**Preparation and Spectroscopic Identification of Methyl-*Se*-nitrososelenol**

Lijuan Song, Felix Keul, and Artur Mardyukov*

Institute of Organic Chemistry, Justus Liebig University, Heinrich-Buff-Ring 17, 35392 Giessen, Germany.

# Table of Contents

## Synthesis of 2,5-Selenohexane

2.000 g (25.3 mmol, 1.00 equiv.) selenium powder was dissolved in 60 mL dry THF under a nitrogen atmosphere. The solution was frozen in a liquid nitrogen bath and 17.2 mL (27.8 mmol, 1.10 equiv.) of an ethereal solution of 1.6 M methyl-lithium was slowly added. The mixture was allowed to warm up to room temperature with stirring, then 1.00 mL (12.7 mmol, 0.50 equiv.) 1,2-dichloroethane was added. The resulting solution was stirred for 1 h at room temperature and refluxed for 15 min. After cooling to room temperature, the mixture was hydrolysed with 25 mL water, the organic phases are separated, washed with saturated $NaHCO_3$ solution and brine and dried with $MgSO_4$. The solvent was distilled and the residue fractioned in vacuum (boiling point: 82 °C, 2 mbar) (0.315 g, 1.46 mmol, 12%). $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$/ppm = 2.84 (s, 4H), 2.04 (s, 6H); $^{13}$C-NMR (100MHz, $CDCl_3$): $\delta$/ppm = 25.0, 4.3; $^{77}$Se-NMR ($CDCl_3$): $\delta$/ppm = 120.4

2,5-Selenohexane-$d_6$ was prepared in analogy. (0.302 g, 1.36 mmol, 7%); $^1$H-NMR (400 MHz, $CDCl_3$): $\delta$/ppm = 2.82 (s, 4H); $^{13}$C-NMR (100MHz, $CDCl_3$): $\delta$/ppm = 24.8

$^{77}$Se-NMR ($CDCl_3$): $\delta$/ppm = 114.0;

## Computational methods

All computations were carried out with Gaussian16[1] and Orca 4.1[2] program package. All the structures are optimized by DFT with B3LYP/6-311++G(3df,3pd)[3,4] inclusion of London dispersion[5] corrections at 298.15 K. Local minima were confirmed by vibrational frequency analysis. An intrinsic reaction coordinate (IRC) calculation was performed to identify each transition state uniquely connecting the reactant to product.[6] The two radical pairs CH$_3$Se•⋯•ON in the open-shell singlet state were computed by broken-symmetry approach (using keyword guess=mix and stable=opt). No contamination of the singlet wave function was found, with the calculated large S2 operators in CH$_3$Se•⋯•ON of 0.03 for both (*syn* and *anti*) conformers. Vertical transitions were computed with time-dependent (TD) DFT[7] at the same level (B3LYP-D3/6-311++G(3df,3pd)). CASSCF(10,8)/def2-TZVPP[8] calculations were performed based on the DFT optimized structures single point energies for all minimum and transition states. Five roots with equal state weights are used NEVPT2 calculations[9] were performed to include the dynamic electron correlation. The DFT and (TD) DFT computations were performed using the Gaussian16 software package. The CASSCF with NEVPT2 computations were performed using Orca 4.1 package.

