(A-G)[a] | Δ(C-G)[b] |
|---|---|---|---|---|---|---|
| 1 | $R_{1\text{-}2}$ | 1.437 | 1.433 | 1.434 | -0.003 | -0.002 |
| 2 | $R_{1\text{-}9}$ | 1.385 | 1.390 | 1.387 | 0.005 | 0.002 |
| 3 | $R_{9\text{-}10}$ | 1.748 | 1.760 | 1.736 | 0.012 | -0.011 |
| 4 | $R_{10\text{-}11}$ | 1.747 | 1.759 | 1.738 | 0.012 | -0.010 |
| 5 | $R_{2\text{-}3}$ | 1.439 | 1.436 | 1.430 | -0.003 | -0.009 |
| 6 | $R_{2\text{-}11}$ | 1.385 | 1.390 | 1.386 | 0.005 | 0.001 |
| 7 | $R_{11\text{-}12}$ | 1.883 | 1.894 | 1.894 | 0.011 | 0.011 |
| 8 | $R_{12\text{-}13}$ | 1.883 | 1.893 | 1.866 | 0.010 | -0.017 |
| 9 | $R_{3\text{-}4}$ | 1.437 | 1.434 | 1.420 | -0.003 | -0.017 |
| 10 | $R_{3\text{-}13}$ | 1.385 | 1.390 | 1.401 | 0.005 | 0.016 |
| 11 | $R_{13\text{-}14}$ | 1.747 | 1.759 | 1.752 | 0.012 | 0.004 |
| 12 | $R_{14\text{-}15}$ | 1.747 | 1.759 | 1.751 | 0.012 | 0.003 |
| 13 | $R_{4\text{-}5}$ | 1.439 | 1.436 | 1.429 | -0.003 | -0.009 |
| 14 | $R_{4\text{-}15}$ | 1.385 | 1.390 | 1.402 | 0.005 | 0.017 |
| 15 | $R_{15\text{-}16}$ | 1.883 | 1.893 | 1.867 | 0.010 | -0.016 |
| 16 | $R_{16\text{-}17}$ | 1.883 | 1.893 | 1.895 | 0.010 | 0.012 |
| 17 | $R_{5\text{-}6}$ | 1.437 | 1.433 | 1.434 | -0.003 | -0.002 |
| 18 | $R_{5\text{-}17}$ | 1.385 | 1.390 | 1.387 | 0.005 | 0.002 |
| 19 | $R_{17\text{-}18}$ | 1.748 | 1.760 | 1.736 | 0.012 | -0.011 |
| 20 | $R_{18\text{-}19}$ | 1.747 | 1.759 | 1.738 | 0.012 | -0.010 |
| 21 | $R_{6\text{-}7}$ | 1.439 | 1.436 | 1.430 | -0.003 | -0.009 |
| 22 | $R_{6\text{-}19}$ | 1.385 | 1.390 | 1.386 | 0.005 | 0.001 |
| 23 | $R_{19\text{-}20}$ | 1.883 | 1.894 | 1.894 | 0.011 | 0.011 |
| 24 | $R_{20\text{-}21}$ | 1.883 | 1.893 | 1.866 | 0.010 | -0.017 |
| 25 | $R_{7\text{-}8}$ | 1.437 | 1.434 | 1.420 | -0.003 | -0.017 |
| 26 | $R_{7\text{-}21}$ | 1.385 | 1.390 | 1.401 | 0.005 | 0.016 |
| 27 | $R_{21\text{-}22}$ | 1.747 | 1.759 | 1.752 | 0.012 | 0.004 |

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|---|---|---|---|---|---|---|
| 28 | $R_{22\text{-}23}$ | 1.747 | 1.759 | 1.751 | 0.012 | 0.003 |
| 29 | $R_{8\text{-}1}$ | 1.439 | 1.436 | 1.429 | -0.003 | -0.009 |
| 30 | $R_{8\text{-}23}$ | 1.385 | 1.390 | 1.402 | 0.005 | 0.017 |
| 31 | $R_{23\text{-}24}$ | 1.883 | 1.893 | 1.867 | 0.010 | -0.016 |
| 32 | $R_{24\text{-}9}$ | 1.883 | 1.893 | 1.895 | 0.010 | 0.012 |

[a] the bond length difference between the anionic and neutral geometries. [b] the bond length difference between the cationic and neutral geometries.

Table S2. Optimized bond lengths of ground, anionic and cationic states for the $C_{16}S_4Se_4$ molecule at the B3P86/6-31G (d,p) level

