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Supporting Information

Divergent Reactivity of a Dinuclear (NHC)Nickel(I) Catalyst versus Nickel(0) Enables Chemoselective Trifluoromethylselenolation

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1. General experimental details

Reagents. All Reagents were purchased at reagent grade from Acros, Aldrich, ABCR, TCI and Fluka, and used as received unless otherwise stated. Selenium powder was purchased from Aldrich and converted to Se_8 according to a modified literature procedure.[1] $NiI_2(dme)_2$ was prepared from NiI_2 according to a literature procedure.[2]

Solvents. THF, toluene, hexane and DCM were purified by solvent purification system (Innovative Technology PS-MD-5). All other anhydrous solvents were purchased from Aldrich and used as received unless stated otherwise. Extraction solvents and column chromatography eluents, *n*-hexane, *n*-pentane, diethyl ether and ethyl acetate were received in technical grade and distilled prior to use.

Experimental Techniques. All reactions were carried out under argon atmosphere unless stated otherwise. All reactions involving the $(Me_4N)SeCF_3$ reagent were carried out in oven-dried amber glassware under argon atmosphere.
Flash column chromatography was carried out with SiO_2 60 (particle size 0.040–0.063 mm, 230–400 mesh). Thin-layer chromatography (TLC) was conducted on aluminum sheets coated with SiO_2 60 F254 obtained from Merck KGaA, Germany. Compounds were visualized under UV light at 254 nm and by an appropriate stain.

Characterization. All ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded at ambient temperature either on Varian V-NMRS 600, Varian V-NMRS 400 or Varian Mercury 300 spectrometer. Chemical shifts (δ) are quoted in parts per million (ppm) and were referenced to the residual solvent peak in the case of ^{1}H (7.26 ppm for $CDCl_3$, 5.32 ppm for CD_2Cl_2, and 7.16 ppm for C_6D_6) and ^{13}C (77.0 ppm for $CDCl_3$, 54.0 ppm for CD_2Cl_2 and 128.06 for C_6D_6) NMR spectra, and added α,α,α-trifluorotoluene (δ = -62.73 ppm) in the case of ^{19}F NMR. Coupling constants (*J*) are given in Hz. The resonance multiplicity is described as s (singlet), d (doublet), t (triplet), q (quartet), quint. (quintet), hept. (heptet), m (multiplet), dd (doublet of doublets) and br. (broad). ^{13}C and ^{19}F NMR spectra are proton decoupled.
Mass spectrometric analysis was performed on Finnigan MAT 95 apparatus using EI ionization. GC-MS analyses were performed using an Agilent Technologies 5975 series MSD mass spectrometer coupled with an Agilent Technologies 7820A gas chromatograph equipped with an Agilent 19091s-433 HP-SMS column (30 m × 0.250 µm × 0.25 µm).
Melting points were measured with a LLG Labware MPM-H2 apparatus.

2. General experimental procedures

2.1 Conversion of grey selenium to red selenium[1]

Grey selenium (1.70 g, 21.5 mmol, 1.0 equiv.) was added to conc. sulfuric acid (100 mL) and the reaction mixture stirred at 180°C for 6 h. The reaction mixture was filtered through a sintered funnel directly onto ice (250 mL) and the resulting solution left to recrystallize at 4°C overnight. The mixture was then filtered and the obtained red solid was washed with cold water (3 x 20 mL) and Et_2O (3 x 20 mL). The resulting red powder was then dried overnight *in vacuo* to give 1.65 g (97%) of Se_8.

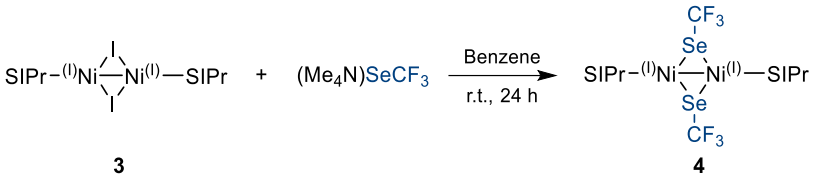
2.2 Synthesis of $(Me_4N)SeCF_3$

Red selenium (Se(red), 1.25 g, 15.8 mmol, 1.0 equiv.) and trifluoromethyl(trimethyl)silane (2.48 g, 17.4 mmol, 1.1 equiv.) were added to anhydrous THF (100 mL). The reaction mixture was stirred at −65°C under strict exclusion of light for 1 hour. Tetramethylammonium fluoride (1.46 g, 15.8 mmol, 1.0 equiv.) was then added in one portion and the reaction mixture was allowed to warm to room temperature and stirred for 12 h in darkness. The solvent was filtered through a short plug of celite and the filtrate was discarded. The plug of celite was then washed with 30 mL of dry MeCN. The filtrate was concentrated to approximately 10 mL. Addition of 90 mL of dry Et_2O resulted in precipitation of a white solid. Filtration gave the product as a white powder. (3.0 g, 86%). ^{1}H NMR (400 MHz, acetone-d_6) δ 3.20 (12H, s, N-CH_3). ^{19}F NMR (376 MHz, acetone-d_6) δ -6.57. These data are in agreement with those reported previously in the literature.[3]

2.3 Procedure for the synthesis of $[(SIPr)Ni(\mu\text{-}I)]_2$ (3)

A 20-mL scintillation vial equipped with a stir bar was charged with $Ni(cod)_2$ (126 mg, 0.46 mmol), $NiI_2(dme)_2$ (213 mg, 0.46 mmol), and SIPr (355 mg, 0.91 mmol). 8 mL of benzene were added and the resulting suspension was stirred *vigorously* at room temperature for 14 hours. The solution turns dark during this time. The reaction mixture was filtered over a pad of celite (~ 2 cm) on a narrow fritted funnel (Por. 4, 2 cm diameter, 10 cm length) and concentrated to ~2-3 mL under vacuum, 16 mL of hexane was added and the mixture was cooled to –25 °C. The product precipitated overnight as a yellow powder which was then isolated by filtration over a medium frit and washed with 3 x 2 mL of cold hexane to yield 402 mg of complex **3** (80% yield). ^{1}H NMR (600 MHz, C_6D_6) δ 7.2-7.12 (m, 12H, H_{Ar}), 3.62 – 3.50 (m, 8H, CHMe$_2$), 2.96 (s, 8H, NCH_2CH_2N), 2.35 (d, J = 6.7 Hz, 24H, CHMe_2), 1.16 (d, J = 6.8 Hz, 24H, CHMe_2). ^{13}C NMR (151 MHz, C_6D_6) δ 210.7, 147.1, 137.6, 128.7, 124.4, 52.5, 29.0, 25.8. Crystals suitable for X-Ray diffraction analysis were obtained *via* slow evaporation of Et_2O at room temperature.

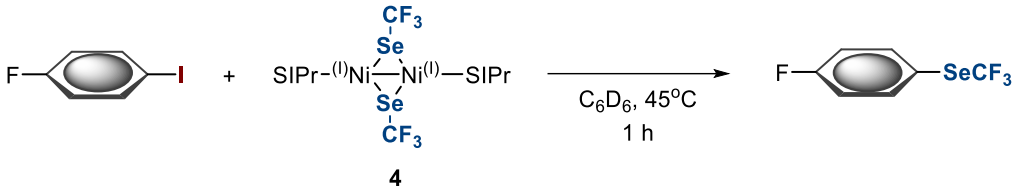
2.4 General procedure for the synthesis of [(SIPr)Ni(μ-SeCF$_3$)]$_2$ (4)



3 4

[(SIPr)Ni(μ-I)]$_2$ (164 mg, 0.15 mmol, 1.0 equiv.), (Me$_4$N)SeCF$_3$ (138 mg, 0.62 mmol, 4.0 equiv.) and dry benzene (8.0 mL) were added in an oven-dried, amber-colored reaction vial equipped with a stirring bar. The reaction was stirred vigorously for 24 h at ambient temperature, then filtered over a pad of celite (~ 2 cm) on a narrow fritted funnel (Por. 4, 2 cm diameter, 10 cm length) and the solvent evaporated completely to give 174 mg of [(SIPr)Ni(μ-SeCF$_3$)]$_2$ as a reddish solid in 94% isolated yield. ^{1}H NMR (600 MHz, C$_6$D$_6$) δ 7.28 (dd, *J* = 7.6, 7.6 Hz, 4H, *H*$_{Ar}$), 7.20 (d, *J* = 7.6 Hz, 8H, *H*$_{Ar}$), 3.49 (m, 8H, C*H*Me$_2$), 3.32 (s, 8H, NC*H*$_2$C*H*$_2$N), 1.65 (d, *J* = 6.8 Hz, 24H, CH*Me*$_2$), 1.14 (d, *J* = 6.9 Hz, 24H, CH*Me*$_2$). ^{13}C NMR (151 MHz, C$_6$D$_6$) δ 214.7, 147.3, 137.8, 128.8, 124.7, 53.5, 28.9, 26.1, 24.6. ^{19}F NMR (564 MHz, C$_6$D$_6$) δ -21.47. Crystals suitable for X-Ray diffraction analysis were obtained *via* slow evaporation of Et$_2$O at room temperature.

2.5 Kinetic studies



4

Inside a glovebox an NMR tube was charged with 0.3 mL of a solution of [(SIPr)Ni(μ-$SeCF_3$)]$_2$ **4** (varying concentration in C_6D_6, see Figure S1) and frozen at -25°C. Then, 0.3 mL of 1-iodo-4-fluorobenzene (constant concentration: 0.33 M) containing a known amount of internal standard 4-trifluoromethoxyanisole in C_6D_6 was added, and the contents of the tube were again frozen in the freezer. The reaction mixture was then, still in the frozen state, submitted to the NMR spectrometer which was preheated to 45°C. The reaction was monitored *in situ* using ^{19}F NMR (relaxation delay: 10 s; pulse angle 90°) for one hour.

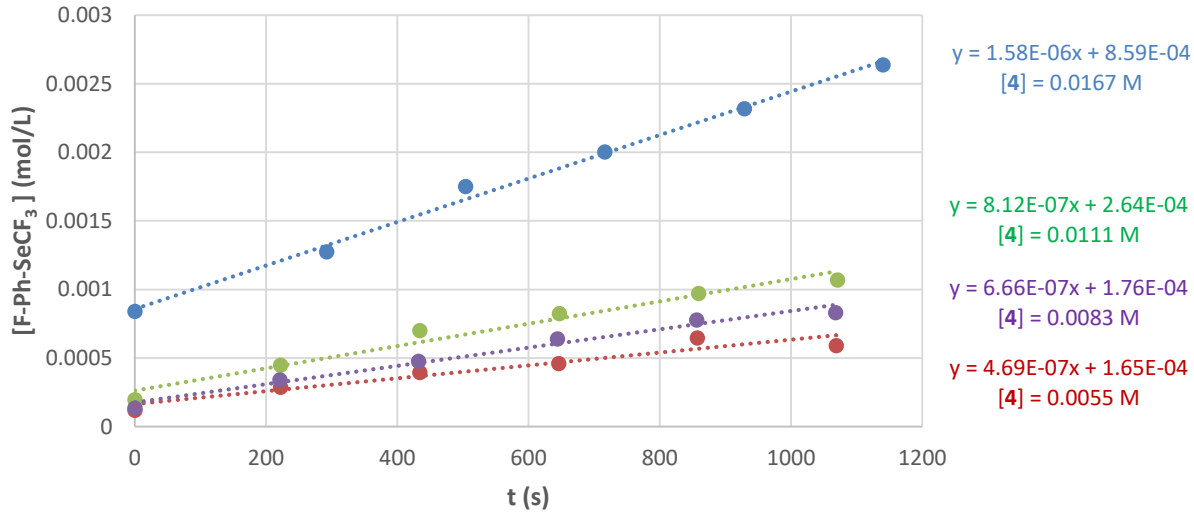


Figure S1. Product formation over time depending on different concentrations of **4.**

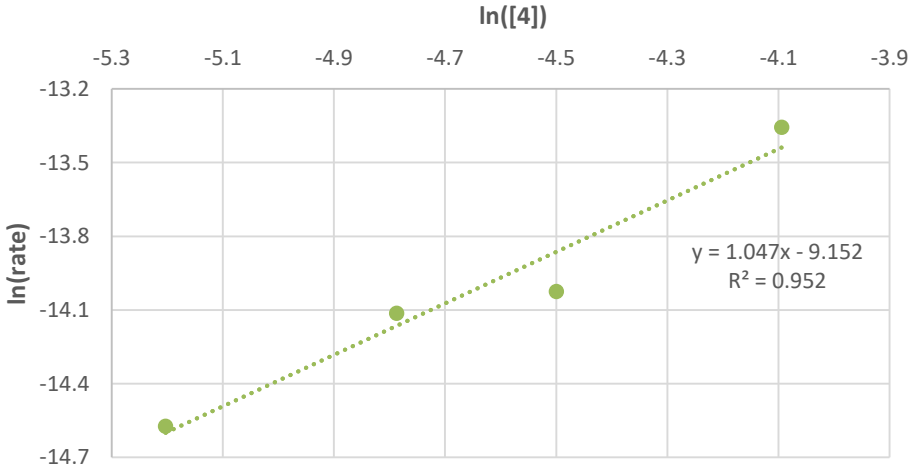
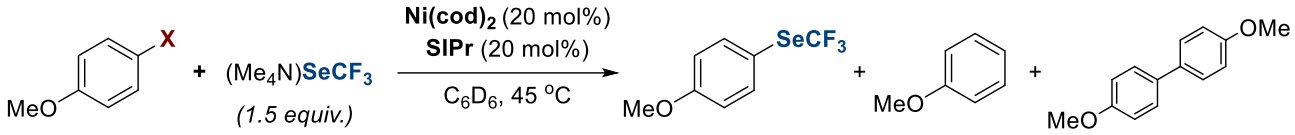


Figure S2. First order dependence of reaction rate in the concentration of the $SeCF_3$-bridged Ni(I) dimer **4**.

2.6 Catalysis with Ni(0) – productive coupling, homocoupling and further sidereactions



Inside an Ar-filled glovebox, $Ni(cod)_2$ and SIPr were dissolved in 0.5 mL of C_6D_6 and stirred for 5 minutes, after which the solution was added to a mixture of 4-haloanisole (23.4 mg, 0.1 mmol, 1.0 equiv.) and $(Me_4N)SeCF_3$ (33.2 mg, 0.15 mmol, 1.5 equiv.) in 0.5 mL of C_6D_6 in an amber vial equipped with a stirring bar.

All reactions were performed in duplicate, and were analyzed by quantitative ^1H NMR after 30 minutes (Figures S3 and S4), and after 18 hours. Virtually no changes in the composition of the mixture were observed when comparing these two time-points.

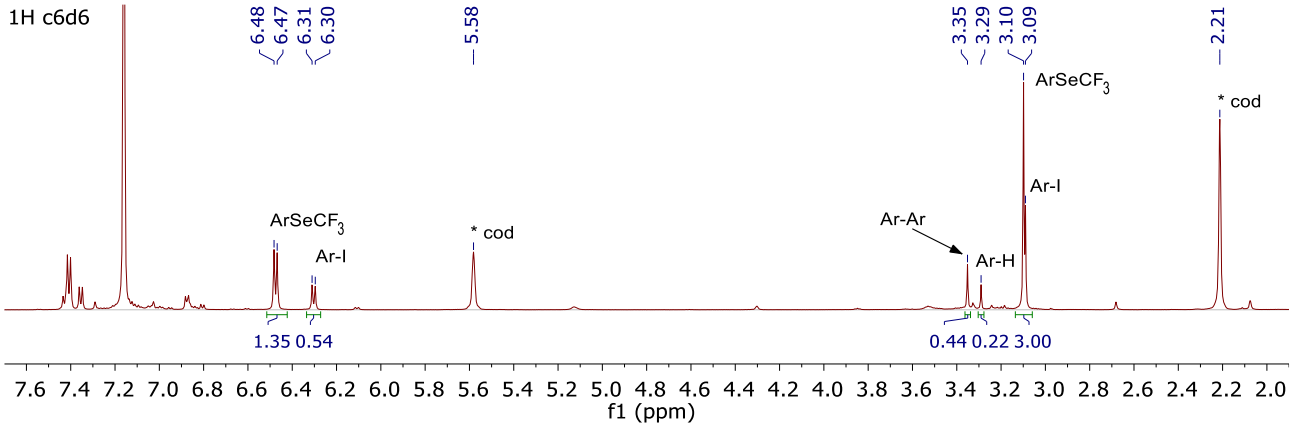


Figure S3. ^1H NMR spectrum of Ni(0)-catalyzed reaction with 4-iodoanisole after 30 minutes.

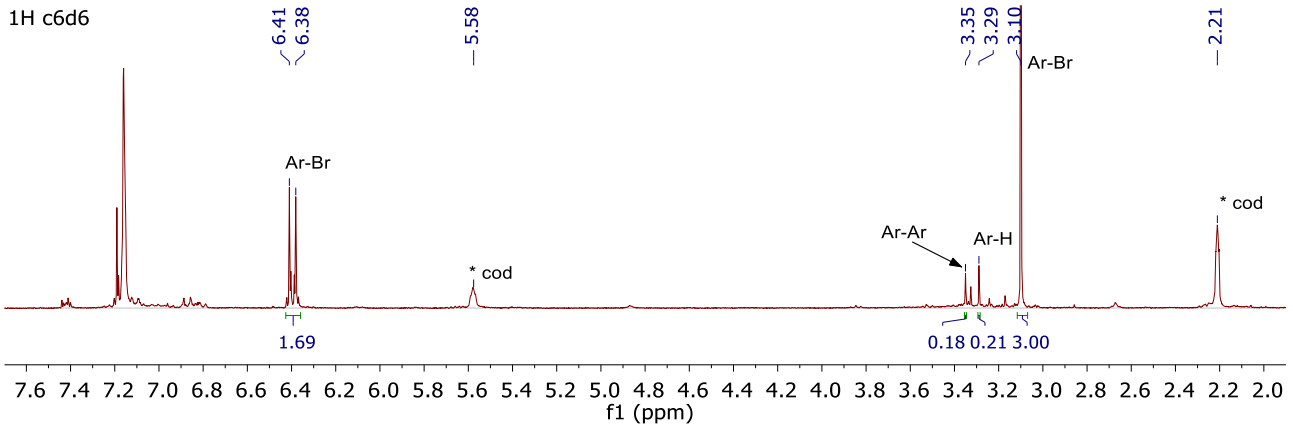
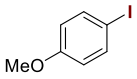
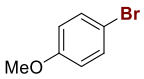


Figure S4. ^1H NMR spectrum of Ni(0)-catalyzed reaction with 4-bromoanisole after 30 minutes.

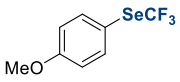
^{1}H NMR shifts of the involved anisole derivatives were also measured independently in C_6D_6 as reference:



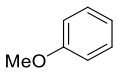
^{1}H NMR (300 MHz, C_6D_6) δ 7.35 (d, *J* = 8.8 Hz, 2H), 6.31 (d, *J* = 8.8 Hz, 2H), 3.10 (s, 3H).



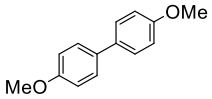
^{1}H NMR (300 MHz, C_6D_6) δ 7.17 (d, *J* = 8.9 Hz, 2H), 6.40 (d, *J* = 8.9 Hz, 2H), 3.10 (s, 3H).



^{1}H NMR (300 MHz, C_6D_6) δ 7.41 (d, *J* = 8.8 Hz, 2H), 6.48 (d, *J* = 8.8 Hz, 2H), 3.11 (s, 3H).



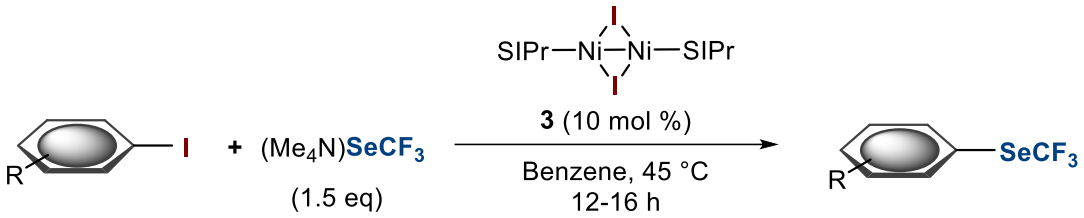
^{1}H NMR (300 MHz, C_6D_6) δ 7.16 – 7.08 (m, 2H), 6.90 – 6.75 (m, 3H), 3.30 (s, 3H).



^{1}H NMR (600 MHz, C_6D_6) δ 7.43 (d, *J* = 8.7 Hz, 4H), 6.87 (d, *J* = 8.7 Hz, 4H), 3.35 (s, 6H).

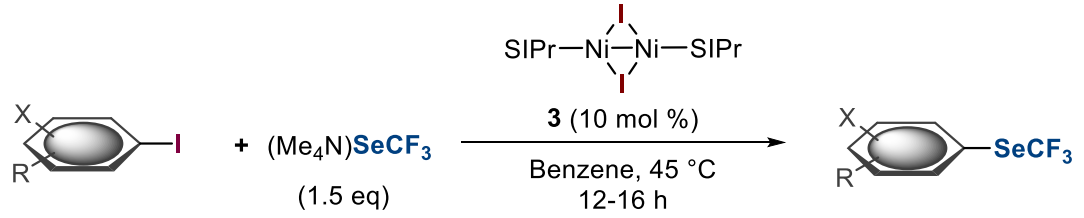
For full data of the generated products, see below in the compound characterization section.

2.7 General procedure for trifluoromethylselenolation of aryl iodides (procedure A)



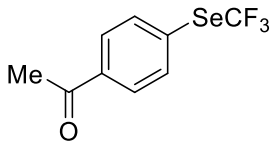
Inside a glovebox, aryl iodide (0.1 mmol, 1.0 equiv.), $(Me_4N)SeCF_3$ (33.3 mg, 0.15 mmol, 1.5 equiv.) and Ni-I-dimer **3** (10.9 mg, 0.01 mmol, 10 mol%) were added to a dry, amber reaction vial equipped with a stirring bar. Followingly, benzene (1.0 ml) was added and the reaction was stirred in the glovebox for 12-16 h at 45 °C. The flask was removed from the glovebox and the mixture was subsequently diluted with Et_2O and filtered through a short pad of silica gel using Et_2O as eluent. The product was purified by flash column chromatography using the indicated eluent mixture. Conversion to the desired coupling product was determined by quantitative ^{19}F NMR analysis using α,α,α-trifluorotoluene as an internal standard, unless stated otherwise.

2.8 General procedure for trifluoromethylselenolation of polyhalogenated arenes (procedure B)

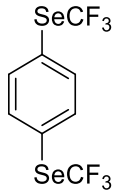


Inside a glovebox, aryl iodide (0.2 mmol, 1.0 equiv.), $(Me_4N)SeCF_3$ (66.5 mg, 0.3 mmol, 1.5 equiv.) and Ni-I-dimer **3** (21.9 mg, 0.02 mmol, 10 mol%) were added in a dry, amber reaction vial equipped with a stirring bar. Then benzene (2.0 ml) was added to the reaction mixture. The reaction was stirred in the glovebox for 12-16 h at 45 °C. The flask was removed from the glovebox and the mixture was subsequently filtered through a short pad of silica gel. The product was purified by flash column chromatography using the indicated eluent mixture. In case of volatile coupling products, careful evaporation of solvents was key to ensuring high isolated yields.

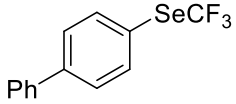
3. Compound Characterization Data



1-(4-(trifluoromethylseleno)phenyl)ethanone (5a): Prepared following procedure A. The residue was purified by flash chromatography on silica gel using as eluent a mixture of pentane/Et_2O (99:1), to afford the title compound as a colorless oil (25 mg, 92%). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.95 (d, *J* = 8.6 Hz, 2H), 7.85 (d, *J* = 8.5 Hz, 2H), 2.60 (s, 3H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 197.6, 138.4, 137.2, 129.6, 128.5, 123.1 (q, *J* = 332.6 Hz), 27.1. ^{19}F NMR (376 MHz, CD_2Cl_2) δ -35.83 (s). MS (70eV, EI): *m/z* 368 (59, ^{80}Se) 266 (29, ^{78}Se) [M^+], 253 (100, ^{80}Se) 251 (49, ^{78}Se), 184 (79, ^{80}Se) 182 (39, ^{78}Se), 169 (22), 156 (33, ^{80}Se) 154 (16, ^{78}Se), 145 (29). These data are in agreement with those reported previously in the literature.[4]

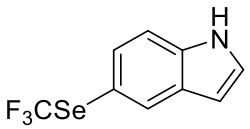


1,4-bis[(trifluoromethyl)seleno]-benzene (5b): Prepared following procedure B. The residue was purified by flash chromatography on silica gel using as eluent pure pentane, to afford the title compound as a white solid (74 mg, 99%). M.p. 48 – 49°C. ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.78 (s, 4H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 138.2, 125.9, 123.1 (q, *J* = 332.7 Hz). ^{19}F NMR (564 MHz, CD_2Cl_2) δ -36.02. MS (70eV, EI): *m/z* (%): 376 (31, ^{82}Se/^{80}Se) 374 (100, ^{80}Se/^{80}Se, ^{82}Se/^{78}Se) 372 (89, ^{82}Se/^{76}Se, ^{80}Se/^{78}Se) 370 (54, ^{80}Se/^{76}Se, ^{78}Se/^{78}Se) [M^+], 307 (23, ^{82}Se/^{80}Se) 305 (74, ^{80}Se/^{80}Se, ^{82}Se/^{78}Se) 303 (66, ^{82}Se/^{76}Se, ^{80}Se/^{78}Se) 301 (40, ^{80}Se/^{76}Se, ^{78}Se/^{78}Se), 275 (30, *also with Se isotopes*), 238 (21, ^{82}Se/^{80}Se) 236 (69, ^{80}Se/^{80}Se, ^{82}Se/^{78}Se) 234 (61, ^{82}Se/^{76}Se, ^{80}Se/^{78}Se) 232 (37, ^{80}Se/^{76}Se, ^{78}Se/^{78}Se), 156 (40, *also with Se isotopes*), 117 (14), 69 (19). HRMS (EI) calculated for $C_8H_4F_6{}^{80}Se_2$: 373.8542 [M^+], found: 373.8537.

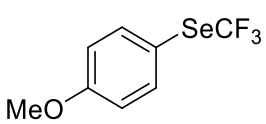


4-[(trifluoromethyl)seleno]biphenyl (5c): Prepared following procedure A. The residue was purified by flash chromatography on silica gel using hexane as eluent, to afford the title compound as a white solid (30 mg, 99%). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.62 (d, *J* = 7.4 Hz, 2H), 7.50 – 7.45 (m, 2H), 7.43 – 7.37 (m, 1H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 143.9, 140.2, 138.0, 129.5, 128.8, 128.7, 127.7, 123.3 (q, J = 332.8 Hz), 121.8. ^{19}F NMR (376 MHz, CD_2Cl_2) δ -36.63. MS (70eV, EI): *m/z* (%) 302 (84, ^{80}Se) 300 (41, ^{78}Se) [M^+], 233 (100, ^{80}Se) 231 (50, ^{78}Se), 152 (96). These data are in agreement with those reported previously in the literature.[5]

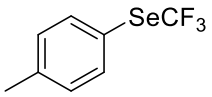
4-[(trifluoromethyl)seleno]-1-indanone (5d): Prepared following procedure A. The residue was purified by flash chromatography on silica gel using as eluent mixture hexane/Et_2O (95:5), to afford the title compound as yellow oil (27 mg, 96%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.5 Hz, 1H), 7.89 (d, *J* = 7.5 Hz, 1H), 7.46 – 7.42 (m, 1H), 3.29 – 3.24 (m, 2H), 2.78 – 2.73 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 206.0, 160.0, 144.1, 138.5, 128.8, 126.4, 122.5 (q, *J* = 333.3 Hz), 121.7, 36.1, 27.5. ^{19}F NMR (564 MHz, $CDCl_3$) δ -34.75. MS (70eV, EI): *m/z* (%): 280 (100, ^{80}Se) 278 (50, ^{78}Se) [M^+], 211 (80, ^{80}Se) 209 (40, ^{78}Se), 183 (56), 102 (69), 91 (22). These data are in agreement with those reported previously in the literature.[5]



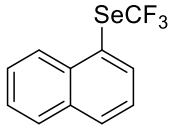
5-[(trifluoromethyl)seleno]indole (5e): Prepared following procedure A. The residue was purified by flash chromatography on silica gel using as eluent a gradient mixture of pentane/Et_2O (from pure pentane to 1:1), to afford the title compound as a colorless oil (24 mg, 89%). ^{1}H (600 MHz, $CDCl_3$) δ 8.30 (br, 1H), 8.08 (s, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.29–7.26 (m, 1H), 6.62–6.59 (m, 1H). ^{13}C (151 MHz, $CDCl_3$) δ 136.4, 130.8, 130.5, 128.9, 125.4, 122.7 (q, *J* = 333.2 Hz), 112.5, 112.0, 103.1. ^{19}F NMR (564 MHz, $CDCl_3$) δ -37.25. MS (70eV, EI): *m/z* (%): 265 (79, ^{80}Se) 263 (39, ^{78}Se) [M^+], 196 (100, ^{80}Se) 194 (51, ^{78}Se), 166 (18), 116 (18), 89 (15). These data are in agreement with those reported previously in the literature.[5]



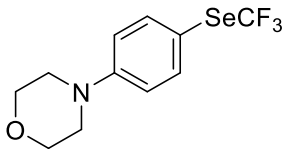
1-methoxy-4-[(trifluoromethyl)seleno]benzene (5f): Procedure A was followed for the synthesis of the product **5c**. The residue was purified by flash chromatography on silica gel using pure pentane as eluent, to afford the title compound as a colourless oil (25 mg, 98%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.6 Hz, 2H), 6.91 (d, *J* = 8.6 Hz, 2H), 3.83 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.4, 138.9, 122.1 (q, *J* = 332.7), 115.2, 112.9, 55.4. ^{19}F (564 MHz, $CDCl_3$) -37.20. MS (70eV, EI): *m/z* (%): 256 (76, ^{80}Se) 254 (37, ^{78}Se) [M^+], 187 (100, ^{80}Se) 185 (49, ^{78}Se), 172 (27), 157 (21), 144 (17). These data are in agreement with those reported previously in the literature.[5]



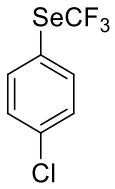
1-methyl-4-[(trifluoromethyl)seleno]benzene (5g): Prepared following procedure A. The residue was purified by flash chromatography on silica gel using pentane as eluent, to afford the title compound as a colourless oil (21 mg, 88%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (151 MHz, CDCl3) δ 140.7, 137.1, 130.4, 122.5 (q, *J* = 332.8 Hz), 119.0, 21.3. ^{19}F (564 MHz, $CDCl_3$) -36.55. MS (70eV, EI): *m/z* (%): 240 (97, ^{80}Se) 238 (47, ^{78}Se) [M^+], 171 (100, ^{80}Se) 169 (57, ^{78}Se), 141 (25), 91 (70). These data are in agreement with those reported previously in the literature.[5]



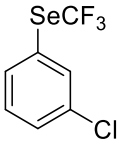
2-[(trifluoromethyl)seleno]naphthalene (5h): Prepared following procedure A. The residue was purified by flash chromatography on silica gel using pure pentane as eluent, to afford the title compound as a light yellow oil (19 mg, 70%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.5 Hz, 1H), 8.08 (d, *J* = 7.1 Hz, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.59 – 7.55 (m, 1H), 7.50 – 7.46 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.5, 135.3, 134.2, 132.0, 128.6, 128.1, 127.6, 126.7, 125.8, 122.5 (d, *J* = 334.0 Hz), 122.1. ^{19}F NMR (564 MHz, $CDCl_3$) δ -35.44. MS (70eV, EI): *m/z* (%): 276 (75, ^{80}Se) 274 (37, ^{78}Se) [M^+], 207 (100, ^{80}Se) 205 (50, ^{78}Se), 126 (30), 115 (69). These data are in agreement with those reported previously in the literature.[5]



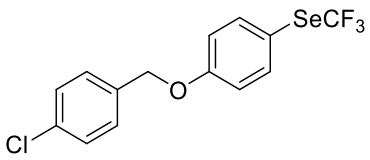
1-morpholino-4-[(trifluoromethyl)seleno]benzene (5i): Prepared following procedure A. The residue was purified by flash chromatography on silica gel using as eluent a gradient mixture of hexane/Et_2O (from pure hexane to 9:1), to afford the title compound as a yellow oil (28 mg, 90%). ^{1}H (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.9 Hz, 2H), 6.86 (d, *J* = 8.9 Hz, 2H), 3.88–3.83 (m, 4H), 3.26–3.20 (m, 4H). ^{13}C (151 MHz, $CDCl_3$) δ 152.5, 138.6, 122.5 (q, *J* = 333.6 Hz), 115.5, 111.0, 66.7, 48.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -37.34. MS (70eV, EI): *m/z* (%): 311 (92, ^{80}Se) 309 (46, ^{78}Se) [M^+], 253 (21, ^{80}Se) 251 (10, ^{78}Se), 242 (100, ^{80}Se) 240 (50, ^{78}Se), 184 (71, ^{80}Se) 182 (35, ^{78}Se), 156 (11). These data are in agreement with those reported previously in the literature.[5]



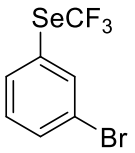
1-[(trifluoromethyl)seleno]-4-chlorobenzene (6a): Prepared following procedure B. The residue was purified by flash chromatography on silica gel using as eluent pure pentane, to afford the title compound as a colorless oil (39 mg, 75%). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 139.0, 137.7, 130.5, 123.1 (q, *J* = 332.6 Hz), 121.2. ^{19}F NMR (376 MHz, CD_2Cl_2) δ -36.72. MS (70eV, EI): *m/z* (%): 262 (39, ^{80}Se/^{37}Cl, ^{82}Se/^{35}Cl) 260 (90, ^{80}Se/^{35}Cl, ^{78}Se/^{37}Cl) 258 (42, ^{78}Se/^{35}Cl, ^{76}Se/^{37}Cl) [M^+], 193 (44, ^{80}Se/^{37}Cl, ^{82}Se/^{35}Cl) 191 (100, ^{80}Se/^{35}Cl, ^{78}Se/^{37}Cl) 189 (47, ^{78}Se/^{35}Cl, ^{76}Se/^{37}Cl), 161 (18), 156 (41), 75 (20). These data are in agreement with those reported previously in the literature.[6]



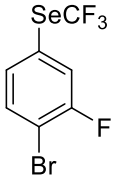
1-[(trifluoromethyl)seleno]-3-chlorobenzene (6b): Prepared following procedure B. The residue was purified by flash chromatography on silica gel using as eluent pure pentane, to afford the title compound as a colorless oil (40 mg, 76%). ^{1}H NMR (600 MHz, CD_2Cl_2) δ 7.78 (s, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.53 – 7.45 (m, 1H), 7.41 – 7.31 (dd, *J* = 8.0, 7.9 Hz, 1H). ^{13}C NMR (151 MHz, CD_2Cl_2) δ 137.1, 135.7, 135.5, 131.3, 131.2, 124.1, 123.1 (q, *J* = 332.7 Hz). ^{19}F NMR (376 MHz, CD_2Cl_2) δ -36.34. MS (70eV, EI): *m/z* (%): 262 (37, ^{80}Se/^{37}Cl, ^{82}Se/^{35}Cl) 260 (85, ^{80}Se/^{35}Cl, ^{78}Se/^{37}Cl) 258 (41, ^{78}Se/^{35}Cl, ^{76}Se/^{37}Cl) [M^+], 193 (44, ^{80}Se/^{37}Cl, ^{82}Se/^{35}Cl) 191 (100, ^{80}Se/^{35}Cl, ^{78}Se/^{37}Cl) 189 (47, ^{78}Se/^{35}Cl, ^{76}Se/^{37}Cl), 156 (41), 75 (21). HRMS (EI) calculated for $C_7H_4F_3{}^{35}Cl{}^{80}Se$: 259.9113 [$M^+$], found: 259.9118.



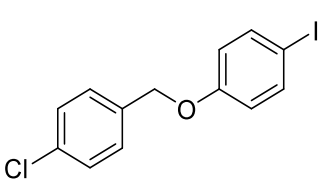
1-chloro-4-[(4-[(trifluoromethyl)seleno]phenoxy)methyl]benzene (6c): Prepared following procedure A. The residue was purified by flash chromatography on silica gel using as eluent pure pentane, to afford the title compound as a white solid (29 mg, 80%). M.p. 51 - 52 °C ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 – 7.62 (m, 2H), 7.41 – 7.34 (m, 4H), 7.00 – 6.92 (m, 2H), 5.05 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.3, 139.0, 134.8, 134.1, 128.9, 128.8, 122.5 (q, *J* = 333.2 Hz), 116.0, 113.5, 69.3. ^{19}F NMR (564 MHz, $CDCl_3$) δ -37.06. HRMS (EI) calculated for $C_{14}H_{10}OF_3{}^{35}Cl{}^{80}Se$: 365.9530 [$M^+$], found: 365.9532.



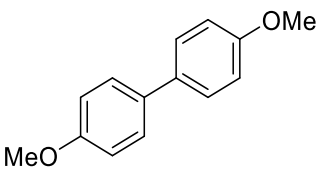
1-bromo-3-[(trifluoromethyl)seleno]benzene (7a): Prepared following procedure B. The residue was purified by flash chromatography on silica gel using as eluent pure pentane, to afford the title compound as a colorless oil (56 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.36 – 7.27 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.5, 135.6, 133.7, 131.0, 124.0, 123.2, 122.5 (q, *J* = 332.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -35.70. HRMS (EI) calculated for $C_7H_4{}^{79}BrF_3{}^{80}Se$: 303.8608 [$M^+$], found: 303.8604.



1-bromo-2-fluoro-4-[(trifluoromethyl)seleno]benzene (7b): Prepared following procedure B. The residue was purified by flash chromatography on silica gel using as eluent pure pentane, to afford the title compound as a colorless oil (64 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 8.2, 7.0 Hz, 1H), 7.53 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.41 (dd, *J* = 8.3, 1.9 Hz, 1H). ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 159.0 (d, *J* = 252.7 Hz, C_{Ar}-F), 134.6, 133.8, 124.9 (d, ^{2}J = 23.2 Hz, Br-C_{Ar}-C_{Ar}-F), 122.5, 122.3 (q, *J* = 333.0 Hz, Ar-SeCF_3), 112.6 (d, ^{2}J = 20.8 Hz, H-C_{Ar}-C_{Ar}-F). ^{13}C{^{1}H,^{19}F} NMR (101 MHz, $CDCl_3$) δ 159.0, 134.6, 133.8, 124.9, 122.5, 112.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -35.73 (-SeCF_3), -104.31 (C_{Ar}-*F*). HRMS (EI) calculated for $C_7H_3F_4{}^{79}Br{}^{80}Se$: 321.8514 [$M^+$], found: 321.8514.



1-chloro-4-[(4-iodophenoxy)methyl]benzene: 4-iodophenol (300 mg, 1.36 mmol, 1 equiv.) and K_2CO_3 (282 mg, 2.04 mmol, 1.5 equiv.) were dissolved in 30 mL DMF. 4-chloro-benzylbromide (336 mg, 1.63 mmol, 1.2 equiv.) was added and the reaction was stirred at room temperature for 14 hours. Then, Et_2O was added (20 mL) and the organic phase was washed with water (40 mL), 1M NaOH (40 mL) and brine (40 mL). The ether phase was dried over Na_2SO_4 and evaporated. The residue was purified by flash chromatography on silica gel using as eluent pure pentane to afford the title compound as a white solid (375 mg, 80%). M.p. 108-109 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 – 7.33 (m, 2H), 7.37 – 7.33 (m, 4H), 6.75 – 6.69 (m, 2H), 5.00 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.5, 138.4, 135.1, 134.1, 129.0, 128.9, 117.4, 83.4, 69.4. HRMS (EI) calculated for $C_{13}H_{10}O{}^{35}ClI$: 343.9460 [M^+], found: 343.9461.

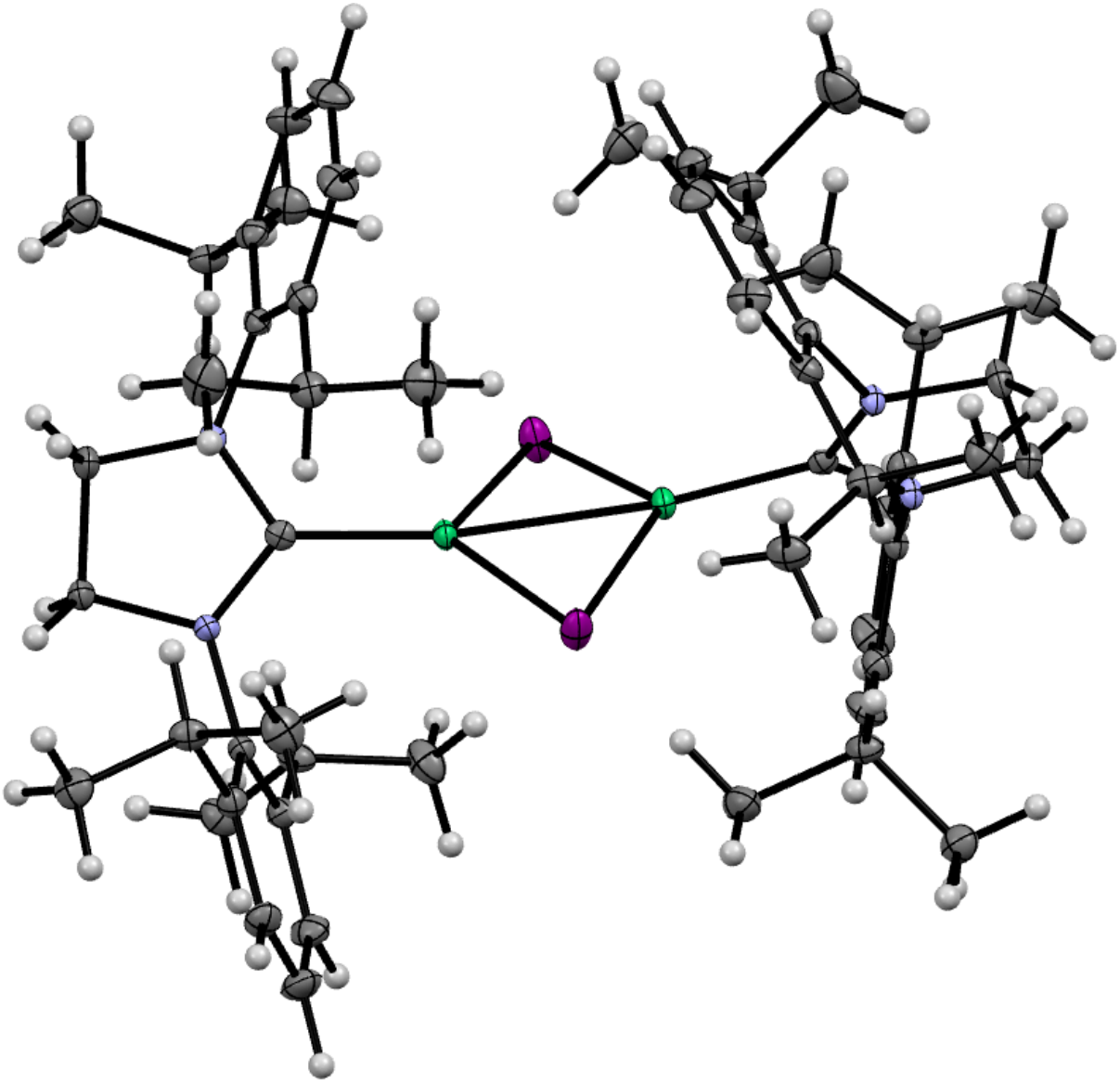


4,4'-dimethoxy-1,1'-biphenyl: Prepared according to a published procedure from 4-iodoanisole (0.5 mmol) and 4-methoxyphenylboronic acid.[7] The title compound was obtained as a white solid in 82% yield (88 mg). ^{1}H NMR (600 MHz, C_6D_6) δ 7.43 (d, *J* = 8.7 Hz, 4H), 6.87 (d, *J* = 8.7 Hz, 4H), 3.35 (s, 6H). ^{13}C NMR (151 MHz, C_6D_6) δ 159.4, 134.0, 128.2, 114.6, 54.9. MS (70eV, EI): *m/z* (%): 214 (100), 199 (90), 171 (33), 156 (13), 128 (25).