## Matrix Apparatus Design.

For the matrix isolation studies, we used an APD Cryogenics HC-2 cryostat with a closed-cycle refrigerator system, equipped with an inner CsI window for IR measurements. Spectra were recorded with a Bruker IFS 55 FT-IR spectrometer with a spectral range of 4500–400 cm$^{-1}$ and a resolution of 0.7 cm$^{-1}$ and UV/vis spectra were recorded with a JASCO V-670 spectrophotometer equipped with an sapphire windows. Matrices were generated by co-deposition of **3** (evaporated at 0 °C from a storage bulb) with a large excess of argon (typically 60–120 mbar from a 2000 mL storage bulb) on the surface of the matrix window at 10 K (20 K). A high-pressure mercury lamp (HBO 200, Osram) with a monochromator (Bausch & Lomb) was used for irradiation.
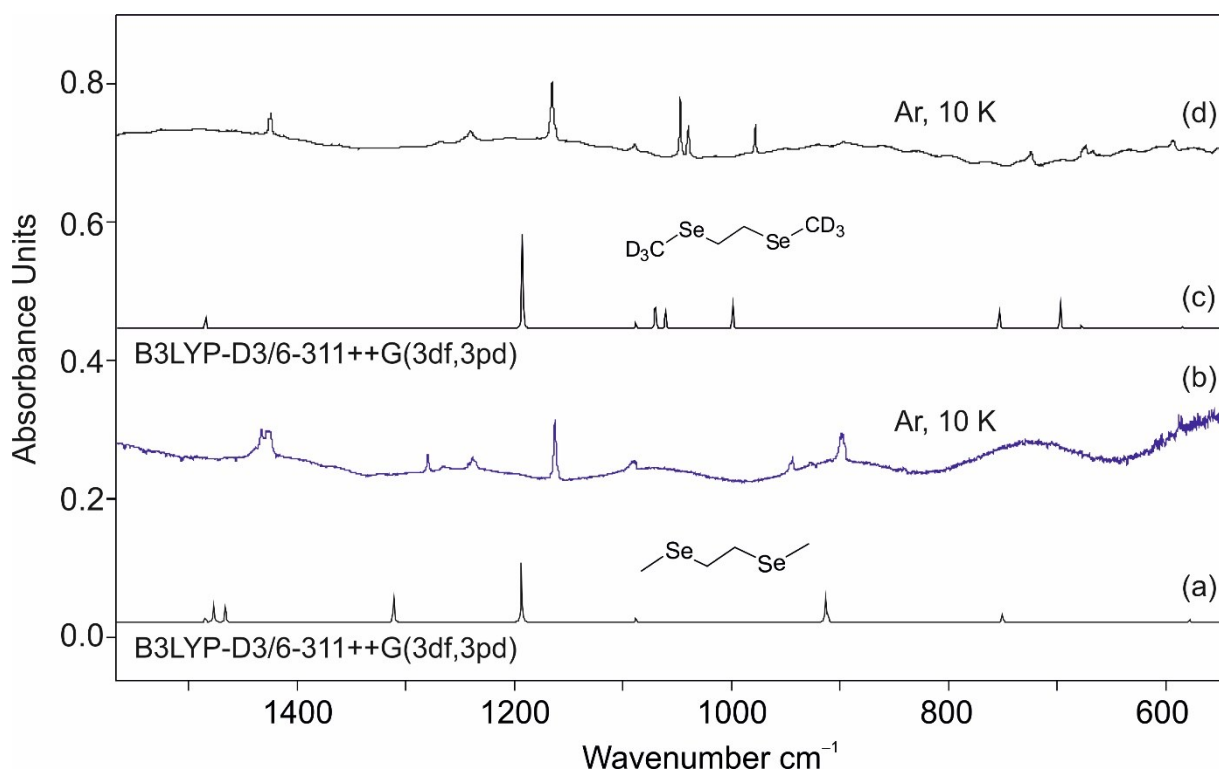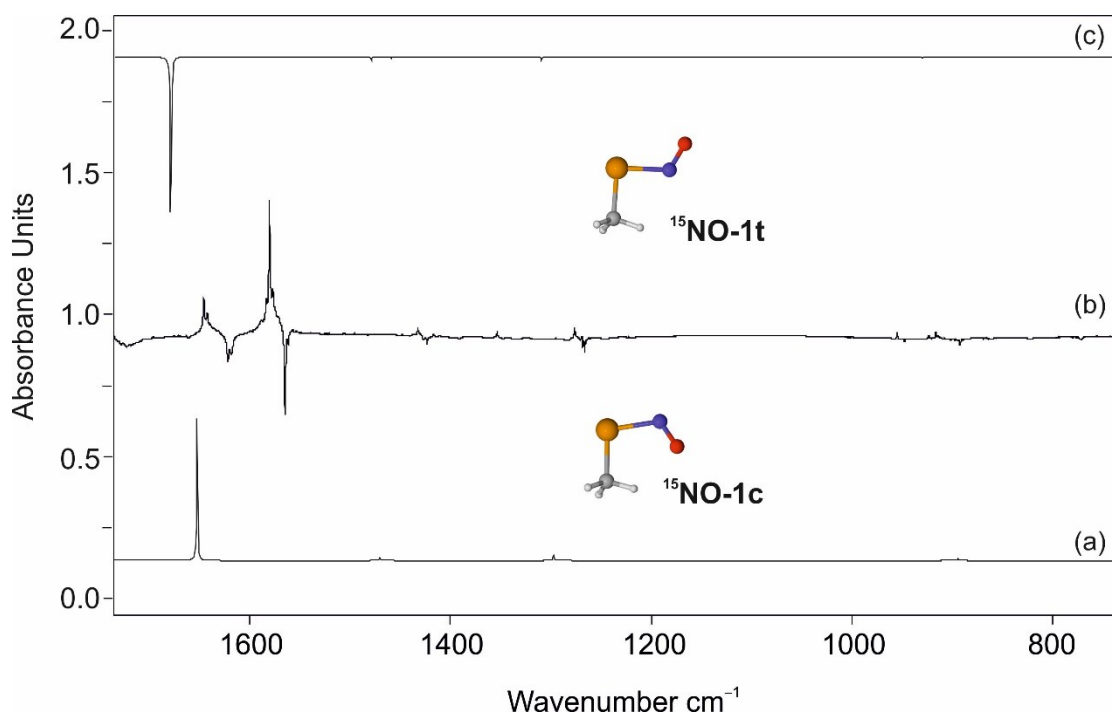