| Index | Bond length | Ground state | Anion state | Cation state | Δ(A-G)[a] | Δ(C-G)[b] |
|---|---|---|---|---|---|---|
| 1 | $R_{1\text{-}2}$ | 1.442 | 1.439 | 1.437 | -0.004 | -0.005 |
| 2 | $R_{1\text{-}9}$ | 1.386 | 1.391 | 1.397 | 0.005 | 0.011 |
| 3 | $R_{9\text{-}10}$ | 1.853 | 1.863 | 1.837 | 0.010 | -0.017 |
| 4 | $R_{10\text{-}11}$ | 1.853 | 1.863 | 1.856 | 0.010 | 0.003 |
| 5 | $R_{2\text{-}3}$ | 1.442 | 1.439 | 1.439 | -0.004 | -0.003 |
| 6 | $R_{2\text{-}11}$ | 1.386 | 1.391 | 1.385 | 0.005 | -0.001 |
| 7 | $R_{11\text{-}12}$ | 1.853 | 1.863 | 1.850 | 0.010 | -0.003 |
| 8 | $R_{12\text{-}13}$ | 1.853 | 1.863 | 1.838 | 0.010 | -0.016 |
| 9 | $R_{3\text{-}4}$ | 1.442 | 1.439 | 1.429 | -0.004 | -0.013 |
| 10 | $R_{3\text{-}13}$ | 1.386 | 1.391 | 1.392 | 0.005 | 0.006 |
| 11 | $R_{13\text{-}14}$ | 1.853 | 1.863 | 1.864 | 0.010 | 0.011 |
| 12 | $R_{14\text{-}15}$ | 1.853 | 1.863 | 1.844 | 0.010 | -0.009 |
| 13 | $R_{4\text{-}5}$ | 1.442 | 1.439 | 1.427 | -0.004 | -0.015 |
| 14 | $R_{4\text{-}15}$ | 1.386 | 1.391 | 1.405 | 0.005 | 0.019 |
| 15 | $R_{15\text{-}16}$ | 1.853 | 1.863 | 1.850 | 0.010 | -0.003 |
| 16 | $R_{16\text{-}17}$ | 1.853 | 1.863 | 1.862 | 0.010 | 0.009 |
| 17 | $R_{5\text{-}6}$ | 1.442 | 1.439 | 1.437 | -0.004 | -0.005 |
| 18 | $R_{5\text{-}17}$ | 1.386 | 1.391 | 1.397 | 0.005 | 0.011 |
| 19 | $R_{17\text{-}18}$ | 1.853 | 1.863 | 1.837 | 0.010 | -0.017 |
| 20 | $R_{18\text{-}19}$ | 1.853 | 1.863 | 1.856 | 0.010 | 0.003 |
| 21 | $R_{6\text{-}7}$ | 1.442 | 1.439 | 1.439 | -0.004 | -0.003 |
| 22 | $R_{6\text{-}19}$ | 1.386 | 1.391 | 1.385 | 0.005 | -0.001 |
| 23 | $R_{19\text{-}20}$ | 1.853 | 1.863 | 1.850 | 0.010 | -0.003 |
| 24 | $R_{20\text{-}21}$ | 1.853 | 1.863 | 1.838 | 0.010 | -0.016 |
| 25 | $R_{7\text{-}8}$ | 1.442 | 1.439 | 1.429 | -0.004 | -0.013 |
| 26 | $R_{7\text{-}21}$ | 1.386 | 1.391 | 1.392 | 0.005 | 0.006 |
| 27 | $R_{21\text{-}22}$ | 1.853 | 1.863 | 1.864 | 0.010 | 0.011 |
| 28 | $R_{22\text{-}23}$ | 1.853 | 1.863 | 1.844 | 0.010 | -0.009 |
| 29 | $R_{8\text{-}1}$ | 1.442 | 1.439 | 1.427 | -0.004 | -0.015 |
| 30 | $R_{8\text{-}23}$ | 1.386 | 1.391 | 1.405 | 0.005 | 0.019 |
| 31 | $R_{23\text{-}24}$ | 1.853 | 1.863 | 1.850 | 0.010 | -0.003 |
| 32 | $R_{24\text{-}9}$ | 1.853 | 1.863 | 1.862 | 0.010 | 0.009 |

[a] the bond length difference between the anionic and neutral geometries. [b] the bond length difference between the cationic and neutral geometries.

Figure S1. Bond-length variations of the $C_{16}S_4Se_4$ upon oxidation and reduction

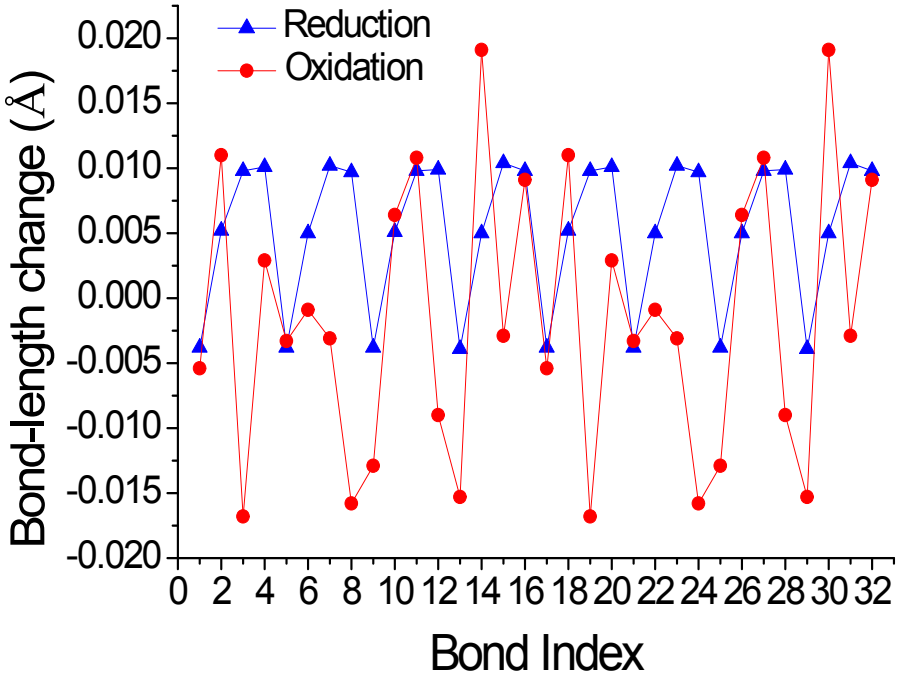

Figure S2. Bond-length variations of the $C_{16}Se_8$ upon oxidation and reduction