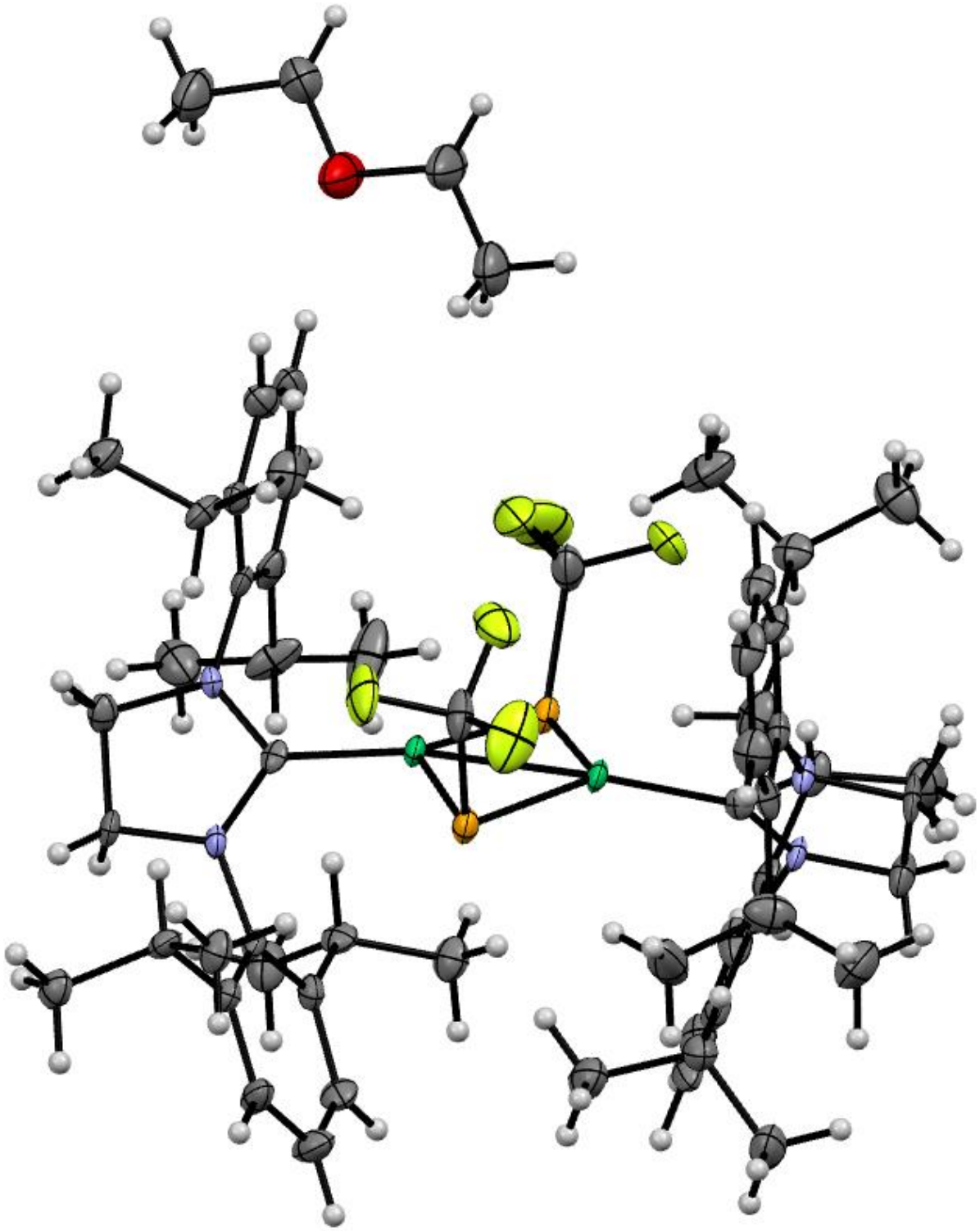
4. Crystallographic Data for [(SIPr)Ni(μ-I)]$_2$ (3) and [(SIPr)Ni(μ-SeCF$_3$)]$_2$ (4)

	[(SIPr)Ni(μ-I)]$_2$	**[(SIPr)Ni(μ-SeCF$_3$)]$_2$·Et$_2$O**
Chemical formula	C_{54} H_{76} I_2 N_4 Ni_2	C_{60} H_{84} F_6 N_4 Ni_2 O Se_2
M_r (g/mol)	1152.40	1266.65
Crystal description	orange block	brown block
Crystal size (mm^3)	0.28x0.26x0.26	0.30x0.24x0.20
Crystal system, space group	monoclinic, I 2/a	Triclinic, $P\bar{1}$
T (K)	100(2)	100(2)
a, b, c (Å)	19.7206(10) 12.3114(6) 23.0533(16)	11.792(5) 11.948(5) 22.207(8)
α, ß, γ (°)	90 111.0560(10) 90	98.093(6) 95.887(6) 95.172(6)
V (Å^3)	5223.4(5)	3064(2)
Z	4	2
μ (mm^{-1})	1.941	1.862
Total/unique reflections	36224, 6633	26059, 11413
R_{int}	0.0354	0.0763
$R(F^2>2\sigma(F^2))$	0.0220	0.0563
$wR(F^2)$	0.0528	0.1439
GoF	1.029	1.020
No. of reflections	6633	11413
No. of parameters	288	694
No. of restraints	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.805, -0.369	1.160, -1.126
CCDC Number	CCDC 1558598	CCDC 1558599

Crystal structure of [(SIPr)Ni(I)]$_2$



Crystal structure of $[(SIPr)Ni(SeCF_3)]_2 \cdot Et_2O$



5. Computational details

General Information

All calculations were performed with the Gaussian 09 program package.[8] Structural optimizations and frequency calculations were performed with B3LYP (and ωB97XD) along with 6-31G(d) basis set on C, H, N, Se, Br, Cl and F atoms, and the effective core potential (ECP) SDD on Ni and I atoms. Single point energy calculations were performed with M06L, M06, PBE0-D3 and PBE0 functionals, and def2-TZVP basis set on all atoms. Solvent effects of benzene were taken into account using the CPCM solvation model. Frequency calculations were performed to confirm whether the structure is a minimum or a transition state. Intrinsic reaction coordinate (IRC) analysis was used to confirm that the obtained transition states connect the correct minima. All energies were corrected to 1M standard state with the addition of 1.89 kcal/mol to the energy of each species.[9] D3 corrections were applied using the original D3 damping functions proposed by Grimme and co-workers.[10]

5.1 Ni(0) pathway and its selectivity

Table S1. Selectivity of oxidative addition of Ar-X to [Ni^0], relative to the barrier with PhI, as predicted by M06L, M06 and PBE0-D3. Calculated using CPCM (Benzene) DFT/def2-TZVP // B3LYP/6-31G(d) (SDD).

Ph-X	**ΔΔG‡ (vs PhI)**		
	M06L	M06	PBE0-D3
PhBr	4.5	5.0	4.9
PhCl	5.0	5.3	4.5
$PhSeCF_3$	-6.3	-4.0	-6.6

The selectivity of oxidative addition was also analyzed based on structures optimized at the ωB97XD/6-31G(d) (SDD) level of theory. As illustrated by Figure S3, the choice of optimization method however did not seem to affect the outcome, and $PhSeCF_3$ was still found to be more reactive than the aryl halides (as shown in Figure 3 in the manuscript, as well as in Table S1).

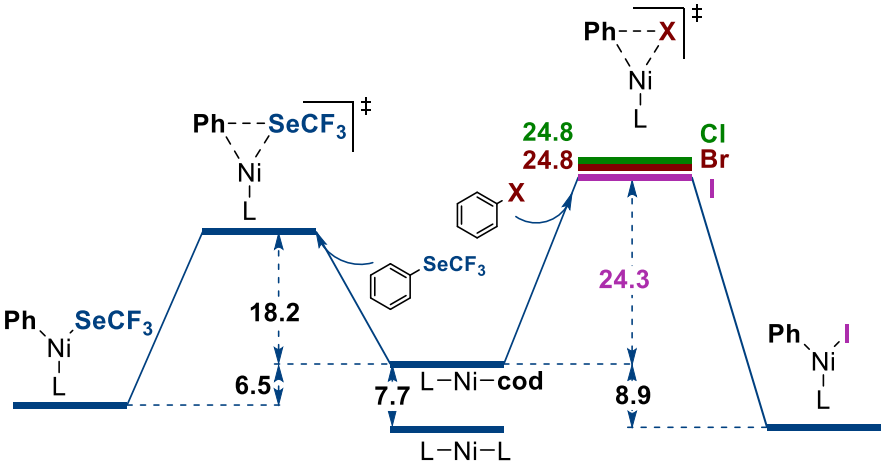
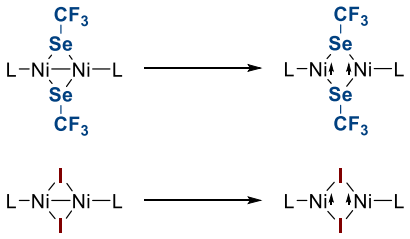


Figure S3. Ni^0/Ni^{II} mechanism for the trifluoromethylselenolation of aryl halides, calculated at CPCM (Benzene) M06L/def2-TZVP // ωB97XD/6-31G(d) (SDD) level of theory.

5.2 DFT methods *vs* the electron structure of Ni(I) dimers

A number of DFT methods, such as the pure functional M06L, and also hybrid methods M06, PBE0-D3, and PBE0 were tested for their ability to reproduce the experimentally observed singlet closed shell state Ni(↑↓)Ni of our prepared Ni(I) dimers **3** and **4** (Table S2). In agreement with our experimental data, the M06L method suggests the $SeCF_3$-bridged dimer to be in the closed shell singlet states. The I-bridged dimer, however, is still predicted to be in the triplet state, by 2.6 kcal/mol. As expected, the introduction of Hartree-Fock exchange in case of hybrid methods leads to substantial favouring of the open shell triplet state, Ni(↑)Ni(↑).[11]

Table S2. Comparison of DFT methods for the prediction of singlet-triplet gaps of SIPr-Ni(I) dimers. Calculated using CPCM (Benzene) DFT/def2-TZVP // B3LYP/6-31G(d) (SDD).



	ΔG (T - S)			
	M06L	M06	PBE0-D3	PBE0
	3.6	-11.4	-18.7	-22.4
	-2.6	-16.2	-25.5	-30.1

5.3 Oxidative addition with Ni(I) dimers

It has to be noted that while in this context pure DFT functionals would be able to more realistically describe the energy differences between singlet and triplet ground state structures, this trend might not hold true for transition states when spin-crossover processes are involved. To illustrate that we computed the absolute barriers of oxidative addition of iodobenzene to a mixed I-$SeCF_3$-bridged dimer (in closed shell singlet state). As shown by Figure S4, the absolute barriers in the closed shell singlet state are relatively unaffected by the choice of the method. In triplet state, however, the barriers range from as low as 5.9 kcal/mol to as high as 28.7 kcal/mol. This suggests that in relative terms pure DFT methods may overestimate the barrier heights of processes where spin-crossover from closed to open shell would occur. Hybrid methods on the other hand may overestimate the stability of triplet state structures.

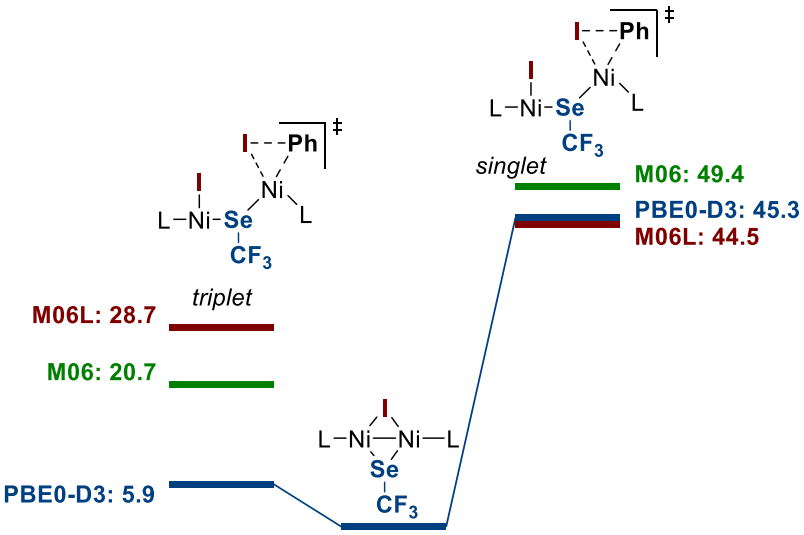


Figure S4. Comparison of triplet and singlet state oxidative addition transition states between PhI and the mixed I-$SeCF_3$ Ni(I) dimer **8**. Calculated using CPCM (Benzene) DFT/def2-TZVP // B3LYP/6-31G(d) (SDD).

To gain insights into the nature of the computed triplet state transition state we performed spin density analysis on it. As illustrated by Figure S5, this analysis indicates that both Ni centers bear a relatively equal degree of open shell character. This suggests that transition state to be of Ni^{I}-Ni^{I}, rather than of Ni^{II}-Ni^{0} type.

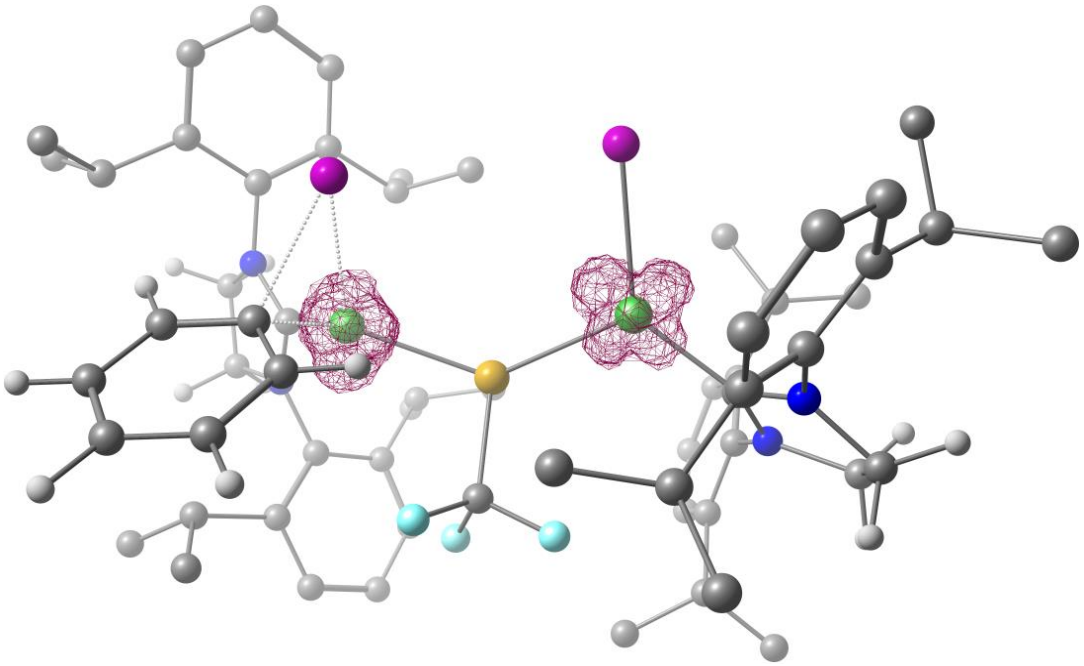


Figure S5. Spin density analysis of a triplet state oxidative addition transition state between PhI and the mixed I-$SeCF_3$ Ni(I) dimer **8**.

With all of the above in mind, the potential energy surface of the reaction can only be constructed in a qualitative manner, as the absolute energy values are highly affected by the different strengths and weaknesses of chosen computational methods to describe triplet or singlet states adequately. Despite that, the relative energies of transition states and intermediates, within one spin state are still comparable, regardless of the method. Two functionals, M06L and PBE0-D3 were used to calculate all of the intermediates in the dimeric pathway. Various structural isomers were considered for the intermediates and transition states (*i.e.* I-bridged or $SeCF_3$-bridged), with only the lowest energy species reported below.

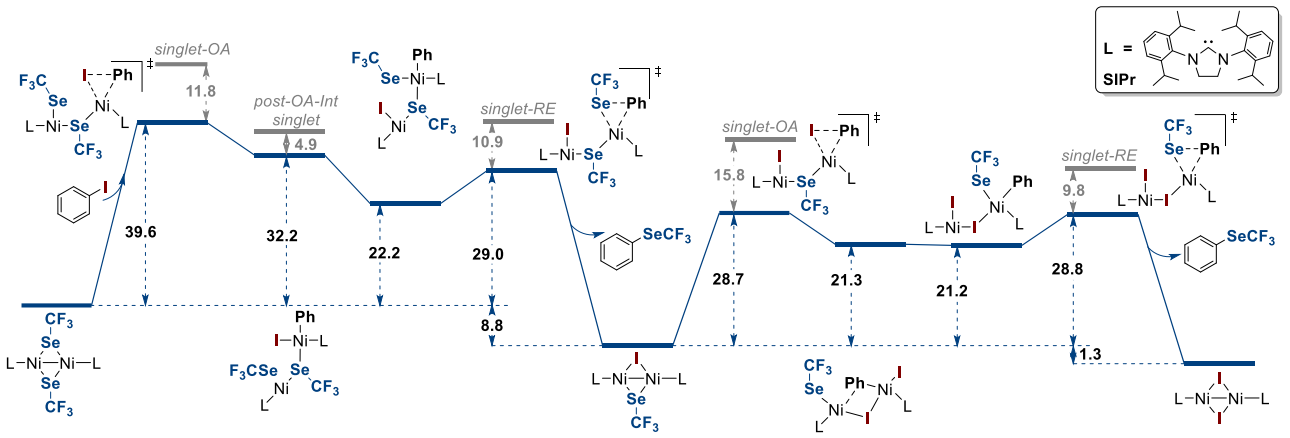


Figure S6. Potential energy surface of a dimeric pathway of trifluoromethylselenolation of iodobenzene, calculated at the CPCM (Benzene) M06L/def2-TZVP // B3LYP/6-31G(d) (SDD for Ni, I) level of theory.

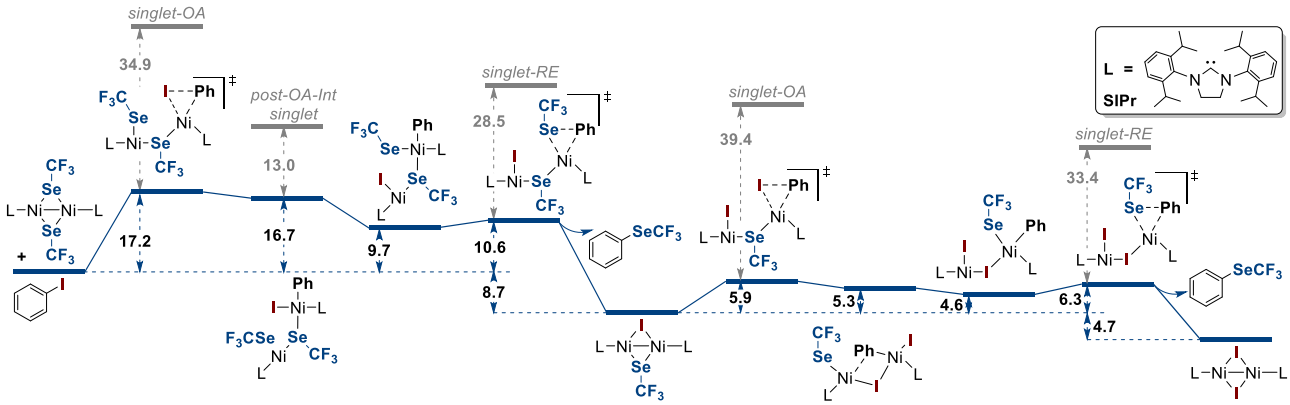
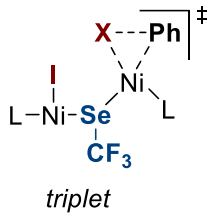


Figure S7. Potential energy surface of a dimeric pathway of trifluoromethylselenolation of iodobenzene, calculated at the CPCM (Benzene) PBE0-D3/def2-TZVP // B3LYP/6-31G(d) (SDD for Ni, I) level of theory.

Table S3. Selectivity of oxidative addition of Ar-X to mixed I-$SeCF_3$ Ni(I) dimer **8**, relative to the barrier with PhI. Calculated using CPCM (Benzene) DFT/def2-TZVP // B3LYP/6-31G(d) (SDD).

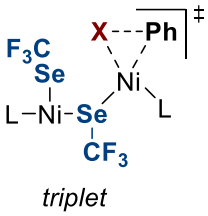


triplet

Ph-X	**ΔΔG‡ (*vs* PhI)**	
	M06L	PBE0-D3
PhBr	0.0	1.6
PhCl	3.1	3.1
$PhSeCF_3$	9.0	13.5

In analogy to the more reactive (in terms of absolute barriers) mixed I-$SeCF_3$-bridged Ni(I) dimer, the selectivity of oxidative addition was also computed for the bis-$SeCF_3$-bridged Ni(I) dimer. The data, presented in Table S4 indicate similar reactivity trends.

Table S4. Selectivity of oxidative addition of Ar-X to the SCF_3-bridged Ni(I) dimer **4**, relative to the barrier with PhI. Calculated using CPCM (Benzene) DFT/def2-TZVP // B3LYP/6-31G(d) (SDD).



triplet

Ph-X	**ΔΔG‡ (*vs* PhI)**	
	M06L	PBE0-D3
PhBr	1.6	2.1
PhCl	5.2	8.2
$PhSeCF_3$	4.4	7.8

5.4 XYZ coordinates and energies of computed structures

SIPr-Ni-cod

Ni	0.043404000000	-0.133720000000	1.278018000000
C	-1.321441000000	0.549061000000	2.732809000000
H	-2.044693000000	1.097607000000	2.131488000000
C	-0.125865000000	1.170319000000	3.028150000000
H	0.042103000000	2.158314000000	2.601078000000
C	0.868894000000	0.720313000000	4.081255000000
H	0.345758000000	0.262759000000	4.927470000000
H	1.387795000000	1.596049000000	4.490929000000
C	1.934588000000	-0.263571000000	3.520757000000
H	2.732004000000	0.318024000000	3.041862000000
H	2.413240000000	-0.799505000000	4.356988000000
C	1.404634000000	-1.237377000000	2.488284000000
H	2.138042000000	-1.550073000000	1.746002000000
C	0.211977000000	-1.923030000000	2.533058000000
H	0.063360000000	-2.717687000000	1.803871000000
C	-0.822129000000	-1.823430000000	3.637311000000
H	-0.330821000000	-1.664765000000	4.602817000000
H	-1.352971000000	-2.779528000000	3.726840000000
C	-1.873689000000	-0.702914000000	3.385599000000
H	-2.656439000000	-1.097094000000	2.726056000000
H	-2.375467000000	-0.458915000000	4.336525000000
C	-0.010993000000	0.083080000000	-0.594853000000
C	-0.777679000000	0.208655000000	-2.860004000000
C	0.720916000000	0.534625000000	-2.829521000000
H	-1.368747000000	0.976648000000	-3.369123000000
H	1.302337000000	-0.074123000000	-3.529460000000
H	-0.983304000000	-0.754200000000	-3.350118000000
H	0.919307000000	1.592160000000	-3.058017000000
N	-1.107988000000	0.149470000000	-1.425341000000
N	1.073080000000	0.222304000000	-1.434101000000
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C	3.121154000000	-1.091361000000	-1.134409000000
C	3.109560000000	1.307055000000	-0.573233000000
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C	-3.147830000000	1.346280000000	-0.779084000000
C	-3.136560000000	-1.115923000000	-0.834580000000
C	-4.487821000000	1.305046000000	-0.374457000000
C	-4.478647000000	-1.103561000000	-0.432725000000
C	-5.149716000000	0.093062000000	-0.196858000000
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H	-3.509157000000	3.833794000000	0.556366000000
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H	2.850495000000	3.167002000000	-2.609588000000
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 Thermal correction to Gibbs Free Energy=         0.703605
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 Sum of electronic and thermal Energies=             -1643.419340
 Sum of electronic and thermal Enthalpies=           -1643.418396
 Sum of electronic and thermal Free Energies=        -1643.535208
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CPCM (Benzene) M06L/def2TZVP E = -2981.95222346
CPCM (Benzene) M06/def2TZVP E = -2981.00047727
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SIPr2-Ni

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C	1.351561000000	-3.976115000000	-0.245191000000
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H	-0.691098000000	-4.755688000000	-0.478912000000
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C	3.759549000000	-1.732787000000	-0.263389000000
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H	5.924339000000	-1.015035000000	-2.820448000000
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C	-2.347446000000	-2.793634000000	2.094531000000
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H	-5.738757000000	-2.840307000000	1.692931000000
C	3.919990000000	-1.860061000000	1.258249000000
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H	-1.511106000000	-2.678108000000	-1.848854000000
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H	-2.768291000000	-4.010197000000	-3.506152000000
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H	-1.151143000000	4.761062000000	-0.754805000000
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C	-3.618836000000	2.069723000000	0.080546000000
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C	-5.057675000000	1.859130000000	-1.869384000000
H	-4.142145000000	2.218346000000	-3.775872000000
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H	-6.040191000000	1.667964000000	-2.293838000000
C	2.024059000000	2.426340000000	1.169095000000
C	3.068727000000	2.533823000000	0.221931000000
C	2.296092000000	2.168392000000	2.532322000000
C	4.379646000000	2.292079000000	0.649838000000
C	3.625248000000	1.942791000000	2.911883000000
C	4.659208000000	1.989791000000	1.980184000000
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H	3.855524000000	1.739420000000	3.954231000000
H	5.684997000000	1.814532000000	2.295537000000
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C	1.187848000000	0.940805000000	4.479679000000
H	2.110688000000	0.842350000000	5.064172000000
H	0.353995000000	0.988369000000	5.190185000000
H	1.069564000000	0.037955000000	3.875635000000
C	1.332234000000	3.462853000000	4.476110000000
H	2.269374000000	3.451145000000	5.046029000000
H	1.324848000000	4.380508000000	3.877198000000
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H	-4.156199000000	3.305505000000	3.292945000000
H	-4.053222000000	4.222639000000	1.776519000000
H	-5.389951000000	3.096872000000	2.041029000000
C	-3.856875000000	0.758639000000	2.241578000000
H	-4.905162000000	0.496456000000	2.056382000000
H	-3.233725000000	-0.046380000000	1.846011000000
H	-3.713785000000	0.803436000000	3.328368000000
H	-2.432305000000	2.288317000000	1.836891000000
C	2.817817000000	2.967272000000	-1.219694000000
C	-1.578119000000	2.805810000000	-3.127022000000
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C	-1.798606000000	4.221244000000	-3.701508000000
H	-1.904411000000	4.971517000000	-2.909766000000
H	-0.953976000000	4.514740000000	-4.336888000000
H	-2.707413000000	4.260879000000	-4.314240000000
C	-1.393345000000	1.791069000000	-4.268965000000
H	-2.258911000000	1.774952000000	-4.942302000000
H	-0.514857000000	2.052821000000	-4.871055000000
H	-1.250385000000	0.780903000000	-3.877117000000
C	3.285971000000	1.918242000000	-2.240201000000
H	4.368394000000	1.755484000000	-2.188187000000
H	2.793871000000	0.958357000000	-2.066503000000
H	3.048932000000	2.249730000000	-3.259109000000
C	3.469419000000	4.336517000000	-1.506093000000
H	3.223444000000	4.672460000000	-2.520913000000
H	3.130311000000	5.105448000000	-0.801842000000
H	4.562000000000	4.280798000000	-1.430610000000
H	1.737708000000	3.075593000000	-1.351208000000

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Zero-point correction=                           1.194704 (Hartree/Particle)
 Thermal correction to Energy=                    1.259468
 Thermal correction to Enthalpy=                  1.260412
 Thermal correction to Gibbs Free Energy=         1.093899
 Sum of electronic and zero-point Energies=          -2492.244377
 Sum of electronic and thermal Energies=             -2492.179613
 Sum of electronic and thermal Enthalpies=           -2492.178669
 Sum of electronic and thermal Free Energies=        -2492.345182
CPCM (Benzene) PBE0-D3/def2TZVP E = -3828.77462064
CPCM (Benzene) M06L/def2TZVP E = -3831.35983603
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SIPr

N	-1.070341000000	-0.007154000000	0.579157000000
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C	-0.745920000000	-0.160741000000	2.008264000000
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C	0.746087000000	0.160808000000	2.008239000000
H	0.953444000000	1.191015000000	2.329899000000
C	-2.421042000000	-0.145823000000	0.142359000000
C	-2.899417000000	-1.405199000000	-0.245219000000
C	-4.238281000000	-1.506027000000	-0.631377000000
H	-4.634185000000	-2.465814000000	-0.950968000000
C	-5.070152000000	-0.395416000000	-0.618225000000
H	-6.109877000000	-0.493812000000	-0.917077000000
C	-4.574757000000	0.846555000000	-0.234658000000
H	-5.235118000000	1.707926000000	-0.242389000000
C	-3.242939000000	0.994424000000	0.148535000000
C	-1.980090000000	-2.612816000000	-0.326072000000
H	-1.065765000000	-2.382865000000	0.230718000000
C	-1.567659000000	-2.845710000000	-1.786508000000
H	-2.444874000000	-3.063871000000	-2.407474000000
H	-0.874502000000	-3.691207000000	-1.863341000000
H	-1.074397000000	-1.952794000000	-2.182936000000
C	-2.589833000000	-3.874125000000	0.295270000000
H	-2.913790000000	-3.694891000000	1.326230000000
H	-1.849644000000	-4.682029000000	0.303476000000
H	-3.455845000000	-4.232877000000	-0.272407000000
C	-2.651176000000	2.356473000000	0.477397000000
H	-1.865772000000	2.207977000000	1.227242000000
C	-1.971259000000	2.934497000000	-0.773783000000
H	-1.227289000000	2.235266000000	-1.167525000000
H	-1.471360000000	3.882362000000	-0.539588000000
H	-2.712801000000	3.122859000000	-1.559090000000
C	-3.660213000000	3.347942000000	1.062181000000
H	-3.140953000000	4.251600000000	1.399082000000
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H	-4.400695000000	3.661416000000	0.317405000000
C	2.421038000000	0.145946000000	0.142173000000
C	3.242616000000	-0.994522000000	0.148358000000
C	4.574488000000	-0.847000000000	-0.234809000000
H	5.234635000000	-1.708532000000	-0.242505000000

C	5.070238000000	0.394856000000	-0.618282000000
H	6.110006000000	0.492991000000	-0.917075000000
C	4.238670000000	1.505699000000	-0.631427000000
H	4.634845000000	2.465384000000	-0.950986000000
C	2.899759000000	1.405205000000	-0.245360000000
C	2.650468000000	-2.356373000000	0.477406000000
H	1.865042000000	-2.207502000000	1.227163000000
C	1.970471000000	-2.934468000000	-0.773696000000
H	1.226553000000	-2.235219000000	-1.167510000000
H	1.470492000000	-3.882257000000	-0.539368000000
H	2.711984000000	-3.123003000000	-1.558990000000
C	3.659150000000	-3.348038000000	1.062487000000
H	4.399586000000	-3.661914000000	0.317839000000
H	3.139583000000	-4.251465000000	1.399538000000
H	4.195609000000	-2.922228000000	1.917326000000
C	1.980692000000	2.612997000000	-0.326429000000
H	1.066259000000	2.383321000000	0.230310000000
C	1.568483000000	2.845757000000	-1.786944000000
H	2.445849000000	3.063481000000	-2.407851000000
H	0.875644000000	3.691491000000	-1.863997000000
H	1.074940000000	1.952939000000	-2.183249000000
C	2.590657000000	3.874278000000	0.294747000000
H	2.914563000000	3.695136000000	1.325739000000
H	1.850619000000	4.682321000000	0.302823000000
H	3.456742000000	4.232794000000	-0.272969000000
H	1.339535000000	-0.517161000000	2.628066000000
H	-0.953187000000	-1.191068000000	2.329592000000

```
Zero-point correction=                           0.603082 (Hartree/Particle)
 Thermal correction to Energy=                    0.632860
 Thermal correction to Enthalpy=                  0.633804
 Thermal correction to Gibbs Free Energy=         0.543675
 Sum of electronic and zero-point Energies=          -1160.292740
 Sum of electronic and thermal Energies=             -1160.262963
 Sum of electronic and thermal Enthalpies=           -1160.262019
 Sum of electronic and thermal Free Energies=        -1160.352147
CPCM (Benzene) PBE0-D3/def2TZVP E = -1160.29644025
CPCM (Benzene) M06L/def2TZVP E = -1161.49059718
```

1,5-cyclooctadiene (cod)

C	-1.083205000000	-1.107768000000	0.665235000000
C	1.923352000000	0.011316000000	-0.024461000000
C	0.007978000000	1.704749000000	-0.218086000000
C	-1.923415000000	-0.010876000000	-0.024290000000
C	-1.215227000000	1.236097000000	-0.495433000000
H	-1.771795000000	-1.910180000000	0.958605000000
H	-2.741047000000	0.283487000000	0.653768000000
H	-0.666355000000	-0.724888000000	1.600205000000
H	0.291717000000	2.634824000000	-0.711800000000
H	-2.425665000000	-0.455621000000	-0.896380000000
C	-0.007776000000	-1.704827000000	-0.218204000000
H	-0.290785000000	-2.635346000000	-0.711489000000
C	1.215478000000	-1.236011000000	-0.495150000000
H	1.822532000000	-1.841673000000	-1.170423000000
H	2.424611000000	0.456531000000	-0.896905000000
H	2.741756000000	-0.282836000000	0.652758000000
H	-1.821805000000	1.841441000000	-1.171403000000
C	1.082851000000	1.107462000000	0.665827000000
H	0.665549000000	0.723609000000	1.600171000000
H	1.771066000000	1.909803000000	0.960263000000

```
Zero-point correction=                           0.181195 (Hartree/Particle)
 Thermal correction to Energy=                    0.188619
 Thermal correction to Enthalpy=                  0.189563
 Thermal correction to Gibbs Free Energy=         0.149669
 Sum of electronic and zero-point Energies=           -311.843270
 Sum of electronic and thermal Energies=              -311.835846
 Sum of electronic and thermal Enthalpies=            -311.834902
 Sum of electronic and thermal Free Energies=         -311.874796
CPCM (Benzene) PBE0-D3/def2TZVP E = -311.764136766
CPCM (Benzene) M06L/def2TZVP E = -312.092526515
CPCM (Benzene) M06/def2TZVP E = -311.88505561
```

$PhSeCF_3$

C	1.585587000000	-0.166584000000	1.213092000000
C	2.896718000000	0.312311000000	1.209954000000
C	3.552000000000	0.551261000000	-0.000067000000
C	2.896741000000	0.311938000000	-1.210026000000
C	1.585609000000	-0.166956000000	-1.213041000000
C	0.929822000000	-0.402109000000	0.000055000000
H	1.069711000000	-0.353501000000	2.149120000000
H	3.404425000000	0.497972000000	2.152439000000
H	4.573304000000	0.922269000000	-0.000115000000
H	3.404465000000	0.497308000000	-2.152560000000
H	1.069751000000	-0.354161000000	-2.149020000000
Se	-0.871642000000	-1.093380000000	0.000137000000
C	-1.764462000000	0.666811000000	-0.000088000000
F	-1.452422000000	1.399541000000	1.081275000000
F	-3.092792000000	0.459486000000	-0.000114000000
F	-1.452334000000	1.399305000000	-1.081584000000

Zero-point correction= 0.105525 (Hartree/Particle)
Thermal correction to Energy= 0.115597
Thermal correction to Enthalpy= 0.116541
Thermal correction to Gibbs Free Energy= 0.066628
Sum of electronic and zero-point Energies= -2968.081121
Sum of electronic and thermal Energies= -2968.071049
Sum of electronic and thermal Enthalpies= -2968.070105
Sum of electronic and thermal Free Energies= -2968.120018
CPCM (Benzene) PBE0-D3/def2TZVP E = -2970.18846689
CPCM (Benzene) M06L/def2TZVP E = -2970.89831173
CPCM (Benzene) M06/def2TZVP E = -2970.68552777

PhI

C	1.267766000000	-1.216253000000	-0.000001000000
C	2.665372000000	-1.207349000000	-0.000002000000
C	3.365511000000	0.000001000000	-0.000003000000
C	2.665364000000	1.207353000000	-0.000002000000
C	1.267764000000	1.216252000000	-0.000001000000
C	0.586989000000	-0.000004000000	0.000000000000
H	0.726135000000	-2.155854000000	-0.000001000000
H	3.202585000000	-2.151943000000	-0.000003000000
H	4.451780000000	0.000007000000	-0.000004000000
H	3.202581000000	2.151946000000	-0.000002000000
H	0.726123000000	2.155847000000	-0.000001000000
I	-1.570223000000	0.000000000000	0.000001000000

Zero-point correction= 0.090272 (Hartree/Particle)
Thermal correction to Energy= 0.096172
Thermal correction to Enthalpy= 0.097116
Thermal correction to Gibbs Free Energy= 0.058488
Sum of electronic and zero-point Energies= -242.963140
Sum of electronic and thermal Energies= -242.957240
Sum of electronic and thermal Enthalpies= -242.956295
Sum of electronic and thermal Free Energies= -242.994923
CPCM (Benzene) PBE0-D3/def2TZVP E = -529.172397515
CPCM (Benzene) M06L/def2TZVP E = -529.569787555
CPCM (Benzene) M06/def2TZVP E = -529.3083291

PhBr

C	0.000000000000	0.000000000000	-2.882060000000
C	0.000000000000	1.207928000000	-2.181629000000
C	0.000000000000	-1.207928000000	-2.181629000000
H	0.000000000000	2.152195000000	-2.719225000000
H	0.000000000000	-2.152195000000	-2.719225000000
C	0.000000000000	1.215909000000	-0.785115000000
C	0.000000000000	-1.215909000000	-0.785115000000
H	0.000000000000	2.150008000000	-0.234210000000
H	0.000000000000	-2.150008000000	-0.234210000000
C	0.000000000000	0.000000000000	-0.103074000000
H	0.000000000000	0.000000000000	-3.968276000000
Br	0.000000000000	0.000000000000	1.811054000000

Zero-point correction= 0.090894 (Hartree/Particle)
Thermal correction to Energy= 0.096582
Thermal correction to Enthalpy= 0.097526
Thermal correction to Gibbs Free Energy= 0.060679
Sum of electronic and zero-point Energies= -2802.956583
Sum of electronic and thermal Energies= -2802.950895
Sum of electronic and thermal Enthalpies= -2802.949951
Sum of electronic and thermal Free Energies= -2802.986797
CPCM (Benzene) PBE0-D3/def2TZVP E = -2805.31268014
CPCM (Benzene) M06L/def2TZVP E = -2805.7574672
CPCM (Benzene) M06/def2TZVP E = -2805.60791816

PhCl

C	0.000000000000	0.000000000000	-2.275083000000
C	0.000000000000	1.207858000000	-1.574512000000
C	0.000000000000	-1.207858000000	-1.574512000000
H	0.000000000000	2.151777000000	-2.112625000000
H	0.000000000000	-2.151777000000	-2.112625000000
C	0.000000000000	1.216367000000	-0.178285000000
C	0.000000000000	-1.216367000000	-0.178285000000
H	0.000000000000	2.149638000000	0.374753000000
H	0.000000000000	-2.149638000000	0.374753000000
C	0.000000000000	0.000000000000	0.504171000000
H	0.000000000000	0.000000000000	-3.361260000000
Cl	0.000000000000	0.000000000000	2.264473000000

```
Zero-point correction=                           0.091242 (Hartree/Particle)
 Thermal correction to Energy=                    0.096738
 Thermal correction to Enthalpy=                  0.097682
 Thermal correction to Gibbs Free Energy=         0.062115
 Sum of electronic and zero-point Energies=           -691.745505
 Sum of electronic and thermal Energies=              -691.740009
 Sum of electronic and thermal Enthalpies=            -691.739065
 Sum of electronic and thermal Free Energies=         -691.774632
CPCM (Benzene) PBE0-D3/def2TZVP E = -691.518328308
CPCM (Benzene) M06L/def2TZVP E = -691.903231885
CPCM (Benzene) M06/def2TZVP E = -691.737090695
```

TS-OA-Ni(0)-PhSeCF$_3$

Ni	-0.271785000000	0.585478000000	-0.281420000000
C	0.346197000000	-1.158583000000	-0.117234000000
C	1.723777000000	-3.081221000000	-0.374055000000
C	0.323326000000	-3.530773000000	0.069552000000
N	-0.442799000000	-2.272453000000	0.005708000000
N	1.624777000000	-1.613358000000	-0.277561000000
H	0.320662000000	-3.933750000000	1.091772000000
H	2.520376000000	-3.465175000000	0.271439000000
C	-1.827642000000	-2.230956000000	0.389258000000
C	-2.844629000000	-2.390448000000	-0.581118000000
C	-2.146317000000	-2.060120000000	1.759847000000
C	-4.177174000000	-2.325175000000	-0.144495000000
C	-3.493195000000	-2.014817000000	2.136742000000
C	-4.506693000000	-2.136679000000	1.192531000000
H	-4.971536000000	-2.428016000000	-0.880303000000
H	-3.749817000000	-1.878830000000	3.183772000000
H	-5.549009000000	-2.087984000000	1.496893000000
C	2.786968000000	-0.786656000000	-0.435877000000
C	3.563571000000	-0.483334000000	0.705542000000
C	3.168572000000	-0.342209000000	-1.722162000000
C	4.708294000000	0.305653000000	0.539424000000
C	4.322494000000	0.443636000000	-1.834265000000
C	5.085110000000	0.771723000000	-0.716685000000
H	5.313819000000	0.554528000000	1.406838000000
H	4.630774000000	0.799106000000	-2.813679000000
H	5.977360000000	1.383008000000	-0.826567000000
C	-2.663802000000	-2.700907000000	-2.073531000000
H	-3.564747000000	-2.291255000000	-2.549779000000
C	-2.708413000000	-4.226083000000	-2.316611000000
H	-2.701593000000	-4.442131000000	-3.392022000000
H	-1.840913000000	-4.728058000000	-1.871712000000
H	-3.609275000000	-4.674536000000	-1.883841000000
C	-1.475673000000	-2.068488000000	-2.814534000000
H	-0.532373000000	-2.576767000000	-2.594801000000
H	-1.647304000000	-2.148452000000	-3.895441000000
H	-1.351053000000	-1.012017000000	-2.558273000000
C	2.394440000000	-0.720792000000	-2.980340000000
H	1.477264000000	-1.226086000000	-2.667405000000
C	3.205702000000	-1.702736000000	-3.851349000000
H	4.129022000000	-1.238727000000	-4.218769000000
H	3.489944000000	-2.600587000000	-3.290083000000
H	2.619701000000	-2.017611000000	-4.723325000000
C	1.967183000000	0.509280000000	-3.802033000000
H	1.365188000000	1.192587000000	-3.195201000000
H	2.830793000000	1.062955000000	-4.189771000000
H	1.362906000000	0.196947000000	-4.662147000000
C	3.208284000000	-1.002788000000	2.095318000000
H	2.274327000000	-1.565830000000	2.009465000000
C	4.289086000000	-1.966248000000	2.626460000000
H	4.459931000000	-2.801065000000	1.936601000000
H	5.248151000000	-1.453481000000	2.766442000000
H	3.989848000000	-2.381671000000	3.596369000000
C	2.953376000000	0.141343000000	3.093955000000
H	2.157013000000	0.802978000000	2.741469000000
H	2.657870000000	-0.265366000000	4.069119000000
H	3.853930000000	0.748073000000	3.249090000000
C	-1.078812000000	-1.957451000000	2.846648000000
H	-0.100293000000	-1.934534000000	2.360615000000
C	-1.114421000000	-3.188388000000	3.776165000000
H	-0.305852000000	-3.134676000000	4.515323000000
H	-2.062548000000	-3.246829000000	4.323763000000
H	-1.001238000000	-4.123125000000	3.214480000000
C	-1.196667000000	-0.655076000000	3.659482000000
H	-0.387967000000	-0.596083000000	4.398091000000
H	-1.124078000000	0.219623000000	3.006605000000
H	-2.146704000000	-0.600878000000	4.204596000000
C	-0.154187000000	2.801693000000	0.588406000000
C	-1.010226000000	2.841814000000	1.702452000000
C	1.185923000000	3.210124000000	0.728218000000
C	-0.516527000000	3.262995000000	2.939335000000
H	-2.047165000000	2.543232000000	1.613278000000
C	1.664604000000	3.618307000000	1.970380000000
H	1.847574000000	3.201363000000	-0.132473000000
C	0.815976000000	3.652415000000	3.082134000000
H	-1.185940000000	3.283429000000	3.795558000000
H	2.704152000000	3.920519000000	2.066310000000
H	1.190132000000	3.983079000000	4.046864000000
H	1.949472000000	-3.384696000000	-1.405413000000
H	-0.105570000000	-4.289617000000	-0.591162000000
Se	-0.790914000000	2.494624000000	-1.264031000000
C	-2.737195000000	2.986002000000	-1.022712000000
F	-2.900173000000	4.208589000000	-0.492455000000
F	-3.420739000000	2.115433000000	-0.254941000000
F	-3.293074000000	2.979995000000	-2.247257000000

```
Zero-point correction=                           0.702165 (Hartree/Particle)
 Thermal correction to Energy=                    0.746368
 Thermal correction to Enthalpy=                  0.747312
 Thermal correction to Gibbs Free Energy=         0.620590
 Sum of electronic and zero-point Energies=          -4299.678672
 Sum of electronic and thermal Energies=             -4299.634469
```

```
 Sum of electronic and thermal Enthalpies=           -4299.633525
 Sum of electronic and thermal Free Energies=        -4299.760247
CPCM (Benzene) PBE0-D3/def2TZVP E = -5638.62463139
CPCM (Benzene) M06L/def2TZVP E = -5640.72932305
CPCM (Benzene) M06/def2TZVP E = -5639.77364403
```