**Figure S1.** (a) IR spectrum of **3** computed at B3LYP-D3/6-311++G(3df,3pd) (unscaled). (b) IR spectrum of **3** in argon at 10 K. (c) IR spectrum of $d_6$−**3** computed at B3LYP-D3/6-311++G(3df,3pd) (unscaled). (d) IR spectrum of $d_6$−**3** in argon at 10 K.
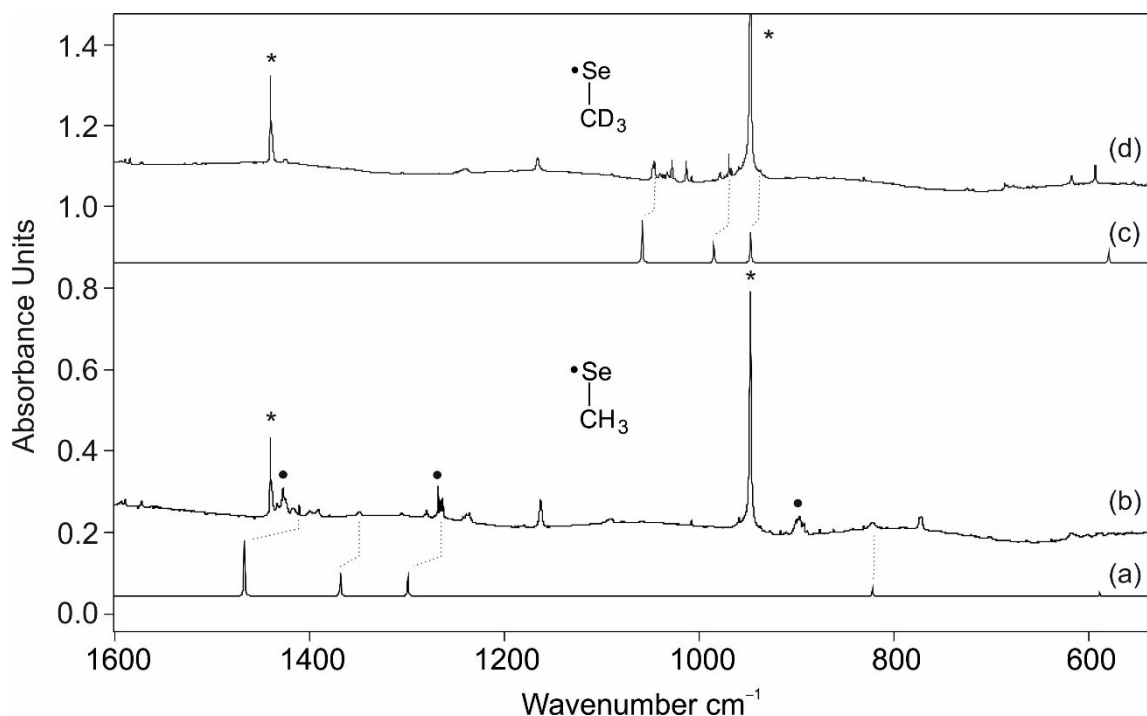
**Figure S2.** (a) IR spectrum of **2** computed at UB3LYP-D3/6-311++G(3df,3pd) (unscaled). (b) IR spectra showing the products of the pyrolysis of **3** in argon with subsequent trapping in an argon matrix at 10 K. (c) IR spectrum of d$_3$-**2** computed at UB3LYP-D3/6-311++G(3df,3pd) (unscaled). (b) IR spectra showing the products of the pyrolysis of d$_6$-**3** in argon with subsequent trapping in an argon matrix at 10 K. Bands attributed to ethylene are marked with an asterisk. Bands attributed to dimethyl diselenide (MeSeSeMe; **5**) are marked with a dot.
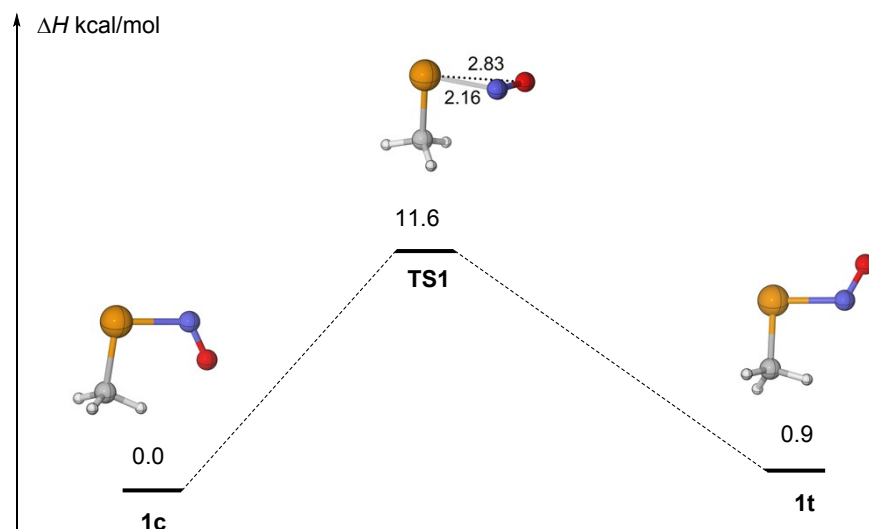


**Figure S3.** Theoretical isomerization pathway between two isomers of methy-Se-nitrososelenols (**1c** and **1t**). Stationary points and transition state were computed by use B3LYP-D3/6-311++G(3df,3pd) method.

**Figure S4.** (a) IR spectrum of [15]NO–**1c** computed at B3LYP-D3/6-311++G(3df,3pd) (unscaled). (b) IR difference spectra showing the photochemistry of [15]NO–**1c** after irradiation at λ = 365 nm in argon at 10 K. Bands pointing downwards assigned to [15]NO–**1c** disappear and bands pointing upwards assigned to [15]NO–**1t** appear after 30 min of irradiation time. (c) IR spectrum of [15]NO–**1t** computed at B3LYP-D3/6-311++G(3df,3pd) (unscaled).
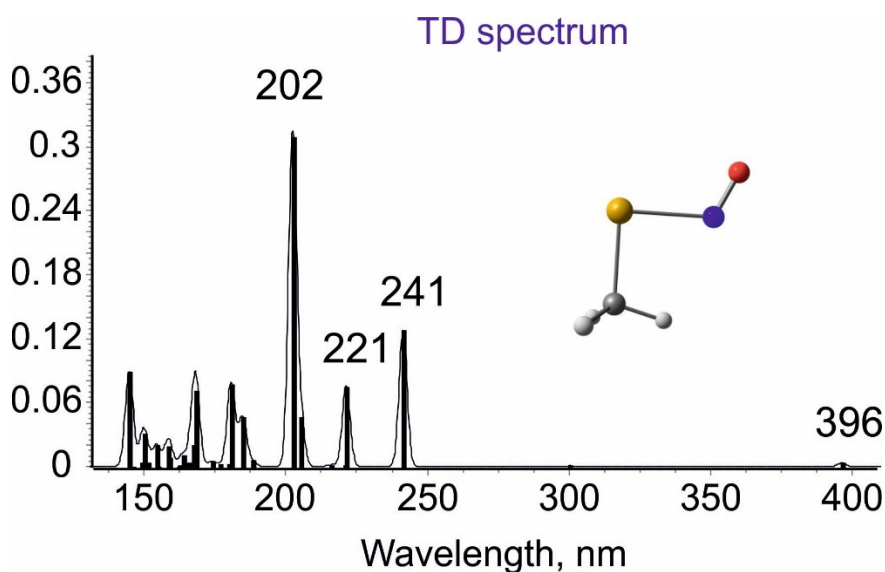


**Figure S5**. TD-UB3LYP-D3/6-311++G(3df,3pd) electronic transitions for **1t**.
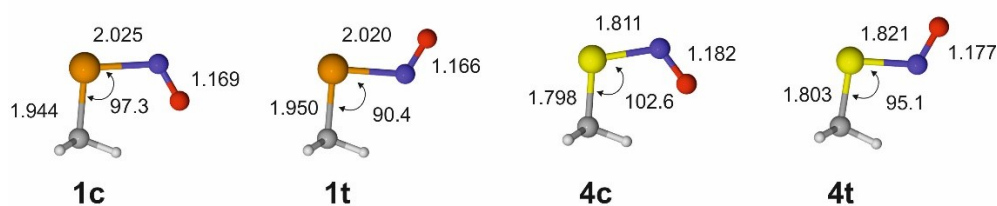
**Figure S6**. Selected bond lengths (Å) and angles of **1** and **4** at the B3LYP-D3/6-311++G(3df,3pd) level.
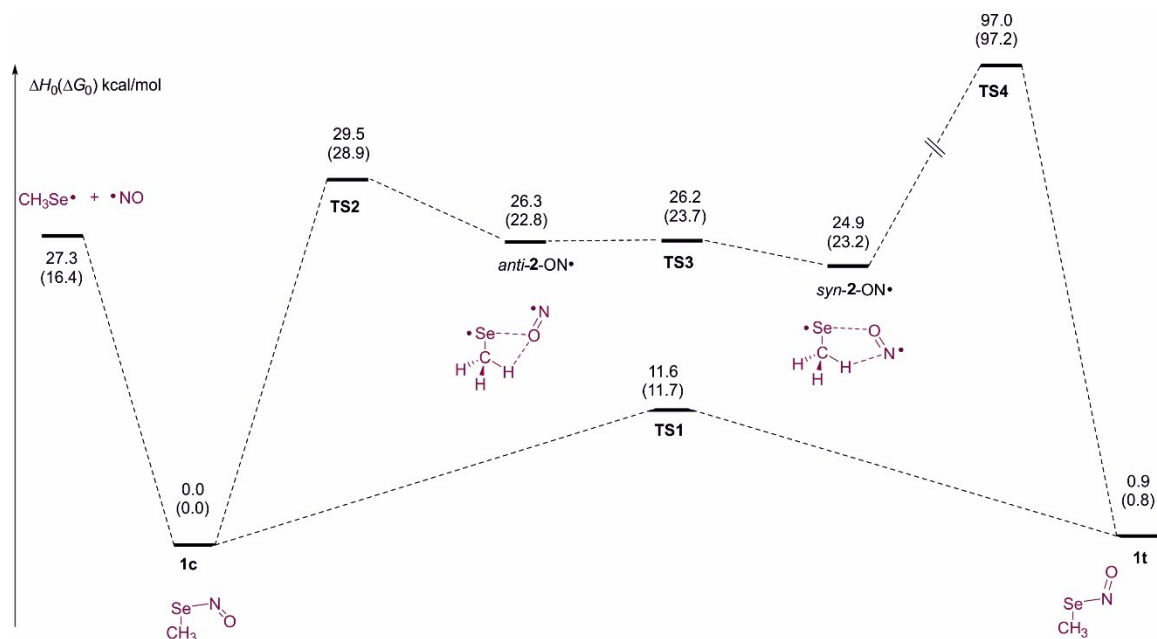