SIPr-Ni-Ph-$SeCF_3$

Ni	-0.464830000000	0.565276000000	0.461381000000	H	-0.675132000000	0.885951000000	-4.433415000000
N	-0.375939000000	-2.071013000000	-0.695820000000	H	-2.157658000000	-1.811783000000	-4.986467000000
N	1.662612000000	-1.566602000000	-0.104458000000	H	-0.426500000000	-1.510105000000	-5.207328000000
C	-2.717632000000	-2.415620000000	-0.046373000000	H	-0.975786000000	-2.856880000000	-4.188926000000
C	-4.078060000000	-2.295224000000	-0.355248000000	H	0.404387000000	-3.331236000000	-2.213002000000
C	-4.494959000000	-1.715759000000	-1.549802000000	H	2.584176000000	-3.120135000000	-1.237745000000
C	-3.554358000000	-1.248779000000	-2.464249000000	H	5.678145000000	0.666615000000	-0.345484000000
C	-2.180771000000	-1.346711000000	-2.209750000000	H	5.860882000000	0.811498000000	2.111975000000
C	-1.779175000000	-1.928499000000	-0.984502000000	H	4.107350000000	-0.169383000000	3.547006000000
C	-2.301278000000	-3.069112000000	1.268490000000	H	2.747301000000	-0.840820000000	-2.133444000000
C	-2.898174000000	-2.341823000000	2.489519000000	H	3.820115000000	0.772094000000	-3.637948000000
C	-2.667626000000	-4.567185000000	1.289153000000	H	4.907546000000	1.321994000000	-2.357890000000
C	-1.184937000000	-0.869222000000	-3.263296000000	H	3.159738000000	1.603857000000	-2.216049000000
C	-1.440857000000	0.582539000000	-3.709905000000	H	4.677309000000	-2.466543000000	-1.911671000000
C	-1.185449000000	-1.820394000000	-4.479524000000	H	4.701946000000	-1.599638000000	-3.461235000000
C	0.385400000000	-3.264848000000	-1.118476000000	H	5.805974000000	-1.131101000000	-2.158405000000
C	1.772742000000	-2.985238000000	-0.518910000000	H	1.049769000000	-1.899675000000	2.232242000000
C	0.396460000000	-1.102425000000	-0.156499000000	H	0.762153000000	0.330822000000	3.285772000000
C	2.786476000000	-0.903081000000	0.503491000000	H	0.489655000000	-0.983198000000	4.445845000000
C	3.792626000000	-0.368978000000	-0.333789000000	C	2.488663000000	-2.694268000000	3.603947000000
C	4.894143000000	0.243197000000	0.275390000000	H	3.297946000000	-2.365358000000	4.266297000000
C	5.000670000000	0.324478000000	1.660443000000	H	1.731602000000	-3.189073000000	4.224099000000
C	4.008875000000	-0.224987000000	2.466531000000	H	2.907286000000	-3.439408000000	2.917096000000
C	2.889608000000	-0.857927000000	1.911826000000	C	-1.614821000000	1.743032000000	1.291915000000
C	3.740258000000	-0.471072000000	-1.856701000000	C	-2.966786000000	1.548730000000	0.942373000000
C	3.918227000000	0.891845000000	-2.552281000000	C	-1.324262000000	2.450403000000	2.473571000000
C	4.788983000000	-1.478899000000	-2.374811000000	C	-3.994419000000	1.981334000000	1.788999000000
C	1.867342000000	-1.504648000000	2.842768000000	C	-2.350175000000	2.886015000000	3.315090000000
C	1.245757000000	-0.491482000000	3.822080000000	C	-3.686380000000	2.648234000000	2.976299000000
H	-4.819648000000	-2.656753000000	0.351384000000	H	-3.225561000000	1.058849000000	0.004892000000
H	-5.555629000000	-1.628910000000	-1.770405000000	H	-0.290245000000	2.663254000000	2.733108000000
H	-3.891690000000	-0.802320000000	-3.394910000000	H	-5.032871000000	1.813895000000	1.510691000000
H	-1.211860000000	-2.994850000000	1.348897000000	H	-2.109825000000	3.420243000000	4.231929000000
H	-2.655185000000	-1.274305000000	2.479662000000	H	-4.483817000000	2.998402000000	3.627426000000
H	-2.507865000000	-2.777116000000	3.417158000000	Se	0.820605000000	2.115810000000	-0.550997000000
H	-3.990276000000	-2.432746000000	2.516972000000	H	1.999828000000	-0.062353000000	4.492132000000
H	-2.217368000000	-5.105342000000	0.446639000000	C	-0.260632000000	3.722256000000	-0.876980000000
H	-2.319056000000	-5.034838000000	2.217622000000	F	-1.461796000000	3.456187000000	-1.444120000000
H	-3.752718000000	-4.711107000000	1.230127000000	F	-0.506997000000	4.467248000000	0.217968000000
H	-0.184906000000	-0.890962000000	-2.819898000000	F	0.416208000000	4.512059000000	-1.744382000000
H	-1.396083000000	1.276951000000	-2.866941000000	H	-0.075583000000	-4.177299000000	-0.728771000000
H	-2.415631000000	0.690722000000	-4.200325000000	H	1.986135000000	-3.608631000000	0.358532000000

```
Zero-point correction=                           0.703148 (Hartree/Particle)
 Thermal correction to Energy=                    0.747871
 Thermal correction to Enthalpy=                  0.748815
 Thermal correction to Gibbs Free Energy=         0.620407
 Sum of electronic and zero-point Energies=          -4299.721182
 Sum of electronic and thermal Energies=             -4299.676459
 Sum of electronic and thermal Enthalpies=           -4299.675515
 Sum of electronic and thermal Free Energies=        -4299.803923
CPCM (Benzene) PBE0-D3/def2TZVP E = -5638.66904741
CPCM (Benzene) M06L/def2TZVP E = -5640.76230228
CPCM (Benzene) M06/def2TZVP E = -5639.80366804
```

TS-OA-Ni(0)-PhI

Ni	0.111498000000	-0.787713000000	-0.483613000000	H	5.893658000000	-2.450828000000	0.962247000000
C	0.717388000000	0.841411000000	0.069853000000	C	-1.395933000000	2.171716000000	0.033031000000
C	0.864816000000	3.175469000000	0.509554000000	C	-2.252999000000	2.191404000000	1.156699000000
C	2.216320000000	2.524901000000	0.830583000000	C	-1.892798000000	2.389635000000	-1.272150000000
N	2.033024000000	1.156930000000	0.311660000000	C	-3.619516000000	2.412038000000	0.946667000000
N	0.012627000000	2.002020000000	0.248075000000	C	-3.268434000000	2.602547000000	-1.428661000000
H	2.417988000000	2.502419000000	1.911114000000	C	-4.127370000000	2.614556000000	-0.333269000000
H	0.470159000000	3.773781000000	1.336929000000	H	-4.294877000000	2.424679000000	1.797973000000
C	3.074261000000	0.177944000000	0.467307000000	H	-3.670280000000	2.771568000000	-2.424372000000
C	4.037696000000	-0.004958000000	-0.552327000000	H	-5.191064000000	2.788258000000	-0.476729000000
C	3.140356000000	-0.562839000000	1.673856000000	C	4.147688000000	0.770951000000	-1.871827000000
C	5.038686000000	-0.965744000000	-0.340430000000	H	4.648217000000	0.073968000000	-2.557595000000
C	4.164309000000	-1.503519000000	1.830375000000	C	5.100741000000	1.977312000000	-1.722611000000
C	5.108137000000	-1.711165000000	0.830530000000	H	5.270936000000	2.453135000000	-2.696295000000
H	5.777821000000	-1.128962000000	-1.121676000000	H	4.684426000000	2.737047000000	-1.050781000000
H	4.220058000000	-2.083732000000	2.747490000000	H	6.071517000000	1.671932000000	-1.317248000000

C	2.847175000000	1.187459000000	-2.576526000000
H	2.384823000000	2.061279000000	-2.109331000000
H	3.074242000000	1.452170000000	-3.617013000000
H	2.107171000000	0.381141000000	-2.576259000000
C	-0.986984000000	2.430381000000	-2.497870000000
H	0.030141000000	2.203339000000	-2.169805000000
C	-0.974358000000	3.833808000000	-3.137740000000
H	-1.963318000000	4.109038000000	-3.523509000000
H	-0.677233000000	4.602826000000	-2.414914000000
H	-0.269481000000	3.865244000000	-3.977314000000
C	-1.367312000000	1.355937000000	-3.533817000000
H	-1.303810000000	0.355562000000	-3.092293000000
H	-2.383977000000	1.503103000000	-3.918498000000
H	-0.680869000000	1.392962000000	-4.388344000000
C	-1.736737000000	1.982165000000	2.576766000000
H	-0.655123000000	1.830386000000	2.515413000000
C	-1.986661000000	3.218831000000	3.462736000000
H	-1.542411000000	4.122643000000	3.029191000000
H	-3.058438000000	3.409322000000	3.594280000000
H	-1.552303000000	3.070615000000	4.458817000000
C	-2.332950000000	0.714409000000	3.216479000000
H	-2.118693000000	-0.169404000000	2.608365000000
H	-1.910618000000	0.558309000000	4.217150000000
H	-3.421543000000	0.791827000000	3.323460000000
C	2.147829000000	-0.369008000000	2.817675000000
H	1.412328000000	0.377710000000	2.509223000000
C	2.846535000000	0.158699000000	4.087076000000
H	2.110732000000	0.348089000000	4.878146000000
H	3.573430000000	-0.563690000000	4.476685000000
H	3.384610000000	1.093880000000	3.891845000000
C	1.361663000000	-1.659883000000	3.114782000000
H	0.627326000000	-1.483657000000	3.910388000000
H	0.826751000000	-1.992145000000	2.218636000000
H	2.022608000000	-2.470910000000	3.443294000000
I	-0.543491000000	-2.951548000000	-1.484504000000
C	-2.298396000000	-2.334321000000	-0.167587000000
C	-2.419222000000	-2.943605000000	1.079759000000
C	-3.325522000000	-1.569983000000	-0.716492000000
C	-3.604113000000	-2.765609000000	1.802019000000
H	-1.612969000000	-3.545032000000	1.486448000000
C	-4.500222000000	-1.397821000000	0.021982000000
H	-3.216530000000	-1.103904000000	-1.689455000000
C	-4.643848000000	-1.996063000000	1.276104000000
H	-3.708989000000	-3.235141000000	2.777001000000
H	-5.300394000000	-0.788152000000	-0.388986000000
H	-5.563320000000	-1.865332000000	1.839910000000
H	0.913844000000	3.819656000000	-0.379757000000
H	3.055657000000	3.028023000000	0.342749000000

```
Zero-point correction=                           0.687053 (Hartree/Particle)
 Thermal correction to Energy=                    0.727170
 Thermal correction to Enthalpy=                  0.728114
 Thermal correction to Gibbs Free Energy=         0.610748
 Sum of electronic and zero-point Energies=          -1574.542903
 Sum of electronic and thermal Energies=             -1574.502786
 Sum of electronic and thermal Enthalpies=           -1574.501841
 Sum of electronic and thermal Free Energies=        -1574.619208
CPCM (Benzene) PBE0-D3/def2TZVP E = -3197.59638181
CPCM (Benzene) M06L/def2TZVP E = -3199.38902415
CPCM (Benzene) M06/def2TZVP E = -3198.38842323
```

TS-OA-Ni(0)-PhBr

Ni	0.159344000000	-0.411702000000	-1.050115000000
C	0.623096000000	0.561334000000	0.419358000000
C	0.598801000000	2.207988000000	2.104976000000
C	1.952884000000	1.501307000000	2.124261000000
N	1.891613000000	0.724967000000	0.886033000000
N	-0.163814000000	1.348257000000	1.198776000000
H	2.057024000000	0.830197000000	2.989538000000
H	0.126081000000	2.270577000000	3.089083000000
C	2.974249000000	-0.115972000000	0.487992000000
C	3.962870000000	0.378904000000	-0.379176000000
C	3.024260000000	-1.430932000000	0.989659000000
C	5.007576000000	-0.481545000000	-0.729845000000
C	4.092206000000	-2.245252000000	0.614535000000
C	5.080479000000	-1.776883000000	-0.239537000000
H	5.777633000000	-0.121365000000	-1.408124000000
H	4.146471000000	-3.263847000000	0.989416000000
H	5.902124000000	-2.424615000000	-0.531069000000
C	-1.558762000000	1.563919000000	0.993635000000
C	-2.457306000000	0.920015000000	1.862226000000
C	-1.995090000000	2.431578000000	-0.017775000000
C	-3.819637000000	1.154466000000	1.688810000000
C	-3.370694000000	2.634439000000	-0.157184000000
C	-4.274371000000	2.006122000000	0.687706000000
H	-4.538674000000	0.663725000000	2.336925000000
H	-3.735892000000	3.303302000000	-0.932172000000
H	-5.340173000000	2.179296000000	0.566679000000
C	4.038284000000	1.793282000000	-0.952235000000
H	4.571599000000	1.679020000000	-1.904650000000
C	4.920043000000	2.684985000000	-0.062611000000
H	5.063727000000	3.667393000000	-0.526881000000
H	4.457113000000	2.843245000000	0.917940000000
H	5.903825000000	2.233555000000	0.101962000000
C	2.720986000000	2.500900000000	-1.290582000000
H	2.236590000000	2.909033000000	-0.398774000000
H	2.928947000000	3.339675000000	-1.965283000000
H	2.010501000000	1.827963000000	-1.781571000000
C	-1.024709000000	3.161874000000	-0.929377000000
H	-0.015458000000	2.824809000000	-0.684400000000
C	-1.081849000000	4.677354000000	-0.692465000000
H	-2.061235000000	5.088496000000	-0.963856000000
H	-0.899615000000	4.920767000000	0.360340000000
H	-0.324619000000	5.186932000000	-1.298920000000
C	-1.255684000000	2.816579000000	-2.404810000000
H	-1.144654000000	1.739667000000	-2.570182000000
H	-2.253581000000	3.121443000000	-2.742516000000
H	-0.518941000000	3.330571000000	-3.032537000000
C	-1.946066000000	-0.050299000000	2.915239000000
H	-0.941729000000	0.274743000000	3.209040000000
C	-2.802151000000	-0.084544000000	4.184773000000
H	-2.964902000000	0.919316000000	4.591940000000
H	-3.781349000000	-0.541807000000	4.003008000000
H	-2.304038000000	-0.688278000000	4.951112000000
C	-1.806366000000	-1.452522000000	2.308672000000
H	-1.166441000000	-1.436681000000	1.421009000000
H	-1.375128000000	-2.147046000000	3.040548000000
H	-2.784554000000	-1.837210000000	2.001489000000
C	1.946288000000	-1.997482000000	1.902294000000
H	1.194563000000	-1.223544000000	2.079150000000
C	2.516146000000	-2.404728000000	3.267278000000
H	1.712548000000	-2.754090000000	3.925597000000
H	3.247324000000	-3.215982000000	3.174380000000
H	3.016819000000	-1.560948000000	3.755504000000
C	1.219245000000	-3.165350000000	1.223251000000
H	0.410005000000	-3.536499000000	1.861873000000
H	0.783951000000	-2.833055000000	0.274317000000
H	1.902218000000	-3.998116000000	1.018943000000
Br	-0.455483000000	-1.444001000000	-2.978930000000
C	-1.933167000000	-1.720128000000	-1.456908000000
C	-2.006215000000	-3.010840000000	-0.944420000000
C	-3.007660000000	-0.839914000000	-1.402889000000
C	-3.188718000000	-3.415987000000	-0.330126000000
H	-1.159816000000	-3.684369000000	-1.019801000000
C	-4.177116000000	-1.262499000000	-0.776667000000
H	-2.928558000000	0.160977000000	-1.811168000000
C	-4.275632000000	-2.547917000000	-0.247117000000
H	-3.257809000000	-4.418523000000	0.082592000000
H	-5.013123000000	-0.573870000000	-0.704180000000
H	-5.196365000000	-2.872425000000	0.228066000000
H	0.669518000000	3.223943000000	1.690515000000
H	2.796427000000	2.195224000000	2.121580000000

```
Zero-point correction=                           0.697547 (Hartree/Particle)
 Thermal correction to Energy=                    0.735728
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```
 Thermal correction to Enthalpy=                  0.736672
 Thermal correction to Gibbs Free Energy=         0.627563
 Sum of electronic and zero-point Energies=          -4134.159563
 Sum of electronic and thermal Energies=             -4134.121382
 Sum of electronic and thermal Enthalpies=           -4134.120438
 Sum of electronic and thermal Free Energies=        -4134.229547
CPCM (Benzene) PBE0-D3/def2TZVP E = -5473.7441425
CPCM (Benzene) M06L/def2TZVP E = -5475.58346736
CPCM (Benzene) M06/def2TZVP E = -5474.69464536
```

TS-OA-Ni(0)-PhCl

Ni	0.068947000000	-0.224341000000	-1.286899000000	H	-1.069661000000	4.673403000000	1.122035000000
C	0.576478000000	0.455809000000	0.298075000000	H	-0.554566000000	5.314429000000	-0.452079000000
C	0.526998000000	1.762605000000	2.269411000000	C	-1.447823000000	3.214003000000	-2.027703000000
C	1.886260000000	1.072247000000	2.165313000000	H	-1.317711000000	2.201763000000	-2.424656000000
N	1.842775000000	0.541358000000	0.803837000000	H	-2.459458000000	3.560959000000	-2.270559000000
N	-0.217901000000	1.089427000000	1.208175000000	H	-0.737645000000	3.870766000000	-2.542634000000
H	1.988804000000	0.254031000000	2.894052000000	C	-1.908779000000	-0.695019000000	2.638903000000
H	0.046609000000	1.627401000000	3.243232000000	H	-0.871290000000	-0.441428000000	2.878330000000
C	2.938230000000	-0.209090000000	0.285735000000	C	-2.649127000000	-0.892087000000	3.965480000000
C	3.950934000000	0.442098000000	-0.438450000000	H	-2.724944000000	0.045929000000	4.526103000000
C	2.989450000000	-1.593488000000	0.540393000000	H	-3.663429000000	-1.278502000000	3.813446000000
C	5.023916000000	-0.330262000000	-0.893613000000	H	-2.116067000000	-1.621054000000	4.585625000000
C	4.083213000000	-2.317227000000	0.067185000000	C	-1.871110000000	-1.993387000000	1.822776000000
C	5.098700000000	-1.692494000000	-0.643363000000	H	-1.344213000000	-1.843884000000	0.874047000000
H	5.815525000000	0.155140000000	-1.460118000000	H	-1.363296000000	-2.786925000000	2.385098000000
H	4.138796000000	-3.386777000000	0.252240000000	H	-2.886483000000	-2.332325000000	1.591406000000
H	5.943580000000	-2.268244000000	-1.010080000000	C	1.888175000000	-2.324006000000	1.295484000000
C	-1.621269000000	1.275581000000	1.061413000000	H	1.115285000000	-1.601522000000	1.568915000000
C	-2.475956000000	0.433100000000	1.792836000000	C	2.413574000000	-2.953842000000	2.592204000000
C	-2.113840000000	2.296030000000	0.234589000000	H	1.592032000000	-3.422684000000	3.146263000000
C	-3.851287000000	0.625947000000	1.672559000000	H	3.162991000000	-3.727548000000	2.388857000000
C	-3.499030000000	2.450683000000	0.139785000000	H	2.879245000000	-2.202343000000	3.239666000000
C	-4.360529000000	1.626856000000	0.852397000000	C	1.211554000000	-3.366918000000	0.397250000000
H	-4.535263000000	-0.016309000000	2.219463000000	H	0.385786000000	-3.854290000000	0.927845000000
H	-3.907434000000	3.234788000000	-0.492625000000	H	0.804334000000	-2.878983000000	-0.494959000000
H	-5.435011000000	1.766811000000	0.770264000000	H	1.917718000000	-4.142996000000	0.079318000000
C	4.015815000000	1.936844000000	-0.750238000000	Cl	-0.581882000000	-0.785686000000	-3.283081000000
H	4.580092000000	1.999624000000	-1.689904000000	C	-1.848356000000	-1.491308000000	-2.197948000000
C	4.852585000000	2.672836000000	0.308961000000	C	-1.798809000000	-2.862731000000	-1.956891000000
H	4.996472000000	3.721529000000	0.024462000000	C	-2.951649000000	-0.720369000000	-1.835240000000
H	4.354235000000	2.658676000000	1.284611000000	C	-2.875135000000	-3.467709000000	-1.315167000000
H	5.837468000000	2.210146000000	0.431223000000	H	-0.932962000000	-3.439265000000	-2.262912000000
C	2.693274000000	2.671389000000	-1.003170000000	C	-4.014106000000	-1.346141000000	-1.193508000000
H	2.176456000000	2.914168000000	-0.070001000000	H	-2.968118000000	0.346858000000	-2.024428000000
H	2.901967000000	3.615843000000	-1.519783000000	C	-3.985391000000	-2.716274000000	-0.939548000000
H	2.008420000000	2.077542000000	-1.616898000000	H	-2.842124000000	-4.534524000000	-1.115524000000
C	-1.185875000000	3.233734000000	-0.518057000000	H	-4.865900000000	-0.748867000000	-0.886087000000
H	-0.163333000000	2.876811000000	-0.373622000000	H	-4.824941000000	-3.195208000000	-0.445141000000
C	-1.277330000000	4.658461000000	0.046189000000	H	0.595273000000	2.841211000000	2.065889000000
H	-2.276813000000	5.083629000000	-0.104737000000	H	2.724386000000	1.759685000000	2.301560000000

```
Zero-point correction=                           0.697608 (Hartree/Particle)
 Thermal correction to Energy=                    0.735669
 Thermal correction to Enthalpy=                  0.736613
 Thermal correction to Gibbs Free Energy=         0.628131
 Sum of electronic and zero-point Energies=          -2022.900586
 Sum of electronic and thermal Energies=             -2022.862526
 Sum of electronic and thermal Enthalpies=           -2022.861582
 Sum of electronic and thermal Free Energies=        -2022.970063
CPCM (Benzene) PBE0-D3/def2TZVP E = -3359.9480567
CPCM (Benzene) M06L/def2TZVP E = -3361.7291304
CPCM (Benzene) M06/def2TZVP E = -3360.82253603
```

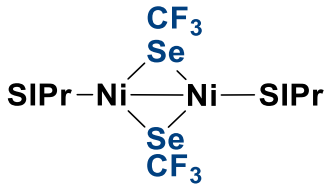
SIPr-Ni-Ph-I

Ni	-0.605802000000	-0.877511000000	-0.265412000000	C	-4.619376000000	2.304391000000	-0.110671000000
C	0.234076000000	0.735624000000	0.581813000000	H	-5.085804000000	1.489916000000	1.818523000000
C	1.584255000000	2.299932000000	1.714594000000	H	-3.866882000000	3.075032000000	-1.964897000000
C	0.217444000000	2.934131000000	1.448672000000	H	-5.660978000000	2.454605000000	-0.381761000000
N	-0.558483000000	1.769668000000	0.965046000000	C	2.661609000000	0.194586000000	0.830065000000
N	1.500222000000	1.042193000000	0.934396000000	C	3.653029000000	0.522064000000	-0.123416000000
H	0.262342000000	3.703539000000	0.668315000000	C	2.820581000000	-0.887812000000	1.722390000000
H	2.419216000000	2.917008000000	1.377869000000	C	4.790497000000	-0.289560000000	-0.190899000000
C	-1.945949000000	1.915581000000	0.595297000000	C	3.972251000000	-1.675736000000	1.599839000000
C	-2.960644000000	1.558339000000	1.517788000000	C	4.947199000000	-1.386276000000	0.651623000000
C	-2.258581000000	2.469658000000	-0.670099000000	H	5.562437000000	-0.063764000000	-0.920710000000
C	-4.291624000000	1.764379000000	1.129034000000	H	4.110026000000	-2.522870000000	2.265843000000
C	-3.608416000000	2.652256000000	-0.998577000000	H	5.833615000000	-2.010166000000	0.573733000000

C	-2.749097000000	0.915322000000	2.893438000000
H	-3.741562000000	0.936034000000	3.361796000000
C	-1.819973000000	1.669908000000	3.861745000000
H	-1.943058000000	1.266204000000	4.873594000000
H	-0.765973000000	1.555234000000	3.594701000000
H	-2.058275000000	2.739225000000	3.899891000000
C	-2.356825000000	-0.571407000000	2.791112000000
H	-1.359383000000	-0.695379000000	2.353799000000
H	-2.339004000000	-1.028806000000	3.788259000000
H	-3.063221000000	-1.128989000000	2.169178000000
C	1.826140000000	-1.205109000000	2.835734000000
H	0.993345000000	-0.499858000000	2.762013000000
C	2.468346000000	-1.008704000000	4.224791000000
H	3.295663000000	-1.709477000000	4.385488000000
H	2.867200000000	0.005561000000	4.343764000000
H	1.728640000000	-1.179704000000	5.016035000000
C	1.233709000000	-2.620263000000	2.699966000000
H	0.738862000000	-2.750189000000	1.732074000000
H	2.008781000000	-3.390527000000	2.786762000000
H	0.494648000000	-2.801728000000	3.489563000000
C	3.546829000000	1.735322000000	-1.044207000000
H	2.537312000000	2.146685000000	-0.940045000000
C	4.555844000000	2.829043000000	-0.631571000000
H	4.443398000000	3.122699000000	0.418888000000
H	5.586590000000	2.478829000000	-0.761760000000
H	4.427415000000	3.724560000000	-1.251415000000
C	3.732396000000	1.375338000000	-2.530384000000
H	3.016364000000	0.609198000000	-2.839481000000
H	3.579077000000	2.265707000000	-3.152300000000
H	4.743788000000	1.004465000000	-2.734001000000
C	-1.196443000000	2.898103000000	-1.681729000000
H	-0.218152000000	2.573873000000	-1.315317000000
C	-1.164386000000	4.434470000000	-1.829695000000
H	-0.360425000000	4.735093000000	-2.511679000000
H	-2.108273000000	4.810568000000	-2.241515000000
H	-1.003089000000	4.937299000000	-0.868775000000
C	-1.394437000000	2.227390000000	-3.055113000000
H	-0.586056000000	2.523639000000	-3.733495000000
H	-1.375318000000	1.137116000000	-2.971693000000
H	-2.341528000000	2.525735000000	-3.519541000000
I	0.717706000000	-1.456484000000	-2.306772000000
C	-1.805419000000	-2.231177000000	-0.636006000000
C	-1.610746000000	-3.593575000000	-0.348134000000
C	-3.115656000000	-1.770623000000	-0.868911000000
C	-2.704054000000	-4.452981000000	-0.210000000000
H	-0.602654000000	-3.983803000000	-0.233102000000
C	-4.209928000000	-2.632763000000	-0.728893000000
H	-3.291451000000	-0.735094000000	-1.157702000000
C	-4.004734000000	-3.973249000000	-0.395021000000
H	-2.541222000000	-5.501424000000	0.030524000000
H	-5.218164000000	-2.260421000000	-0.898269000000
H	-4.852692000000	-4.647161000000	-0.299551000000
H	1.738213000000	2.060825000000	2.775415000000
H	-0.239389000000	3.372039000000	2.337856000000

```
Zero-point correction=                           0.688846 (Hartree/Particle)
 Thermal correction to Energy=                    0.729065
 Thermal correction to Enthalpy=                  0.730009
 Thermal correction to Gibbs Free Energy=         0.613043
 Sum of electronic and zero-point Energies=          -1574.606165
 Sum of electronic and thermal Energies=             -1574.565946
 Sum of electronic and thermal Enthalpies=           -1574.565002
 Sum of electronic and thermal Free Energies=        -1574.681968
CPCM (Benzene) PBE0-D3/def2TZVP E = -3197.66014718
CPCM (Benzene) M06L/def2TZVP E = -3199.44175535
```

[(SIPr)Ni(SeCF$_3$)]$_2$ (4) *singlet*



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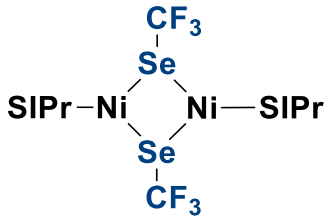
Se	0.135221000000	1.942289000000	-0.365030000000
Ni	-1.205919000000	0.090641000000	0.004419000000
Ni	1.211646000000	-0.070488000000	0.053320000000
N	-3.738394000000	1.289927000000	0.787235000000
N	-4.071445000000	-0.385410000000	-0.572547000000
N	3.730918000000	-0.715412000000	1.350433000000
N	4.082705000000	0.055033000000	-0.662352000000
C	-3.102496000000	0.322823000000	0.065723000000
C	-5.209864000000	1.158390000000	0.768958000000
H	-5.687350000000	2.126624000000	0.600808000000
H	-5.564349000000	0.764844000000	1.731211000000
C	-5.426285000000	0.175404000000	-0.382126000000
H	-6.142803000000	-0.614957000000	-0.144911000000
H	-5.758749000000	0.674755000000	-1.300811000000
C	-3.139662000000	2.203177000000	1.722928000000
C	-2.772039000000	1.745797000000	3.009407000000
C	-2.259182000000	2.680238000000	3.918634000000
H	-1.968237000000	2.350110000000	4.911898000000
C	-2.127708000000	4.022994000000	3.578635000000
H	-1.730148000000	4.731594000000	4.300780000000
C	-2.514449000000	4.458349000000	2.314695000000
H	-2.415485000000	5.509543000000	2.059266000000
C	-3.028857000000	3.567239000000	1.365522000000
C	-3.476143000000	4.100123000000	0.006526000000
H	-3.703488000000	3.239389000000	-0.630382000000
C	-2.372545000000	4.908328000000	-0.701722000000
H	-2.144773000000	5.837758000000	-0.166120000000
H	-2.697527000000	5.181931000000	-1.712463000000
H	-1.451353000000	4.326448000000	-0.781721000000
C	-4.757388000000	4.950796000000	0.139296000000
H	-5.573337000000	4.396400000000	0.617562000000
H	-5.103245000000	5.281094000000	-0.847650000000
H	-4.572342000000	5.845983000000	0.745110000000
C	-2.958641000000	0.299337000000	3.460321000000
H	-3.249205000000	-0.294313000000	2.589578000000
C	-1.658011000000	-0.319055000000	4.004295000000
H	-0.850294000000	-0.254696000000	3.269551000000
H	-1.813462000000	-1.377660000000	4.242565000000
H	-1.322284000000	0.180608000000	4.920559000000
C	-4.088523000000	0.190411000000	4.505982000000
H	-3.837641000000	0.744057000000	5.418766000000
H	-4.253244000000	-0.857416000000	4.784922000000
H	-5.034280000000	0.594438000000	4.126191000000
C	-3.920497000000	-1.565949000000	-1.382375000000
C	-4.125143000000	-2.827812000000	-0.775629000000
C	-4.071439000000	-3.966753000000	-1.587114000000
H	-4.216713000000	-4.946431000000	-1.140420000000
C	-3.836772000000	-3.866615000000	-2.954502000000
H	-3.798532000000	-4.763370000000	-3.567631000000
C	-3.653418000000	-2.616634000000	-3.536080000000
H	-3.477975000000	-2.547856000000	-4.605420000000
C	-3.694038000000	-1.443796000000	-2.771396000000
C	-3.544479000000	-0.092935000000	-3.464503000000
H	-3.372613000000	0.664918000000	-2.694272000000
C	-4.835697000000	0.279467000000	-4.225071000000
H	-5.036984000000	-0.440226000000	-5.028001000000
H	-4.739768000000	1.272604000000	-4.680346000000
H	-5.712355000000	0.290121000000	-3.567167000000
C	-2.337455000000	-0.050262000000	-4.419228000000
H	-1.418128000000	-0.344750000000	-3.908825000000
H	-2.198760000000	0.966763000000	-4.800483000000

H	-2.481152000000	-0.711245000000	-5.282111000000
C	-4.446054000000	-2.988477000000	0.708746000000
H	-4.360720000000	-2.003731000000	1.178533000000
C	-5.894616000000	-3.481543000000	0.912310000000
H	-6.031984000000	-4.487736000000	0.498786000000
H	-6.624192000000	-2.825278000000	0.423160000000
H	-6.138778000000	-3.524722000000	1.980716000000
C	-3.457030000000	-3.919516000000	1.435374000000
H	-3.708099000000	-3.971880000000	2.502099000000
H	-2.429844000000	-3.558954000000	1.341530000000
H	-3.495841000000	-4.940240000000	1.037419000000
C	3.105987000000	-0.241668000000	0.235078000000
C	5.202492000000	-0.602113000000	1.285146000000
H	5.681687000000	-1.520751000000	1.631263000000
H	5.544820000000	0.223696000000	1.923281000000
C	5.434143000000	-0.329897000000	-0.201888000000
H	6.150427000000	0.474406000000	-0.386879000000
H	5.774845000000	-1.222855000000	-0.740570000000
C	3.936093000000	0.658709000000	-1.961137000000
C	4.127922000000	2.055644000000	-2.079414000000
C	4.067947000000	2.623546000000	-3.357249000000
H	4.201972000000	3.695586000000	-3.470488000000
C	3.840997000000	1.840476000000	-4.484121000000
H	3.797213000000	2.301297000000	-5.467621000000
C	3.672720000000	0.466326000000	-4.350471000000
H	3.503737000000	-0.137374000000	-5.237054000000
C	3.719187000000	-0.154885000000	-3.095882000000
C	3.586038000000	-1.672266000000	-3.006594000000
H	3.398185000000	-1.934152000000	-1.960940000000
C	2.400387000000	-2.211984000000	-3.826803000000
H	2.566737000000	-2.095140000000	-4.904245000000
H	1.471511000000	-1.701732000000	-3.563783000000
H	2.264057000000	-3.279908000000	-3.627138000000
C	4.893590000000	-2.365096000000	-3.447666000000
H	5.108682000000	-2.156711000000	-4.502927000000
H	4.810143000000	-3.452364000000	-3.330437000000
H	5.757147000000	-2.025348000000	-2.864545000000
C	4.441472000000	2.952621000000	-0.883670000000
H	4.347585000000	2.348097000000	0.023818000000
C	5.891924000000	3.476934000000	-0.951844000000
H	6.620368000000	2.660886000000	-1.026161000000
H	6.130371000000	4.065303000000	-0.057443000000
H	6.036523000000	4.124288000000	-1.824984000000
C	3.455286000000	4.127585000000	-0.745657000000
H	3.519950000000	4.812919000000	-1.599041000000
H	3.686177000000	4.705357000000	0.157911000000
H	2.423986000000	3.774483000000	-0.674110000000
C	3.116251000000	-1.037618000000	2.610064000000
C	3.002326000000	-2.397600000000	2.981537000000
C	2.476396000000	-2.695278000000	4.244085000000
H	2.375816000000	-3.733200000000	4.548054000000
C	2.077124000000	-1.686201000000	5.115440000000
H	1.669847000000	-1.938772000000	6.091144000000
C	2.206814000000	-0.353326000000	4.737788000000
H	1.902980000000	0.428844000000	5.427912000000
C	2.733071000000	0.001659000000	3.488725000000
C	2.914658000000	1.479854000000	3.153217000000
H	3.202868000000	1.557775000000	2.101481000000
C	4.044519000000	2.102500000000	4.000469000000
H	3.799181000000	2.075221000000	5.068987000000
H	4.201332000000	3.151031000000	3.719712000000
H	4.993238000000	1.569320000000	3.867592000000
C	1.611952000000	2.283729000000	3.315046000000
H	1.286461000000	2.326643000000	4.361125000000
H	0.799645000000	1.846495000000	2.727245000000
H	1.758571000000	3.314484000000	2.972418000000
C	3.457031000000	-3.535825000000	2.071781000000
H	3.661230000000	-3.107571000000	1.085253000000
C	4.757068000000	-4.182262000000	2.596909000000
H	5.563244000000	-3.450237000000	2.722979000000
H	5.107399000000	-4.957492000000	1.904731000000
H	4.592029000000	-4.655654000000	3.572368000000
C	2.371349000000	-4.612083000000	1.883780000000
H	2.170580000000	-5.151951000000	2.816813000000
H	2.698606000000	-5.349241000000	1.141169000000
H	1.435215000000	-4.167557000000	1.538571000000
C	-0.082905000000	-2.998170000000	-0.963682000000
C	0.081370000000	2.125980000000	-2.330203000000
F	1.160653000000	-3.508613000000	-1.157581000000
F	-0.423002000000	-2.352990000000	-2.099944000000
F	-0.917139000000	-4.053122000000	-0.846228000000
F	0.875846000000	3.133389000000	-2.752027000000
F	0.466712000000	1.016336000000	-2.995044000000
F	-1.174516000000	2.423726000000	-2.753653000000

```
Zero-point correction=                           1.227867 (Hartree/Particle)
 Thermal correction to Energy=                    1.306937
 Thermal correction to Enthalpy=                  1.307881
 Thermal correction to Gibbs Free Energy=         1.108151
 Sum of electronic and zero-point Energies=          -8136.428102
 Sum of electronic and thermal Energies=             -8136.349032
 Sum of electronic and thermal Enthalpies=           -8136.348087
 Sum of electronic and thermal Free Energies=        -8136.547817
CPCM (Benzene) PBE0-D3/def2TZVP E = -10814.5230821
CPCM (Benzene) PBE0/def2TZVP E = -10814.3532175
CPCM (Benzene) M06L/def2TZVP E = -10818.2444619
CPCM (Benzene) M06/def2TZVP E = -10816.6259851
```

[(SIPr)Ni(SeCF$_3$)]$_2$ (4) *triplet*



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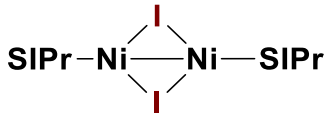
Se	0.123579000000	1.677149000000	-0.142194000000
Ni	-1.509810000000	-0.219983000000	0.069603000000
Ni	1.523261000000	-0.371379000000	-0.011213000000
N	-3.891154000000	1.353197000000	0.974180000000
N	-4.395845000000	-0.218054000000	-0.454119000000
N	4.136413000000	-0.660153000000	1.230257000000
N	4.346894000000	0.496945000000	-0.606322000000
C	-3.365235000000	0.364987000000	0.206539000000
C	-5.370431000000	1.373274000000	0.961163000000
H	-5.747234000000	2.387752000000	0.810855000000
H	-5.754352000000	1.005115000000	1.921995000000
C	-5.699278000000	0.432269000000	-0.203368000000
H	-6.461575000000	-0.311313000000	0.046211000000
H	-6.029467000000	0.973406000000	-1.098086000000
C	-3.194015000000	2.140184000000	1.956598000000
C	-2.854476000000	1.562985000000	3.201085000000
C	-2.232702000000	2.378087000000	4.156130000000
H	-1.957854000000	1.954526000000	5.118297000000
C	-1.974173000000	3.721157000000	3.901228000000
H	-1.495682000000	4.336899000000	4.658557000000
C	-2.334445000000	4.276024000000	2.676826000000
H	-2.130534000000	5.325633000000	2.485880000000
C	-2.946672000000	3.504790000000	1.682248000000
C	-3.338220000000	4.159384000000	0.360557000000
H	-3.635085000000	3.361820000000	-0.327944000000
C	-2.161049000000	4.905419000000	-0.295041000000
H	-1.860785000000	5.782257000000	0.291299000000