**Figure S7**. Potential energy profile (298.15 K) for CH₃SeNO isomers calculated at the B3LYP-D3/6-311++G(3df,3pd) level. The relative enthalpies and free energies (in parentheses) are given.
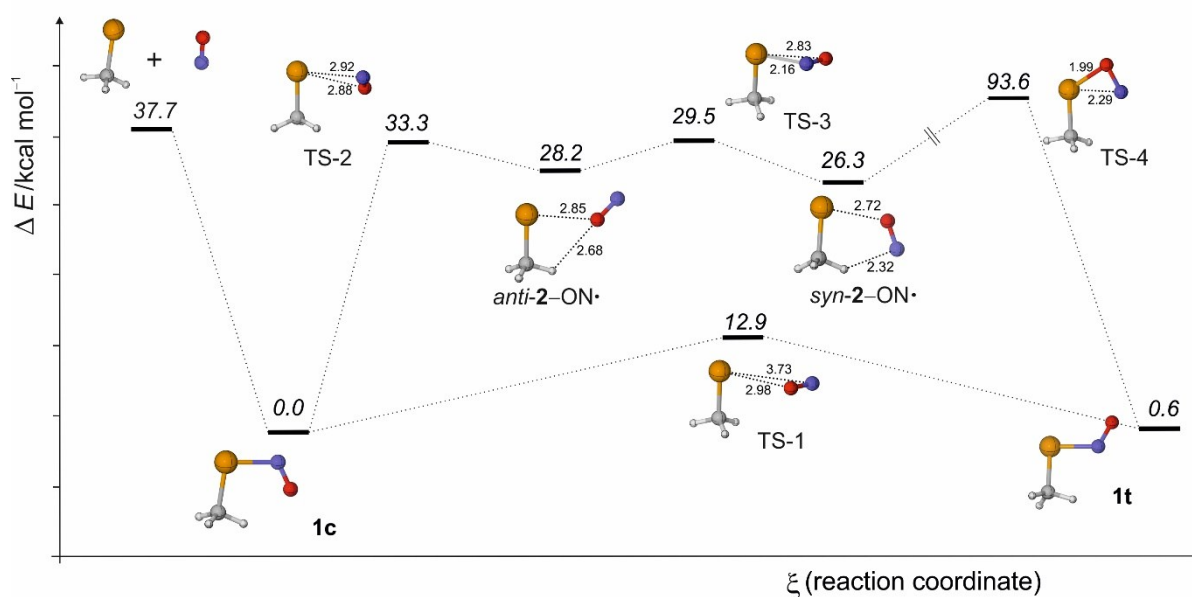


**Figure S8**. Potential energy profile (298.15 K) for CH₃SeNO isomers calculated at the CASSCF(10,8)/def2-TZVPP level with NEVPT2, based on the geometries from B3LYP-D3/6-

311++G(3df,3pd) level. The relative energies (kcal mol$^{-1}$) and selected distances (Å) are depicted.
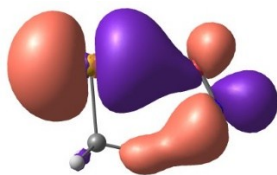


**Figure S9**. HOMO-1 orbitals of *syn*-**2**–ON• depicting non-covalent interactions.

**Table S1.** Experimental (Ar matrix, 10 K) and computed IR frequencies of **2**, band origins in cm$^{-1}$, computed intensities (km mol$^{-1}$) in parentheses.

| Mode | **2** Computed[a] | **2** Ar, 10 K[b] | $d_3$-**2** Computed[a] | $d_3$-**2** Ar, 10 K[b] | Assignment |
|------|-------------------|-------------------|------------------------|-------------------------|------------|
| 9 | 3132 (0.3) | 2931 | 2314 (0.03) | | CH$_3$ asym. str. |
| 8 | 3118 (9.1) | - | 2307 (4.1) | | CH$_3$ asym. str. |
| 7 | 3039 (6.1) | 2797 | 2175 (4.1) | - | CH$_3$ sym. str. |
| 6 | 1467 (11.7) | 1410 | 1067 (5.6) | 1046 | CH$_3$ def. |
| 5 | 1368 (5.9) | 1348 | 986 (2.1) | 937 | CH$_3$ def. |
| 4 | 1299 (4.8) | 1263 | 975 (3.4) | 969 | CH$_3$ rock. |
| 3 | 823 (1.5) | 820 | 619 (0.1) | 617 | CH$_3$ rock. |
| 2 | 590 (0.7) | 574 | 547 (0.7) | 533 | C–Se str. |
| 1 | 515 (24) | - | 392 (11.8) | - | CH$_3$ twist |

[a]UB3LYP-D3/6-311++G(3df,3pd), harmonic approximation, unscaled frequencies, intensities (in parentheses) in km mol$^{-1}$. [b]Experiment: argon matrix, 10 K.; approximate relative intensities ( w: weak, s: strong).