H	-2.449438000000	5.258922000000	-1.291901000000
H	-1.293974000000	4.249436000000	-0.398722000000
C	-4.539970000000	5.110847000000	0.542502000000
H	-5.406813000000	4.604004000000	0.982796000000
H	-4.846424000000	5.530427000000	-0.423350000000
H	-4.282341000000	5.947842000000	1.202738000000
C	-3.167484000000	0.112483000000	3.558459000000
H	-3.613641000000	-0.365746000000	2.682261000000
C	-1.896258000000	-0.685874000000	3.902838000000
H	-1.177752000000	-0.655724000000	3.077465000000
H	-2.146405000000	-1.736007000000	4.094602000000
H	-1.402525000000	-0.291139000000	4.798711000000
C	-4.195992000000	0.029297000000	4.705310000000
H	-3.799167000000	0.461374000000	5.631499000000
H	-4.455867000000	-1.016219000000	4.910563000000
H	-5.118656000000	0.568136000000	4.459448000000
C	-4.316438000000	-1.351262000000	-1.339289000000
C	-4.502483000000	-2.645579000000	-0.799850000000
C	-4.496456000000	-3.733926000000	-1.679879000000
H	-4.627402000000	-4.737746000000	-1.285885000000
C	-4.324841000000	-3.552622000000	-3.048115000000
H	-4.322302000000	-4.410994000000	-3.714853000000
C	-4.154177000000	-2.271223000000	-3.561972000000
H	-4.023050000000	-2.139751000000	-4.631854000000
C	-4.146056000000	-1.146526000000	-2.727503000000
C	-3.992200000000	0.241081000000	-3.342901000000
H	-3.792310000000	0.949288000000	-2.533199000000
C	-5.293448000000	0.676185000000	-4.051185000000
H	-5.521541000000	0.011568000000	-4.893403000000
H	-5.193117000000	1.694541000000	-4.445568000000
H	-6.156753000000	0.656210000000	-3.375786000000
C	-2.802979000000	0.325299000000	-4.317763000000
H	-1.875400000000	-0.004724000000	-3.845768000000
H	-2.662546000000	1.361369000000	-4.644368000000
H	-2.971132000000	-0.284489000000	-5.213315000000
C	-4.740341000000	-2.894882000000	0.687133000000
H	-4.613475000000	-1.943084000000	1.211811000000
C	-6.182429000000	-3.379344000000	0.945150000000
H	-6.365684000000	-4.349930000000	0.469127000000
H	-6.925159000000	-2.675315000000	0.551244000000
H	-6.361864000000	-3.496544000000	2.020804000000
C	-3.719398000000	-3.880956000000	1.286578000000
H	-3.881294000000	-3.978325000000	2.367296000000
H	-2.693063000000	-3.540963000000	1.120670000000
H	-3.819379000000	-4.880875000000	0.847933000000
C	3.446728000000	-0.126328000000	0.189034000000
C	5.569836000000	-0.304785000000	1.230270000000
H	6.192112000000	-1.188263000000	1.398590000000
H	5.779091000000	0.418093000000	2.029650000000
C	5.746796000000	0.298079000000	-0.168932000000
H	6.290699000000	1.246120000000	-0.163068000000
H	6.258402000000	-0.385107000000	-0.858560000000
C	4.087960000000	1.176274000000	-1.848319000000
C	4.085698000000	2.589813000000	-1.852857000000
C	3.924303000000	3.244183000000	-3.079110000000
H	3.910987000000	4.330114000000	-3.105226000000
C	3.770162000000	2.528862000000	-4.262141000000
H	3.641656000000	3.055744000000	-5.204110000000
C	3.774713000000	1.137985000000	-4.237558000000
H	3.652183000000	0.588284000000	-5.166172000000
C	3.936930000000	0.431192000000	-3.039280000000
C	3.979398000000	-1.094039000000	-3.072895000000
H	3.931391000000	-1.457652000000	-2.042112000000
C	2.774022000000	-1.695908000000	-3.819070000000
H	2.802547000000	-1.457846000000	-4.889147000000
H	1.828747000000	-1.326435000000	-3.413895000000
H	2.778055000000	-2.787012000000	-3.722753000000
C	5.303005000000	-1.596116000000	-3.687585000000
H	5.399373000000	-1.274007000000	-4.731477000000
H	5.342988000000	-2.691971000000	-3.669816000000
H	6.175880000000	-1.214900000000	-3.144163000000
C	4.268292000000	3.417940000000	-0.583485000000
H	4.298817000000	2.726658000000	0.264954000000
C	5.600643000000	4.195692000000	-0.609722000000
H	6.460390000000	3.532112000000	-0.761992000000
H	5.749647000000	4.734879000000	0.333683000000
H	5.610762000000	4.934479000000	-1.419843000000
C	3.086041000000	4.374911000000	-0.338013000000
H	3.002454000000	5.124508000000	-1.133750000000
H	3.228593000000	4.911699000000	0.608227000000
H	2.141588000000	3.827194000000	-0.286523000000
C	3.547008000000	-1.316997000000	2.365793000000
C	3.579540000000	-2.727989000000	2.428836000000
C	3.027502000000	-3.348881000000	3.555631000000
H	3.032986000000	-4.433020000000	3.623011000000
C	2.467793000000	-2.602564000000	4.588189000000
H	2.040751000000	-3.104643000000	5.452516000000
C	2.460182000000	-1.212587000000	4.515785000000
H	2.030882000000	-0.637367000000	5.331429000000
C	3.001874000000	-0.540080000000	3.413205000000
C	3.020833000000	0.986038000000	3.403650000000
H	3.379067000000	1.315109000000	2.424142000000
C	3.996322000000	1.530819000000	4.468210000000
H	3.673391000000	1.255816000000	5.479404000000
H	4.045489000000	2.625256000000	4.418900000000
H	5.010135000000	1.137312000000	4.328596000000
C	1.618118000000	1.591916000000	3.591803000000
H	1.201786000000	1.352127000000	4.577164000000
H	0.922264000000	1.224848000000	2.831765000000
H	1.661832000000	2.683719000000	3.507018000000
C	4.214753000000	-3.583309000000	1.336115000000
H	4.478043000000	-2.921050000000	0.505024000000
C	5.514177000000	-4.245278000000	1.841176000000
H	6.233298000000	-3.503868000000	2.209603000000
H	5.993926000000	-4.814259000000	1.035727000000
H	5.308798000000	-4.940086000000	2.664241000000
C	3.245745000000	-4.644176000000	0.781168000000
H	2.964560000000	-5.374497000000	1.549108000000
H	3.723288000000	-5.195787000000	-0.037755000000
H	2.330701000000	-4.185509000000	0.398173000000
C	-0.202074000000	-3.009947000000	-1.417331000000
C	-0.073261000000	2.010792000000	-2.056704000000
F	0.967415000000	-3.605508000000	-1.766404000000
F	-0.497687000000	-2.133158000000	-2.405424000000
F	-1.148529000000	-3.971939000000	-1.453121000000
F	0.722582000000	3.019730000000	-2.478545000000
F	0.218521000000	0.938825000000	-2.834422000000
F	-1.345848000000	2.378412000000	-2.377569000000

```
Zero-point correction=                           1.225941 (Hartree/Particle)
 Thermal correction to Energy=                    1.306365
 Thermal correction to Enthalpy=                  1.307309
 Thermal correction to Gibbs Free Energy=         1.099876
 Sum of electronic and zero-point Energies=          -8136.456611
 Sum of electronic and thermal Energies=             -8136.376187
 Sum of electronic and thermal Enthalpies=           -8136.375243
 Sum of electronic and thermal Free Energies=        -8136.582677
CPCM (Benzene) PBE0-D3/def2TZVP E = -10814.5445798
CPCM (Benzene) PBE0/def2TZVP E = -10814.3806999
CPCM (Benzene) M06L/def2TZVP E = -10818.2305149
CPCM (Benzene) M06/def2TZVP E = -10816.6359309
```

[(SIPr)Ni(I)]$_2$ (3) *singlet*



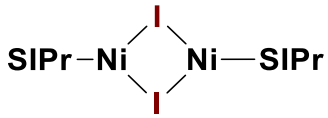
Ni	1.238287000000	-0.000021000000	-0.000007000000
I	-0.002832000000	0.343976000000	2.191909000000
N	3.968334000000	0.976055000000	0.488658000000
N	3.968321000000	-0.976081000000	-0.488677000000
C	3.154468000000	-0.000008000000	-0.000010000000
C	5.395319000000	0.741598000000	0.184898000000
H	6.026373000000	0.970616000000	1.046371000000
H	5.709350000000	1.380429000000	-0.652106000000
C	5.395309000000	-0.741641000000	-0.184922000000
H	6.026359000000	-0.970668000000	-1.046396000000
H	5.709334000000	-1.380474000000	0.652083000000
C	3.553115000000	2.239567000000	1.036215000000
C	3.108089000000	3.269252000000	0.176833000000
C	3.083660000000	3.126647000000	-1.342884000000
H	3.258097000000	2.075741000000	-1.589835000000
C	4.219219000000	3.953913000000	-1.983171000000
H	4.084575000000	5.025548000000	-1.792721000000
H	4.233963000000	3.806348000000	-3.069874000000
H	5.201699000000	3.670436000000	-1.587222000000
C	1.723696000000	3.508072000000	-1.954640000000
H	1.491753000000	4.568963000000	-1.802246000000
H	0.915330000000	2.910696000000	-1.524414000000
H	1.734359000000	3.325011000000	-3.035449000000
C	2.736549000000	4.490569000000	0.754281000000
H	2.384660000000	5.295164000000	0.115103000000
C	2.820679000000	4.697133000000	2.127468000000
H	2.526365000000	5.652908000000	2.553474000000
C	3.294875000000	3.682347000000	2.953641000000
H	3.371531000000	3.856873000000	4.023164000000
C	3.673064000000	2.440380000000	2.431011000000
C	4.239806000000	1.376131000000	3.367707000000
H	4.346496000000	0.450112000000	2.793600000000
C	3.311510000000	1.063320000000	4.556485000000
H	3.180574000000	1.934197000000	5.209318000000
H	3.741263000000	0.258383000000	5.165151000000
H	2.323229000000	0.744530000000	4.213929000000
C	5.637702000000	1.784692000000	3.881221000000
H	5.578010000000	2.686793000000	4.501729000000
H	6.331827000000	1.999589000000	3.060325000000
H	6.071764000000	0.985683000000	4.494517000000
C	3.553077000000	-2.239587000000	-1.036228000000
C	3.108034000000	-3.269251000000	-0.176832000000
C	3.083652000000	-3.126630000000	1.342884000000
H	3.258080000000	-2.075718000000	1.589816000000
C	1.723718000000	-3.508075000000	1.954695000000
H	0.915326000000	-2.910715000000	1.524496000000
H	1.734421000000	-3.325006000000	3.035503000000
H	1.491787000000	-4.568971000000	1.802319000000
C	4.219251000000	-3.953870000000	1.983137000000
H	4.084618000000	-5.025508000000	1.792699000000
H	4.234028000000	-3.806296000000	3.069839000000
H	5.201712000000	-3.670378000000	1.587153000000
C	2.736440000000	-4.490559000000	-0.754263000000
H	2.384529000000	-5.295136000000	-0.115074000000
C	2.820537000000	-4.697134000000	-2.127451000000
H	2.526177000000	-5.652899000000	-2.553446000000
C	3.294761000000	-3.682372000000	-2.953638000000
H	3.371393000000	-3.856910000000	-4.023161000000
C	3.673001000000	-2.440413000000	-2.431024000000
C	4.239766000000	-1.376194000000	-3.367741000000
H	4.346530000000	-0.450180000000	-2.793639000000
C	5.637623000000	-1.784836000000	-3.881298000000
H	6.331759000000	-1.999769000000	-3.060420000000
H	6.071711000000	-0.985852000000	-4.494608000000
H	5.577863000000	-2.686935000000	-4.501801000000
C	3.311445000000	-1.063329000000	-4.556484000000
H	3.180432000000	-1.934200000000	-5.209311000000
H	3.741223000000	-0.258418000000	-5.165167000000
H	2.323194000000	-0.744483000000	-4.213892000000

Ni	-1.228427000000	-0.000008000000	-0.000001000000
I	-0.002845000000	-0.344027000000	-2.191911000000
N	-3.952321000000	0.854410000000	-0.680205000000
N	-3.952341000000	-0.854333000000	0.680239000000
C	-3.139897000000	0.000026000000	0.000010000000
C	-5.379990000000	0.686170000000	-0.336458000000
H	-6.009183000000	0.727956000000	-1.227950000000
H	-5.697335000000	1.485600000000	0.346738000000
C	-5.380006000000	-0.686059000000	0.336491000000
H	-6.009203000000	-0.727827000000	1.227980000000
H	-5.697369000000	-1.485482000000	-0.346705000000
C	-3.539417000000	1.969720000000	-1.490333000000
C	-3.100865000000	3.165521000000	-0.876635000000
C	-3.067808000000	3.354832000000	0.637771000000
H	-3.166303000000	2.371530000000	1.106039000000
C	-4.260410000000	4.221152000000	1.098488000000
H	-4.199294000000	5.231084000000	0.674854000000
H	-4.266941000000	4.314980000000	2.191220000000
H	-5.220564000000	3.792326000000	0.787963000000
C	-1.742658000000	3.957996000000	1.137928000000
H	-1.603027000000	4.986160000000	0.782800000000
H	-0.885329000000	3.360546000000	0.816571000000
H	-1.735844000000	3.985736000000	2.233623000000
C	-2.748167000000	4.237680000000	-1.706799000000
H	-2.404933000000	5.165399000000	-1.258660000000
C	-2.840805000000	4.142913000000	-3.091564000000
H	-2.561397000000	4.988175000000	-3.715346000000
C	-3.303657000000	2.968071000000	-3.676026000000
H	-3.386490000000	2.906870000000	-4.757510000000
C	-3.664946000000	1.863711000000	-2.895540000000
C	-4.221526000000	0.618114000000	-3.581762000000
H	-4.306511000000	-0.169726000000	-2.826223000000
C	-3.299700000000	0.081702000000	-4.692939000000
H	-3.207411000000	0.793123000000	-5.521946000000
H	-3.710912000000	-0.848340000000	-5.104142000000
H	-2.296094000000	-0.125532000000	-4.311719000000
C	-5.630965000000	0.889158000000	-4.151941000000
H	-5.593054000000	1.646952000000	-4.943672000000
H	-6.323068000000	1.255181000000	-3.384708000000
H	-6.054210000000	-0.025509000000	-4.584631000000
C	-3.539464000000	-1.969666000000	1.490351000000
C	-3.100947000000	-3.165463000000	0.876628000000
C	-3.067905000000	-3.354740000000	-0.637783000000
H	-3.166381000000	-2.371422000000	-1.106023000000
C	-1.742774000000	-3.957920000000	-1.137966000000
H	-0.885427000000	-3.360509000000	-0.816588000000
H	-1.735963000000	-3.985615000000	-2.233662000000
H	-1.603172000000	-4.986102000000	-0.782880000000
C	-4.260531000000	-4.221018000000	-1.098514000000
H	-4.199443000000	-5.230958000000	-0.674894000000
H	-4.267064000000	-4.314830000000	-2.191247000000
H	-5.220673000000	-3.792170000000	-0.787983000000
C	-2.748262000000	-4.237646000000	1.706767000000
H	-2.405053000000	-5.165364000000	1.258606000000
C	-2.840882000000	-4.142902000000	3.091534000000
H	-2.561482000000	-4.988182000000	3.715297000000
C	-3.303702000000	-3.968062000000	3.676025000000
H	-3.386516000000	-2.906877000000	4.757511000000
C	-3.664980000000	-1.863681000000	2.895563000000
C	-4.221522000000	-0.618085000000	3.581819000000
H	-4.306513000000	0.169770000000	2.826298000000
C	-5.630948000000	-0.889122000000	4.152033000000
H	-6.323080000000	-1.255125000000	3.384816000000
H	-6.054171000000	0.025541000000	4.584754000000
H	-5.593020000000	-1.646932000000	4.943748000000
C	-3.299663000000	-0.081707000000	4.692985000000
H	-3.207365000000	-0.793144000000	5.521979000000
H	-3.710852000000	0.848332000000	5.104215000000
H	-2.296063000000	0.125522000000	4.311746000000

```
Zero-point correction=                           1.198077 (Hartree/Particle)
 Thermal correction to Energy=                    1.269178
 Thermal correction to Enthalpy=                  1.270122
 Thermal correction to Gibbs Free Energy=         1.085645
 Sum of electronic and zero-point Energies=          -2686.190395
 Sum of electronic and thermal Energies=             -2686.119294
 Sum of electronic and thermal Enthalpies=           -2686.118350
```

```
 Sum of electronic and thermal Free Energies=          -2686.302827
CPCM (Benzene) PBE0-D3/def2TZVP E = -5932.5064647
CPCM (Benzene) PBE0/def2TZVP E = -5932.35405853
CPCM (Benzene) M06L/def2TZVP E = -5935.59730855
CPCM (Benzene) M06/def2TZVP E = -5933.88709631
```

[(SIPr)Ni(I)]$_2$ (3) *triplet*

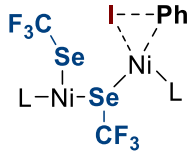


Ni	1.711688000000	-0.253309000000	0.006287000000
I	-0.000363000000	1.855759000000	-0.000323000000
N	4.323948000000	0.951174000000	-0.812409000000
N	4.524589000000	-0.699904000000	0.600462000000
C	3.620575000000	0.050734000000	-0.081647000000
C	5.785649000000	0.736669000000	-0.743959000000
H	6.313267000000	1.680328000000	-0.584073000000
H	6.141434000000	0.301555000000	-1.687530000000
C	5.915877000000	-0.234803000000	0.434922000000
H	6.587997000000	-1.072728000000	0.230106000000
H	6.257783000000	0.261576000000	1.353170000000
C	3.789731000000	1.879766000000	-1.772048000000
C	3.385395000000	1.418414000000	-3.044015000000
C	3.474782000000	-0.046376000000	-3.463066000000
H	3.828490000000	-0.625955000000	-2.605356000000
C	4.496452000000	-0.236589000000	-4.603382000000
H	4.185281000000	0.291997000000	-5.512175000000
H	4.595324000000	-1.299578000000	-4.854352000000
H	5.487452000000	0.141638000000	-4.324930000000
C	2.099794000000	-0.621131000000	-3.853259000000
H	1.679730000000	-0.103531000000	-4.724003000000
H	1.387446000000	-0.532732000000	-3.026952000000
H	2.192198000000	-1.683542000000	-4.108915000000
C	2.911862000000	2.363066000000	-3.963411000000
H	2.585505000000	2.031565000000	-4.945240000000
C	2.857933000000	3.716522000000	-3.645970000000
H	2.488128000000	4.432345000000	-4.375549000000
C	3.282488000000	4.153548000000	-2.394356000000
H	3.240678000000	5.212563000000	-2.155673000000
C	3.754309000000	3.251362000000	-1.434270000000
C	4.229726000000	3.775647000000	-0.082010000000
H	4.458336000000	2.910351000000	0.548588000000
C	3.143732000000	4.589216000000	0.647772000000
H	2.888951000000	5.504158000000	0.099865000000
H	3.502220000000	4.888999000000	1.640302000000
H	2.227975000000	4.003734000000	0.771859000000
C	5.520577000000	4.608402000000	-0.230264000000
H	5.341687000000	5.510057000000	-0.828062000000
H	6.319264000000	4.042135000000	-0.724216000000
H	5.887394000000	4.927953000000	0.752723000000
C	4.203409000000	-1.702849000000	1.579473000000
C	3.843468000000	-1.310550000000	2.888281000000
C	3.783676000000	0.150070000000	3.326859000000
H	4.008912000000	0.775991000000	2.458308000000
C	2.378026000000	0.551586000000	3.812399000000
H	1.632937000000	0.402471000000	3.024699000000
H	2.363713000000	1.611299000000	4.093985000000
H	2.072944000000	-0.031712000000	4.689456000000
C	4.847196000000	0.450155000000	4.403431000000
H	4.659642000000	-0.119127000000	5.321516000000
H	4.835566000000	1.515125000000	4.664561000000
H	5.855887000000	0.194788000000	4.057174000000
C	3.558899000000	-2.317769000000	3.818841000000
H	3.269264000000	-2.041905000000	4.828987000000
C	3.644806000000	-3.663598000000	3.475365000000
H	3.419109000000	-4.428698000000	4.213616000000
C	4.023145000000	-4.029662000000	2.186689000000
H	4.091312000000	-5.082694000000	1.928555000000
C	4.309312000000	-3.063932000000	1.214716000000
C	4.741331000000	-3.505550000000	-0.180523000000
H	4.821757000000	-2.608540000000	-0.802904000000
C	6.128833000000	-4.179685000000	-0.145380000000
H	6.887911000000	-3.525787000000	0.300428000000
H	6.455870000000	-4.439400000000	-1.159471000000
H	6.105020000000	-5.103994000000	0.444042000000
C	3.704958000000	-4.428017000000	-0.850556000000
H	3.595220000000	-5.373764000000	-0.306825000000
H	4.021552000000	-4.670321000000	-1.872460000000
H	2.721163000000	-3.951051000000	-0.897777000000

Ni	-1.711699000000	-0.254496000000	-0.005986000000
I	0.000187000000	-2.335741000000	0.001171000000
N	-4.524519000000	-0.699018000000	-0.601806000000
N	-4.324005000000	0.950354000000	0.813062000000
C	-3.620589000000	0.050639000000	0.081490000000
C	-5.915735000000	-0.233722000000	-0.436233000000
H	-6.588257000000	-1.071693000000	-0.232965000000
H	-6.257022000000	0.264165000000	-1.353905000000
C	-5.785700000000	0.735991000000	0.744092000000
H	-6.313317000000	1.679872000000	0.585558000000
H	-6.141575000000	0.299418000000	1.686965000000
C	-4.203153000000	-1.701261000000	-1.581464000000
C	-3.842524000000	-1.308039000000	-2.889809000000
C	-3.782290000000	0.152912000000	-3.327246000000
H	-4.007523000000	0.778224000000	-2.458259000000
C	-4.845581000000	0.454006000000	-4.403774000000
H	-4.657965000000	-0.114642000000	-5.322241000000
H	-4.833723000000	1.519167000000	-4.664114000000
H	-5.854372000000	0.198554000000	-4.057875000000
C	-2.376491000000	0.554513000000	-3.812241000000
H	-2.071347000000	-0.028167000000	-4.689688000000
H	-1.631591000000	0.404694000000	-3.024498000000
H	-2.361933000000	1.614435000000	-4.093023000000
C	-3.557699000000	-2.314591000000	-3.821003000000
H	-3.267535000000	-2.038008000000	-4.830800000000
C	-3.644041000000	-3.660666000000	-3.478596000000
H	-3.418143000000	-4.425253000000	-4.217318000000
C	-4.023064000000	-4.027638000000	-2.190382000000
H	-4.091587000000	-5.080856000000	-1.933099000000
C	-4.309504000000	-3.062600000000	-1.217803000000
C	-4.742315000000	-3.505185000000	0.176882000000
H	-4.822879000000	-2.608627000000	0.799899000000
C	-3.706472000000	-4.428365000000	0.846762000000
H	-3.596643000000	-5.373731000000	0.302388000000
H	-4.023634000000	-4.671361000000	1.868324000000
H	-2.722610000000	-3.951625000000	0.894838000000
C	-6.129943000000	-4.178996000000	0.140526000000
H	-6.106032000000	-5.102833000000	-0.449629000000
H	-6.888659000000	-3.524576000000	-0.305134000000
H	-6.457536000000	-4.439453000000	1.154247000000
C	-3.789771000000	1.878104000000	1.773502000000
C	-3.385596000000	1.415688000000	3.045140000000
C	-3.475232000000	-0.049409000000	3.463064000000
H	-3.828830000000	-0.628310000000	2.604849000000
C	-2.100373000000	-0.624589000000	3.853117000000
H	-1.387850000000	-0.535689000000	3.027020000000
H	-2.192930000000	-1.687172000000	4.107995000000
H	-1.680439000000	-0.107649000000	4.724317000000
C	-4.497146000000	-0.240389000000	4.603023000000
H	-4.186101000000	0.287436000000	5.512302000000
H	-4.596186000000	-1.303566000000	4.853131000000
H	-5.488048000000	0.138169000000	4.324668000000
C	-2.912025000000	2.359556000000	3.965319000000
H	-2.585865000000	2.027259000000	4.946944000000
C	-2.857855000000	3.713251000000	3.648929000000
H	-2.488000000000	4.428450000000	4.379095000000
C	-3.282258000000	4.151319000000	2.397631000000
H	-3.240294000000	5.210516000000	2.159783000000
C	-3.754177000000	3.249961000000	1.436813000000
C	-4.229777000000	3.775392000000	0.085065000000
H	-4.458405000000	2.910633000000	-0.546259000000
C	-5.520732000000	4.607849000000	0.234292000000
H	-6.319219000000	4.041050000000	0.727957000000
H	-5.887810000000	4.928163000000	-0.748348000000
H	-5.341821000000	5.509023000000	0.832807000000
C	-3.144041000000	4.589736000000	-0.644218000000
H	-2.889126000000	5.504147000000	-0.095490000000
H	-3.502848000000	4.890489000000	-1.636341000000
H	-2.228292000000	4.004425000000	-0.769174000000

```
Zero-point correction=                           1.196159 (Hartree/Particle)
 Thermal correction to Energy=                    1.268536
 Thermal correction to Enthalpy=                  1.269481
 Thermal correction to Gibbs Free Energy=         1.076361
 Sum of electronic and zero-point Energies=          -2686.237803
 Sum of electronic and thermal Energies=             -2686.165426
 Sum of electronic and thermal Enthalpies=           -2686.164481
 Sum of electronic and thermal Free Energies=        -2686.357601
CPCM (Benzene) PBE0-D3/def2TZVP E = -5932.53782537
CPCM (Benzene) PBE0/def2TZVP E = -5932.3927131
CPCM (Benzene) M06L/def2TZVP E = -5935.59218137
CPCM (Benzene) M06/def2TZVP E = -5933.90369117
```

TS-OA-bis-SeCF$_3$-PhI *triplet*



Ni	-1.97633800	0.32733600	-0.26457500
Ni	2.19636400	0.08602900	-0.46820300
C	-3.52483400	-0.90606600	0.35673400
C	-5.54978000	-1.84672200	1.14623600
C	-4.61074000	-2.97385200	0.72892700
C	3.86419900	0.35338300	0.52591800
C	5.71803900	0.03084500	1.96323900
C	5.91960900	1.32910000	1.18794900
N	-3.35421100	-2.24633700	0.44562500
N	-4.81885600	-0.64236200	0.68175500
N	4.60210800	1.49899400	0.53711400
N	4.54782800	-0.55731200	1.27296500
H	-4.95106000	-3.48850400	-0.17647100
H	-6.53108900	-1.91199200	0.67537200
H	6.70450200	1.24249300	0.42611700
H	6.57777800	-0.64137300	1.92310700
C	-2.16185900	-3.01690700	0.16102000
C	-1.36200000	-3.48953400	1.22958400
C	-1.86789200	-3.36067900	-1.18452800
C	-0.21290500	-4.22496700	0.90038900
C	-0.71462400	-4.10946400	-1.44201000
C	0.12037500	-4.52436500	-0.41238900
H	0.44042500	-4.55589800	1.70346400
H	-0.45272200	-4.34949200	-2.46590500
H	1.03112300	-5.07336500	-0.63283500
C	-5.48647500	0.63141300	0.80962000
C	-6.40938000	1.02191100	-0.19490800
C	-5.31203900	1.40467400	1.98356200
C	-7.09948300	2.22883500	-0.02385900
C	-6.03500900	2.59963100	2.10086700
C	-6.91299000	3.01719500	1.10706000
H	-7.80140400	2.55100700	-0.78666200
H	-5.91063400	3.20676500	2.99211500
H	-7.46151300	3.94887400	1.21851500
C	4.32312200	2.70716500	-0.19926500
C	4.65007100	2.78571800	-1.57531800
C	3.81515700	3.82791500	0.50080400
C	4.37569400	3.98351600	-2.24817800
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C	3.83334700	5.07981600	-1.58581900
H	4.60267500	4.06103400	-3.30671700
H	3.18487700	5.87614600	0.29758600
H	3.63232500	5.99951600	-2.12949600
C	4.21303200	-1.93919800	1.51126700
C	3.64832300	-2.30970400	2.75270200
C	4.57089200	-2.91296200	0.54302700
C	3.44925400	-3.67288500	3.01194100
C	4.33417200	-4.25801500	0.85175000
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H	3.02515800	-3.97586600	3.96513200
H	4.59153100	-5.02324800	0.12815800
H	3.62892400	-5.69351600	2.29332600
C	-1.61732200	-3.38513800	2.74229500
H	-0.61383200	-3.31951100	3.18103700
C	-2.23127300	-4.70383700	3.26725600
H	-2.29199100	-4.68646300	4.36232400
H	-3.24671600	-4.86046900	2.88230200
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C	-2.38120600	-2.17936100	3.30131300
H	-3.45247300	-2.21729100	3.08472200
H	-2.27740900	-2.17373400	4.39351800
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C	-4.42424300	0.97118700	3.14601100
H	-3.78156800	0.15977000	2.80026100
C	-5.28502600	0.43107200	4.30944500
H	-5.92353300	1.22095700	4.72338200
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H	-4.35973200	-3.98279300	-3.53194700
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C	3.59899600	3.82735300	2.01231100
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C	4.74179600	4.58759000	2.72226100
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H	4.62403900	4.52951800	3.81118800
C	2.24568200	4.42632400	2.43514700
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C	5.37523500	1.66802700	-2.32240100
H	5.27177400	0.74740800	-1.74062100
C	6.88158200	1.99801800	-2.43337800
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C	4.80007300	1.38760900	-3.72228500
H	5.29352800	0.50959600	-4.15436900
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H	4.97253200	2.22713600	-4.40676700
C	5.23577100	-2.54680300	-0.78621100
H	4.79276700	-1.60678400	-1.13135100
C	6.75563700	-2.32968300	-0.61687600
H	7.23717400	-3.24204700	-0.24379100

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H	3.94435800	-3.81436600	-2.02295100
H	5.36686800	-3.18250300	-2.84970800
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H	3.32915100	-0.29706700	3.39419700
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H	5.27813400	-1.22805700	4.73659400
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H	1.53628000	-0.66553200	4.98578400
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C	-0.46920000	4.13941100	-0.55116300
H	-0.04415600	2.34699700	-1.66864300
C	-1.42550200	4.85694000	0.17568400
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H	0.52441900	4.54867600	-0.71149600
H	-1.17983400	5.83581800	0.57819200
H	-5.69330700	-1.79342500	2.23179400
H	-4.45636700	-3.72054400	1.51007300
H	6.15560000	2.17876600	1.83117400
H	5.47946100	0.21890100	3.01647000
Se	1.29745700	-0.00034000	-2.66406800
C	1.98232200	-1.68163700	-3.35469100
F	3.30592200	-1.63587000	-3.67286900
F	1.33887700	-2.06239300	-4.48557400
F	1.85207300	-2.72355500	-2.48293400
Se	0.12854200	-0.15738200	0.98052400
C	0.14545900	1.14519400	2.43708100
F	1.40488000	1.39104700	2.88355700
F	-0.55504400	0.71367400	3.52271200
F	-0.38728600	2.34829300	2.11047500

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Zero-point correction=                           1.318762 (Hartree/Particle)
 Thermal correction to Energy=                    1.405043
 Thermal correction to Enthalpy=                  1.405987
 Thermal correction to Gibbs Free Energy=         1.188620
 Sum of electronic and zero-point Energies=          -8379.362146
 Sum of electronic and thermal Energies=             -8379.275865
 Sum of electronic and thermal Enthalpies=           -8379.274921
 Sum of electronic and thermal Free Energies=        -8379.492288
CPCM (Benzene) PBE0-D3/def2TZVP E = -11343.6870853
CPCM (Benzene) M06L/def2TZVP E = -11347.7701324
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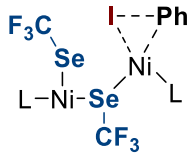
TS-OA-bis-SeCF$_3$-PhI *singlet*



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C	4.54963400	2.98557800	0.31832300
C	-3.38603400	-0.13135700	0.33121000
C	-5.61778500	0.59730200	0.60539100
C	-5.61451300	-0.88384700	0.24286300
N	3.24686300	2.29482800	0.22450700
N	4.67085600	0.65533200	0.44854600
N	-4.18587300	-1.24056200	0.40367000
N	-4.19344200	0.96620200	0.42687200
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H	6.42377800	1.85047000	0.23720400
H	-5.91738900	-1.04438700	-0.79766300
H	-6.25255600	1.19423300	-0.05285000
C	2.07643100	3.09951800	-0.03091400
C	1.41175200	3.72849600	1.04937100
C	1.67491200	3.32908600	-1.37305200
C	0.28432900	4.50918400	0.74886900
C	0.55401700	4.13322000	-1.60484600
C	-0.15012900	4.70806000	-0.55363600
H	-0.26707900	4.96481100	1.56722900
H	0.22549900	4.30621500	-2.62418000
H	-1.03512300	5.30596900	-0.74677900
C	5.35482900	-0.61423500	0.49880900
C	6.09808800	-1.03175300	-0.63696000
C	5.39832100	-1.35127000	1.70832500
C	6.80411100	-2.23917800	-0.55986100
C	6.12795500	-2.54792000	1.72683300
C	6.81262900	-2.99985200	0.60416200
H	7.36559700	-2.58227100	-1.42324200
H	6.16700900	-3.13065200	2.64162000
H	7.36679400	-3.93412400	0.64166000
C	-3.83764500	-2.62771000	0.65425700
C	-3.90565000	-3.58464600	-0.38802300
C	-3.60470400	-3.04498000	1.99567400
C	-3.70479200	-4.93703500	-0.07254900
C	-3.39623900	-4.40673100	2.24409000
C	-3.44641700	-5.35163200	1.22539900
H	-3.76336400	-5.67551600	-0.86567500
H	-3.20704500	-4.73813300	3.25842700
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C	-3.58774600	2.79928700	1.98815800
C	-4.01515200	3.30225300	-0.37986400
C	-3.45581900	4.17404600	2.22391300
C	-3.88488600	4.66525900	-0.08113500
C	-3.60983400	5.10686500	1.20614200
H	-3.25472500	4.51779600	3.23403000
H	-4.01678400	5.39203400	-0.87714500
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H	2.15080400	1.62445300	2.92394600
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C	6.23300500	-0.19125600	-1.90680900
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C	7.60527500	0.52109000	-1.94663000
H	7.79646100	1.12673300	-1.05494000
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C	6.06620800	-1.00619900	-3.20439700
H	5.14637500	-1.59445200	-3.19826100

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C	3.37277200	3.91092200	-3.15071400
H	3.96797700	3.51979400	-3.98497600
H	2.77753100	4.75061800	-3.52883100
H	4.06226800	4.31275200	-2.40033300
C	1.53879300	2.27911500	-3.70379500
H	2.14144500	1.75806500	-4.45802400
H	0.77783800	1.58794700	-3.33106100
H	1.02386500	3.09740200	-4.22127900
C	-3.64687800	-2.09308500	3.19047900
H	-3.24204500	-1.13202500	2.86599300
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H	-5.73838200	-1.43102100	2.91256500
H	-5.54671700	-2.82952700	3.97691900
H	-5.11026200	-1.20972300	4.54914100
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H	-3.60296000	3.21014400	-3.83171700
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H	-2.13598300	1.37516600	4.82127600
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C	0.19350900	-4.14439900	0.11110300
H	-0.39486300	-2.66170900	-1.34388600
C	1.23719800	-4.65942100	0.88852500
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Se	-1.50813900	-0.34906300	-2.54480600
C	-3.16120100	-0.19549800	-3.57544900
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F	-3.32432000	-1.23568800	-4.42967400
F	-3.18277700	0.91297400	-4.35380800
Se	0.06547900	0.46861800	1.23761500
C	0.19473200	-0.81075800	2.73484200
F	-0.73813400	-0.52630100	3.67455800
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Zero-point correction=                           1.320601 (Hartree/Particle)
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 Sum of electronic and thermal Energies=            -8379.214494
 Sum of electronic and thermal Enthalpies=          -8379.213550
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CPCM (Benzene) PBE0-D3/def2TZVP E = -11343.6372255
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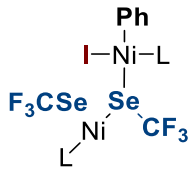
post-OA-*bis*-SeCF$_3$ *triplet*



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N	-3.337467000000	-2.145005000000	0.692163000000
N	-4.716706000000	-0.457339000000	0.864536000000
N	4.542355000000	1.643900000000	0.344168000000
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H	-5.022173000000	-3.364457000000	0.301581000000
H	-6.471754000000	-1.642077000000	1.092411000000
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H	6.628539000000	-0.246407000000	1.927076000000
C	-2.185796000000	-2.983093000000	0.430975000000
C	-1.321844000000	-3.334338000000	1.496460000000
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C	-0.854996000000	-4.282821000000	-1.116246000000
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H	0.954699000000	-5.128627000000	-0.319539000000
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C	-6.328874000000	1.117904000000	-0.135746000000
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H	-7.740674000000	2.580736000000	-0.835157000000
H	-5.721366000000	3.624785000000	2.783997000000
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C	4.229933000000	2.740666000000	-0.538041000000
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C	3.730330000000	3.940918000000	0.021275000000
C	4.250479000000	3.744874000000	-2.733406000000
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C	3.756072000000	-1.993489000000	2.888829000000
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H	-0.476046000000	-2.969839000000	3.382976000000
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H	6.799384000000	2.534910000000	-3.569932000000
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C	4.529558000000	0.922942000000	-3.819730000000
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H	4.593914000000	1.659143000000	-4.629999000000
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H	5.023294000000	-1.539054000000	-0.983638000000
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H	3.344179000000	0.051181000000	3.349796000000
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H	3.965572000000	-0.022467000000	5.755519000000
H	4.230506000000	-1.771381000000	5.661660000000
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H	1.539352000000	-0.253964000000	4.942674000000
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C	-0.347929000000	4.153164000000	-1.285983000000
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H	-3.261580000000	5.113882000000	0.194628000000
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H	-1.130874000000	6.070470000000	-0.677235000000
H	-5.526639000000	-1.415726000000	2.572337000000
H	-4.419791000000	-3.458742000000	1.966542000000
H	6.076434000000	2.522097000000	1.537803000000
H	5.484897000000	0.667625000000	2.926583000000
Se	1.071763000000	-0.532285000000	-2.500446000000
C	1.821700000000	-2.272930000000	-2.942882000000
F	3.017896000000	-2.189177000000	-3.583016000000
F	1.007563000000	-2.985550000000	-3.761247000000
F	2.044016000000	-3.064871000000	-1.854189000000
Se	0.133353000000	-0.003552000000	0.959453000000
C	0.155478000000	1.410292000000	2.322395000000
F	1.425986000000	1.665544000000	2.729205000000
F	-0.530240000000	1.057666000000	3.442947000000
F	-0.366073000000	2.585921000000	1.918169000000

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Zero-point correction=                           1.319050 (Hartree/Particle)
 Thermal correction to Energy=                    1.406180
 Thermal correction to Enthalpy=                  1.407124
 Thermal correction to Gibbs Free Energy=         1.186984
 Sum of electronic and zero-point Energies=          -8379.365846
 Sum of electronic and thermal Energies=             -8379.278716
 Sum of electronic and thermal Enthalpies=           -8379.277772
 Sum of electronic and thermal Free Energies=        -8379.497912
CPCM (Benzene) PBE0-D3/def2TZVP E = -11343.6862555
CPCM (Benzene) M06L/def2TZVP E = -11347.7753004
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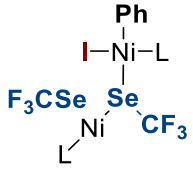
post-OA-*bis*-SeCF$_3$ *singlet*



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C	-5.12448600	-2.31515700	0.55126900
C	-4.24626100	-3.08436200	-0.42654000
C	3.53312800	-0.03384200	0.68583100
C	5.41971700	-0.88482100	1.81472800
C	5.41727600	0.63879200	1.93003000
N	-3.03136800	-2.24237500	-0.48222700
N	-4.46696900	-0.98790900	0.58766800
N	4.29100800	1.02553700	1.05069500
N	4.11947400	-1.16296700	1.15694800
H	-4.69499500	-3.15514600	-1.42396800
H	-6.15656600	-2.23283400	0.21516400
H	6.34541200	1.09994500	1.58596000
H	6.23470900	-1.26490900	1.18894300
C	-1.87680400	-2.78255800	-1.16108200
C	-0.97540700	-3.61406200	-0.45103200
C	-1.73799600	-2.58608500	-2.56098900
C	0.12428500	-4.13271900	-1.15307900
C	-0.63508100	-3.15598700	-3.20789800
C	0.30230400	-3.90890900	-2.51140600
H	0.84666400	-4.73745300	-0.61207000
H	-0.51352300	-3.00643600	-4.27542300
H	1.15825600	-4.33453100	-3.02855600
C	-5.17097400	0.08821500	1.25463000
C	-6.28710900	0.68003800	0.60482000
C	-4.83595000	0.44630000	2.58556500
C	-6.99963100	1.67513100	1.28507600
C	-5.58565100	1.45220000	3.21049500
C	-6.64998300	2.07266300	2.56876800
H	-7.84564600	2.14672800	0.79537000
H	-5.33801200	1.74583600	4.22458900
H	-7.21391100	2.85268600	3.07375800
C	4.20718400	2.38085100	0.54692800
C	4.78620800	2.66911900	-0.71505000
C	3.67509500	3.40279100	1.36681900
C	4.70457800	3.98402500	-1.18744400
C	3.62908400	4.70127900	0.84334200
C	4.11548300	4.98861600	-0.42733700
H	5.12178600	4.22682500	-2.15962200
H	3.20476200	5.49876700	1.44399100
H	4.05711700	6.00162100	-0.81632400
C	3.80505700	-2.55350800	0.90284900
C	3.34769900	-3.34643900	1.98278900
C	4.12817700	-3.13684000	-0.34871300
C	3.16699700	-4.71894000	1.76907900
C	3.92860700	-4.51510800	-0.50170700
C	3.44975800	-5.30294700	0.53962000
H	2.81434000	-5.34025300	2.58693200
H	4.17141900	-4.98133900	-1.45122100
H	3.31243100	-6.37166700	0.39681200
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H	-0.04432700	-4.18421900	1.34243900
C	-1.59309700	-5.60299400	0.97094200
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C	-1.84825700	-3.34147300	2.05061400
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H	-1.63548800	-3.77243600	3.03687000
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C	-3.76725900	-0.27393300	3.40722000
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H	-3.63802300	-1.97122500	4.77878200
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H	-2.52303300	1.48956300	3.80395500
H	-3.61653200	1.07195500	5.13814700
H	-2.18152700	0.09612300	4.83889400
C	-6.80837500	0.25103900	-0.76718400
H	-6.03403600	-0.35062600	-1.25270200
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H	-7.97179600	-1.45883700	0.04306400
H	-8.90957000	0.00914200	-0.21253800
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C	-2.78313400	-1.87284400	-3.41504000
H	-3.41958200	-1.27500500	-2.75864700
C	-3.66764300	-2.90701200	-4.14856300
H	-4.46357400	-2.39796100	-4.70524000
H	-3.07571500	-3.48859100	-4.86621500
H	-4.13697200	-3.62034700	-3.46147500
C	-2.16959700	-0.90243200	-4.44085200
H	-2.96861100	-0.33879000	-4.93437700
H	-1.50525700	-0.18036300	-3.96177300
H	-1.60922500	-1.43250100	-5.22088400
C	3.25020800	3.16835000	2.81431200
H	3.06181200	2.09922700	2.94429400
C	4.38957100	3.58505300	3.77400800
H	5.33634200	3.07962500	3.55362600
H	4.57390200	4.66358800	3.70336000
H	4.11584500	3.35981500	4.81188200
C	1.96099300	3.91281600	3.20536700
H	1.15670600	3.74543100	2.48794300
H	1.62145100	3.57002900	4.18917600
H	2.12869500	4.99379300	3.28062700
C	5.60599200	1.65200800	-1.50867300
H	5.37735400	0.65300400	-1.12820300
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H	7.71229100	1.13691100	-1.79201100
H	7.40920300	2.87983800	-1.67685300
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C	5.31031200	1.64246100	-3.01870100
H	5.87026300	0.83121100	-3.49924600
H	4.25054600	1.49443200	-3.22883500
H	5.62300700	2.57645700	-3.49924300
C	4.76382800	-2.36520300	-1.50295700
H	4.58833100	-1.29928400	-1.34032200
C	6.29084800	-2.59713800	-1.54052300
H	6.51792300	-3.65259000	-1.73224500
H	6.74784700	-2.00407100	-2.34159300
H	6.77733100	-2.32343400	-0.59808300
C	4.15490700	-2.71133000	-2.87397900
H	4.42640200	-3.72355000	-3.19676300
H	3.06488200	-2.63535800	-2.86235000
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C	3.09635400	-2.79209000	3.38245300
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C	1.66243900	-3.07322500	3.86697700
H	0.92441000	-2.69919400	3.15505500
H	1.48959300	-4.14648600	4.00979200
H	1.48433800	-2.57809000	4.82824100
I	-3.31506200	1.71266600	-1.98343700
C	-1.49313200	2.48180600	0.35293300
C	-2.29536000	3.11460400	1.31867400
C	-0.44616700	3.22329200	-0.21022600
C	-2.03692700	4.42635900	1.73489500
H	-3.15804800	2.60019000	1.73713900
C	-0.19634100	4.54072300	0.18567300
H	0.16552500	2.79061300	-0.99282200
C	-0.98798300	5.14911400	1.16438700
H	-2.67747500	4.88971700	2.48325100
H	0.61855700	5.09194200	-0.27905700
H	-0.79936600	6.17700300	1.46616300
H	-5.12766400	-2.75538800	1.55549700
H	-4.00366700	-4.09418500	-0.08852600
H	5.22074400	0.97681900	2.95194700
H	5.47332600	-1.38257300	2.78423900
Se	0.12756800	-0.33719800	0.74236100
C	0.44669300	0.24281300	2.60060600
F	1.74338200	0.09060100	2.98380000
F	-0.28894500	-0.53308600	3.43545600

F	0.11863600	1.51303600	2.85765700
Se	1.49720900	-0.06753500	-2.70163700
C	1.40497000	1.76955000	-3.41084900
F	1.94737700	2.70107700	-2.59638500
F	0.14126500	2.13558300	-3.65994700
F	2.08783700	1.82644200	-4.57751800

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Zero-point correction=                           1.321202 (Hartree/Particle)
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 Thermal correction to Enthalpy=                  1.408332
 Thermal correction to Gibbs Free Energy=         1.194012
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 Sum of electronic and thermal Energies=             -8379.256526
 Sum of electronic and thermal Enthalpies=           -8379.255582
 Sum of electronic and thermal Free Energies=        -8379.469902
CPCM (Benzene) PBE0-D3/def2TZVP E = -11343.6724422
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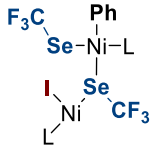
pre-RE-*bis*-SeCF$_3$ *triplet*



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N	3.121450000000	2.476664000000	-0.182508000000
N	4.558128000000	1.088217000000	0.712488000000
N	-4.568722000000	-1.211653000000	0.786848000000
N	-4.550612000000	0.972264000000	0.861490000000
H	4.764815000000	3.499045000000	-1.039430000000
H	6.268804000000	2.313220000000	0.385393000000
H	-6.649913000000	-1.435771000000	1.185625000000
H	-6.657575000000	0.906250000000	0.630809000000
C	1.944691000000	3.063334000000	-0.790039000000
C	1.028268000000	3.782735000000	0.013365000000
C	1.777138000000	2.970526000000	-2.196034000000
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C	-0.347489000000	4.127253000000	-1.974546000000
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H	0.448270000000	3.408863000000	-3.827879000000
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C	4.965214000000	-0.460194000000	2.604040000000
C	6.839761000000	-1.852573000000	1.039367000000
C	5.671741000000	-1.555378000000	3.119742000000
C	6.595877000000	-2.250756000000	2.349063000000
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H	5.497689000000	-1.861459000000	4.146054000000
H	7.131625000000	-3.097103000000	2.770748000000
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C	-4.562661000000	-3.031171000000	-0.880754000000
C	-3.904960000000	-3.491200000000	1.455549000000
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C	-3.761255000000	-4.844273000000	1.118446000000
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C	4.824011000000	1.253864000000	4.452886000000
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H	-3.599908000000	-1.978628000000	2.931624000000
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H	-5.645509000000	-1.147689000000	2.616108000000
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F	0.264767000000	0.461450000000	3.592918000000
F	0.156279000000	-1.565496000000	2.843601000000
Se	2.993286000000	-0.991835000000	-1.952096000000
C	2.697058000000	-2.806022000000	-2.677441000000
F	3.326244000000	-2.830371000000	-3.875312000000
F	1.415813000000	-3.122819000000	-2.887943000000
F	3.248788000000	-3.775466000000	-1.923283000000
I	-1.468910000000	-0.255171000000	-3.004905000000

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Zero-point correction=                           1.320265 (Hartree/Particle)
 Thermal correction to Energy=                    1.406885
 Thermal correction to Enthalpy=                  1.407829
 Thermal correction to Gibbs Free Energy=         1.190534
 Sum of electronic and zero-point Energies=          -8379.374073
 Sum of electronic and thermal Energies=             -8379.287453
 Sum of electronic and thermal Enthalpies=           -8379.286509
 Sum of electronic and thermal Free Energies=        -8379.503805
CPCM (Benzene) PBE0-D3/def2TZVP E = -11343.7009667
CPCM (Benzene) M06L/def2TZVP E = -11347.7997794
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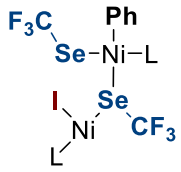
pre-RE-*bis*-SeCF$_3$ *singlet*



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C	-5.682029000000	0.697617000000	1.272915000000
C	-5.613041000000	-0.810860000000	1.484246000000
N	3.018670000000	2.445978000000	-0.161589000000
N	4.363054000000	1.051077000000	0.847364000000
N	-4.405730000000	-1.180155000000	0.709343000000
N	-4.309096000000	1.013576000000	0.810161000000
H	4.737427000000	3.433602000000	-0.910856000000
H	6.109865000000	2.245912000000	0.631545000000
H	-6.488661000000	-1.345828000000	1.112298000000
H	-6.401913000000	0.986966000000	0.497873000000
C	1.902730000000	3.067916000000	-0.836404000000
C	0.929299000000	3.765228000000	-0.082261000000
C	1.862860000000	3.065476000000	-2.256637000000
C	-0.153437000000	4.325647000000	-0.778840000000
C	0.771505000000	3.667835000000	-2.892089000000
C	-0.246203000000	4.269850000000	-2.161898000000
H	-0.933423000000	4.824929000000	-0.211334000000
H	0.718420000000	3.661884000000	-3.975634000000
H	-1.098679000000	4.711960000000	-2.670258000000
C	5.007965000000	-0.113719000000	1.411868000000
C	5.981060000000	-0.799294000000	0.639945000000
C	4.770292000000	-0.461894000000	2.763705000000
C	6.671897000000	-1.858370000000	1.241367000000
C	5.497831000000	-1.526185000000	3.312359000000
C	6.436474000000	-2.224217000000	2.562016000000
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H	5.325590000000	-1.808527000000	4.346334000000
H	6.987872000000	-3.048676000000	3.006622000000
C	-4.205899000000	-2.557004000000	0.306668000000
C	-4.540374000000	-2.936533000000	-1.019708000000
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C	-4.393341000000	-4.283425000000	-1.371020000000
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H	-4.622864000000	-4.597577000000	-2.383321000000
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C	-3.687224000000	3.185426000000	1.764107000000
C	-4.174434000000	3.016999000000	-0.649499000000
C	-3.534579000000	4.568693000000	1.609758000000
C	-4.009401000000	4.405480000000	-0.742108000000
C	-3.695219000000	5.178723000000	0.370276000000
H	-3.301309000000	5.176695000000	2.479141000000
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C	0.948223000000	4.123940000000	1.413894000000
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C	1.408244000000	5.592119000000	1.580243000000
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H	2.458180000000	5.716265000000	1.286653000000
H	0.812397000000	6.274841000000	0.966212000000
C	1.696647000000	3.237100000000	2.415585000000
H	2.782488000000	3.345334000000	2.346101000000
H	1.412051000000	3.538442000000	3.431333000000
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H	3.167499000000	0.921993000000	3.027851000000

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H	7.696821000000	1.244054000000	-0.200596000000
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C	2.528664000000	1.746626000000	-4.357196000000
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H	1.832633000000	0.953989000000	-4.076397000000
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C	-3.563774000000	-3.177910000000	2.738704000000
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H	-6.321726000000	3.532107000000	-2.391760000000
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H	-2.088858000000	2.366973000000	4.751306000000
C	1.503108000000	-2.328383000000	0.324114000000
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H	0.860447000000	-5.956085000000	1.655782000000
H	5.076832000000	2.678963000000	2.002930000000
H	4.001957000000	4.212157000000	0.501525000000
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Se	-0.314222000000	0.435425000000	0.836722000000
C	-0.651374000000	-0.274594000000	2.641653000000
F	-1.966846000000	-0.218335000000	2.988287000000
F	0.015991000000	0.472411000000	3.556966000000
F	-0.260291000000	-1.544016000000	2.823627000000
I	-1.209026000000	-0.449590000000	-2.917851000000
Se	2.794143000000	-0.910004000000	-2.012885000000
C	2.810748000000	-2.785092000000	-2.600445000000
F	3.480625000000	-3.617449000000	-1.769678000000
F	3.458158000000	-2.828507000000	-3.792666000000
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Zero-point correction=                           1.320910 (Hartree/Particle)
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 Thermal correction to Enthalpy=                  1.408033
 Thermal correction to Gibbs Free Energy=         1.193418
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 Sum of electronic and thermal Energies=             -8379.257485
 Sum of electronic and thermal Enthalpies=           -8379.256541
 Sum of electronic and thermal Free Energies=        -8379.471156
CPCM (Benzene) PBE0-D3/def2TZVP E = -11343.6760589
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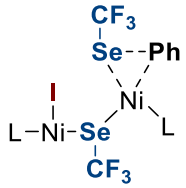
TS-RE-I/SeCF$_3$-PhSeCF$_3$ *triplet*



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C	-5.94075200	0.85479400	1.26151200
C	-5.87591700	-0.63118400	1.60509500
N	3.14618800	2.51784600	-0.37459100
N	4.61681600	1.23432800	0.60932700
N	-4.66733300	-1.06626400	0.86873400
N	-4.57369400	1.11306400	0.75901800
H	4.76192300	3.50014300	-1.32686600
H	6.30198600	2.46705800	0.18162600
H	-6.75512900	-1.19299000	1.28204200
H	-6.67489000	1.07468200	0.47576800
C	1.96850300	3.00808800	-1.05628700
C	1.04614100	3.82195600	-0.35849800

C	1.80158800	2.71447200	-2.43457800
C	-0.09674900	4.24326300	-1.05535100
C	0.64394800	3.17262100	-3.07256100
C	-0.31027200	3.91412000	-2.38647400
H	-0.84205600	4.83058400	-0.52646400
H	0.48181500	2.93096700	-4.11695600
H	-1.21938400	4.23407300	-2.88736400
C	5.28708300	0.10900000	1.21617900
C	6.25020000	-0.59799800	0.45219000
C	5.04853100	-0.20656500	2.57584300
C	6.93097200	-1.65529400	1.06760600
C	5.76273200	-1.27396200	3.13733100
C	6.68914300	-1.99741000	2.39415100
H	7.66632100	-2.21625400	0.49915100
H	5.59369600	-1.53673400	4.17663300
H	7.23020700	-2.82176600	2.85125200
C	-4.41789000	-2.47365800	0.67438000
C	-4.71116400	-3.05780600	-0.58521700
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C	-4.52797200	-4.43890400	-0.72392400
C	-3.84423500	-4.64165200	1.57488100
C	-4.10045600	-5.22722400	0.34085600
H	-4.73017100	-4.90835300	-1.68009000
H	-3.52452900	-5.26383300	2.40569600
H	-3.97490200	-6.29883800	0.20766200
C	-4.22255600	2.47041900	0.42848000
C	-3.70065700	3.30252000	1.44654000
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H	-3.08277600	5.30914600	1.91942400
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H	-3.58701800	6.22283200	-0.32155900
C	1.16506800	4.40029800	1.06111800
H	0.12828000	4.46536400	1.41298600
C	1.68795500	5.85412400	0.99405000
H	1.65521100	6.31814700	1.98748800
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H	1.08681400	6.46382200	0.31160100
C	1.91136500	3.61154400	2.14563200
H	2.99693300	3.62331700	2.01132200
H	1.70707900	4.07508300	3.11875700
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C	4.10121100	0.59603000	3.46431500
H	3.43612300	1.17710300	2.82010500
C	4.89499800	1.58912700	4.34152500
H	5.55509700	1.05334700	5.03447500
H	5.52204200	2.25964400	3.74324800
H	4.21002100	2.20486500	4.93586800
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H	2.66540400	-1.03638700	3.76921400
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H	2.47193300	0.32863300	4.87183100
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H	8.79365800	-0.18832600	-0.70018200
H	8.22512600	0.83702600	-2.02763400
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C	3.73828700	3.03448400	-4.01966900
H	4.53512900	2.52883000	-4.57854900
H	3.13368100	3.60228400	-4.73673400
H	4.20417400	3.75964400	-3.34315200
C	2.26706000	1.01138600	-4.29602000
H	3.06938200	0.40485800	-4.73213000
H	1.53479400	0.34097600	-3.83957100
H	1.77467400	1.53667900	-5.12265600
C	-3.74033100	-2.68597700	3.16123900
H	-3.69226600	-1.59717400	3.07249000
C	-4.89044800	-3.05419900	4.12482300
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C	-2.39770700	-3.14107200	3.76245800
H	-1.56362000	-2.93662200	3.08960700
H	-2.21158100	-2.60755100	4.70190000
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C	-5.27055400	-2.25125400	-1.75869500
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C	-6.80752900	-2.13063700	-1.66189200
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C	-4.88917600	-2.81991000	-3.13612200
H	-5.17775900	-2.10672800	-3.91594500
H	-3.81087000	-2.97739800	-3.21872500
H	-5.40749800	-3.76304300	-3.35090400
C	-5.20486100	2.15135400	-1.94348300
H	-5.21366900	1.10737200	-1.61788700
C	-6.66966800	2.59559200	-2.14908800
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H	-4.41606500	3.21387200	-3.69496600
H	-3.41165600	1.84264300	-3.16080300
H	-4.93063400	1.55284800	-4.01382800
C	-3.42410000	2.79637000	2.85937100
H	-3.50116000	1.70638100	2.84441600
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H	-1.79753600	2.65404300	4.29697900
C	1.75594000	-2.29815900	0.28403800
C	2.65310000	-2.86953400	1.19842500
C	0.50921800	-2.88423000	0.03237800
C	2.24453400	-3.97491600	1.95340300
H	3.65278400	-2.46738400	1.32929900
C	0.12690800	-4.00110700	0.77395200
H	-0.15565900	-2.46142500	-0.71397900
C	0.98782400	-4.54035500	1.73777500
H	2.92510400	-4.40664500	2.68293800
H	-0.84952100	-4.44525100	0.60029700
H	0.68282200	-5.41472800	2.30697800
H	5.35608400	2.95596700	1.59871600
H	4.12062100	4.35208900	0.08885000
H	-5.74262800	-0.79247600	2.68022000
H	-6.16507700	1.48460100	2.12555300
Se	-0.15070000	0.57734200	0.77079100
C	-0.31263400	-0.05253900	2.61674300
F	-1.60455700	-0.09337500	3.02949700
F	0.32977300	0.77888000	3.48626000
F	0.20364400	-1.28419800	2.84123500
Se	2.84004700	-1.45439500	-1.75112100
C	2.76520300	-3.36739200	-2.30140900
F	3.45850800	-3.40373600	-3.46042600
F	3.36554500	-4.21056500	-1.44604900
F	1.53567000	-3.83092300	-2.54415000
I	-1.52293000	-0.73196500	-2.94201800

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Zero-point correction=                           1.318893 (Hartree/Particle)
 Thermal correction to Energy=                    1.405289
 Thermal correction to Enthalpy=                  1.406233
 Thermal correction to Gibbs Free Energy=         1.187794
 Sum of electronic and zero-point Energies=          -8379.371016
 Sum of electronic and thermal Energies=             -8379.284619
 Sum of electronic and thermal Enthalpies=           -8379.283675
 Sum of electronic and thermal Free Energies=        -8379.502115
CPCM (Benzene) PBE0-D3/def2TZVP E = -11343.6967467
CPCM (Benzene) M06L/def2TZVP E = -11347.7862146
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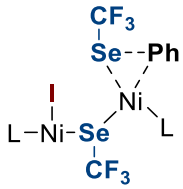
TS-RE-I/SeCF$_3$-PhSeCF$_3$ *singlet*



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C	4.43240200	3.49361400	-0.31283100
C	-3.63641200	-0.55773600	0.68570300
C	-5.48715900	-0.65494500	2.12970100
C	-4.97750300	-2.07008400	1.89281700
N	3.23761400	2.63084800	-0.18948600
N	4.89784500	1.26830600	0.17886100
N	-3.70627800	-1.82121500	1.17512700
N	-4.73062400	0.12187900	1.12216300
H	4.59905900	3.75141200	-1.36570600
H	6.44846000	2.62818400	-0.35199400
H	-5.64839100	-2.66391400	1.25968600
H	-6.56112100	-0.54815900	1.97622600
C	1.96351300	3.23817100	-0.48118800
C	1.32620400	4.01938000	0.51145500
C	1.44103600	3.15963000	-1.79949500
C	0.11635300	4.64411200	0.16778900
C	0.22979000	3.80167200	-2.07512600
C	-0.43969200	4.53054200	-1.09839400
H	-0.39505800	5.23356400	0.92482900
H	-0.19774200	3.73168500	-3.06928400
H	-1.38619500	5.01151700	-1.32898100
C	5.75418200	0.14722400	0.44493700
C	6.61516200	-0.29102600	-0.59055800
C	5.84254000	-0.38553100	1.74998800
C	7.54772100	-1.29282900	-0.29645500
C	6.79232600	-1.38714200	1.98894300
C	7.63947000	-1.83819200	0.98163300
H	8.21516300	-1.64523700	-1.07827800
H	6.87263600	-1.81449100	2.98468000
H	8.37506400	-2.61036200	1.19284800
C	-2.89825200	-2.97274700	0.85125000
C	-3.05609600	-3.61215000	-0.40166800
C	-2.08635600	-3.52594600	1.86972600
C	-2.32299500	-4.78398900	-0.63143200
C	-1.39771200	-4.71144800	1.58857800
C	-1.49910800	-5.32966100	0.34608900
H	-2.41299800	-5.28430200	-1.59050600
H	-0.77701800	-5.15959300	2.35892800
H	-0.94474400	-6.24208000	0.14396300
C	-5.26724500	1.39822400	0.70339800
C	-4.85791100	2.58617200	1.34614100
C	-6.30444100	1.39957800	-0.26289900
C	-5.45102300	3.78955700	0.94119900
C	-6.86139800	2.63069000	-0.62519200
C	-6.43236600	3.81843600	-0.04261900
H	-5.14641300	4.71760700	1.41413600
H	-7.64763400	2.65751900	-1.37358900
H	-6.87604300	4.76416500	-0.34271500
C	1.81503000	4.35030500	1.93395600
H	0.89687100	4.37453000	2.53301900
C	2.39458400	5.78325400	1.98553300
H	2.62020700	6.06484700	3.02145300
H	3.32445000	5.86794800	1.41028800
H	1.69029500	6.51612800	1.57885400
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H	3.77890000	3.41970500	2.30200500
H	2.77661700	3.65179300	3.72777200
H	2.40408000	2.34357100	2.59973700
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H	4.28564800	0.85788800	2.50323100
C	5.82147400	0.78369900	3.99507100
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H	6.41894300	1.60948200	3.59083300
H	5.17468800	1.18714400	4.78326000
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H	3.48166300	-1.48309800	2.72340100
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H	3.44763300	-0.61850300	4.27132800
C	6.58161700	0.30157100	-1.99959900
H	5.79753200	1.06424900	-2.02429300
C	7.91893700	0.98461000	-2.35471200
H	8.20142200	1.74054700	-1.61283000
H	8.73706700	0.25665300	-2.40703400
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H	6.22197400	-0.28488900	-4.06542700
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C	2.18802000	2.49065800	-2.95239700
H	2.92924800	1.80672600	-2.52903900
C	2.93551600	3.54843700	-3.79654900
H	3.51683300	3.06365600	-4.59063300
H	2.22523000	4.23503800	-4.27263000
H	3.62150100	4.15531500	-3.19567200
C	1.27158900	1.66481600	-3.87498700
H	1.87919700	1.09680900	-4.58931700
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H	0.60027600	2.30438300	-4.45907700
C	-1.97221200	-2.91705900	3.26539400
H	-2.46202500	-1.93953400	3.24665900
C	-2.67831000	-3.79820000	4.31892800
H	-3.72747300	-3.99308500	4.06831600
H	-2.18218300	-4.77175300	4.41014700
H	-2.64795000	-3.31567300	5.30318200
C	-0.51051300	-2.67546200	3.68496200
H	0.02815200	-2.10134600	2.92881800
H	-0.47727300	-2.11635300	4.62689500
H	0.02517400	-3.61882200	3.84275800
C	-4.04580500	-3.14582600	-1.46839000
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C	-5.29476200	-4.05566600	-1.47103300
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H	-3.18265900	-4.08603000	-3.25571000
C	-6.89769000	0.12610300	-0.86526100
H	-6.25176400	-0.71428800	-0.59173600
C	-8.30459800	-0.14355900	-0.28464800
H	-9.00444700	0.64552300	-0.58365800
H	-8.69745500	-1.09715600	-0.65750400
H	-8.30825800	-0.17982400	0.81081400
C	-6.97407700	0.15411900	-2.40383100
H	-7.67369100	0.91954800	-2.75950300
H	-5.99491000	0.35290100	-2.84556600
H	-7.33466700	-0.81319400	-2.77456100
C	-3.87084300	2.59798000	2.50823500
H	-3.31316900	1.65826800	2.49819600
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H	-3.31528400	4.72168400	2.51108900
H	-2.10316600	3.64181300	3.20647400
C	2.77044700	-2.30551000	-0.30121600
C	4.11231600	-2.74507200	-0.30245400
C	1.84406300	-3.00065500	0.50584400
C	4.53238500	-3.76536500	0.54487100
H	4.82650700	-2.28890800	-0.97464200
C	2.27957700	-4.02315000	1.35328200
H	0.79317000	-2.74868600	0.48309600
C	3.61845300	-4.40921100	1.38446000
H	5.57553400	-4.06714700	0.53334800
H	1.55136400	-4.52904900	1.98005500
H	3.94348600	-5.21616500	2.03592900
H	5.79486900	2.83935900	1.28147800
H	4.30327400	4.42118300	0.24668800
H	-4.79720400	-2.62108600	2.81625900
H	-5.24014000	-0.28758500	3.13350700
Se	2.22260700	-1.37028000	-2.13997100
C	0.67781300	-2.59135500	-2.46732600
F	-0.37438600	-2.32434200	-1.66143500
F	0.96261300	-3.89661400	-2.32728500
F	0.27603100	-2.39226200	-3.73693200
I	-3.06933400	1.01882100	-2.50236400
Se	-0.10313700	-0.04430400	0.64360000

C	-0.18821600	0.78911300	2.41781600		F	-0.24689600	2.13754600	2.39771900
F	-1.27744300	0.37284900	3.11887800		F	0.89567300	0.46210500	3.16200600

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Zero-point correction=                           1.318666 (Hartree/Particle)
 Thermal correction to Energy=                    1.405135
 Thermal correction to Enthalpy=                  1.406079
 Thermal correction to Gibbs Free Energy=         1.187973
 Sum of electronic and zero-point Energies=          -8379.318467
 Sum of electronic and thermal Energies=             -8379.231999
 Sum of electronic and thermal Enthalpies=           -8379.231054
 Sum of electronic and thermal Free Energies=        -8379.449161
CPCM (Benzene) PBE0-D3/def2TZVP E = -11343.6514302
CPCM (Benzene) M06L/def2TZVP E = -11347.7689492
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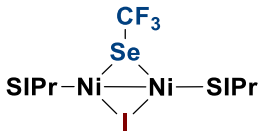