**Table S2.** Experimental (Ar matrix, 10 K) and computed IR frequencies of **1c** and [15]NO-**1c**, band origins in cm$^{-1}$, computed intensities (km mol$^{-1}$) in parentheses.

| Mode | **1c** Computed[a] | **1c** Computed[a] scaled 0.97 | **1c** Ar, 10 K[b] | [15]NO-**1c** Computed[a] | [15]NO-**1c** Computed[a] scaled 0.97 | [15]NO-**1c** Ar, 10 K[b] | Assignment |
|---|---|---|---|---|---|---|---|
| 12 | 1687 (644) | 1637 (644) | 1591 (s) | 1658 (619) | 1609 (619) | 1564 (s) | N=O str. |
| 11 | 1470 (13.1) | 1426 (13.1) | 1423 (w) | 1470 (14) | 1426 (14) | 1423 (w) | CH$_3$ def. |
| 10 | 1467 (4.4) | 1423 (4.4) | - | 1467 (4.4) | 1423 (4.4) | - | CH$_3$ def. |
| 9 | 1301 (21.2) | 1262 (21.2) | 1266 (w) | 1301 (22.6) | 1262 (22.6) | 1266 (w) | CH$_3$ def. |
| 8 | 912 (2.7) | 883 (2.7) | 897 (w) | 912 (2.7) | 883 (2.7) | 897 (w) | CH$_3$ rock |
| 7 | 909 (8.8) | 883 (8.8) | 893 (w) | 909 (8.1) | 882 (8.1) | 892 (w) | CH$_3$ rock |
| 6 | 629 (79.5) | 611 (79.5) | 603 (m) | 615 (71.1) | 598 (71.1) | 589 (m) | Se−N str. |
| 5 | 597 (1.9) | 578 (1.9) | 560 (w) | 597 (2.8) | 590 (2.8) | 546 (s) | C−Se str. |

[a]B3LYP-D3/6-311++G(3df,3pd), harmonic approximation, unscaled and scaled frequencies, intensities (in parentheses) in km mol$^{-1}$. [b]Experiment: argon matrix, 10 K.; approximate relative intensities (w: weak, m: moderate, s: strong).

**Table S3.** Experimental (Ar matrix, 10 K) and computed IR frequencies of **1t** and [15]NO-**1t**, band origins in cm$^{-1}$, computed intensities (km mol$^{-1}$) in parentheses.

| Mode | **1t** Computed[a] | **1t** Computed[a] Scaled 0.97 | **1t** Ar, 10 K[b] | [15]NO-**1t** Computed[a] | [15]NO-**1t** Computed[a] Scaled 0.97 | [15]NO-**1t** Ar, 10 K[b] | Assignment |
|---|---|---|---|---|---|---|---|
| 12 | 1708 (813) | 1659 (813) | 1607 (s) | 1678 (781) | 1678 (781) | 1580 (s) | N=O str. |
| 11 | 1479 (10.7) | 1434 (10.7) | 1432 (w) | 1479 (10.8) | 1479 (10.8) | 1432 (w) | CH$_3$ def. |
| 10 | 1460 (4.2) | 1415 (4.2) | 1416 (w) | 1460 (4.2) | 1460 (4.2) | 1416 (w) | CH$_3$ def. |
| 9 | 1310 (13.8) | 1270 (13.8) | 1275 (w) | 1310 (14.1) | 1310 (14.1) | 1275 (w) | CH$_3$ def. |
| 8 | 931 (3.0) | 902 (3.0) | 916 (m) | 931 (3.0) | 931 (3.0) | 916 (m) | CH$_3$ rock |
| 7 | 912 (0.7) | 882 (0.7) | - | 912 (0.6) | 912 (0.6) | - | CH$_3$ rock |
| 6 | 622 (71.4) | 605 (71.4) | 592 (m) | 609 (56) | 609 (56) | 580 (m) | Se−N str. |
| 5 | 598 (3.9) | 580 (3.9) | - | 597 (12.9) | 597 (12.9) | - | C−Se str. |

[a]B3LYP-D3/6-311++G(3df,3pd), harmonic approximation, unscaled and scaled frequencies, intensities (in parentheses) in km mol$^{-1}$. [b]Experiment: argon matrix, 10 K.; approximate relative intensities (w: weak, m: moderate, s: strong).

**Table S4.** Experimental (Ar matrix, 10 K) and computed IR frequencies of *syn***2-ON ,***syn***2-O$^{15}$N**, and *anti***2-ON ,** *anti***2-O$^{15}$N** band origins in cm$^{-1}$, computed intensities (km mol$^{-1}$) in parentheses.

| Mode | 2-NO Ar, 10 K[b] | 2-$^{15}$NO Ar, 10 K[b] | syn-2-NO Computed[a] | syn2-$^{15}$NO Computed[a] | anti2-NO Computed[a] | anti2-$^{15}$NO Computed[a] | Assignment |
|---|---|---|---|---|---|---|---|
| 15 | - | - | 3146 (1.6) | 3146 (1.8) | 3147 (1.6) | 3147 (1.6) | CH$_3$ asym str. |
| 14 | - | - | 3096 (10.8) | 3096 (10.8) | 3121 (8.4) | 3121 (8.4) | CH$_3$ sym str. |
| 13 | - | - | 2984 (7.7) | 2984 (7.7) | 3042 (13.6) | 3042 (13.6) | CH$_3$ sym. str. |
| 12 | 1820 (s) | 1788 (s) | 1924 (464) | 1890 (447) | 1936 (285) | 1901 (274) | N=O str. |
| 11 | 1419 (m) | 1419 (m) | 1470 (9.2) | 1470 (9.2) | 1471 (7.4) | 1471 (7.4) | CH$_3$ def. |
| 10 | 1400 (w) | 1400 (w) | 1447 (3.3) | 1447 (3.3) | 1444 (13.4) | 1444 (4.6) | CH$_3$ def. |
| 9 | 1278 (m) | 1278 (m) | 1308 (16.5) | 1308 (16.6) | 1300 (26.3) | 1300 (13.4) | CH$_3$ def. |
| 8 | 883 (w) | 883 (w) | 895 (6.5) | 895 (6.5) | 884 (8.1) | 884 (8.1) | CH$_3$ rock |
| 7 | 852 (w) | 852 (w) | 860 (1.3) | 860 (1.3) | 844 (0.3) | 844 (0.3) | CH$_3$ rock |
| 6 | | - | 599 (0.8) | 599 (0.8) | 589 (1.2) | 589 (1.2) | C−Se str. |