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N	4.039662000000	-0.043258000000	-0.861422000000		C	3.405273000000	-3.204589000000	2.466531000000
N	3.757755000000	-0.565795000000	1.241877000000		H	3.555392000000	-2.971555000000	1.407756000000
C	3.097803000000	-0.189308000000	0.108409000000		C	4.718459000000	-3.793986000000	3.025439000000
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H	5.688913000000	-1.419520000000	1.530397000000		H	2.151634000000	-4.628378000000	3.571666000000
H	5.636964000000	0.353110000000	1.597212000000		H	2.533488000000	-5.119802000000	1.917781000000
C	3.850232000000	0.425804000000	-2.209448000000		H	1.329972000000	-3.850474000000	2.208243000000
C	3.483089000000	-0.480021000000	-3.228879000000		Ni	-1.244453000000	0.119987000000	-0.108170000000
C	3.245604000000	-1.962962000000	-2.962878000000		N	-4.092731000000	-0.575174000000	-0.398270000000
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H	4.310429000000	-3.859396000000	-3.167004000000		H	-6.144089000000	-0.798716000000	0.129459000000
H	5.387925000000	-2.473015000000	-2.908579000000		H	-5.840965000000	0.236591000000	-1.280714000000
C	1.968159000000	-2.489028000000	-3.641559000000		C	-5.268213000000	1.159860000000	0.628465000000
H	2.065624000000	-2.508144000000	-4.733708000000		H	-5.827486000000	2.040979000000	0.306608000000
H	1.102535000000	-1.873736000000	-3.384460000000		H	-5.538194000000	0.943103000000	1.671078000000
H	1.763890000000	-3.511946000000	-3.308886000000		C	-3.876897000000	-1.835519000000	-1.055389000000
C	3.382881000000	0.009318000000	-4.537600000000		C	-3.623523000000	-1.869219000000	-2.444159000000
H	3.099169000000	-0.667942000000	-5.337414000000		C	-3.518790000000	-0.607054000000	-3.294950000000
C	3.644734000000	1.343152000000	-4.833954000000		H	-3.576248000000	0.258063000000	-2.627944000000
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C	4.022688000000	2.216920000000	-3.818947000000		H	-4.670175000000	-1.333586000000	-5.015111000000
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C	4.611245000000	2.767175000000	-1.427875000000		C	-2.167045000000	-0.514647000000	-4.027136000000
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C	3.712755000000	4.015013000000	-1.332978000000		H	-1.335963000000	-0.536818000000	-3.316711000000
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C	6.079539000000	3.179193000000	-1.667033000000		C	-3.621353000000	-4.299580000000	-2.327751000000
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H	6.745884000000	2.309937000000	-1.717928000000		C	-3.885512000000	-4.245922000000	-0.962218000000
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C	3.164798000000	1.947538000000	2.684420000000		H	-4.315240000000	-1.966386000000	1.528359000000
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C	1.890504000000	2.811508000000	2.666791000000		H	-3.358870000000	-4.867107000000	1.783739000000
H	1.093395000000	2.329460000000	2.093421000000		H	-3.612625000000	-3.716365000000	3.102747000000
H	2.099391000000	3.780880000000	2.199158000000		H	-2.336516000000	-3.427540000000	1.902227000000
H	1.518555000000	3.005164000000	3.680162000000		C	-5.795434000000	-3.522890000000	1.436502000000
C	4.304065000000	2.667153000000	3.436599000000		H	-5.889796000000	-4.576116000000	1.146248000000
H	4.033409000000	2.858715000000	4.481806000000		H	-6.540213000000	-2.958558000000	0.862920000000
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H	5.226199000000	2.073833000000	3.439039000000		C	-3.221010000000	2.518255000000	1.180109000000
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H	2.202812000000	1.359827000000	5.133247000000		C	-2.782806000000	1.071919000000	3.274362000000
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H	-1.490709000000	-0.333044000000	4.319049000000
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H	-3.571464000000	1.925881000000	5.132900000000
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H	-4.830332000000	1.418891000000	3.999688000000
C	-2.181812000000	3.518475000000	3.113814000000
H	-1.781814000000	3.435480000000	4.120304000000
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C	-2.701648000000	4.874958000000	1.192862000000
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C	-5.199361000000	4.745839000000	-0.742204000000
H	-5.901773000000	4.267861000000	-0.049571000000
H	-5.685271000000	4.821131000000	-1.722579000000
H	-5.024869000000	5.764990000000	-0.376817000000
C	-2.932505000000	4.669348000000	-1.853149000000
H	-2.706894000000	5.696616000000	-1.543536000000
H	-3.409936000000	4.722597000000	-2.839206000000
H	-1.986118000000	4.131794000000	-1.957862000000
Se	-0.120392000000	-1.580443000000	0.942580000000
C	-0.005546000000	-3.080385000000	-0.352307000000
F	-0.482837000000	-2.792204000000	-1.577419000000
F	1.284058000000	-3.476943000000	-0.515731000000
F	-0.683728000000	-4.162106000000	0.092880000000

```
Zero-point correction=                           1.212953 (Hartree/Particle)
 Thermal correction to Energy=                   1.288055
 Thermal correction to Enthalpy=                 1.288999
 Thermal correction to Gibbs Free Energy=        1.096041
 Sum of electronic and zero-point Energies=          -5411.311047
 Sum of electronic and thermal Energies=             -5411.235945
 Sum of electronic and thermal Enthalpies=           -5411.235001
 Sum of electronic and thermal Free Energies=        -5411.427959
CPCM (Benzene) PBE0-D3/def2TZVP E = -8373.51707297
CPCM (Benzene) M06L/def2TZVP E = -8376.92598502
CPCM (Benzene) M06/def2TZVP E = -8375.25900232
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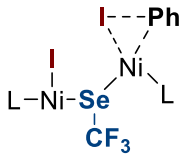
TS-OA-I/SeCF$_3$-PhI *triplet*



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C	-5.968517000000	1.700856000000	-0.164063000000
C	-6.231553000000	0.669314000000	0.927687000000
N	4.742345000000	-0.097197000000	-1.140065000000
N	4.130101000000	1.850252000000	-0.355289000000
N	-5.071118000000	-0.227729000000	0.771231000000
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C	4.699914000000	-1.429132000000	-1.702174000000
C	3.814031000000	-1.708836000000	-2.770096000000
C	5.641521000000	-2.386078000000	-1.256666000000
C	3.850611000000	-2.990636000000	-3.332812000000
C	5.639801000000	-3.646952000000	-1.864210000000
C	4.746299000000	-3.955285000000	-2.884533000000
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C	3.545779000000	3.454934000000	1.436809000000
C	2.565884000000	3.684511000000	-0.815148000000
C	2.897600000000	4.641101000000	1.804072000000
C	1.933773000000	4.857741000000	-0.389300000000
C	2.098569000000	5.337915000000	0.905241000000
C	-5.063967000000	-1.501364000000	1.443670000000
C	-4.465510000000	-1.624706000000	2.716941000000
C	-5.748178000000	-2.583128000000	0.840649000000
C	-4.540213000000	-2.865792000000	3.361964000000
C	-5.793233000000	-3.799590000000	1.530592000000
C	-5.192595000000	-3.945842000000	2.777045000000
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C	2.110982000000	-0.997144000000	4.580496000000
C	3.468880000000	-0.906873000000	4.896981000000
Se	-0.231363000000	0.519007000000	0.363897000000
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C	8.096035000000	-1.976245000000	-0.780565000000
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H	-5.236016000000	-4.901170000000	3.293693000000
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I	2.056470000000	-2.837451000000	0.511131000000
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C	3.024915000000	4.289525000000	-3.232386000000
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H	6.305521000000	3.684832000000	1.719020000000
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Zero-point correction=                           1.302494 (Hartree/Particle)
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 Thermal correction to Enthalpy=                  1.386619
 Thermal correction to Gibbs Free Energy=         1.171490
 Sum of electronic and zero-point Energies=          -5654.268999
 Sum of electronic and thermal Energies=             -5654.185818
 Sum of electronic and thermal Enthalpies=           -5654.184874
 Sum of electronic and thermal Free Energies=        -5654.400003
CPCM (Benzene) PBE0-D3/def2TZVP E = -8902.69400066
CPCM (Benzene) M06L/def2TZVP E = -8906.46391884
CPCM (Benzene) M06/def2TZVP E = -8904.54841525
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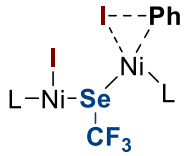
TS-OA-I/SeCF$_3$-PhI *triplet* (wB97XD opt.)



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N	-4.584561000000	0.261720000000	1.101725000000
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C	3.801419000000	-1.353371000000	-2.213209000000
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C	-4.612411000000	-2.942549000000	2.990563000000
C	-6.240665000000	-3.041662000000	1.229267000000
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Se	-0.084846000000	0.888378000000	0.387625000000
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H	2.082877000000	0.215107000000	-5.294321000000
H	1.712568000000	1.756322000000	-4.502229000000
H	-2.821587000000	-0.066279000000	2.775550000000
H	-2.055873000000	-2.770308000000	3.993050000000
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H	-1.479267000000	-2.105733000000	2.453772000000
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H	3.083490000000	2.528106000000	-2.087629000000
C	3.513684000000	4.567845000000	-2.550774000000
C	1.230264000000	3.579636000000	-2.138480000000
H	0.650410000000	2.821626000000	-1.604807000000
H	0.808649000000	4.556650000000	-1.881537000000
H	1.086109000000	3.435547000000	-3.214420000000
H	3.144751000000	5.576427000000	-2.332590000000
H	3.413157000000	4.400815000000	-3.629040000000
H	4.580143000000	4.547876000000	-2.299037000000
C	4.449488000000	1.785703000000	2.736379000000
H	4.408710000000	0.833396000000	2.201808000000
C	3.759746000000	1.577652000000	4.088672000000
C	5.928664000000	2.147184000000	2.933597000000
H	6.444046000000	2.280348000000	1.976095000000
H	6.028190000000	3.083161000000	3.496126000000
H	6.442805000000	1.356882000000	3.492446000000
H	3.846311000000	2.461455000000	4.730821000000
H	4.227699000000	0.743118000000	4.616613000000
H	2.698147000000	1.348890000000	3.959383000000

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Zero-point correction=                           1.320636 (Hartree/Particle)
 Thermal correction to Energy=                    1.400890
 Thermal correction to Enthalpy=                  1.401834
 Thermal correction to Gibbs Free Energy=         1.200411
 Sum of electronic and zero-point Energies=          -5653.536076
 Sum of electronic and thermal Energies=             -5653.455821
 Sum of electronic and thermal Enthalpies=           -5653.454877
 Sum of electronic and thermal Free Energies=        -5653.656301
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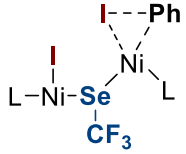
TS-OA-I/SeCF$_3$-PhI *singlet*



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C	4.72082700	2.76816400	0.53038000
C	-3.62369100	-0.04231200	0.43418300
C	-5.49397500	0.77032900	1.63888100
C	-5.78258000	-0.65523600	1.18464900
N	3.39290100	2.17918400	0.26150900
N	4.62660800	0.44816000	0.77603500
N	-4.46906200	-1.09087500	0.65963900
N	-4.22913700	1.07122800	0.93201500
H	5.18229700	3.09614500	-0.40822900
H	6.48594300	1.48995300	0.77933100
H	-6.53274800	-0.69086700	0.38658600
H	-6.27259700	1.48146200	1.35441200
C	2.33195400	3.04380400	-0.19487300
C	1.55235000	3.75128700	0.74982300
C	2.14530800	3.23782800	-1.58815100
C	0.51699400	4.56296800	0.26101700

C	1.10407900	4.07060200	-2.01202400
C	0.27871700	4.71451400	-1.09741700
H	-0.12109400	5.07718800	0.97445900
H	0.93434300	4.21201000	-3.07404800
H	-0.54369300	5.33513800	-1.44183700
C	5.14402200	-0.87798100	0.99864500
C	6.03582000	-1.42766100	0.04146400
C	4.86056400	-1.55879900	2.20755700
C	6.58419400	-2.69156700	0.29473600
C	5.44034500	-2.81901200	2.40720100
C	6.28605200	-3.38842900	1.46114200
H	7.26156500	-3.13260100	-0.43024200
H	5.23309200	-3.35811100	3.32644100
H	6.72297700	-4.36783900	1.63835200
C	-4.29611100	-2.48373600	0.31497800
C	-4.61290100	-2.93823500	-0.99023100
C	-3.94790800	-3.39713400	1.34206400
C	-4.46261500	-4.30407400	-1.26550100
C	-3.82656700	-4.75274200	1.00999900
C	-4.06155100	-5.20428500	-0.28424500
H	-4.68228800	-4.67013600	-2.26296400
H	-3.55340500	-5.46597900	1.78182100
H	-3.95662800	-6.25968100	-0.52275100
C	-3.80351000	2.44926600	0.87413800
C	-3.30943700	3.05951500	2.04950700
C	-4.04246600	3.20160000	-0.30282200
C	-3.05192000	4.43653200	2.02459900
C	-3.75312300	4.57145900	-0.27323600
C	-3.27002400	5.18931100	0.87684500
H	-2.67920000	4.92263200	2.92209500
H	-3.92375100	5.16816400	-1.16302500
H	-3.07042100	6.25813500	0.87783800
C	1.73943000	3.82570300	2.27354500
H	0.72062700	3.92941300	2.66615100
C	2.47840100	5.13020200	2.65334300
H	2.50444900	5.24959700	3.74355300
H	3.51543800	5.12553500	2.29580100
H	1.98740000	6.00991900	2.22449300
C	2.34933900	2.63272800	3.02141900
H	3.43344400	2.56535200	2.89547700
H	2.16177300	2.75830900	4.09521300
H	1.90366400	1.68799200	2.71147000
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H	3.43566100	-0.12739700	2.89964200
C	4.91917400	-0.38133800	4.43690800
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H	3.50843000	-2.75682800	4.47002000
H	2.35982900	-1.42722100	4.64242100
C	6.47378100	-0.67892900	-1.21674000
H	5.79116900	0.16524200	-1.35719900
C	7.90953800	-0.12849000	-1.05710200
H	8.02673900	0.49524300	-0.16465400
H	8.62959500	-0.95127600	-0.97375600
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C	6.40838600	-1.54100900	-2.49238500
H	5.42081000	-1.98808800	-2.62653700
H	6.62359700	-0.92065800	-3.37071600
H	7.15166800	-2.34647200	-2.47606700
C	3.08244600	2.65169100	-2.64217000
H	3.60030500	1.79485100	-2.20055500
C	4.14463600	3.69438600	-3.06099800
H	4.85009100	3.25714600	-3.77853100
H	3.66753500	4.55619600	-3.54308200
H	4.71845300	4.07485700	-2.20922200
C	2.34343300	2.15206300	-3.89840800
H	3.03062000	1.57835000	-4.53253400
H	1.49068700	1.51738900	-3.64433700
H	1.97305100	2.98563500	-4.50670800
C	-3.79385900	-2.98862800	2.80607400
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C	-5.04370400	-3.40244000	3.61667500
H	-5.97231100	-3.00320000	3.19405000
H	-5.14366600	-4.49418000	3.64258100
H	-4.96256200	-3.04920400	4.65183600
C	-2.53980800	-3.57909100	3.47698400
H	-1.63497000	-3.35706400	2.91104400
H	-2.42402300	-3.15515000	4.48142900
H	-2.61838600	-4.66664200	3.59273800
C	-5.21760600	-2.03915300	-2.06750300
H	-4.97119800	-1.00043700	-1.82662400
C	-6.75759300	-2.18641800	-2.07700200
H	-7.20183600	-1.49328400	-2.80141400
H	-7.04355300	-3.20459000	-2.36744400
H	-7.20731200	-1.98982000	-1.09825200
C	-4.68084100	-2.32281000	-3.48212100
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H	-3.58962000	-2.30292500	-3.51329100
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C	-4.65623000	2.59228200	-1.56238000
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H	-6.62742500	2.24254900	-2.43141600
H	-6.63348700	2.19863300	-0.66142700
C	-4.11928400	3.21245100	-2.86412900
H	-4.47482600	4.24043700	-3.00824200
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H	-3.88696500	2.13862500	5.36386800
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C	1.57993100	-2.54343900	-0.98157100
C	2.48272100	-3.15931300	-0.10648400
C	0.25480700	-2.98458500	-1.09802200
C	2.01949600	-4.19400000	0.71733500
H	3.52517000	-2.86846000	-0.08227700
C	-0.18225300	-4.01736300	-0.27262600
H	-0.42065100	-2.51394000	-1.80453000
C	0.69735100	-4.62505600	0.63315500
H	2.71339800	-4.66842500	1.40605300
H	-1.21496600	-4.34706500	-0.33932000
H	0.34977700	-5.44053100	1.26181500
H	5.52389100	1.67467600	2.25508800
H	4.63798100	3.63415100	1.19018000
H	-6.11314000	-1.30434600	1.99649400
H	-5.34816700	0.83785400	2.72302000
Se	-0.14981800	0.37194300	0.63294600
C	-0.30308200	-0.63666700	2.31456100
F	-1.55924300	-0.60286900	2.82951900
F	0.50908700	-0.12441000	3.27548600
F	0.02871600	-1.94230900	2.19950900
I	-1.67936800	0.07785500	-3.15832900

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Zero-point correction=                           1.304845 (Hartree/Particle)
 Thermal correction to Energy=                    1.386723
 Thermal correction to Enthalpy=                  1.387667
 Thermal correction to Gibbs Free Energy=         1.180755
 Sum of electronic and zero-point Energies=          -5654.206184
 Sum of electronic and thermal Energies=             -5654.124307
 Sum of electronic and thermal Enthalpies=           -5654.123363
 Sum of electronic and thermal Free Energies=        -5654.330274
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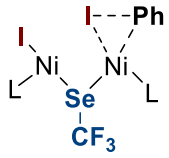
TS-OA-I/SeCF$_3$-PhI *singlet* (wB97XD opt.)



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C	-5.422287000000	0.574852000000	0.487038000000
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N	-4.033549000000	-1.254561000000	0.111843000000
N	-3.993719000000	0.904813000000	0.384069000000
H	4.797187000000	3.109843000000	-0.635827000000
H	6.182284000000	1.646861000000	0.694191000000
H	-5.815115000000	-0.981693000000	-0.981844000000
H	-6.012411000000	1.223332000000	-0.161524000000
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C	1.612236000000	3.144478000000	-1.581436000000
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C	0.462112000000	3.841726000000	-1.940454000000
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H	-0.652677000000	4.768832000000	1.109282000000
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C	5.026412000000	-1.487975000000	1.726745000000
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C	5.680363000000	-2.721497000000	1.698421000000
C	6.264778000000	-3.194527000000	0.533269000000
H	6.693661000000	-2.811027000000	-1.525901000000
H	5.731055000000	-3.321813000000	2.601451000000
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C	-3.643776000000	2.279499000000	0.615711000000
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C	-3.176109000000	4.075289000000	2.147829000000
C	-3.713759000000	4.567243000000	-0.134793000000
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H	-3.884042000000	5.295471000000	-0.922867000000
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C	1.426926000000	3.753109000000	2.280568000000
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C	2.339591000000	2.743380000000	2.982859000000
H	3.397395000000	2.947488000000	2.796302000000
H	2.187420000000	2.835213000000	4.064418000000
H	2.126358000000	1.712675000000	2.705271000000
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H	3.729505000000	-0.172466000000	2.784613000000
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C	3.629819000000	-2.058317000000	3.772430000000
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H	6.824047000000	1.331378000000	-1.122789000000
H	7.777522000000	0.035766000000	-1.857766000000
H	6.867214000000	1.164290000000	-2.879340000000
C	5.649312000000	-1.182037000000	-3.202931000000
H	4.906163000000	-1.982689000000	-3.177748000000
H	5.429137000000	-0.540366000000	-4.063180000000
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H	3.134694000000	1.814206000000	-2.259050000000
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C	-3.178325000000	-2.442431000000	2.636729000000
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C	-4.457710000000	-1.871090000000	3.265079000000
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C	-2.398116000000	-3.222132000000	3.700307000000
H	-1.503106000000	-3.688056000000	3.278508000000
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H	-3.015360000000	-3.998839000000	4.166943000000
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H	-4.138725000000	-1.749754000000	-2.305416000000
C	-5.731778000000	-3.126229000000	-2.778599000000
H	-5.969918000000	-2.618012000000	-3.719521000000
H	-5.885478000000	-4.201265000000	-2.930318000000
H	-6.450972000000	-2.798626000000	-2.020133000000
C	-3.316563000000	-3.340880000000	-3.450622000000
H	-3.484684000000	-2.795531000000	-4.385002000000
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C	-4.278695000000	2.805725000000	-1.824573000000
H	-4.214042000000	1.716850000000	-1.903595000000
C	-5.725549000000	3.239642000000	-2.111464000000
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C	-4.523399000000	1.760934000000	3.912866000000
H	-5.390006000000	1.492064000000	3.302531000000
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C	2.251239000000	-2.865065000000	0.169653000000
C	-0.002153000000	-2.924469000000	-0.738383000000
C	1.936899000000	-3.950562000000	0.989640000000
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C	-0.293074000000	-4.004900000000	0.079306000000
H	-0.736672000000	-2.557010000000	-1.445779000000
C	0.670669000000	-4.518568000000	0.950563000000
H	2.707864000000	-4.357970000000	1.637699000000
H	-1.272354000000	-4.463184000000	0.012555000000
H	0.434728000000	-5.376481000000	1.573565000000
H	5.102821000000	1.778416000000	2.094149000000
H	4.310410000000	3.753474000000	0.951518000000
H	-6.052217000000	-1.522473000000	0.693724000000
H	-5.766085000000	0.715724000000	1.516642000000
Se	-0.056289000000	0.565639000000	1.379294000000
C	0.151627000000	-0.669595000000	2.877839000000
F	-0.894326000000	-0.576290000000	3.725382000000
F	1.242622000000	-0.337682000000	3.596171000000
F	0.268571000000	-1.957409000000	2.550484000000
I	-1.752370000000	0.032450000000	-2.741027000000

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Zero-point correction=                           1.326785 (Hartree/Particle)
 Thermal correction to Energy=                    1.404452
 Thermal correction to Enthalpy=                  1.405396
 Thermal correction to Gibbs Free Energy=         1.215483
 Sum of electronic and zero-point Energies=          -5653.462584
 Sum of electronic and thermal Energies=             -5653.384917
 Sum of electronic and thermal Enthalpies=           -5653.383973
 Sum of electronic and thermal Free Energies=        -5653.573886
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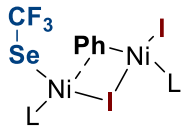
post-OA-I/SeCF$_3$ *triplet*



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C	5.79072300	0.94527100	1.19861000
C	5.38561100	2.14008000	0.34395100
C	-3.55282200	-0.06724300	0.63523100
C	-5.40953300	1.02384600	1.57869400
C	-5.79440500	-0.42742700	1.28066500
N	3.99576500	1.79795500	-0.02722500
N	4.78147200	-0.06548100	0.80915900
N	-4.59075300	-0.93637900	0.58101800
N	-3.95113500	1.04256700	1.30021500
H	5.99703200	2.22758300	-0.56259400
H	6.80101800	0.60019900	0.98598700
H	-6.67164900	-0.50839300	0.63603800
H	-5.90983800	1.73142900	0.90969600
C	3.18981100	2.80562900	-0.67852900
C	2.54794900	3.80016700	0.10159700
C	3.13166800	2.84018600	-2.09598400
C	1.76953200	4.75244200	-0.57575400
C	2.34070500	3.81981900	-2.70779600
C	1.64803400	4.76196500	-1.95815100
H	1.24704500	5.50486200	0.01024600
H	2.27524900	3.84693800	-3.79033300
H	1.02781700	5.50712500	-2.44911600
C	4.91519900	-1.41375300	1.31132300
C	5.92207700	-2.25462000	0.77073800
C	4.10969000	-1.84833900	2.39274900
C	6.04435800	-3.55130700	1.28346900
C	4.27049800	-3.16162900	2.85486600
C	5.21762900	-4.01394900	2.30063800
H	6.80031500	-4.21220300	0.87148300
H	3.65710700	-3.51365200	3.67845400
H	5.32514900	-5.02931800	2.67346600
C	-4.53749900	-2.35152000	0.26453400
C	-5.19254100	-2.83217400	-0.89491900
C	-3.95872600	-3.24748700	1.20086700
C	-5.21939800	-4.21578300	-1.11364100
C	-4.01243300	-4.61891800	0.92345700
C	-4.63361500	-5.10504100	-0.22079600
H	-5.71811000	-4.60015200	-1.99789900
H	-3.57276400	-5.31810000	1.62799000
H	-4.67013700	-6.17463200	-0.41058800
C	-3.16879800	2.10435000	1.91591800
C	-2.81439700	1.95341800	3.27998900
C	-2.90093100	3.30904000	1.22746800
C	-2.14176900	3.00381700	3.91456700
C	-2.23273600	4.33033700	1.91623800
C	-1.84577800	4.18399700	3.24223300
H	-1.85461400	2.89604700	4.95658800
H	-2.01967900	5.25939200	1.39767600
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C	2.63974900	4.05888500	1.61814400
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C	3.61970500	5.22406500	1.89361300
H	3.59561500	5.49955900	2.95511200
H	4.65261200	4.95113100	1.64541000
H	3.36506000	6.11067100	1.30425100
C	2.91390400	2.90223400	2.58801200
H	3.94654700	2.54747100	2.55284800
H	2.73473600	3.25690800	3.61084800
H	2.24811300	2.05651300	2.40951300
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H	2.94096100	-0.06166000	2.51773100
C	3.85551900	-0.39309700	4.42907500
H	4.08415600	-1.21543100	5.11805400
H	4.79872500	0.11530500	4.19994600
H	3.20536200	0.31781600	4.95337100
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H	1.15476300	-0.82397900	3.95864300
C	6.92971800	-1.80016600	-0.28578700
H	6.54985800	-0.87985400	-0.74086600
C	8.30357900	-1.51439400	0.36711800
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H	8.73994900	-2.44140300	0.75787200
H	9.00171300	-1.10364900	-0.37239000
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H	6.17919500	-3.08780000	-1.88866400
H	7.77453400	-2.37773000	-2.19878400
H	7.62397400	-3.72979900	-1.07491000
C	3.96709500	1.92619100	-2.98849100
H	4.28620500	1.05922600	-2.40629300
C	5.23259100	2.66913500	-3.47332600
H	5.86319400	1.99652300	-4.06704600
H	4.96739400	3.52696800	-4.10355300
H	5.83378900	3.05012600	-2.63961600
C	3.18742000	1.38184600	-4.19906400
H	3.78935800	0.62626600	-4.71387200
H	2.25422700	0.90280400	-3.89080500
H	2.95158300	2.17029700	-4.92432000
C	-3.36116300	-2.81144900	2.53623900
H	-3.24563700	-1.72644300	2.52217000
C	-4.31529800	-3.17067800	3.69646200
H	-5.31336700	-2.73935300	3.55772000
H	-4.43702600	-4.25698600	3.78001900
H	-3.91567700	-2.80488900	4.64979400
C	-1.96267400	-3.40106400	2.79565500
H	-1.26636300	-3.14928600	1.99155500
H	-1.55992000	-3.00485800	3.73430400
H	-1.99091100	-4.49291700	2.88842100
C	-5.91906300	-1.92904100	-1.88503700
H	-5.66401500	-0.89511900	-1.65046100
C	-7.44974600	-2.08745800	-1.75037900
H	-7.96324000	-1.38594400	-2.41805400
H	-7.76792600	-3.10148100	-2.02081200
H	-7.79769600	-1.89919500	-0.72777400
C	-5.48905100	-2.18768200	-3.34170100
H	-6.00013700	-1.48835800	-4.00957400
H	-4.41291300	-2.03942300	-3.46818900
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C	-3.34761600	3.56122700	-0.20241500
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H	-4.43244500	5.43201400	0.15310100
H	-4.99024900	4.51579500	-1.26288700
H	-5.43007400	3.98833500	0.37188800
C	-2.24737300	4.19514600	-1.07216700
H	-2.02195600	5.22307900	-0.76258200
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C	-3.15216500	0.72141200	4.11410800
H	-3.68474200	0.00997400	3.47909700
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H	-4.37314700	0.16119200	5.83325700
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C	0.65520000	-3.08949000	-0.16925600
C	-0.29280700	-1.63377200	-1.83198100
C	-0.30330600	-4.05870200	-0.47276100
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C	-1.25081600	-2.62399600	-2.15430800
H	-0.18721800	-0.77628000	-2.49628300
C	-1.26508200	-3.83398600	-1.46597900
H	-0.29373400	-5.00770100	0.06017100
H	-1.95986900	-2.43694500	-2.95544700
H	-2.00195900	-4.59438100	-1.70397800
H	5.71665000	1.14645500	2.27493000
H	5.42701900	3.09041300	0.87854400
H	-5.97453800	-1.02005100	2.18533300
H	-5.60623400	1.32128400	2.61092100
I	0.15345200	0.84853700	0.69219200
I	3.46088800	-1.89533100	-2.25528200
Se	-2.57171500	0.61876000	-2.73543300
C	-4.35236500	1.41740500	-2.85391400
F	-5.11632800	1.29862000	-1.72339400
F	-5.07378900	0.85917300	-3.85025600
F	-4.30946200	2.74328600	-3.12839800

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Zero-point correction=                           1.305626 (Hartree/Particle)
 Thermal correction to Energy=                    1.388148
 Thermal correction to Enthalpy=                  1.389092
 Thermal correction to Gibbs Free Energy=         1.179479
 Sum of electronic and zero-point Energies=          -5654.258739
 Sum of electronic and thermal Energies=             -5654.176217
 Sum of electronic and thermal Enthalpies=           -5654.175273
 Sum of electronic and thermal Free Energies=        -5654.384886
CPCM (Benzene) PBE0-D3/def2TZVP E = -8902.70288706
CPCM (Benzene) M06L/def2TZVP E = -8906.48379898
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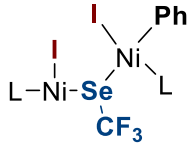
post-OA-I/SeCF$_3$ *singlet*



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C	5.17104100	1.87708800	1.14674100
C	4.36311700	2.94165600	0.41584200
C	-3.51918800	-0.16895600	0.44397500
C	-5.49515300	0.44287900	1.55983400
C	-5.41736800	-1.07698100	1.48783600
N	3.09900400	2.23030600	0.12552900
N	4.42620700	0.63826700	0.82186000
N	-4.27098500	-1.28860000	0.57194900
N	-4.15131700	0.84874300	1.08025900
H	4.83791000	3.25283200	-0.52087200
H	6.20105700	1.81612300	0.79872700
H	-6.31894500	-1.54523600	1.08942300
H	-6.26018000	0.86111700	0.89510500
C	1.99915900	3.00272800	-0.40454000
C	1.09989200	3.64006400	0.48497400
C	1.91026800	3.21403300	-1.80630300
C	0.03783700	4.36885300	-0.07434900
C	0.84253800	3.97296700	-2.29849600
C	-0.10347000	4.52832600	-1.44558800
H	-0.68696200	4.82606200	0.59362000
H	0.75336000	4.12749300	-3.36841300
H	-0.93770400	5.09755700	-1.84703000
C	5.04596500	-0.62206400	1.17379100
C	6.10737500	-1.11164400	0.36675100
C	4.69432600	-1.27551800	2.38244700
C	6.74750300	-2.29303400	0.76081800
C	5.37131300	-2.45508700	2.72092500
C	6.38091100	-2.96981200	1.91714400
H	7.55143900	-2.68679000	0.14730100
H	5.10986200	-2.97257200	3.63782900
H	6.89007500	-3.88779800	2.19910900
C	-4.13893800	-2.56151600	-0.10945200
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C	-3.75079000	-3.70568700	0.62581400
C	-4.49864600	-3.91618300	-2.07583600
C	-3.73762800	-4.93985600	-0.03743400
C	-4.09374300	-5.04781600	-1.37514200
H	-4.79138600	-4.01546100	-3.11507600
H	-3.43365400	-5.82809600	0.50663400
H	-4.06563700	-6.01397900	-1.87186500
C	-3.83312700	2.26051900	1.14067900
C	-3.45640500	2.80712400	2.39198400
C	-4.07814000	3.09446400	0.02128200
C	-3.26985100	4.19212900	2.48217500
C	-3.87534500	4.47262200	0.17328900
C	-3.47155500	5.02179200	1.38498700
H	-2.97783200	4.62630800	3.43391000
H	-4.05791500	5.12878100	-0.67154700
H	-3.33137600	6.09568600	1.47775000
C	1.18476500	3.75933600	2.01716700
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C	1.74848300	5.15057900	2.39321100
H	1.70549100	5.29942900	3.47928800
H	2.79645700	5.25316000	2.08517200
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C	1.89560900	2.67827200	2.83997200
H	2.98289200	2.71682500	2.73831000
H	1.66861800	2.83974200	3.90123400
H	1.55711100	1.67655600	2.57717300
C	3.68053600	-0.70989400	3.37538100
H	3.01906100	-0.02748700	2.83659100
C	4.40244300	0.09792400	4.47732400
H	5.05410600	-0.55581000	5.06991500
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H	3.67407400	0.55547700	5.15769500
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H	2.28626500	-2.40323600	3.28565300
H	3.37573700	-2.44683700	4.68540600
H	2.03188300	-1.30801300	4.65125200
C	6.64475800	-0.39130300	-0.87039100
H	5.90719700	0.35715800	-1.17640500
C	7.98537600	0.31465000	-0.55584400
H	7.92546000	0.99934500	0.29710800
H	8.75965400	-0.42445600	-0.31786800
H	8.32776900	0.88692600	-1.42646400
C	6.86112700	-1.33276300	-2.07245900
H	5.96594200	-1.92024000	-2.28381600
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H	7.70166500	-2.01671700	-1.90416100
C	2.97673600	2.74712900	-2.79444900
H	3.56477700	1.95601400	-2.32226300
C	3.92050700	3.91985400	-3.15008500
H	4.72721900	3.57199700	-3.80653800
H	3.37416400	4.70959300	-3.68029800
H	4.37605500	4.37879100	-2.26536700
C	2.38979300	2.15866700	-4.09094500
H	3.19296500	1.71465900	-4.68910800

H	1.65969300	1.37425200	-3.88016000
H	1.91029000	2.93030900	-4.70606600
C	-3.40162000	-3.67928900	2.11198800
H	-3.21738600	-2.64178700	2.40129200
C	-4.57334000	-4.22683500	2.95861800
H	-5.51224900	-3.69105500	2.78022000
H	-4.75384000	-5.28308600	2.72672100
H	-4.33807700	-4.15575800	4.02743100
C	-2.12147100	-4.47411300	2.43711900
H	-1.29848800	-4.21228600	1.77023000
H	-1.81077400	-4.26903600	3.46782600
H	-2.28997700	-5.55454200	2.35850100
C	-5.14708900	-1.48406100	-2.24422400
H	-4.69495000	-0.56063900	-1.87199600
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H	-7.09015700	-0.53771800	-2.56116600
H	-7.17137400	-2.29886200	-2.37166100
H	-6.93043400	-1.26812100	-0.95641100
C	-4.86244600	-1.53289000	-3.75553700
H	-5.17144800	-0.58747200	-4.21546700
H	-3.79831200	-1.67456000	-3.96139200
H	-5.42511100	-2.33145500	-4.25319100
C	-4.63801700	2.58943700	-1.30614900
H	-4.48541700	1.50795000	-1.35560500
C	-6.15702200	2.85892800	-1.39185900
H	-6.36113300	3.93622000	-1.37931800
H	-6.56453600	2.45075800	-2.32430900
H	-6.70742600	2.41203300	-0.55672100
C	-3.93132000	3.20077100	-2.53013700
H	-4.16548100	4.26614400	-2.64242500
H	-2.84677400	3.08503600	-2.46756000
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C	-3.30340900	1.97463000	3.66228200
H	-3.39845700	0.92139000	3.39307500
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H	-5.41499100	2.19192300	4.26798000
H	-4.32622000	1.65848400	5.56345100
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C	-1.91701700	2.15083300	4.30860500
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I	3.07878500	-1.14431400	-2.42874400
C	1.28562100	-2.45103900	-0.32730600
C	2.07225200	-3.31949200	0.44816300
C	0.21121000	-2.99854600	-1.03991900
C	1.76213200	-4.68098400	0.55342900
H	2.95775100	-2.94973800	0.96139700
C	-0.09253400	-4.36074500	-0.95083700
H	-0.37988700	-2.37011300	-1.69975900
C	0.67719100	-5.20861900	-0.14867300
H	2.38912800	-5.32984500	1.16234400
H	-0.93010100	-4.75871700	-1.51916500
H	0.44669900	-6.26995800	-0.08878800
H	5.18643500	2.02695900	2.23275500
H	4.17602400	3.83376600	1.01828000
H	-5.19559300	-1.52108000	2.46315500
H	-5.67364100	0.81460300	2.56939700
Se	-0.18123800	0.23420100	0.75523900
C	-0.54760900	-0.77686600	2.41234300
F	-1.85901400	-0.71661200	2.76991800
F	0.15182000	-0.22308500	3.43305200
F	-0.21979100	-2.07214800	2.37214500
I	-1.37736700	0.22873600	-3.07628900

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Zero-point correction=                           1.306515 (Hartree/Particle)
 Thermal correction to Energy=                    1.388450
 Thermal correction to Enthalpy=                  1.389394
 Thermal correction to Gibbs Free Energy=         1.183978
 Sum of electronic and zero-point Energies=          -5654.235422
 Sum of electronic and thermal Energies=             -5654.153487
 Sum of electronic and thermal Enthalpies=           -5654.152543
 Sum of electronic and thermal Free Energies=        -5654.357959
CPCM (Benzene) PBE0-D3/def2TZVP E = -8902.67426249
CPCM (Benzene) M06L/def2TZVP E = -8906.46723012
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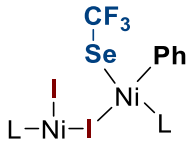
pre-RE-I/SeCF$_3$ *triplet*



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C	5.19038900	2.52218700	0.64563700
C	4.41177100	3.19132500	-0.48505900
C	-4.05377300	0.03053400	0.53424200
C	-6.04896000	0.98518700	1.38886400
C	-6.10970600	-0.53484500	1.57180500
N	3.19425800	2.35101000	-0.57251700
N	4.52713200	1.19858200	0.72949300
N	-4.89316100	-0.98340900	0.86369400
N	-4.66805000	1.18694600	0.89923700
H	4.94756600	3.15106400	-1.44062300
H	6.25277800	2.41564100	0.42568800
H	-7.00345000	-0.98299400	1.13042700
H	-6.76750400	1.34627700	0.64264500
C	2.10167800	2.77603700	-1.42439000
C	1.14010300	3.68834100	-0.92716400
C	2.05752500	2.32027000	-2.76660900
C	0.06713900	4.01442900	-1.77123800
C	0.96672400	2.69367700	-3.55909300
C	-0.03800500	3.51239100	-3.06056900
H	-0.70856700	4.67341700	-1.39021900
H	0.90090100	2.33060400	-4.57880800
H	-0.89389500	3.76648600	-3.67916600
C	5.05571200	0.18927500	1.61949900
C	6.20329800	-0.54166000	1.21912600
C	4.48076600	0.00778800	2.90202700
C	6.71711100	-1.49639200	2.10421900
C	5.03523000	-0.96962800	3.74021200
C	6.13476600	-1.72341800	3.34662700
H	7.58983700	-2.07278500	1.81362500
H	4.60533600	-1.12902400	4.72400000
H	6.54774900	-2.47581700	4.01327300
C	-4.60767200	-2.39142500	0.76206700
C	-5.13019100	-3.11769300	-0.33266400
C	-3.89122600	-3.02781700	1.80184300
C	-4.88152500	-4.49464400	-0.38412800
C	-3.67261900	-4.40710900	1.69890600
C	-4.15583600	-5.13513700	0.61583100
H	-5.26487300	-5.07313900	-1.21923400
H	-3.11964000	-4.91788800	2.48160600
H	-3.97458900	-6.20531800	0.55510300
C	-4.16619200	2.52445900	0.73188700
C	-3.62233000	3.18540200	1.85907300
C	-4.31613300	3.18403900	-0.50986600
C	-3.19170900	4.50899200	1.70556600
C	-3.86989800	4.50892800	-0.60645700
C	-3.30881200	5.16674200	0.48410400
H	-2.77193800	5.03552100	2.55826200
H	-3.97797600	5.03729700	-1.54909500
H	-2.97836900	6.19802800	0.38689600
C	1.14559100	4.48315000	0.39139800
H	0.08403500	4.58783600	0.64903200

C	1.67184100	5.91457300	0.12981600
H	1.56449300	6.53148900	1.03050700
H	2.73435000	5.91019200	-0.14438200
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C	1.81076800	3.90138500	1.64494900
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H	1.52601700	4.51511300	2.50867700
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C	3.35849400	0.88836900	3.44742400
H	2.87000000	1.38264300	2.60568400
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H	4.42813400	1.54980300	5.24027900
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C	2.26852800	0.10542900	4.20278200
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H	1.44292200	0.77908100	4.45707600
C	6.94682000	-0.29164000	-0.09258400
H	6.30361400	0.31679000	-0.73684300
C	8.25487400	0.48977100	0.17061300
H	8.08664000	1.41558100	0.73196300
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H	6.37423300	-2.16965100	-1.06208100
H	7.72885600	-1.32683100	-1.83285800
H	7.99024200	-2.21164900	-0.32855400
C	3.18999300	1.53492500	-3.42413100
H	3.80751400	1.08885900	-2.63985200
C	4.08999500	2.48822100	-4.24386000
H	4.93490000	1.93875600	-4.67652800
H	3.52567100	2.94062500	-5.06783800
H	4.49118000	3.30713000	-3.63529700
C	2.69669800	0.38595400	-4.32286300
H	3.54579300	-0.23626600	-4.62735100
H	1.97588000	-0.25137300	-3.80540700
H	2.22391600	0.76256000	-5.23703000
C	-3.41090000	-2.28698500	3.04775100
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C	-4.26664900	-2.67369200	4.27380700
H	-5.33458200	-2.49390000	4.10255600
H	-4.14826200	-3.73689000	4.51456000
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C	-1.91797000	-2.51700200	3.34445500
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C	-5.99652000	-2.47182600	-1.41103100
H	-5.90892300	-1.38589500	-1.30344400
C	-7.48031100	-2.85333000	-1.21244600
H	-8.11056700	-2.33946100	-1.94827900
H	-7.62623100	-3.93240000	-1.34240000
H	-7.84483500	-2.59347100	-0.21140200
C	-5.54337900	-2.82401100	-2.83963800
H	-6.15543700	-2.27756200	-3.56741700
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H	-6.93913700	2.61396700	-2.71879900
H	-7.03475100	3.00286400	-0.98942000
C	-4.19579600	2.68449800	-3.01279200
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H	-1.82200700	3.62287800	4.04439700
H	-2.13316300	2.06528600	4.81949100
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C	0.40700600	-2.96170000	-0.17279000
C	1.61110700	-4.16425200	2.05309700
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C	-0.05366400	-4.19358100	0.30279000
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C	0.54481500	-4.79557800	1.41342700
H	2.09337500	-4.62930100	2.91004200
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H	0.18601700	-5.75706400	1.77241700
H	5.08687900	3.04695200	1.60281600
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H	-6.06296900	-0.83424700	2.62625300
H	-6.21884200	1.53546300	2.31775300
Se	3.61195700	-1.48167800	-1.41617900
C	3.31910300	-3.37287000	-1.91597600
F	4.29383500	-3.66479700	-2.81023400
F	2.14261100	-3.59646100	-2.51516500
F	3.44231100	-4.23789400	-0.89888900
I	-1.89198400	-0.80329300	-2.95853500
I	-0.09512600	0.51888200	0.89084400

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Zero-point correction=                           1.304082 (Hartree/Particle)
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 Thermal correction to Enthalpy=                  1.388383
 Thermal correction to Gibbs Free Energy=         1.173497
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 Sum of electronic and thermal Energies=             -5654.181065
 Sum of electronic and thermal Enthalpies=           -5654.180121
 Sum of electronic and thermal Free Energies=        -5654.395008
CPCM (Benzene) PBE0-D3/def2TZVP E = -8902.69812381
CPCM (Benzene) M06L/def2TZVP E = -8906.47790308
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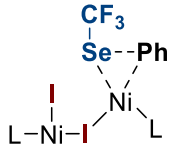
TS-RE-I_2-PhSeCF_3 *triplet*



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C	5.17521200	2.58708000	0.63123600
C	4.28454100	3.31470300	-0.37290200
C	-4.06812600	-0.04384000	0.53551600
C	-6.15852300	0.82210500	1.25177700
C	-6.11384100	-0.67892400	1.55790800
N	3.09854100	2.43117700	-0.43872600
N	4.55162100	1.24101800	0.68534700
N	-4.83866500	-1.08830800	0.93340500
N	-4.78272600	1.08775000	0.77946300
H	4.74414400	3.38504400	-1.36501200
H	6.21473900	2.51860800	0.30911600
H	-6.95313600	-1.22950400	1.12485300
H	-6.87974400	1.06881500	0.46257600
C	1.92600800	2.85979000	-1.17477300
C	0.94960800	3.65995700	-0.53313300
C	1.81143100	2.52024700	-2.54835400
C	-0.20615700	3.97397000	-1.26423100
C	0.64091300	2.88175000	-3.22453100
C	-0.37601800	3.57623800	-2.58258600
H	-0.99356700	4.53948200	-0.77385000
H	0.51993400	2.60281700	-4.26520800
H	-1.29421600	3.81593100	-3.11084700
C	5.21460000	0.22807600	1.47441000
C	6.33553700	-0.43832700	0.91758900
C	4.82410500	0.01252600	2.81838000
C	7.02575100	-1.35193100	1.72388200
C	5.55595300	-0.91148300	3.57618200
C	6.64226600	-1.59270300	3.03913400
H	7.88140800	-1.87954500	1.31388900
H	5.26906800	-1.09376600	4.60719400
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C	-3.82714900	-3.08401800	1.96785800
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C	-3.54228500	-4.45360700	1.89430300
C	-3.90468100	-5.20739300	0.78205200
H	-4.86644700	-5.20205100	-1.13485100
H	-3.03504300	-4.93680300	2.72426700
H	-3.67264700	-6.26878300	0.74424100
C	-4.41250900	2.43424900	0.43406700
C	-3.93449100	3.28879100	1.45469500
C	-4.63287500	2.90600800	-0.88086300
C	-3.64875300	4.61918700	1.12350900
C	-4.32478200	4.24444300	-1.15864100
C	-3.83640500	5.09518800	-0.17139600
H	-3.28543800	5.29394200	1.89369600
H	-4.48701800	4.62874200	-2.16152200
H	-3.61573700	6.13336600	-0.40758000
C	1.02069300	4.35659100	0.83700500
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C	1.46284100	5.82675100	0.64341700
H	1.39879900	6.37218300	1.59293900
H	2.50014800	5.89316300	0.29190400
H	0.83475600	6.34129300	-0.09077900
C	1.80597500	3.71777400	1.98859400
H	2.88941000	3.77406300	1.85220300
H	1.57491200	4.26036600	2.91374900
H	1.51989300	2.67507400	2.13180900
C	3.68193200	0.76747500	3.49043400
H	3.09793100	1.26272700	2.71328800
C	4.23115200	1.85775300	4.43524600
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H	3.40669900	2.43098900	4.87501600
C	2.71643200	-0.16173000	4.25049200
H	2.34842700	-0.96736600	3.60949700
H	3.19053400	-0.61116900	5.13134100
H	1.84986500	0.41055700	4.59902800
C	6.85738900	-0.17552500	-0.49454900
H	6.10658400	0.41644100	-1.02856300
C	8.17516800	0.63056200	-0.45537500
H	8.08017400	1.56794300	0.10411100
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H	8.50433100	0.87345200	-1.47255400
C	7.07304500	-1.47078200	-1.30151300
H	6.16260400	-2.07331700	-1.33135400
H	7.35326400	-1.22361800	-2.33221000
H	7.88109300	-2.08053500	-0.88143600
C	2.93801300	1.87113000	-3.34951800
H	3.61686600	1.37138000	-2.65230900
C	3.74348300	2.95257600	-4.10607700
H	4.58294600	2.49699200	-4.64538500
H	3.10823600	3.46130000	-4.84064400
H	4.14579800	3.72117300	-3.43607700
C	2.44307500	0.80607900	-4.34600400
H	3.29594200	0.24543600	-4.74530200
H	1.75876200	0.09847700	-3.87192300
H	1.92625200	1.26137200	-5.19891200
C	-3.47264200	-2.31519900	3.23789300
H	-3.59560600	-1.24713100	3.03124300
C	-4.43131300	-2.69224000	4.38867800
H	-5.48175400	-2.53299500	4.11876300
H	-4.32011800	-3.74925200	4.65904400
H	-4.21434700	-2.09376800	5.28191100
C	-2.01124900	-2.52512100	3.67423900
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H	-1.78117100	-1.88094200	4.53141600
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C	-5.69917800	-2.64072600	-1.40246300
H	-5.66858800	-1.55137000	-1.29987200
C	-7.17572000	-3.08511400	-1.31444500
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H	-7.62800200	-2.83028100	-0.34862800
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C	-6.70190100	2.50504300	-2.26765100
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H	-7.32283000	2.50532300	-1.36390800
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H	-4.35898600	3.03238500	-3.72102200
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C	-4.86451300	3.45395500	3.80046600
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C	3.06127400	-2.76540900	1.34588600
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C	2.81440900	-3.93471400	2.07532400
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C	0.68396600	-4.19005400	0.96177400
H	0.16950400	-2.67895900	-0.48329400
C	1.62900600	-4.64574600	1.88567400
H	3.56691500	-4.29407700	2.77300200
H	-0.24281800	-4.73560200	0.80416500
H	1.44826600	-5.56159600	2.44247800
H	5.15309200	3.04044800	1.62920700
H	4.00195000	4.31923200	-0.05300900
H	-6.08983900	-0.88552600	2.63466800
H	-6.39432400	1.43051500	2.12898100
I	-0.18554700	0.33592500	1.35623500
Se	3.34551100	-1.37811200	-1.65141400
C	2.76613500	-3.06268300	-2.51426800
F	1.46008200	-3.12285100	-2.78826500
F	3.09240000	-4.16101500	-1.81271900
F	3.44110200	-3.11703400	-3.68422100
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Zero-point correction=                           1.304027 (Hartree/Particle)
 Thermal correction to Energy=                    1.386703
 Thermal correction to Enthalpy=                  1.387647
 Thermal correction to Gibbs Free Energy=         1.175257
 Sum of electronic and zero-point Energies=          -5654.262947
 Sum of electronic and thermal Energies=             -5654.180271
 Sum of electronic and thermal Enthalpies=           -5654.179327
 Sum of electronic and thermal Free Energies=        -5654.391718
CPCM (Benzene) PBE0-D3/def2TZVP E = -8902.69708564
CPCM (Benzene) M06L/def2TZVP E = -8906.46755982
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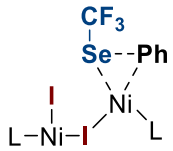
TS-RE-I_2-PhSeCF_3 *singlet*



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C	-3.80430700	-0.05403600	0.47351900
C	-5.88278600	0.74830800	1.24363000
C	-5.94391400	-0.77602600	1.13775500
N	3.19458100	2.39064400	-0.16670500
N	4.58025200	1.06672500	0.88218500
N	-4.53851100	-1.13309800	0.83860000
N	-4.56481500	1.05630200	0.64487300
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H	6.25425700	2.38587800	0.82736500
H	-6.59216800	-1.10495400	0.31955300
H	-6.68071100	1.24668000	0.68925300
C	2.10672700	2.90828000	-0.95990100
C	1.09842000	3.68756500	-0.34566000
C	2.10651500	2.68598000	-2.36193200
C	0.03830900	4.13068200	-1.15366300
C	1.03358200	3.17344800	-3.11537800
C	-0.00819400	3.87219100	-2.51608700
H	-0.77009300	4.68956400	-0.68946900
H	1.01076600	2.99751900	-4.18574400
H	-0.84886600	4.21960000	-3.11060200
C	5.18340300	-0.06285900	1.53992200
C	6.27381300	-0.71399000	0.91105000
C	4.75070800	-0.44353900	2.83285300
C	6.87521700	-1.78998500	1.57663600
C	5.39040700	-1.52501700	3.45234900
C	6.43493100	-2.20172900	2.83063300
H	7.70607300	-2.30909200	1.10803500
H	5.06920900	-1.83591900	4.44217200
H	6.91517200	-3.04027900	3.32844500
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C	-4.46352300	-3.46470300	0.02022600
C	-3.46630300	-2.87921800	2.20351700
C	-4.12549300	-4.80321900	0.26180900
C	-3.15387800	-4.23152200	2.38763400
C	-3.47568800	-5.18742300	1.42905400
H	-4.38397700	-5.55563000	-0.47659600
H	-2.65866800	-4.54189600	3.30188000
H	-3.22701600	-6.23234500	1.59609900
C	-4.17416300	2.44179900	0.51386700
C	-3.66077400	3.12032200	1.64606300
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C	-3.36759200	4.48415800	1.51923400
C	-4.12513400	4.48687600	-0.76540100
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C	6.86038600	-0.24930200	-0.42082600
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C	3.26431700	2.01296300	-3.09637700
H	3.82338100	1.40951800	-2.37581200
C	4.22039500	3.07316300	-3.68883800
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H	4.60809800	3.76016400	-2.92887300
C	2.79919700	1.06785900	-4.21955700
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H	2.43084100	1.62559300	-5.08910600
C	-3.17144000	-1.89254400	3.33244400
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C	-4.30519700	-1.90916700	4.38156500
H	-5.28126000	-1.67162000	3.94443700
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H	-1.82983100	-3.06595200	4.61957800
C	-5.24443900	-3.12327200	-1.24627900
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I	-0.09721300	0.12847100	1.17655700
Se	3.30759200	-1.72932400	-1.79998300
C	2.19326200	-2.45557300	-3.29707600
F	1.00967400	-1.82916200	-3.44382100
F	1.94460900	-3.77186900	-3.19371500
F	2.90231300	-2.26424700	-4.42820200
I	-2.53980700	-0.50761600	-2.76677400

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Zero-point correction=                           1.305141 (Hartree/Particle)
 Thermal correction to Energy=                   1.387068
 Thermal correction to Enthalpy=                 1.388012
 Thermal correction to Gibbs Free Energy=        1.179559
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 Sum of electronic and thermal Energies=             -5654.135811
 Sum of electronic and thermal Enthalpies=           -5654.134866
 Sum of electronic and thermal Free Energies=        -5654.343320
CPCM (Benzene) PBE0-D3/def2TZVP E = -8902.65501574
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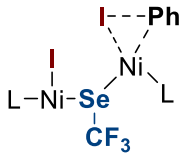
TS-OA-I/SeCF$_3$-PhBr *triplet*



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C	4.143573000000	-0.681233000000	-3.091186000000
C	5.535937000000	-2.320686000000	-1.885208000000
C	4.158840000000	-1.535908000000	-4.200383000000
C	5.521707000000	-3.131271000000	-3.025883000000
C	4.837595000000	-2.749067000000	-4.174402000000
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C	2.848949000000	4.246697000000	3.262518000000
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Se	-0.182531000000	0.653390000000	0.165035000000
C	-0.360714000000	1.354442000000	1.982868000000
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F	0.558301000000	2.311795000000	2.250262000000
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C	6.310143000000	-2.798687000000	-0.659395000000
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C	-4.271455000000	0.497806000000	-4.813157000000
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H	6.082009000000	-4.964819000000	-0.911306000000
H	6.320644000000	-4.451212000000	0.761876000000
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H	1.893469000000	0.120247000000	-4.708867000000
H	1.417538000000	1.431537000000	-3.621123000000
H	1.419739000000	-0.242864000000	-3.041884000000
H	5.192326000000	1.795460000000	-3.816017000000
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H	3.649143000000	2.581317000000	-4.205677000000
H	-4.093101000000	1.126922000000	2.265507000000
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H	-2.807921000000	0.816429000000	4.305610000000
H	-2.788611000000	-0.694337000000	3.380951000000
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H	-0.924130000000	5.477042000000	-0.186294000000
H	-1.890671000000	5.276801000000	1.279246000000
H	-3.969003000000	-0.073216000000	-2.769213000000
H	-1.692739000000	-0.608320000000	-4.744987000000
H	-2.856558000000	-1.783110000000	-4.110960000000
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H	-5.026482000000	1.267194000000	-4.611407000000
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H	-4.792955000000	-0.431667000000	-5.070758000000
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C	2.097382000000	3.937974000000	-1.071466000000
H	1.433521000000	3.091533000000	-0.870815000000
H	1.621703000000	4.838524000000	-0.666124000000
H	2.176983000000	4.065738000000	-2.158019000000
H	4.021321000000	5.849249000000	-0.336702000000
H	4.507297000000	5.064500000000	-1.845798000000
H	5.424402000000	4.774941000000	-0.354381000000
C	4.270527000000	0.731525000000	3.684603000000
H	4.438433000000	-0.015307000000	2.902411000000
C	3.215715000000	0.154852000000	4.647837000000
C	5.608342000000	0.956517000000	4.420118000000
H	6.386360000000	1.338275000000	3.748599000000
H	5.492755000000	1.681727000000	5.234382000000
H	5.967930000000	0.017389000000	4.857370000000
H	3.062760000000	0.807560000000	5.515118000000
H	3.541526000000	-0.820469000000	5.022314000000
H	2.250465000000	0.021797000000	4.150393000000

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Zero-point correction=                           1.302602 (Hartree/Particle)
 Thermal correction to Energy=                    1.385615
 Thermal correction to Enthalpy=                  1.386559
 Thermal correction to Gibbs Free Energy=         1.173575
 Sum of electronic and zero-point Energies=          -8214.262655
 Sum of electronic and thermal Energies=             -8214.179642
 Sum of electronic and thermal Enthalpies=           -8214.178698
 Sum of electronic and thermal Free Energies=        -8214.391682
CPCM (Benzene) PBE0-D3/def2TZVP E = -11178.8316095
CPCM (Benzene) M06L/def2TZVP E = -11182.6515095
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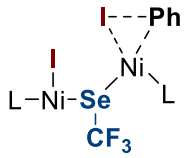
TS-OA-I/SeCF$_3$-PhCl *triplet*



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C	-6.053541000000	1.525591000000	0.097040000000
N	4.956943000000	-0.278643000000	-0.905710000000
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N	-5.113040000000	0.396796000000	0.248026000000
N	-3.965037000000	1.863534000000	-0.890730000000
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C	4.084938000000	-0.677337000000	-3.188797000000
C	5.515159000000	-2.358252000000	-2.089331000000
C	4.063889000000	-1.491444000000	-4.328029000000
C	5.463950000000	-3.126878000000	-3.257658000000
C	4.743238000000	-2.703731000000	-4.368760000000
C	3.931955000000	2.043166000000	1.641336000000
C	3.893940000000	1.765530000000	3.024535000000
C	3.502028000000	3.289246000000	1.124598000000
C	3.405090000000	2.761557000000	3.879994000000
C	3.014390000000	4.242917000000	2.024304000000
C	2.970264000000	3.987798000000	3.390911000000
C	-5.532712000000	-0.767526000000	0.985469000000
C	-5.243932000000	-0.874223000000	2.363308000000
C	-6.313225000000	-1.738229000000	0.316270000000
C	-5.735077000000	-1.989929000000	3.052796000000
C	-6.781242000000	-2.830711000000	1.054247000000
C	-6.494319000000	-2.961366000000	2.409246000000
C	-2.974948000000	2.455311000000	-1.749690000000
C	-2.723250000000	1.897694000000	-3.024705000000
C	-2.349447000000	3.654878000000	-1.333747000000
C	-1.795383000000	2.543938000000	-3.853128000000
C	-1.446786000000	4.268510000000	-2.209351000000
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C	0.964508000000	-2.704615000000	1.837993000000
C	3.454542000000	-3.367765000000	2.956752000000
C	1.035683000000	-3.376595000000	3.060797000000
C	2.272355000000	-3.711465000000	3.619287000000
Se	-0.125839000000	0.565792000000	0.188934000000
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F	-0.128352000000	0.119211000000	2.945291000000
F	-1.484472000000	1.692910000000	2.310645000000
F	0.651734000000	2.060019000000	2.381709000000
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C	7.838852000000	-2.901092000000	-1.220767000000
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C	1.875778000000	0.501214000000	-3.663539000000
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H	-7.038617000000	1.175638000000	-0.219698000000
H	-6.166444000000	2.048291000000	1.056521000000
H	3.505630000000	-1.165232000000	-5.200424000000
H	5.992443000000	-4.075030000000	-3.294457000000
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H	2.668057000000	5.201072000000	1.647627000000
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H	-7.373543000000	-3.593524000000	0.557033000000
H	-6.863007000000	-3.820496000000	2.963725000000
H	-1.583776000000	2.128903000000	-4.834508000000
H	-0.959363000000	5.192185000000	-1.910904000000
H	-0.456753000000	4.208307000000	-4.120977000000
H	4.317452000000	-2.443340000000	1.204450000000
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H	4.419124000000	-3.642534000000	3.376743000000
H	0.111542000000	-3.666213000000	3.553289000000
H	2.315419000000	-4.262043000000	4.555023000000
H	6.171379000000	-2.200340000000	-0.062415000000
H	8.059866000000	-3.596643000000	-2.038510000000
H	8.409571000000	-3.227181000000	-0.343045000000
H	8.211907000000	-1.915460000000	-1.522582000000
H	4.786229000000	-4.303021000000	-0.261566000000
H	6.071341000000	-5.034163000000	-1.231869000000
H	6.390910000000	-4.587304000000	0.447243000000
H	3.342150000000	1.088095000000	-2.233837000000
H	1.788226000000	0.180830000000	-4.708303000000
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H	1.360116000000	-0.237358000000	-3.042814000000
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H	4.101091000000	1.291490000000	-5.197223000000
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H	-8.780227000000	-2.230657000000	-0.969644000000
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H	-4.958710000000	0.200230000000	-5.078163000000
Cl	1.986375000000	-2.481747000000	-0.971484000000
C	3.565949000000	3.642165000000	-0.358808000000
H	3.992110000000	2.789335000000	-0.894759000000
C	4.486553000000	4.852288000000	-0.618169000000
C	2.162543000000	3.885942000000	-0.944876000000
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H	1.691163000000	4.765298000000	-0.490907000000
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H	4.095879000000	5.761033000000	-0.146289000000
H	4.566104000000	5.046014000000	-1.694402000000
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C	4.381419000000	0.450527000000	3.621695000000
H	4.542792000000	-0.255406000000	2.801240000000
C	3.332342000000	-0.174343000000	4.561021000000
C	5.724802000000	0.637551000000	4.357445000000
H	6.498022000000	1.050198000000	3.698714000000
H	5.615768000000	1.323339000000	5.205999000000
H	6.086192000000	-0.321792000000	4.746664000000
H	3.182987000000	0.434542000000	5.460294000000
H	3.660967000000	-1.166571000000	4.885585000000
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Zero-point correction=                           1.302786 (Hartree/Particle)
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 Thermal correction to Enthalpy=                  1.386553
 Thermal correction to Gibbs Free Energy=         1.173057
 Sum of electronic and zero-point Energies=          -6103.042268
 Sum of electronic and thermal Energies=             -6102.959445
 Sum of electronic and thermal Enthalpies=           -6102.958501
 Sum of electronic and thermal Free Energies=        -6103.171997
CPCM (Benzene) PBE0-D3/def2TZVP E = -9065.02749282
CPCM (Benzene) M06L/def2TZVP E = -9068.79039616
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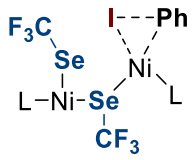
TS-OA-bis-SeCF$_3$-PhBr *triplet*



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C	-4.763171000000	-2.812883000000	0.867631000000
C	3.760024000000	0.477203000000	0.503474000000
C	5.536951000000	0.414854000000	2.064416000000
C	5.726061000000	1.624880000000	1.155264000000
N	-3.484401000000	-2.154799000000	0.521768000000
N	-4.885590000000	-0.484373000000	0.624494000000
N	4.438637000000	1.655859000000	0.426747000000
N	4.445938000000	-0.311585000000	1.376132000000
H	-5.116691000000	-3.403206000000	0.015292000000
H	-6.642938000000	-1.687364000000	0.685166000000
H	6.553015000000	1.491989000000	0.445614000000
H	6.428617000000	-0.208027000000	2.159163000000
C	-2.315164000000	-2.968078000000	0.272880000000
C	-1.509416000000	-3.383208000000	1.359377000000

C	-2.038759000000	-3.385835000000	-1.055382000000
C	-0.370956000000	-4.147903000000	1.062001000000
C	-0.889809000000	-4.150765000000	-1.282203000000
C	-0.050387000000	-4.516204000000	-0.236777000000
H	0.287116000000	-4.440309000000	1.876489000000
H	-0.630587000000	-4.437401000000	-2.294890000000
H	0.857954000000	-5.075594000000	-0.437697000000
C	-5.519097000000	0.810352000000	0.590325000000
C	-6.386326000000	1.113163000000	-0.489508000000
C	-5.366279000000	1.698516000000	1.682322000000
C	-7.051604000000	2.345563000000	-0.474740000000
C	-6.061481000000	2.914748000000	1.643439000000
C	-6.890107000000	3.243114000000	0.575766000000
H	-7.713307000000	2.601428000000	-1.296645000000
H	-5.953434000000	3.612486000000	2.467907000000
H	-7.418005000000	4.193154000000	0.566893000000
C	4.165273000000	2.747207000000	-0.473954000000
C	4.528090000000	2.642785000000	-1.839232000000
C	3.629621000000	3.946083000000	0.054856000000
C	4.269074000000	3.737981000000	-2.673593000000
C	3.406196000000	5.014299000000	-0.823527000000
C	3.707354000000	4.910291000000	-2.178295000000
H	4.526944000000	3.674532000000	-3.726163000000
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C	4.174925000000	-1.686335000000	1.716253000000
C	3.547288000000	-1.985796000000	2.946052000000
C	4.645302000000	-2.713576000000	0.856895000000
C	3.388121000000	-3.333076000000	3.299280000000
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C	-2.391920000000	-4.447995000000	3.472897000000
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C	-2.488879000000	-1.922818000000	3.351430000000
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H	-2.063069000000	-1.015490000000	2.920755000000
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H	-6.072505000000	1.793023000000	4.401206000000
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H	3.379985000000	3.156776000000	2.021276000000
C	4.450675000000	5.021423000000	2.188563000000
H	5.458216000000	4.623849000000	2.022883000000
H	4.429890000000	6.035034000000	1.770253000000
H	4.290760000000	5.102704000000	3.270554000000
C	1.971892000000	4.748870000000	1.832746000000
H	1.171136000000	4.172131000000	1.368049000000
H	1.791460000000	4.764131000000	2.913960000000
H	1.903210000000	5.784195000000	1.477007000000
C	5.273388000000	1.439118000000	-2.412774000000
H	5.183724000000	0.612975000000	-1.701790000000
C	6.775040000000	1.770330000000	-2.566986000000
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H	6.923347000000	2.572072000000	-3.300486000000
H	7.226001000000	2.101418000000	-1.624344000000
C	4.702108000000	0.943870000000	-3.753598000000
H	5.223567000000	0.030097000000	-4.060990000000
H	3.637795000000	0.709098000000	-3.670675000000
H	4.840714000000	1.682509000000	-4.552453000000
C	5.391316000000	-2.417055000000	-0.446443000000
H	4.927933000000	-1.533447000000	-0.897299000000
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C	5.304517000000	-3.549685000000	-1.484437000000
H	5.896788000000	-4.422623000000	-1.182787000000
H	4.274340000000	-3.863514000000	-1.656631000000
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H	3.099931000000	0.052478000000	3.400245000000
C	3.976041000000	-0.834704000000	5.160363000000
H	5.024893000000	-0.659536000000	4.895543000000
H	3.652305000000	-0.024386000000	5.824902000000
H	3.935469000000	-1.770517000000	5.730702000000
C	1.601833000000	-1.124509000000	4.344209000000
H	0.952186000000	-1.218231000000	3.470220000000
H	1.487169000000	-2.023502000000	4.961855000000
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C	-2.023868000000	2.213889000000	-1.170090000000
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C	-1.377648000000	4.854444000000	-0.621769000000
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H	-1.121460000000	5.886511000000	-0.398855000000
H	-5.829866000000	-1.473133000000	2.244811000000
H	-4.634742000000	-3.483705000000	1.719216000000
H	5.890568000000	2.551771000000	1.707063000000
H	5.216209000000	0.710578000000	3.070352000000
Se	1.212877000000	-0.509584000000	-2.628415000000
C	1.962194000000	-2.260902000000	-3.018781000000
F	3.197504000000	-2.203104000000	-3.584330000000
F	1.188060000000	-2.965015000000	-3.884481000000
F	2.101877000000	-3.053910000000	-1.916653000000
Se	0.049039000000	-0.060813000000	0.905866000000
C	0.002701000000	1.381004000000	2.224641000000
F	1.244796000000	1.689226000000	2.681578000000
F	-0.725918000000	1.048409000000	3.325836000000
F	-0.534533000000	2.535627000000	1.763594000000
Br	-2.796827000000	0.687775000000	-2.684500000000

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Zero-point correction=                           1.318583 (Hartree/Particle)
 Thermal correction to Energy=                    1.404922
 Thermal correction to Enthalpy=                  1.405867
 Thermal correction to Gibbs Free Energy=         1.188809
 Sum of electronic and zero-point Energies=         -10939.356262
 Sum of electronic and thermal Energies=            -10939.269922
 Sum of electronic and thermal Enthalpies=          -10939.268978
 Sum of electronic and thermal Free Energies=       -10939.486035
CPCM (Benzene) PBE0-D3/def2TZVP E = -13619.8219461
CPCM (Benzene) M06L/def2TZVP E = -13623.9532794
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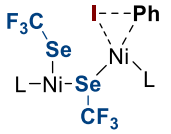
TS-OA-bis-SeCF$_3$-PhCl *triplet*



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N	4.906555000000	0.272546000000	0.688395000000
N	-4.767133000000	-1.068137000000	0.645446000000
N	-4.253985000000	0.892028000000	1.456721000000
H	5.440399000000	3.111678000000	-0.169915000000
H	6.738820000000	1.353374000000	0.794343000000
H	-6.831319000000	-0.989385000000	1.156739000000
H	-6.329030000000	1.329394000000	1.502254000000
C	2.616744000000	2.861967000000	-0.270756000000
C	1.680170000000	3.414927000000	0.632504000000
C	2.588690000000	3.179435000000	-1.654801000000
C	0.648080000000	4.197761000000	0.090797000000
C	1.549381000000	3.987379000000	-2.125898000000
C	0.570753000000	4.474577000000	-1.267309000000
H	-0.112068000000	4.590233000000	0.760702000000
H	1.495182000000	4.221733000000	-3.183678000000
H	-0.249226000000	5.071708000000	-1.656532000000
C	5.484338000000	-1.046867000000	0.761073000000
C	6.380915000000	-1.446820000000	-0.261886000000
C	5.248737000000	-1.860726000000	1.894446000000
C	7.004474000000	-2.695125000000	-0.140900000000
C	5.906541000000	-3.096511000000	1.962940000000
C	6.771300000000	-3.515915000000	0.957556000000
H	7.687948000000	-3.024945000000	-0.917532000000
H	5.739638000000	-3.738616000000	2.821713000000
H	7.268573000000	-4.479428000000	1.033102000000
C	-4.781314000000	-2.259448000000	-0.164808000000
C	-5.448818000000	-2.223558000000	-1.413281000000
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C	-5.467600000000	-3.393344000000	-2.182491000000
C	-4.267338000000	-4.596432000000	-0.475679000000
C	-4.875681000000	-4.567021000000	-1.726623000000
H	-5.960593000000	-3.385948000000	-3.150007000000
H	-3.832215000000	-5.524482000000	-0.116814000000
H	-4.900955000000	-5.463238000000	-2.341274000000
C	-3.689727000000	2.205513000000	1.626088000000
C	-3.023528000000	2.508075000000	2.836042000000
C	-3.922280000000	3.189953000000	0.646045000000
C	-2.576533000000	3.820100000000	3.036140000000
C	-3.445136000000	4.492933000000	0.893652000000
C	-2.781560000000	4.806636000000	2.075595000000
H	-2.068850000000	4.073604000000	3.962475000000
H	-3.614771000000	5.269979000000	0.153795000000
H	-2.435043000000	5.821857000000	2.253503000000
C	1.692047000000	3.362876000000	2.169302000000
H	0.631887000000	3.321897000000	2.449459000000
C	2.244516000000	4.698583000000	2.720967000000
H	2.154084000000	4.726865000000	3.813744000000
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C	2.357081000000	2.185993000000	2.896446000000
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H	4.543210000000	-0.559180000000	5.041908000000
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H	3.978744000000	-3.387437000000	3.987744000000
H	2.723717000000	-2.180507000000	4.281247000000
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H	8.905561000000	-0.829136000000	-1.369906000000
H	8.391212000000	0.667827000000	-2.164013000000
C	6.571384000000	-1.298102000000	-2.805609000000
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C	3.677736000000	2.742786000000	-2.635024000000
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C	3.129187000000	2.288864000000	-4.002130000000
H	3.932772000000	1.824909000000	-4.585841000000
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H	2.756638000000	3.138397000000	-4.587060000000
C	-3.607272000000	-3.552458000000	1.730297000000
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H	-2.366451000000	-5.350308000000	1.523150000000
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C	-4.723400000000	2.942868000000	-0.627351000000
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C	2.055275000000	-2.368285000000	-1.164664000000
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H	-5.652675000000	0.828155000000	3.063207000000
Se	-2.044686000000	-0.490344000000	-2.880622000000
C	-0.766364000000	0.892258000000	-3.360531000000
F	-0.075936000000	0.574969000000	-4.482580000000
F	0.184405000000	1.114676000000	-2.395548000000
F	-1.322185000000	2.108901000000	-3.595365000000
Se	-0.033123000000	0.097759000000	0.702849000000
C	0.024623000000	-1.221280000000	2.142710000000
F	-1.187505000000	-1.380430000000	2.735955000000
F	0.876695000000	-0.846125000000	3.138182000000
F	0.428024000000	-2.452499000000	1.755419000000
Cl	2.889694000000	-0.979062000000	-2.616509000000

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Zero-point correction=                           1.318610 (Hartree/Particle)
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 Thermal correction to Enthalpy=                  1.405874
 Thermal correction to Gibbs Free Energy=         1.189139
 Sum of electronic and zero-point Energies=          -8828.139709
 Sum of electronic and thermal Energies=             -8828.053390
 Sum of electronic and thermal Enthalpies=           -8828.052446
 Sum of electronic and thermal Free Energies=        -8828.269181
CPCM (Benzene) PBE0-D3/def2TZVP E = -11506.0168504
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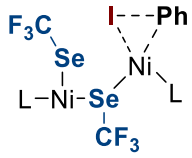
TS-OA-bis-SeCF$_3$-PhSeCF$_3$ *triplet*



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C	5.869103000000	1.368669000000	1.434747000000
N	-3.219465000000	-2.441927000000	0.179515000000
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N	4.541459000000	1.540660000000	0.804231000000
N	4.644373000000	-0.602279000000	1.215566000000
H	-4.820647000000	-3.605730000000	-0.563869000000
H	-6.378812000000	-2.250210000000	0.639087000000
H	6.656224000000	1.443116000000	0.672756000000
H	6.660661000000	-0.632996000000	1.913671000000
C	-2.033153000000	-3.099204000000	-0.325463000000
C	-1.152010000000	-3.739609000000	0.578800000000
C	-1.828029000000	-3.164583000000	-1.728759000000
C	-0.010432000000	-4.352557000000	0.040333000000
C	-0.669764000000	-3.792153000000	-2.198484000000
C	0.241624000000	-4.370042000000	-1.323708000000
H	0.703454000000	-4.811222000000	0.719966000000
H	-0.465853000000	-3.806187000000	-3.262954000000
H	1.151580000000	-4.821656000000	-1.705322000000
C	-5.405445000000	0.251383000000	1.163704000000
C	-6.397311000000	0.751748000000	0.281003000000
C	-5.204927000000	0.824223000000	2.443608000000
C	-7.126726000000	1.877997000000	0.681292000000
C	-5.971650000000	1.945439000000	2.789821000000
C	-6.914653000000	2.477522000000	1.917974000000
H	-7.880877000000	2.285522000000	0.015347000000
H	-5.829878000000	2.404001000000	3.763282000000
H	-7.494402000000	3.350084000000	2.207424000000
C	4.201347000000	2.813820000000	0.219672000000
C	4.515012000000	3.071529000000	-1.136883000000
C	3.653263000000	3.818994000000	1.051770000000
C	4.197803000000	4.333144000000	-1.656734000000
C	3.369241000000	5.066379000000	0.481510000000
C	3.623948000000	5.320801000000	-0.862929000000
H	4.418599000000	4.547134000000	-2.697876000000
H	2.947644000000	5.850997000000	1.102917000000
H	3.391384000000	6.294054000000	-1.287717000000
C	4.426583000000	-2.027391000000	1.209337000000
C	3.869577000000	-2.646879000000	2.350060000000
C	4.886802000000	-2.790669000000	0.103799000000
C	3.767906000000	-4.045092000000	2.364213000000
C	4.747088000000	-4.181891000000	0.169682000000
C	4.198275000000	-4.807892000000	1.286349000000
H	3.347573000000	-4.538288000000	3.236103000000
H	5.078760000000	-4.790309000000	-0.663962000000
H	4.113322000000	-5.891456000000	1.314535000000
C	-1.313917000000	-3.946020000000	2.094195000000
H	-0.287573000000	-3.923928000000	2.481183000000
C	-1.849491000000	-5.368989000000	2.377411000000
H	-1.843981000000	-5.570318000000	3.455599000000
H	-2.880531000000	-5.492824000000	2.023075000000
H	-1.239881000000	-6.132501000000	1.883517000000
C	-2.082382000000	-2.911672000000	2.926078000000
H	-3.164098000000	-2.958852000000	2.771897000000
H	-1.904773000000	-3.115090000000	3.989317000000
H	-1.736774000000	-1.898410000000	2.720300000000
C	-4.245115000000	0.246635000000	3.480557000000
H	-3.560374000000	-0.436590000000	2.972953000000
C	-5.022723000000	-0.563350000000	4.541692000000
H	-5.704945000000	0.085819000000	5.103740000000
H	-5.624942000000	-1.362013000000	4.094373000000
H	-4.328108000000	-1.021325000000	5.255543000000
C	-3.385467000000	1.320881000000	4.173025000000
H	-2.848427000000	1.938205000000	3.448939000000
H	-3.991954000000	1.979182000000	4.805944000000
H	-2.642113000000	0.840642000000	4.815976000000
C	-6.765646000000	0.082305000000	-1.043226000000
H	-5.979300000000	-0.639376000000	-1.289212000000
C	-8.104152000000	-0.681310000000	-0.912592000000
H	-8.103241000000	-1.402160000000	-0.087794000000
H	-8.929232000000	0.016947000000	-0.729196000000
H	-8.325634000000	-1.224862000000	-1.838669000000
C	-6.866942000000	1.071591000000	-2.220535000000
H	-5.954201000000	1.661360000000	-2.324963000000
H	-7.026719000000	0.519471000000	-3.154058000000
H	-7.712933000000	1.758204000000	-2.101656000000
C	-2.847427000000	-2.667593000000	-2.752601000000
H	-3.520124000000	-1.959920000000	-2.258934000000
C	-3.697903000000	-3.847448000000	-3.276230000000
H	-4.463018000000	-3.486645000000	-3.974488000000
H	-3.068298000000	-4.568112000000	-3.811143000000
H	-4.201858000000	-4.392344000000	-2.469769000000
C	-2.205106000000	-1.928461000000	-3.942294000000
H	-2.982448000000	-1.423217000000	-4.526765000000
H	-1.480472000000	-1.180284000000	-3.613229000000
H	-1.688144000000	-2.621331000000	-4.616135000000
C	3.422499000000	3.614720000000	2.546894000000
H	3.474566000000	2.540923000000	2.748580000000
C	4.522507000000	4.319802000000	3.371643000000
H	5.530567000000	3.999583000000	3.085363000000
H	4.475585000000	5.406501000000	3.231160000000
H	4.391740000000	4.114536000000	4.441085000000
C	2.038867000000	4.099674000000	3.015920000000
H	1.234145000000	3.670742000000	2.417268000000
H	1.876303000000	3.806579000000	4.059528000000
H	1.956691000000	5.192320000000	2.967842000000
C	5.263221000000	2.077614000000	-2.022928000000
H	5.251672000000	1.102763000000	-1.527317000000
C	6.738275000000	2.510620000000	-2.178373000000
H	7.297038000000	1.763222000000	-2.754415000000
H	6.809541000000	3.466208000000	-2.711815000000
H	7.236530000000	2.637431000000	-1.210109000000
C	4.616198000000	1.888363000000	-3.406738000000
H	5.150963000000	1.109498000000	-3.962473000000
H	3.571605000000	1.578835000000	-3.318150000000
H	4.662358000000	2.806526000000	-4.004700000000
C	5.553913000000	-2.152885000000	-1.118393000000
H	5.021882000000	-1.220784000000	-1.335537000000
C	7.034986000000	-1.809835000000	-0.844961000000
H	7.598321000000	-2.714069000000	-0.583412000000
H	7.493145000000	-1.377058000000	-1.742342000000
H	7.160482000000	-1.090536000000	-0.031969000000
C	5.480339000000	-3.018186000000	-2.389052000000
H	6.135176000000	-3.895785000000	-2.320291000000
H	4.462519000000	-3.351217000000	-2.595323000000
H	5.816541000000	-2.428187000000	-3.248071000000

C	3.399551000000	-1.867676000000	3.575689000000
H	3.402803000000	-0.803206000000	3.327382000000
C	4.345150000000	-2.089308000000	4.775241000000
H	5.381363000000	-1.823003000000	4.537906000000
H	4.025269000000	-1.484828000000	5.632597000000
H	4.341612000000	-3.140322000000	5.088357000000
C	1.952670000000	-2.221216000000	3.965089000000
H	1.280087000000	-2.093670000000	3.112616000000
H	1.870506000000	-3.255114000000	4.321590000000
H	1.605990000000	-1.563785000000	4.769718000000
Se	-3.198839000000	0.977516000000	-1.969829000000
C	-1.970877000000	2.271520000000	-0.111197000000
C	-2.950391000000	2.942477000000	0.623176000000
C	-0.779989000000	2.914925000000	-0.470471000000
C	-2.691955000000	4.235324000000	1.091163000000
H	-3.903088000000	2.474043000000	0.831502000000
C	-0.541686000000	4.211986000000	-0.011001000000
H	-0.030423000000	2.416663000000	-1.074870000000
C	-1.491478000000	4.871409000000	0.774296000000
H	-3.448616000000	4.748045000000	1.679948000000
H	0.396748000000	4.696593000000	-0.266207000000
H	-1.301866000000	5.883342000000	1.122576000000
H	-5.461305000000	-2.397535000000	2.147220000000
H	-4.219760000000	-4.117935000000	1.023525000000
H	6.048179000000	2.132554000000	2.192996000000
H	5.476189000000	-0.012507000000	3.077999000000
Se	1.209518000000	0.066825000000	-2.552893000000
C	2.064720000000	-1.479935000000	-3.363357000000
F	3.279223000000	-1.196767000000	-3.907845000000
F	1.317822000000	-2.006289000000	-4.367883000000
F	2.287870000000	-2.505661000000	-2.490931000000
Se	0.183921000000	-0.324565000000	1.004752000000
C	0.170254000000	0.687001000000	2.682656000000
F	1.430333000000	0.890077000000	3.146475000000
F	-0.490003000000	0.024455000000	3.671772000000
F	-0.411298000000	1.902702000000	2.599020000000
C	-2.474990000000	2.338803000000	-3.211255000000
F	-3.103006000000	2.122591000000	-4.387934000000
F	-2.750088000000	3.599029000000	-2.835036000000
F	-1.157302000000	2.255938000000	-3.427840000000