[a]UB3LYP-D3/6-311++G(3df,3pd), harmonic approximation, unscaled frequencies, intensities (in parentheses) in km mol$^{-1}$. [b]Experiment: argon matrix, 10 K.; approximate relative intensities (w: weak, m: moderate, s: strong).

**Table S5.** Experimental (Ar matrix, 10 K) and computed (scaled:0.97) IR frequencies of *syn***2-ON ,***syn***2-O$^{15}$N**, and *anti***2-ON ,** *anti***2-O$^{15}$N** band origins in cm$^{-1}$, computed intensities (km mol$^{-1}$) in parentheses.

| Mode | 2-NO Ar, 10 K[b] | 2-$^{15}$NO Ar, 10 K[b] | syn-2-NO Computed[a] Scaled 0.97 | syn2-$^{15}$NO Computed[a] Scaled 0.97 | anti2-NO Computed[a] Scaled 0.97 | anti2-$^{15}$NO Computed[a] Scaled 0.97 | Assignment |
|---|---|---|---|---|---|---|---|
| 12 | 1820 (s) | 1788 (s) | 1866 (464) | 1834 (447) | 1877 (285) | 1845 (274) | N=O str. |
| 11 | 1419 (m) | 1419 (m) | 1427 (9.2) | 1427 (9.2) | 1428 (7.4) | 1426 (7.4) | CH$_3$ def. |
| 10 | 1400 (w) | 1400 (w) | 1405 (3.3) | 1405 (3.3) | 1401 (13.4) | 1402 (4.6) | CH$_3$ def. |
| 9 | 1278 (m) | 1278 (m) | 1270 (16.5) | 1270 (16.6) | 1261 (26.3) | 1261 (13.4) | CH$_3$ def. |
| 8 | 883 (w) | 883 (w) | 867 (6.5) | 867 (6.5) | 858 (8.1) | 857 (8.1) | CH$_3$ rock |
| 7 | 852 (w) | 852 (w) | 834 (1.3) | 834 (1.3) | 819 (0.3) | 818 (0.3) | CH$_3$ rock |
| 6 | | - | 581 (0.8) | 581 (0.8) | 572 (1.2) | 573 (1.2) | C−Se str. |

[a]UB3LYP-D3/6-311++G(3df,3pd), harmonic approximation, scaled frequencies, intensities (in parentheses) in km mol$^{-1}$. [b]Experiment: argon matrix, 10 K.; approximate relative intensities (w: weak, m: moderate, s: strong).

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## Geometric Structures and Electronic energies (Hartree)

| Energies | E(0K) | E (298K) | H (298K) | G (298K) |
|---|---|---|---|---|
| ON• | -129.940481 | -129.935971 | -129.932666 | -129.955954 |
| MeSe• | -2441.456111 | -2441.421126 | -2441.416874 | -2441.446780 |
| **1c** | -2571.443052 | -2571.399350 | -2571.393006 | -2571.428873 |
| **1t** | -2571.441718 | -2571.397965 | -2571.391539 | -2571.427616 |
| *anti-***2**–ON• | -2571.400545 | -2571.358935 | -2571.351108 | -2571.392483 |
| *syn-***2**–ON• | -2571.402734 | -2571.360538 | -2571.353267 | -2571.391980 |
| **TS1** | -2571.423504 | -2571.380623 | -2571.374517 | -2571.410289 |
| **TS2** | -2571.393374 | -2571.352231 | -2571.346045 | -2571.382858 |
| **TS3** | -2571.399734 | -2571.358451 | -2571.351316 | -2571.391049 |
| **TS4** | -2571.285656 | -2571.244685 | -2571.238495 | -2571.273997 |
| MeS• | -438.112666 | -438.077262 | -438.073125 | -438.101530 |
| **4c** | -568.107946 | -568.063420 | -568.057351 | -568.091667 |
| **4t** | -568.106211 | -568.061586 | -568.055446 | -568.089790 |

ON•
N    0.000000000    0.000000000    -0.610471000
O    0.000000000    0.000000000    0.534162000

$CH_3Se$•
C    -0.002091000    1.518691000    0.000000000

| H | 1.045062000 | 1.823414000 | 0.000000000 |
| H | -0.480718000 | 1.899013000 | 0.897204000 |
| H | -0.480718000 | 1.899013000 | -0.897204000 |
| Se | -0.002091000 | -0.433341000 | 0.000000000 |

**1c**

| C | -1.646964000 | -0.309791000 | 0.000000000 |
| H | -2.220907000 | -0.088118000 | 0.893842000 |
| H | -2.220907000 | -0.088118000 | -0.893842000 |
| H | -1.345484000 | -1.359373000 | 0.000000000 |
| Se | -0.000547000 | 0.724616000 | 0.000000000 |
| N | 1.288731000 | -0.838092000 | -0.000001000 |
| O | 0.817609000 | -1.908231000 | 0.000001000 |