```
Zero-point correction=                           1.333748 (Hartree/Particle)
 Thermal correction to Energy=                    1.424148
 Thermal correction to Enthalpy=                  1.425092
 Thermal correction to Gibbs Free Energy=         1.198377
 Sum of electronic and zero-point Energies=         -11104.472318
 Sum of electronic and thermal Energies=            -11104.381919
 Sum of electronic and thermal Enthalpies=          -11104.380975
 Sum of electronic and thermal Free Energies=       -11104.607690
CPCM (Benzene) PBE0-D3/def2TZVP E = -13784.6922876
CPCM (Benzene) M06L/def2TZVP E = -13789.0931929
```

SIPr-Ni-cod (ωB97XD opt.)

Ni	0.000039000000	-0.000289000000	1.149471000000
C	-1.433389000000	0.775811000000	2.442025000000
H	-2.193412000000	1.152989000000	1.756710000000
C	-0.302055000000	1.535888000000	2.621741000000
H	-0.232416000000	2.462307000000	2.055154000000
C	0.731690000000	1.349597000000	3.711271000000
H	0.256410000000	0.988162000000	4.628184000000
H	1.170064000000	2.322108000000	3.964101000000
C	1.876188000000	0.394649000000	3.289057000000
H	2.608990000000	0.957919000000	2.699199000000
H	2.409786000000	0.042945000000	4.185078000000
C	1.433427000000	-0.777396000000	2.441708000000
H	2.193447000000	-1.154066000000	1.756112000000
C	0.302107000000	-1.537608000000	2.620769000000
H	0.232528000000	-2.463576000000	2.053441000000
C	-0.731794000000	-1.352062000000	3.710266000000
H	-0.256612000000	-0.991322000000	4.627508000000
H	-1.170239000000	-2.324744000000	3.962314000000
C	-1.876221000000	-0.396753000000	3.288627000000
H	-2.609066000000	-0.959600000000	2.698426000000
H	-2.409775000000	-0.045580000000	4.184881000000
C	0.000007000000	0.000134000000	-0.718161000000
C	-0.731024000000	-0.222702000000	-2.957590000000
C	0.731025000000	0.224335000000	-2.957456000000
H	-1.366216000000	0.372715000000	-3.619460000000
H	1.366207000000	-0.370664000000	-3.619709000000
H	-0.832986000000	-1.282344000000	-3.235362000000
H	0.832987000000	1.284154000000	-3.234548000000
N	-1.081969000000	-0.019622000000	-1.553057000000
N	1.081979000000	0.020352000000	-1.553053000000
C	2.417000000000	0.071788000000	-1.061867000000
C	3.157783000000	-1.122743000000	-1.021833000000
C	2.944843000000	1.287373000000	-0.600023000000
C	4.436576000000	-1.083697000000	-0.466531000000
C	4.231991000000	1.281655000000	-0.058747000000
C	4.967347000000	0.106528000000	0.018307000000
H	5.027462000000	-1.992442000000	-0.405700000000
H	4.664065000000	2.207737000000	0.310158000000
H	5.962854000000	0.117675000000	0.452787000000
C	-2.416987000000	-0.071172000000	-1.061888000000
C	-3.157623000000	1.123418000000	-1.021212000000
C	-2.944969000000	-1.286944000000	-0.600687000000
C	-4.436417000000	1.084234000000	-0.465916000000
C	-4.232107000000	-1.281360000000	-0.059391000000
C	-4.967323000000	-0.106182000000	0.018296000000
H	-5.027186000000	1.993023000000	-0.404597000000
H	-4.664287000000	-2.207583000000	0.309036000000
H	-5.962823000000	-0.117440000000	0.452789000000
C	2.556186000000	-2.428167000000	-1.522385000000
H	1.800590000000	-2.175864000000	-2.273819000000
C	2.163323000000	2.584589000000	-0.717074000000
H	1.119597000000	2.327351000000	-0.916641000000
C	-2.163619000000	-2.584199000000	-0.718499000000
H	-1.119865000000	-2.326985000000	-0.917963000000
C	-2.555873000000	2.429033000000	-1.521058000000
H	-1.800166000000	2.177035000000	-2.272486000000
C	-2.180082000000	-3.405641000000	0.574672000000
H	-1.891142000000	-2.787231000000	1.428304000000
H	-3.169282000000	-3.832897000000	0.776658000000
H	-1.470984000000	-4.237812000000	0.499494000000
C	-2.683533000000	-3.416984000000	-1.899944000000
H	-2.633728000000	-2.854886000000	-2.838959000000
H	-2.093381000000	-4.333350000000	-2.015761000000
H	-3.729649000000	-3.705390000000	-1.741804000000
C	-3.580329000000	3.348515000000	-2.194084000000
H	-4.296446000000	3.758429000000	-1.472781000000
H	-3.069516000000	4.199087000000	-2.658449000000
H	-4.145419000000	2.821793000000	-2.970644000000
C	-1.824625000000	3.157565000000	-0.384530000000
H	-2.525538000000	3.433184000000	0.412704000000
H	-1.052977000000	2.511366000000	0.044919000000
H	-1.351429000000	4.074498000000	-0.756524000000
C	3.580808000000	-3.347274000000	-2.195676000000
H	4.146065000000	-2.820128000000	-2.971825000000
H	4.296766000000	-3.757562000000	-1.474427000000
H	3.070111000000	-4.197607000000	-2.660605000000
C	1.824796000000	-3.157287000000	-0.386324000000
H	2.525600000000	-3.433251000000	0.410884000000
H	1.053030000000	-2.511355000000	0.043320000000
H	1.351719000000	-4.074070000000	-0.758839000000
C	2.179739000000	3.405286000000	0.576569000000
H	1.890945000000	2.786330000000	1.429854000000
H	3.168887000000	3.832576000000	0.778742000000
H	1.470502000000	4.237386000000	0.501920000000
C	2.683063000000	3.418147000000	-1.898051000000
H	2.633306000000	2.856599000000	-2.837397000000
H	2.092753000000	4.334483000000	-2.013295000000
H	3.729139000000	3.706631000000	-1.739788000000

```
Zero-point correction=                           0.789523 (Hartree/Particle)
 Thermal correction to Energy=                    0.829121
 Thermal correction to Enthalpy=                  0.830066
 Thermal correction to Gibbs Free Energy=         0.719834
 Sum of electronic and zero-point Energies=          -1643.046807
 Sum of electronic and thermal Energies=             -1643.007209
 Sum of electronic and thermal Enthalpies=           -1643.006265
 Sum of electronic and thermal Free Energies=        -1643.116496
CPCM (Benzene) M06L/def2TZVP E = -2981.96067892
```

SIPr$_2$-Ni (ωB97XD opt.)

Ni	-0.033458000000	0.028262000000	0.001351000000
C	0.089712000000	-1.830546000000	0.035155000000
C	-0.443002000000	-4.110370000000	0.472241000000
C	0.999079000000	-4.033722000000	-0.023105000000
N	1.152890000000	-2.609465000000	-0.319221000000
N	-0.820056000000	-2.698121000000	0.562496000000
H	1.178031000000	-4.636062000000	-0.921012000000
H	-1.105792000000	-4.631405000000	-0.231753000000
C	2.315301000000	-2.195000000000	-1.032590000000
C	3.509743000000	-1.897850000000	-0.357626000000
C	2.253766000000	-2.215161000000	-2.441516000000
C	4.628554000000	-1.571152000000	-1.133064000000
C	3.399153000000	-1.896403000000	-3.167434000000
C	4.583820000000	-1.574316000000	-2.517761000000
H	5.557269000000	-1.321217000000	-0.624945000000
H	3.366320000000	-1.894308000000	-4.252916000000
H	5.470280000000	-1.320918000000	-3.092671000000
C	-2.179086000000	-2.436415000000	0.904325000000
C	-3.152193000000	-2.399169000000	-0.109405000000
C	-2.531828000000	-2.387245000000	2.261942000000
C	-4.494188000000	-2.339648000000	0.268025000000
C	-3.886683000000	-2.347891000000	2.593784000000
C	-4.862945000000	-2.337179000000	1.607052000000
H	-5.262525000000	-2.299790000000	-0.499282000000
H	-4.180850000000	-2.309246000000	3.639473000000
H	-5.913639000000	-2.303961000000	1.881102000000
C	3.749649000000	-1.979623000000	1.146527000000
H	4.476150000000	-1.185746000000	1.355431000000
C	4.438398000000	-3.310955000000	1.494898000000
H	4.682449000000	-3.344252000000	2.563044000000
H	3.789005000000	-4.165505000000	1.273177000000
H	5.364868000000	-3.444319000000	0.926521000000
C	2.572066000000	-1.715297000000	2.085357000000
H	1.884604000000	-2.565111000000	2.150960000000
H	2.966194000000	-1.532699000000	3.091528000000
H	1.996370000000	-0.838968000000	1.772878000000
C	-1.478751000000	-2.323326000000	3.352732000000
H	-0.498317000000	-2.412386000000	2.874569000000
C	-1.622244000000	-3.465468000000	4.365855000000
H	-2.570095000000	-3.401120000000	4.912919000000
H	-1.589771000000	-4.442706000000	3.871257000000
H	-0.811512000000	-3.427019000000	5.101981000000
C	-1.523294000000	-0.953166000000	4.042140000000
H	-1.315750000000	-0.155541000000	3.319774000000
H	-2.506934000000	-0.766877000000	4.489950000000
H	-0.775213000000	-0.902387000000	4.840156000000
C	-2.780322000000	-2.393637000000	-1.581471000000
H	-1.699322000000	-2.538452000000	-1.657591000000
C	-3.456969000000	-3.528566000000	-2.359542000000
H	-3.258712000000	-4.503744000000	-1.900491000000
H	-4.544061000000	-3.395944000000	-2.406954000000
H	-3.083021000000	-3.552378000000	-3.389778000000
C	-3.091220000000	-1.022456000000	-2.189786000000
H	-2.519175000000	-0.243738000000	-1.675601000000
H	-2.828517000000	-0.998330000000	-3.253653000000
H	-4.155546000000	-0.777542000000	-2.099505000000
C	0.962816000000	-2.555433000000	-3.168114000000
H	0.310444000000	-3.082110000000	-2.465085000000
C	1.177314000000	-3.489079000000	-4.365144000000
H	0.208888000000	-3.821177000000	-4.755736000000
H	1.702316000000	-2.989802000000	-5.187393000000
H	1.756022000000	-4.375698000000	-4.083693000000
C	0.231110000000	-1.275856000000	-3.586383000000
H	-0.693218000000	-1.521444000000	-4.122909000000
H	-0.029085000000	-0.671658000000	-2.708109000000
H	0.860190000000	-0.668455000000	-4.247883000000
H	-0.536059000000	-4.599199000000	1.447985000000
H	1.718330000000	-4.347894000000	0.741916000000
C	-0.079502000000	1.863043000000	0.228699000000
C	0.590909000000	4.038494000000	0.916444000000
C	-0.849026000000	4.101886000000	0.419052000000
H	1.288933000000	4.540224000000	0.231110000000
H	-1.557687000000	4.266310000000	1.240914000000
N	0.842708000000	2.595642000000	0.933573000000
N	-1.024063000000	2.766475000000	-0.157559000000
H	0.718926000000	4.474009000000	1.911596000000
H	-1.019236000000	4.880075000000	-0.330163000000
C	-2.214768000000	2.484297000000	-0.889135000000
C	-2.156406000000	2.434448000000	-2.296197000000
C	-3.423959000000	2.348720000000	-0.194573000000
C	-3.358385000000	2.313013000000	-2.991406000000
C	-4.602068000000	2.221429000000	-0.934020000000
C	-4.573392000000	2.223992000000	-2.319852000000
H	-3.352205000000	2.271197000000	-4.075424000000
H	-5.550907000000	2.111832000000	-0.415577000000
H	-5.497858000000	2.132088000000	-2.883012000000
C	2.181034000000	2.157010000000	1.161486000000
C	3.077817000000	2.110905000000	0.079028000000
C	2.591743000000	1.874960000000	2.472946000000
C	4.388850000000	1.707417000000	0.329109000000
C	3.919707000000	1.499661000000	2.681529000000
C	4.809604000000	1.405360000000	1.619008000000
H	5.094087000000	1.641855000000	-0.495168000000
H	4.262995000000	1.278567000000	3.688677000000
H	5.839125000000	1.106888000000	1.798173000000
C	-3.471078000000	2.286205000000	1.322241000000
C	1.637692000000	2.024621000000	3.645543000000
H	0.634609000000	2.164738000000	3.230077000000
C	1.596526000000	0.779652000000	4.536388000000
H	2.569497000000	0.580566000000	5.001177000000
H	0.867011000000	0.918638000000	5.342406000000
H	1.304908000000	-0.101577000000	3.960058000000
C	1.997527000000	3.268263000000	4.473025000000
H	2.983466000000	3.153707000000	4.939413000000
H	2.030058000000	4.169981000000	3.851721000000
H	1.263053000000	3.427013000000	5.271027000000
C	-4.326543000000	3.409804000000	1.920521000000
H	-4.284751000000	3.378783000000	3.015214000000
H	-3.982707000000	4.396874000000	1.590741000000
H	-5.377686000000	3.309165000000	1.626106000000
C	-3.948108000000	0.905522000000	1.777108000000
H	-4.972591000000	0.700848000000	1.446318000000
H	-3.296340000000	0.129770000000	1.366467000000
H	-3.924518000000	0.828656000000	2.870250000000
H	-2.450669000000	2.394120000000	1.700227000000
C	2.667626000000	2.540057000000	-1.320854000000
C	-0.818051000000	2.462236000000	-3.023174000000
H	-0.130600000000	1.850820000000	-2.426313000000
C	-0.233001000000	3.877869000000	-3.123654000000
H	-0.071327000000	4.327380000000	-2.140974000000
H	0.735796000000	3.849303000000	-3.636637000000
H	-0.901104000000	4.534192000000	-3.694093000000
C	-0.880602000000	1.839456000000	-4.420315000000
H	-1.430917000000	2.473951000000	-5.125846000000
H	0.133921000000	1.717618000000	-4.814802000000
H	-1.355415000000	0.854210000000	-4.400339000000
C	2.713931000000	1.380250000000	-2.315151000000
H	3.733973000000	1.008405000000	-2.453066000000
H	2.095037000000	0.550992000000	-1.959425000000
H	2.334314000000	1.702730000000	-3.293371000000
C	3.509483000000	3.729176000000	-1.803047000000
H	3.135819000000	4.091122000000	-2.768013000000
H	3.474327000000	4.559839000000	-1.089031000000
H	4.561057000000	3.450324000000	-1.937188000000
H	1.629573000000	2.873928000000	-1.280773000000

```
Zero-point correction=                           1.212174 (Hartree/Particle)
 Thermal correction to Energy=                    1.273877
 Thermal correction to Enthalpy=                  1.274821
 Thermal correction to Gibbs Free Energy=         1.119714
 Sum of electronic and zero-point Energies=          -2491.622353
 Sum of electronic and thermal Energies=             -2491.560650
 Sum of electronic and thermal Enthalpies=           -2491.559705
 Sum of electronic and thermal Free Energies=        -2491.714812
CPCM (Benzene) M06L/def2TZVP E = -3831.37825232
```

SIPr (ωB97XD opt.)

N	-1.070336000000	-0.007179000000	0.579082000000
N	1.070325000000	0.007510000000	0.579073000000
C	0.000007000000	-0.000101000000	-0.244329000000
C	-0.746040000000	-0.160273000000	2.008239000000
H	-1.339391000000	0.517748000000	2.628106000000
C	0.746003000000	0.161151000000	2.008185000000
H	0.953403000000	1.191445000000	2.329527000000
C	-2.421005000000	-0.145770000000	0.142154000000
C	-2.899445000000	-1.405124000000	-0.245376000000
C	-4.238309000000	-1.505903000000	-0.631541000000
H	-4.634258000000	-2.465692000000	-0.951080000000
C	-5.070109000000	-0.395234000000	-0.618484000000
H	-6.109844000000	-0.493591000000	-0.917316000000
C	-4.574630000000	0.846737000000	-0.235012000000
H	-5.234958000000	1.708130000000	-0.242739000000
C	-3.242819000000	0.994529000000	0.148250000000
C	-1.980273000000	-2.612858000000	-0.326021000000
H	-1.065855000000	-2.382860000000	0.230615000000
C	-1.568087000000	-2.846180000000	-1.786441000000
H	-2.445398000000	-3.064515000000	-2.407203000000
H	-0.874943000000	-3.691700000000	-1.863152000000
H	-1.074913000000	-1.953352000000	-2.183179000000
C	-2.590174000000	-3.873872000000	0.295758000000
H	-2.913816000000	-3.694306000000	1.326760000000
H	-1.850181000000	-4.681957000000	0.303960000000
H	-3.456435000000	-4.232530000000	-0.271604000000
C	-2.650923000000	2.356504000000	0.477223000000
H	-1.865451000000	2.207828000000	1.226970000000
C	-1.971107000000	2.934719000000	-0.773909000000
H	-1.226994000000	2.235719000000	-1.167780000000
H	-1.471387000000	3.882648000000	-0.539595000000
H	-2.712692000000	3.123058000000	-1.559186000000
C	-3.659812000000	3.347998000000	1.062277000000
H	-3.140430000000	4.251549000000	1.399278000000
H	-4.196169000000	2.922126000000	1.917146000000
H	-4.400328000000	3.661690000000	0.317627000000
C	2.421040000000	0.145828000000	0.142229000000
C	3.242606000000	-0.994645000000	0.148371000000
C	4.574477000000	-0.847150000000	-0.234787000000
H	5.234604000000	-1.708700000000	-0.242517000000
C	5.070257000000	0.394717000000	-0.618197000000
H	6.110038000000	0.492844000000	-0.916944000000
C	4.238708000000	1.505577000000	-0.631292000000
H	4.634911000000	2.465285000000	-0.950751000000
C	2.899785000000	1.405087000000	-0.245274000000
C	2.650411000000	-2.356499000000	0.477243000000
H	1.864927000000	-2.207702000000	1.226951000000
C	1.970532000000	-2.934442000000	-0.773997000000
H	1.226724000000	-2.235131000000	-1.167893000000
H	1.470425000000	-3.882197000000	-0.539799000000
H	2.712145000000	-3.123008000000	-1.559190000000
C	3.659084000000	-3.348201000000	1.062283000000
H	4.399612000000	-3.661963000000	0.317674000000
H	3.139521000000	-4.251682000000	1.399195000000
H	4.195447000000	-2.922457000000	1.917214000000
C	1.980782000000	2.612943000000	-0.326079000000
H	1.066479000000	2.383266000000	0.230874000000
C	1.568256000000	2.845798000000	-1.786504000000
H	2.445445000000	3.063980000000	-2.407491000000
H	0.875064000000	3.691274000000	-1.863332000000
H	1.075036000000	1.952850000000	-2.182904000000
C	2.590940000000	3.874144000000	0.295033000000
H	2.914926000000	3.694974000000	1.325995000000
H	1.850964000000	4.682245000000	0.303166000000
H	3.457004000000	4.232589000000	-0.272765000000
H	1.339346000000	-0.516648000000	2.628303000000
H	-0.953437000000	-1.190454000000	2.329968000000

```
Zero-point correction=                           0.603083 (Hartree/Particle)
 Thermal correction to Energy=                    0.632861
 Thermal correction to Enthalpy=                  0.633805
 Thermal correction to Gibbs Free Energy=         0.543671
 Sum of electronic and zero-point Energies=          -1160.292740
 Sum of electronic and thermal Energies=             -1160.262962
 Sum of electronic and thermal Enthalpies=           -1160.262018
 Sum of electronic and thermal Free Energies=        -1160.352152
CPCM (Benzene) PBE0-D3/def2TZVP E = -1161.49075582
```

1,5-cyclooctadiene (ωB97XD opt.)

C	-1.095939000000	-1.084968000000	0.669802000000
C	1.915923000000	-0.020769000000	-0.016612000000
C	0.041510000000	1.693905000000	-0.224391000000
C	-1.915920000000	0.020744000000	-0.016623000000
C	-1.185190000000	1.246036000000	-0.501332000000
H	-1.795667000000	-1.875273000000	0.965733000000
H	-2.718759000000	0.340001000000	0.664646000000
H	-0.665169000000	-0.711843000000	1.601228000000
H	0.345665000000	2.611439000000	-0.727501000000
H	-2.429314000000	-0.419520000000	-0.882780000000
C	-0.041521000000	-1.693898000000	-0.224385000000
H	-0.345717000000	-2.611413000000	-0.727504000000
C	1.185173000000	-1.246036000000	-0.501357000000
H	1.777589000000	-1.853882000000	-1.185968000000
H	2.429385000000	0.419462000000	-0.882743000000
H	2.718703000000	-0.340047000000	0.664718000000
H	-1.777634000000	1.853897000000	-1.185906000000
C	1.095961000000	1.084984000000	0.669766000000
H	0.665224000000	0.711911000000	1.601229000000
H	1.795713000000	1.875289000000	0.965641000000

```
Zero-point correction=                           0.183361 (Hartree/Particle)
 Thermal correction to Energy=                    0.190701
 Thermal correction to Enthalpy=                  0.191646
 Thermal correction to Gibbs Free Energy=         0.151915
 Sum of electronic and zero-point Energies=           -311.745607
 Sum of electronic and thermal Energies=              -311.738266
 Sum of electronic and thermal Enthalpies=            -311.737322
 Sum of electronic and thermal Free Energies=         -311.777053
CPCM (Benzene) M06L/def2TZVP E = -312.0931141
```

$PhSeCF_3$ (ωB97XD opt.)

C	0.911163000000	-0.402147000000	-0.101095000000
C	1.535562000000	0.179089000000	-1.204670000000
C	1.592108000000	-0.520259000000	1.110048000000
H	0.998723000000	0.267210000000	-2.143218000000
H	1.098042000000	-0.971297000000	1.964096000000
C	2.840352000000	0.650070000000	-1.091409000000
C	2.898263000000	-0.051369000000	1.217125000000
H	3.323755000000	1.106806000000	-1.949528000000
H	3.426608000000	-0.142142000000	2.161163000000
C	3.521379000000	0.533909000000	0.117847000000
H	4.539639000000	0.901198000000	0.204143000000
Se	-0.879965000000	-1.059643000000	-0.251518000000
C	-1.732401000000	0.649824000000	0.162677000000
F	-1.424666000000	1.599250000000	-0.726073000000
F	-3.057690000000	0.470764000000	0.140830000000
F	-1.391701000000	1.111248000000	1.368780000000

```
Zero-point correction=                           0.107229 (Hartree/Particle)
 Thermal correction to Energy=                    0.117097
 Thermal correction to Enthalpy=                  0.118041
 Thermal correction to Gibbs Free Energy=         0.069072
 Sum of electronic and zero-point Energies=          -2967.935241
 Sum of electronic and thermal Energies=             -2967.925374
 Sum of electronic and thermal Enthalpies=           -2967.924430
 Sum of electronic and thermal Free Energies=        -2967.973399
CPCM (Benzene) M06L/def2TZVP E = -2970.89854866
```

PhI (ωB97XD opt.)

C	0.000000000000	0.000000000000	-0.574224000000
C	0.000000000000	1.212529000000	-1.255361000000
C	0.000000000000	-1.212529000000	-1.255361000000
H	0.000000000000	2.152445000000	-0.714557000000
H	0.000000000000	-2.152445000000	-0.714557000000
C	0.000000000000	1.204240000000	-2.648723000000
C	0.000000000000	-1.204240000000	-2.648723000000
H	0.000000000000	2.147879000000	-3.185957000000
H	0.000000000000	-2.147879000000	-3.185957000000
C	0.000000000000	0.000000000000	-3.346460000000
H	0.000000000000	0.000000000000	-4.432127000000
I	0.000000000000	0.000000000000	1.558609000000