**1t**

| C | -1.874381000 | 0.085614000 | 0.000001000 |
| H | -1.871671000 | -1.004139000 | 0.000004000 |
| H | -2.364927000 | 0.459842000 | 0.892358000 |
| H | -2.364923000 | 0.459837000 | -0.892362000 |
| Se | 0.000113000 | 0.624751000 | 0.000004000 |
| N | 0.574650000 | -1.312800000 | -0.000004000 |
| O | 1.717714000 | -1.544297000 | -0.000001000 |

*anti-***2**–ON•

| C | -1.340464000 | 1.337162000 | -0.000008000 |
| H | -1.912252000 | 1.561695000 | -0.895215000 |
| H | -0.429500000 | 1.935634000 | 0.000004000 |
| H | -1.912262000 | 1.561677000 | 0.895198000 |
| Se | -0.789143000 | -0.538761000 | -0.000024000 |
| N | 2.844809000 | -0.024950000 | 0.000015000 |
| O | 1.851107000 | 0.529402000 | 0.000012000 |

*syn-***2**–ON•

| C | 0.403500000 | 1.578183000 | -0.000437000 |
| H | 0.773821000 | 2.069010000 | 0.894625000 |
| H | -0.690937000 | 1.630058000 | 0.000648000 |
| H | 0.772078000 | 2.069568000 | -0.895911000 |
| Se | 0.894157000 | -0.304374000 | -0.001495000 |
| N | -2.487685000 | 0.159106000 | 0.001762000 |
| O | -1.790958000 | -0.737154000 | 0.000809000 |

**TS1**

| C | 0.983179000 | 1.437243000 | 0.012460000 |
| H | 2.057733000 | 1.505758000 | -0.134590000 |
| H | 0.469087000 | 1.960879000 | -0.787577000 |
| H | 0.726903000 | 1.852863000 | 0.983102000 |
| Se | 0.543818000 | -0.478897000 | -0.032845000 |
| N | -1.475554000 | 0.015448000 | 0.537016000 |

| O | -2.164216000 | 0.278926000 | -0.347259000 |
|---|---|---|---|

**TS2**

| C | -1.716857000 | -0.350395000 | -0.218751000 |
|---|---|---|---|
| H | -1.436179000 | -0.829417000 | 0.717981000 |
| H | -2.547361000 | 0.323433000 | -0.032589000 |
| H | -1.986360000 | -1.115610000 | -0.940393000 |
| Se | -0.167766000 | 0.659255000 | -0.851341000 |
| N | 1.520792000 | -0.875723000 | 0.972751000 |
| O | 1.005263000 | -1.678651000 | 0.352341000 |

**TS3**

| C | -1.100556000 | 1.436134000 | 0.018483000 |
|---|---|---|---|
| H | -0.783728000 | 1.800240000 | -0.954612000 |
| H | -0.532256000 | 1.903199000 | 0.817059000 |
| H | -2.157785000 | 1.663940000 | 0.151208000 |
| Se | -0.934802000 | -0.510689000 | 0.096401000 |
| N | 2.713769000 | 0.221214000 | 0.329256000 |
| O | 1.920793000 | 0.122586000 | -0.482620000 |

**TS4**

| C | -1.617626000 | 0.910919000 | 0.000000000 |
|---|---|---|---|
| H | -2.531075000 | 0.302114000 | -0.000004000 |
| H | -1.560650000 | 1.511829000 | -0.900109000 |
| H | -1.560652000 | 1.511821000 | 0.900114000 |
| N | 1.341218000 | 1.181265000 | 0.000012000 |
| O | 1.713206000 | -0.041695000 | 0.000006000 |
| Se | -0.227531000 | -0.491958000 | -0.000004000 |

MeS•

| C | 1.105702000 | 0.000010000 | -0.008794000 |
|---|---|---|---|
| H | 1.505308000 | -0.896460000 | -0.478221000 |
| H | 1.418839000 | -0.000628000 | 1.039479000 |
| H | 1.505264000 | 0.897032000 | -0.477187000 |
| S | -0.691477000 | 0.000000000 | -0.001957000 |

**4c**

| C | -1.619919000 | -0.320701000 | 0.000003000 |
|---|---|---|---|
| H | -2.193624000 | -0.084098000 | 0.891987000 |
| H | -2.193602000 | -0.084112000 | -0.892000000 |
| H | -1.362162000 | -1.382741000 | 0.000014000 |
| N | 1.168757000 | -0.727254000 | -0.000017000 |
| O | 0.783168000 | -1.845067000 | -0.000004000 |
| S | -0.071286000 | 0.592961000 | 0.000018000 |

**4t**

| C | -1.577483000 | -0.317548000 | -0.000002000 |
|---|---|---|---|
| H | -2.165534000 | -0.113022000 | 0.890276000 |

```
H    -2.165564000    -0.113391000    -0.890344000
H    -1.259077000    -1.360504000     0.000210000
N     1.067042000    -0.727718000     0.000070000
O     2.217054000    -0.473873000     0.000016000
S    -0.079768000     0.687752000    -0.000235000
```