```
Zero-point correction=                           0.091513 (Hartree/Particle)
 Thermal correction to Energy=                    0.097310
 Thermal correction to Enthalpy=                  0.098254
 Thermal correction to Gibbs Free Energy=         0.060505
 Sum of electronic and zero-point Energies=           -242.888371
 Sum of electronic and thermal Energies=              -242.882573
 Sum of electronic and thermal Enthalpies=            -242.881629
 Sum of electronic and thermal Free Energies=         -242.919379
CPCM (Benzene) M06L/def2TZVP E = -529.570349595
```

PhBr (ωB97XD opt.)

C	0.000000000000	0.000000000000	-0.097553000000
C	0.000000000000	1.212437000000	-0.778143000000
C	0.000000000000	-1.212437000000	-0.778143000000
H	0.000000000000	2.146853000000	-0.228040000000
H	0.000000000000	-2.146853000000	-0.228040000000
C	0.000000000000	1.204632000000	-2.170589000000
C	0.000000000000	-1.204632000000	-2.170589000000
H	0.000000000000	2.147876000000	-2.708280000000

H	0.000000000000	-2.147876000000	-2.708280000000
C	0.000000000000	0.000000000000	-2.868384000000
H	0.000000000000	0.000000000000	-3.953939000000
Br	0.000000000000	0.000000000000	1.800200000000

```
Zero-point correction=                           0.092044 (Hartree/Particle)
 Thermal correction to Energy=                    0.097668
 Thermal correction to Enthalpy=                  0.098613
 Thermal correction to Gibbs Free Energy=         0.061883
 Sum of electronic and zero-point Energies=          -2802.899628
 Sum of electronic and thermal Energies=             -2802.894003
 Sum of electronic and thermal Enthalpies=           -2802.893059
 Sum of electronic and thermal Free Energies=        -2802.929789
CPCM (Benzene) M06L/def2TZVP E = -2805.75805909
```

PhCl (ωB97XD opt.)

C	-0.503970000000	0.000000000000	0.000021000000
C	0.176144000000	-1.213011000000	-0.000005000000
H	-0.376197000000	-2.146371000000	0.000019000000
C	1.568464000000	-1.204601000000	-0.000069000000
H	2.106349000000	-2.147717000000	-0.000090000000
C	2.266578000000	-0.000002000000	-0.000101000000
C	1.568463000000	1.204601000000	-0.000066000000
H	2.106354000000	2.147714000000	-0.000086000000
C	0.176149000000	1.213013000000	-0.000005000000
H	-0.376199000000	2.146370000000	0.000022000000
H	3.352102000000	-0.000001000000	-0.000153000000
Cl	-2.254316000000	0.000000000000	0.000096000000

```
Zero-point correction=                           0.092363 (Hartree/Particle)
 Thermal correction to Energy=                    0.097804
 Thermal correction to Enthalpy=                  0.098748
 Thermal correction to Gibbs Free Energy=         0.062620
 Sum of electronic and zero-point Energies=           -691.647479
 Sum of electronic and thermal Energies=              -691.642038
 Sum of electronic and thermal Enthalpies=            -691.641094
 Sum of electronic and thermal Free Energies=         -691.677223
CPCM (Benzene) M06L/def2TZVP E = -691.903835079
```

TS-OA-Ni(0)-PhSeCF$_3$ (ωB97XD opt.)

Ni	-0.166619000000	0.566335000000	-0.396591000000
C	-0.209339000000	-1.229407000000	-0.009866000000
C	0.406097000000	-3.508653000000	0.041963000000
C	-1.022855000000	-3.365911000000	0.569748000000
N	-1.321048000000	-1.973981000000	0.233727000000
N	0.823080000000	-2.109524000000	-0.042974000000
H	-1.080300000000	-3.516258000000	1.658007000000
H	1.058684000000	-4.077981000000	0.710551000000
C	-2.594257000000	-1.395975000000	0.513065000000
C	-3.604540000000	-1.425103000000	-0.463421000000
C	-2.803976000000	-0.809858000000	1.775451000000
C	-4.838519000000	-0.856055000000	-0.135857000000
C	-4.054941000000	-0.259082000000	2.052456000000
C	-5.069105000000	-0.281915000000	1.105925000000
H	-5.631404000000	-0.861047000000	-0.880114000000
H	-4.234178000000	0.202900000000	3.019591000000
H	-6.036286000000	0.158150000000	1.330570000000
C	2.184017000000	-1.742727000000	-0.242805000000
C	3.004392000000	-1.618912000000	0.890570000000
C	2.672383000000	-1.536971000000	-1.541553000000
C	4.339978000000	-1.268359000000	0.698774000000
C	4.016899000000	-1.188958000000	-1.687246000000
C	4.844137000000	-1.055398000000	-0.579138000000
H	4.994930000000	-1.151568000000	1.557500000000
H	4.424393000000	-1.027567000000	-2.681761000000
H	5.888682000000	-0.787655000000	-0.712433000000
C	-3.498916000000	-2.055229000000	-1.851899000000
H	-4.203368000000	-1.482885000000	-2.469144000000
C	-4.018533000000	-3.502025000000	-1.829105000000
H	-4.050254000000	-3.914913000000	-2.843927000000
H	-3.367588000000	-4.146893000000	-1.228135000000
H	-5.025395000000	-3.557109000000	-1.402461000000
C	-2.147851000000	-1.973557000000	-2.573431000000
H	-1.442386000000	-2.727368000000	-2.210711000000
H	-2.303489000000	-2.157968000000	-3.642971000000
H	-1.679118000000	-0.991849000000	-2.450750000000
C	1.784396000000	-1.709559000000	-2.761181000000
H	0.758236000000	-1.836113000000	-2.408008000000
C	2.175821000000	-2.968811000000	-3.547369000000
H	3.186730000000	-2.877678000000	-3.962425000000
H	2.157620000000	-3.858480000000	-2.907815000000
H	1.482212000000	-3.130535000000	-4.380206000000
C	1.790618000000	-0.470887000000	-3.662719000000
H	1.494690000000	0.417390000000	-3.095993000000
H	2.777514000000	-0.290104000000	-4.104778000000
H	1.075564000000	-0.598424000000	-4.483045000000
C	2.436010000000	-1.805590000000	2.287864000000
H	1.487530000000	-2.343265000000	2.192452000000
C	3.344403000000	-2.640652000000	3.196398000000
H	3.588636000000	-3.605714000000	2.739343000000
H	4.285556000000	-2.124823000000	3.417772000000
H	2.845776000000	-2.829488000000	4.153469000000
C	2.112908000000	-0.444202000000	2.915306000000
H	1.459319000000	0.142851000000	2.261113000000
H	1.614081000000	-0.577573000000	3.883145000000
H	3.028602000000	0.133848000000	3.078789000000
C	-1.710681000000	-0.739147000000	2.831303000000
H	-0.803290000000	-1.190832000000	2.421383000000
C	-2.091934000000	-1.525634000000	4.092108000000
H	-1.269502000000	-1.505381000000	4.816423000000
H	-2.975736000000	-1.098191000000	4.579562000000
H	-2.315471000000	-2.572201000000	3.856438000000
C	-1.364581000000	0.718351000000	3.158909000000
H	-0.539014000000	0.765650000000	3.877550000000
H	-1.056354000000	1.243441000000	2.249361000000
H	-2.221832000000	1.247744000000	3.590876000000
C	1.209916000000	2.452064000000	0.038822000000
C	0.918142000000	3.031875000000	1.278436000000
C	2.515051000000	2.010756000000	-0.227859000000
C	1.921334000000	3.161952000000	2.234802000000
H	-0.082185000000	3.374299000000	1.509339000000
C	3.503066000000	2.142601000000	0.737891000000
H	2.753625000000	1.548796000000	-1.180967000000
C	3.215918000000	2.729693000000	1.968927000000
H	1.680673000000	3.609439000000	3.194688000000
H	4.502140000000	1.778045000000	0.522117000000
H	3.993899000000	2.838118000000	2.718528000000
H	0.436828000000	-3.977662000000	-0.951566000000

H	-1.724081000000	-4.053210000000	0.091453000000	F	-0.884740000000	4.924383000000	-0.504716000000
Se	-0.039059000000	2.454481000000	-1.479080000000	F	-2.065057000000	3.295648000000	0.274049000000
C	-1.405963000000	3.731527000000	-0.806701000000	F	-2.296041000000	3.900350000000	-1.790025000000

```
Zero-point correction=                           0.713410 (Hartree/Particle)
 Thermal correction to Energy=                   0.755603
 Thermal correction to Enthalpy=                 0.756547
 Thermal correction to Gibbs Free Energy=        0.638549
 Sum of electronic and zero-point Energies=          -4299.209415
 Sum of electronic and thermal Energies=             -4299.167222
 Sum of electronic and thermal Enthalpies=           -4299.166278
 Sum of electronic and thermal Free Energies=        -4299.284276
CPCM (Benzene) M06L/def2TZVP E = -5640.7383097
```

SIPr-Ni-Ph-SeCF$_3$ (ωB97XD opt.)

Ni	0.485273000000	0.553929000000	-0.224494000000	H	0.058291000000	0.191134000000	4.246280000000
N	0.511435000000	-2.215229000000	0.290786000000	H	2.012227000000	-2.187506000000	4.780932000000
N	-1.542234000000	-1.734551000000	-0.194187000000	H	0.248289000000	-2.260172000000	4.898976000000
C	2.888401000000	-2.104893000000	-0.225225000000	H	1.120254000000	-3.400761000000	3.852156000000
C	4.188577000000	-1.829193000000	0.194284000000	H	-0.231966000000	-3.716727000000	1.573003000000
C	4.447333000000	-1.444570000000	1.504668000000	H	-2.379868000000	-3.552637000000	0.506106000000
C	3.409128000000	-1.313173000000	2.416885000000	H	-5.583804000000	0.286297000000	0.519059000000
C	2.087597000000	-1.561990000000	2.040790000000	H	-5.763550000000	0.964209000000	-1.845770000000
C	1.854287000000	-1.965265000000	0.716170000000	H	-3.981105000000	0.388705000000	-3.447006000000
C	2.585557000000	-2.478098000000	-1.668478000000	H	-2.603989000000	-1.557944000000	1.892539000000
C	2.314610000000	-1.218341000000	-2.505741000000	H	-3.529539000000	-0.223155000000	3.721659000000
C	3.685326000000	-3.328759000000	-2.313304000000	H	-4.651062000000	0.592176000000	2.622545000000
C	0.962637000000	-1.372973000000	3.046494000000	H	-2.904085000000	0.839700000000	2.436721000000
C	0.893232000000	0.076402000000	3.546304000000	H	-4.597608000000	-3.020546000000	1.412666000000
C	1.093652000000	-2.365213000000	4.210295000000	H	-4.540234000000	-2.500658000000	3.111247000000
C	-0.173623000000	-3.493619000000	0.499696000000	H	-5.663190000000	-1.729424000000	1.979186000000
C	-1.549842000000	-3.201217000000	-0.111639000000	H	-0.884749000000	-1.525847000000	-2.488669000000
C	-0.324330000000	-1.210421000000	-0.026787000000	H	-0.685437000000	0.941932000000	-2.818119000000
C	-2.683267000000	-1.006526000000	-0.650910000000	H	-0.203915000000	0.011317000000	-4.254092000000
C	-3.685719000000	-0.690429000000	0.279006000000	C	-2.220381000000	-1.915797000000	-4.105633000000
C	-4.795467000000	0.018475000000	-0.178575000000	H	-3.003474000000	-1.424758000000	-4.694332000000
C	-4.896962000000	0.402936000000	-1.509311000000	H	-1.416599000000	-2.202472000000	-4.793006000000
C	-3.891639000000	0.077493000000	-2.409976000000	H	-2.649421000000	-2.828430000000	-3.677015000000
C	-2.765210000000	-0.637517000000	-2.002271000000	C	1.747366000000	1.812686000000	-0.617838000000
C	-3.588349000000	-1.102589000000	1.739189000000	C	2.922804000000	1.561756000000	0.103031000000
C	-3.672649000000	0.102207000000	2.684833000000	C	1.835899000000	2.493107000000	-1.838709000000
C	-4.656778000000	-2.152071000000	2.079002000000	C	4.167721000000	1.912767000000	-0.422189000000
C	-1.681359000000	-0.985532000000	-3.010377000000	C	3.076582000000	2.852075000000	-2.358116000000
C	-1.048511000000	0.277480000000	-3.608431000000	C	4.245371000000	2.552772000000	-1.655534000000
H	5.010144000000	-1.906459000000	-0.510055000000	H	2.878416000000	1.076776000000	1.076576000000
H	5.467544000000	-1.236024000000	1.813209000000	H	0.929380000000	2.732053000000	-2.388344000000
H	3.625000000000	-0.998450000000	3.434006000000	H	5.072880000000	1.693659000000	0.139097000000
H	1.665949000000	-3.075792000000	-1.671351000000	H	3.136850000000	3.365083000000	-3.314693000000
H	1.423272000000	-0.685302000000	-2.154168000000	H	5.212102000000	2.833339000000	-2.064904000000
H	2.147433000000	-1.482366000000	-3.556589000000	Se	-1.171803000000	1.942889000000	0.321950000000
H	3.153350000000	-0.515572000000	-2.448935000000	H	-1.771600000000	0.837580000000	-4.212362000000
H	3.952474000000	-4.185900000000	-1.686082000000	C	-0.345904000000	3.579410000000	0.972156000000
H	3.341853000000	-3.706433000000	-3.282118000000	F	0.634620000000	3.363322000000	1.869471000000
H	4.594195000000	-2.745833000000	-2.498720000000	F	0.173097000000	4.362827000000	0.015068000000
H	0.011304000000	-1.573949000000	2.544033000000	F	-1.290367000000	4.308969000000	1.598898000000
H	0.733844000000	0.776330000000	2.720482000000	H	0.355790000000	-4.310992000000	0.003070000000
H	1.811685000000	0.363926000000	4.071018000000	H	-1.660739000000	-3.624258000000	-1.118396000000

```
Zero-point correction=                           0.712440 (Hartree/Particle)
 Thermal correction to Energy=                   0.755990
 Thermal correction to Enthalpy=                 0.756934
 Thermal correction to Gibbs Free Energy=        0.633787
 Sum of electronic and zero-point Energies=          -4299.249941
 Sum of electronic and thermal Energies=             -4299.206391
 Sum of electronic and thermal Enthalpies=           -4299.205446
 Sum of electronic and thermal Free Energies=        -4299.328594
CPCM (Benzene) M06L/def2TZVP E = -5640.77292940
```

TS-OA-Ni(0)-PhI (ωB97XD opt.)

Ni	0.123547000000	-0.655134000000	-0.639738000000	C	4.047657000000	0.029889000000	-0.433772000000
C	0.748710000000	0.807584000000	0.201893000000	C	3.012910000000	-0.921947000000	1.578250000000
C	0.916030000000	3.030370000000	0.988662000000	C	5.016205000000	-0.976111000000	-0.364247000000
C	2.215662000000	2.292135000000	1.308039000000	C	4.003969000000	-1.902177000000	1.603728000000
N	2.048396000000	1.060540000000	0.538956000000	C	5.002983000000	-1.931858000000	0.640920000000
N	0.057722000000	1.927437000000	0.560303000000	H	5.794098000000	-1.007029000000	-1.123733000000
H	2.307704000000	2.066638000000	2.381187000000	H	3.989353000000	-2.658114000000	2.384248000000
H	0.493263000000	3.554006000000	1.851293000000	H	5.766369000000	-2.703919000000	0.668644000000
C	3.048365000000	0.044115000000	0.553944000000	C	-1.331213000000	2.127665000000	0.318506000000

C	-2.214675000000	1.993250000000	1.403680000000
C	-1.778773000000	2.486438000000	-0.961937000000
C	-3.571161000000	2.222580000000	1.180121000000
C	-3.147505000000	2.698942000000	-1.142633000000
C	-4.035952000000	2.572978000000	-0.083099000000
H	-4.278686000000	2.120306000000	1.997420000000
H	-3.520183000000	2.979766000000	-2.124335000000
H	-5.096385000000	2.750834000000	-0.240478000000
C	4.204045000000	1.041166000000	-1.568457000000
H	4.703329000000	0.483974000000	-2.372004000000
C	5.167902000000	2.166624000000	-1.158164000000
H	5.368330000000	2.829645000000	-2.007747000000
H	4.742823000000	2.776370000000	-0.353133000000
H	6.121751000000	1.763474000000	-0.802238000000
C	2.925406000000	1.620310000000	-2.186181000000
H	2.497409000000	2.413042000000	-1.565674000000
H	3.164751000000	2.058306000000	-3.162557000000
H	2.155650000000	0.853707000000	-2.322593000000
C	-0.816226000000	2.673069000000	-2.121134000000
H	0.173348000000	2.356560000000	-1.784835000000
C	-0.729993000000	4.150510000000	-2.528467000000
H	-1.690180000000	4.514893000000	-2.913156000000
H	-0.452014000000	4.781892000000	-1.676888000000
H	0.021044000000	4.286209000000	-3.315047000000
C	-1.177237000000	1.784448000000	-3.316045000000
H	-1.198597000000	0.732052000000	-3.014198000000
H	-2.152585000000	2.047968000000	-3.742593000000
H	-0.426275000000	1.893079000000	-4.106823000000
C	-1.699396000000	1.549276000000	2.763216000000
H	-0.648727000000	1.848572000000	2.834877000000
C	-2.437905000000	2.198156000000	3.937944000000
H	-2.475506000000	3.288366000000	3.837985000000
H	-3.466438000000	1.829733000000	4.026224000000
H	-1.928989000000	1.956666000000	4.877471000000
C	-1.735108000000	0.018566000000	2.864999000000
H	-1.212550000000	-0.444169000000	2.020460000000
H	-1.261298000000	-0.315311000000	3.796394000000
H	-2.768488000000	-0.342912000000	2.856039000000
C	1.927215000000	-0.939129000000	2.644135000000
H	1.236580000000	-0.114606000000	2.449610000000
C	2.513379000000	-0.731962000000	4.047053000000
H	1.710776000000	-0.690631000000	4.792514000000
H	3.186956000000	-1.549984000000	4.327716000000
H	3.083308000000	0.202233000000	4.105203000000
C	1.100081000000	-2.228610000000	2.566049000000
H	0.295053000000	-2.211844000000	3.309077000000
H	0.649274000000	-2.323092000000	1.571272000000
H	1.716973000000	-3.115209000000	2.754568000000
I	-0.739429000000	-2.493962000000	-2.012339000000
C	-2.247276000000	-2.129807000000	-0.463981000000
C	-2.330165000000	-3.039145000000	0.585112000000
C	-3.182543000000	-1.113979000000	-0.630540000000
C	-3.395446000000	-2.939522000000	1.477358000000
H	-1.581643000000	-3.814471000000	0.706931000000
C	-4.240609000000	-1.031181000000	0.271667000000
H	-3.086594000000	-0.386933000000	-1.429445000000
C	-4.356819000000	-1.946085000000	1.315006000000
H	-3.471075000000	-3.648418000000	2.296531000000
H	-4.969500000000	-0.236093000000	0.155546000000
H	-5.189085000000	-1.877263000000	2.009028000000
H	1.042923000000	3.757033000000	0.172871000000
H	3.106232000000	2.843224000000	0.996473000000

```
Zero-point correction=                           0.697542 (Hartree/Particle)
 Thermal correction to Energy=                    0.735813
 Thermal correction to Enthalpy=                  0.736757
 Thermal correction to Gibbs Free Energy=         0.627058
 Sum of electronic and zero-point Energies=          -1574.142972
 Sum of electronic and thermal Energies=             -1574.104702
 Sum of electronic and thermal Enthalpies=           -1574.103758
 Sum of electronic and thermal Free Energies=        -1574.213457
CPCM (Benzene) M06L/def2TZVP E = -3199.39742446
```

TS-OA-Ni(0)-PhBr (ωB97XD opt.)

Ni	0.114571000000	-0.437277000000	-1.015820000000
C	0.631511000000	0.574879000000	0.382954000000
C	0.638250000000	2.269781000000	2.028889000000
C	1.983702000000	1.547238000000	2.057712000000
N	1.908498000000	0.746508000000	0.837159000000
N	-0.139978000000	1.391279000000	1.157503000000
H	2.082018000000	0.896169000000	2.939508000000
H	0.176398000000	2.367360000000	3.015835000000
C	2.981903000000	-0.110165000000	0.453062000000
C	3.969440000000	0.359045000000	-0.429182000000
C	3.028640000000	-1.414290000000	0.982798000000
C	5.008278000000	-0.513956000000	-0.766188000000
C	4.090681000000	-2.242332000000	0.621080000000
C	5.077359000000	-1.798626000000	-0.248103000000
H	5.777093000000	-0.172096000000	-1.455454000000
H	4.143099000000	-3.251656000000	1.020822000000
H	5.894707000000	-2.456767000000	-0.528561000000
C	-1.536868000000	1.597561000000	0.970434000000
C	-2.419983000000	0.970887000000	1.867506000000
C	-1.994804000000	2.437985000000	-0.054775000000
C	-3.786040000000	1.199516000000	1.714474000000
C	-3.373127000000	2.633311000000	-0.176041000000
C	-4.260730000000	2.026434000000	0.701670000000
H	-4.491934000000	0.725103000000	2.389166000000
H	-3.753388000000	3.283496000000	-0.959818000000
H	-5.328790000000	2.197429000000	0.597160000000
C	4.047780000000	1.760171000000	-1.033749000000
H	4.571766000000	1.622397000000	-1.988435000000
C	4.943216000000	2.664984000000	-0.171434000000
H	5.085047000000	3.638359000000	-0.655122000000
H	4.491850000000	2.842736000000	0.811103000000
H	5.927287000000	2.212977000000	-0.009476000000
C	2.730494000000	2.467301000000	-1.374232000000
H	2.263057000000	2.905587000000	-0.487541000000
H	2.934166000000	3.283408000000	-2.077757000000
H	2.007161000000	1.782816000000	-1.829016000000
C	-1.040004000000	3.150972000000	-0.996131000000
H	-0.028742000000	2.806101000000	-0.771213000000
C	-1.081875000000	4.668952000000	-0.771922000000
H	-2.065177000000	5.083561000000	-1.023806000000
H	-0.874073000000	4.920190000000	0.274286000000
H	-0.335683000000	5.168626000000	-1.399961000000
C	-1.306418000000	2.794345000000	-2.462545000000
H	-1.198333000000	1.715586000000	-2.617311000000
H	-2.311250000000	3.097612000000	-2.780932000000
H	-0.583139000000	3.300931000000	-3.111603000000
C	-1.886777000000	0.024043000000	2.930941000000
H	-0.870803000000	0.346264000000	3.182997000000
C	-2.703646000000	0.033157000000	4.226423000000
H	-2.841449000000	1.049195000000	4.612022000000
H	-3.694056000000	-0.414931000000	4.086044000000
H	-2.190361000000	-0.557449000000	4.993094000000
C	-1.778180000000	-1.396776000000	2.361067000000
H	-1.196932000000	-1.407383000000	1.432633000000
H	-1.295681000000	-2.064922000000	3.085257000000
H	-2.772706000000	-1.795238000000	2.135357000000
C	1.957904000000	-1.950532000000	1.922125000000
H	1.199342000000	-1.176226000000	2.063743000000
C	2.538728000000	-2.286985000000	3.301865000000
H	1.743198000000	-2.614886000000	3.980982000000
H	3.279505000000	-3.092750000000	3.241812000000
H	3.031894000000	-1.415741000000	3.747453000000
C	1.238553000000	-3.156270000000	1.304423000000
H	0.442545000000	-3.508775000000	1.970007000000
H	0.786611000000	-2.871289000000	0.347822000000
H	1.928443000000	-3.990057000000	1.129029000000
Br	-0.531784000000	-1.511930000000	-2.879947000000
C	-1.976581000000	-1.836772000000	-1.591731000000
C	-2.047520000000	-3.097350000000	-1.005409000000
C	-3.004807000000	-0.907159000000	-1.460609000000
C	-3.175412000000	-3.425809000000	-0.258543000000
H	-1.236414000000	-3.806334000000	-1.128831000000
C	-4.120475000000	-1.253714000000	-0.706128000000
H	-2.927107000000	0.073835000000	-1.914667000000
C	-4.214793000000	-2.510777000000	-0.112956000000
H	-3.238999000000	-4.404854000000	0.206754000000
H	-4.915764000000	-0.526647000000	-0.581694000000
H	-5.094594000000	-2.774022000000	0.466349000000

H	0.719352000000	3.273226000000	1.585628000000
H	2.835233000000	2.231562000000	2.038328000000

```
Zero-point correction=                           0.697554 (Hartree/Particle)
 Thermal correction to Energy=                    0.735732
 Thermal correction to Enthalpy=                  0.736676
 Thermal correction to Gibbs Free Energy=         0.627581
 Sum of electronic and zero-point Energies=          -4134.159556
 Sum of electronic and thermal Energies=             -4134.121378
 Sum of electronic and thermal Enthalpies=           -4134.120434
 Sum of electronic and thermal Free Energies=        -4134.229529
CPCM (Benzene) M06L/def2TZVP E = -5475.58346706
```

TS-OA-Ni(0)-PhCl (ωB97XD opt.)

Ni	0.068989000000	-0.224273000000	-1.287008000000
C	0.576522000000	0.455836000000	0.297973000000
C	0.527032000000	1.762675000000	2.269268000000
C	1.886281000000	1.072294000000	2.165213000000
N	1.842803000000	0.541372000000	0.803755000000
N	-0.217865000000	1.089429000000	1.208077000000
H	1.988801000000	0.254094000000	2.893972000000
H	0.046648000000	1.627538000000	3.243102000000
C	2.938250000000	-0.209127000000	0.285737000000
C	3.951119000000	0.442032000000	-0.438240000000
C	2.989319000000	-1.593542000000	0.540331000000
C	5.024159000000	-0.330366000000	-0.893202000000
C	4.083135000000	-2.317322000000	0.067306000000
C	5.098816000000	-1.692611000000	-0.642986000000
H	5.815899000000	0.155010000000	-1.459548000000
H	4.138614000000	-3.386885000000	0.252318000000
H	5.943738000000	-2.268396000000	-1.009554000000
C	-1.621236000000	1.275532000000	1.061364000000
C	-2.475841000000	0.433137000000	1.792996000000
C	-2.113886000000	2.295865000000	0.234457000000
C	-3.851182000000	0.625949000000	1.672833000000
C	-3.499091000000	2.450461000000	0.139741000000
C	-4.360509000000	1.626721000000	0.852555000000
H	-4.535092000000	-0.016233000000	2.219912000000
H	-3.907572000000	3.234474000000	-0.492733000000
H	-5.435000000000	1.766660000000	0.770508000000
C	4.016079000000	1.936764000000	-0.750093000000
H	4.580418000000	1.999462000000	-1.689727000000
C	4.852801000000	2.672780000000	0.309128000000
H	4.996828000000	3.721429000000	0.024540000000
H	4.354329000000	2.658770000000	1.284719000000
H	5.837621000000	2.210005000000	0.431566000000
C	2.693600000000	2.671368000000	-1.003202000000
H	2.176634000000	2.914185000000	-0.070124000000
H	2.902421000000	3.615813000000	-1.519779000000
H	2.008822000000	2.077557000000	-1.617050000000
C	-1.185983000000	3.233554000000	-0.518291000000
H	-0.163417000000	2.876655000000	-0.373913000000
C	-1.277432000000	4.658288000000	0.045940000000
H	-2.276973000000	5.083385000000	-0.104806000000
H	-1.069560000000	4.673261000000	1.121747000000
H	-0.554807000000	5.314295000000	-0.452477000000
C	-1.448043000000	3.213817000000	-2.027916000000
H	-1.317826000000	2.201611000000	-2.424916000000
H	-2.459743000000	3.560646000000	-2.270684000000
H	-0.737994000000	3.870686000000	-2.542888000000
C	-1.908566000000	-0.694894000000	2.639110000000
H	-0.871197000000	-0.441081000000	2.878814000000
C	-2.649187000000	-0.892284000000	3.965486000000
H	-2.725897000000	0.045777000000	4.525910000000
H	-3.663144000000	-1.279514000000	3.813218000000
H	-2.115767000000	-1.620732000000	4.585929000000
C	-1.870367000000	-1.993162000000	1.822850000000
H	-1.343344000000	-1.843410000000	0.874227000000
H	-1.362438000000	-2.786621000000	2.385183000000
H	-2.885604000000	-2.332355000000	1.591263000000
C	1.887832000000	-2.324043000000	1.295136000000
H	1.114898000000	-1.601557000000	1.568450000000
C	2.412909000000	-2.954001000000	2.591928000000
H	1.591243000000	-3.422975000000	3.145695000000
H	3.162445000000	-3.727627000000	2.388700000000
H	2.878334000000	-2.202551000000	3.239622000000
C	1.211377000000	-3.366864000000	0.396666000000
H	0.385063000000	-3.853790000000	0.926818000000
H	0.804932000000	-2.878955000000	-0.495914000000
H	1.917432000000	-4.143298000000	0.079364000000
Cl	-0.582053000000	-0.785649000000	-3.283113000000
C	-1.848462000000	-1.491173000000	-2.197840000000
C	-1.799041000000	-2.862618000000	-1.956894000000
C	-2.951627000000	-0.720137000000	-1.834937000000
C	-2.875344000000	-3.467520000000	-1.315056000000
H	-0.933306000000	-3.439232000000	-2.263083000000
C	-4.014040000000	-1.345829000000	-1.193059000000
H	-2.968028000000	0.347111000000	-2.024033000000
C	-3.985450000000	-2.715984000000	-0.939205000000
H	-2.842429000000	-4.534356000000	-1.115500000000
H	-4.865736000000	-0.748476000000	-0.885521000000
H	-4.824974000000	-3.194853000000	-0.444691000000
H	0.595306000000	2.841269000000	2.065677000000
H	2.724417000000	1.759724000000	2.301442000000

```
Zero-point correction=                           0.697620 (Hartree/Particle)
 Thermal correction to Energy=                    0.735678
 Thermal correction to Enthalpy=                  0.736622
 Thermal correction to Gibbs Free Energy=         0.628126
 Sum of electronic and zero-point Energies=          -2022.900574
 Sum of electronic and thermal Energies=             -2022.862516
 Sum of electronic and thermal Enthalpies=           -2022.861572
 Sum of electronic and thermal Free Energies=        -2022.970069
CPCM (Benzene) M06L/def2TZVP E = -3361.72912894
```

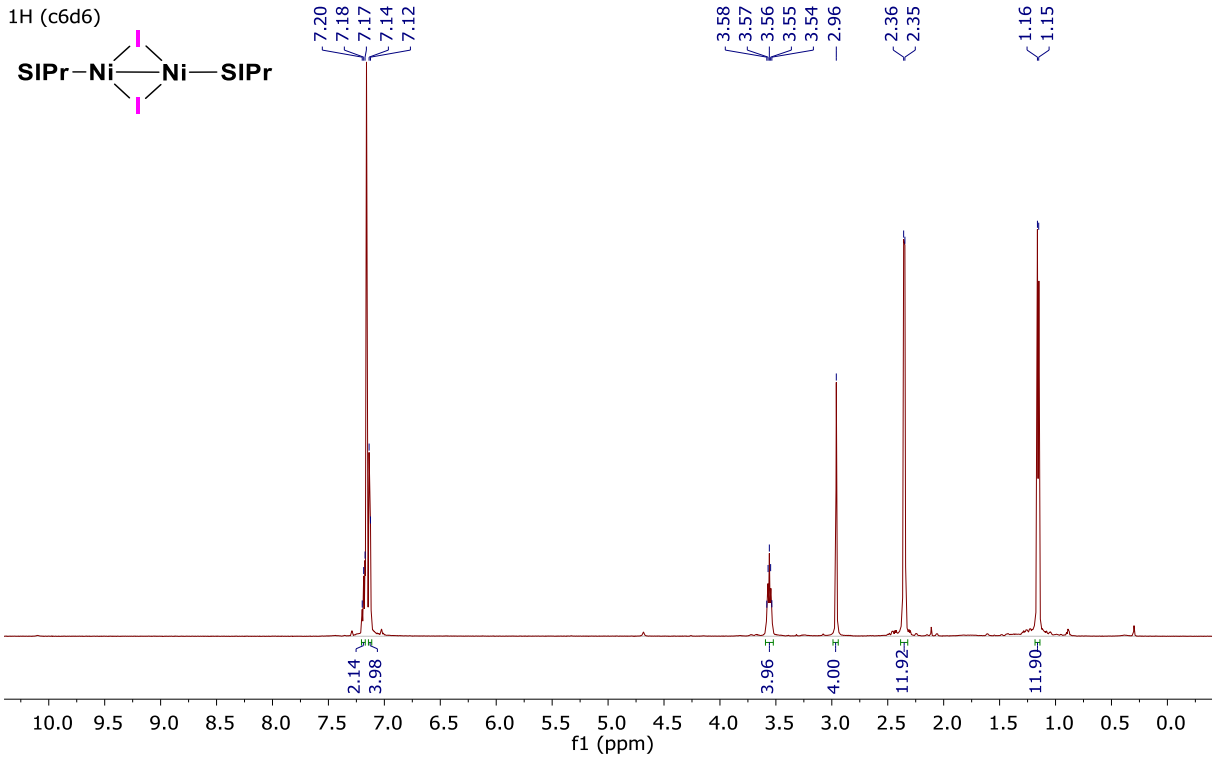
SIPr-Ni-Ph-I (ωB97XD opt.)

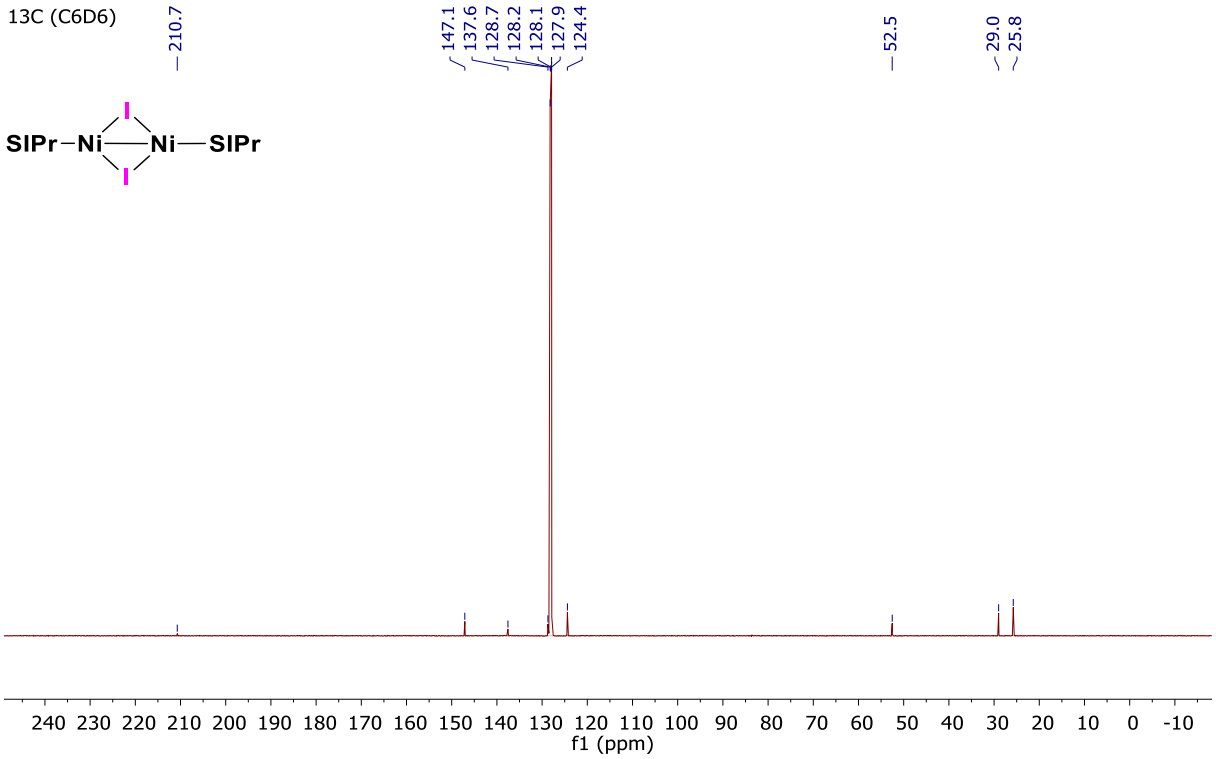
Ni	-0.596170000000	-0.733962000000	-0.388469000000
C	0.252803000000	0.712824000000	0.657673000000
C	1.539460000000	2.120682000000	2.009966000000
C	0.166125000000	2.760421000000	1.799904000000
N	-0.564506000000	1.658667000000	1.163085000000
N	1.493114000000	0.991568000000	1.070190000000
H	0.209989000000	3.622139000000	1.121204000000
H	2.369318000000	2.790917000000	1.776799000000
C	-1.926413000000	1.791387000000	0.741636000000
C	-2.955461000000	1.253784000000	1.537069000000
C	-2.188770000000	2.450616000000	-0.473604000000
C	-4.267537000000	1.420159000000	1.089899000000
C	-3.519759000000	2.597355000000	-0.867608000000
C	-4.552635000000	2.091090000000	-0.091923000000
H	-5.080243000000	1.002663000000	1.677997000000
H	-3.747334000000	3.102559000000	-1.801846000000
H	-5.583010000000	2.209556000000	-0.413768000000
C	2.641631000000	0.165571000000	0.864794000000
C	3.623535000000	0.607845000000	-0.034357000000
C	2.759913000000	-1.037156000000	1.575551000000
C	4.744022000000	-0.198979000000	-0.221223000000
C	3.891363000000	-1.819197000000	1.340472000000
C	4.874254000000	-1.407081000000	0.451450000000
H	5.518118000000	0.113308000000	-0.916216000000

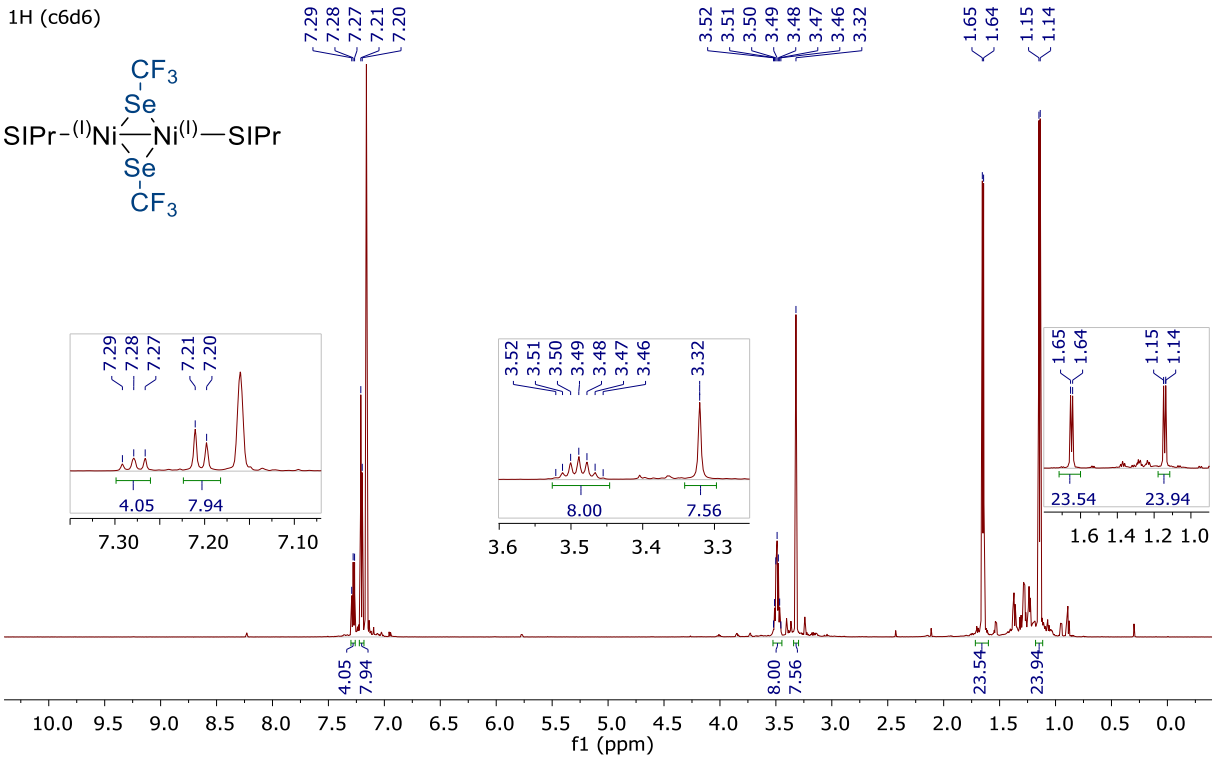
H	4.003516000000	-2.766762000000	1.859922000000
H	5.746807000000	-2.030601000000	0.281018000000
C	-2.746517000000	0.428293000000	2.803471000000
H	-3.736662000000	0.373529000000	3.272966000000
C	-1.807939000000	1.025660000000	3.859176000000
H	-1.951250000000	0.502567000000	4.810808000000
H	-0.756722000000	0.909257000000	3.580264000000
H	-2.013862000000	2.088200000000	4.028695000000
C	-2.342866000000	-1.015534000000	2.468679000000
H	-1.345035000000	-1.052532000000	2.012660000000
H	-2.305069000000	-1.621002000000	3.381932000000
H	-3.045019000000	-1.479113000000	1.769488000000
C	1.713072000000	-1.505094000000	2.574109000000
H	0.937592000000	-0.735716000000	2.647048000000
C	2.311457000000	-1.672374000000	3.977443000000
H	3.070715000000	-2.461919000000	3.997868000000
H	2.784446000000	-0.745813000000	4.321115000000
H	1.528719000000	-1.945435000000	4.694022000000
C	1.029125000000	-2.794336000000	2.101921000000
H	0.590603000000	-2.662899000000	1.106997000000
H	1.745789000000	-3.621366000000	2.042513000000
H	0.233061000000	-3.083330000000	2.797646000000
C	3.497715000000	1.924126000000	-0.784545000000
H	2.500833000000	2.331833000000	-0.585090000000
C	4.537249000000	2.937148000000	-0.281245000000
H	4.463446000000	3.091788000000	0.801394000000
H	5.554580000000	2.588318000000	-0.492758000000
H	4.404594000000	3.905305000000	-0.777114000000
C	3.602463000000	1.739405000000	-2.303437000000
H	2.856018000000	1.023273000000	-2.657947000000
H	3.440151000000	2.698202000000	-2.809303000000
H	4.593187000000	1.374059000000	-2.596641000000
C	-1.081832000000	2.969551000000	-1.379932000000
H	-0.116302000000	2.703480000000	-0.940293000000
C	-1.133335000000	4.498658000000	-1.503858000000
H	-0.297323000000	4.858366000000	-2.113470000000
H	-2.061851000000	4.826879000000	-1.984690000000
H	-1.078084000000	4.984590000000	-0.523063000000
C	-1.130292000000	2.294619000000	-2.757569000000
H	-0.289113000000	2.633977000000	-3.371574000000
H	-1.056622000000	1.206305000000	-2.666598000000
H	-2.056157000000	2.536152000000	-3.292136000000
I	0.959769000000	-1.463739000000	-2.165214000000
C	-1.900504000000	-1.883787000000	-0.938195000000
C	-1.972994000000	-3.254146000000	-0.664809000000
C	-3.082983000000	-1.169321000000	-1.171766000000
C	-3.212229000000	-3.879095000000	-0.547554000000
H	-1.058545000000	-3.825735000000	-0.529154000000
C	-4.324303000000	-1.795983000000	-1.047711000000
H	-3.048405000000	-0.112775000000	-1.434864000000
C	-4.388717000000	-3.149596000000	-0.728850000000
H	-3.264491000000	-4.939979000000	-0.316200000000
H	-5.236343000000	-1.227253000000	-1.211173000000
H	-5.352769000000	-3.642307000000	-0.637236000000
H	1.673874000000	1.738361000000	3.030552000000
H	-0.314947000000	3.071304000000	2.728604000000

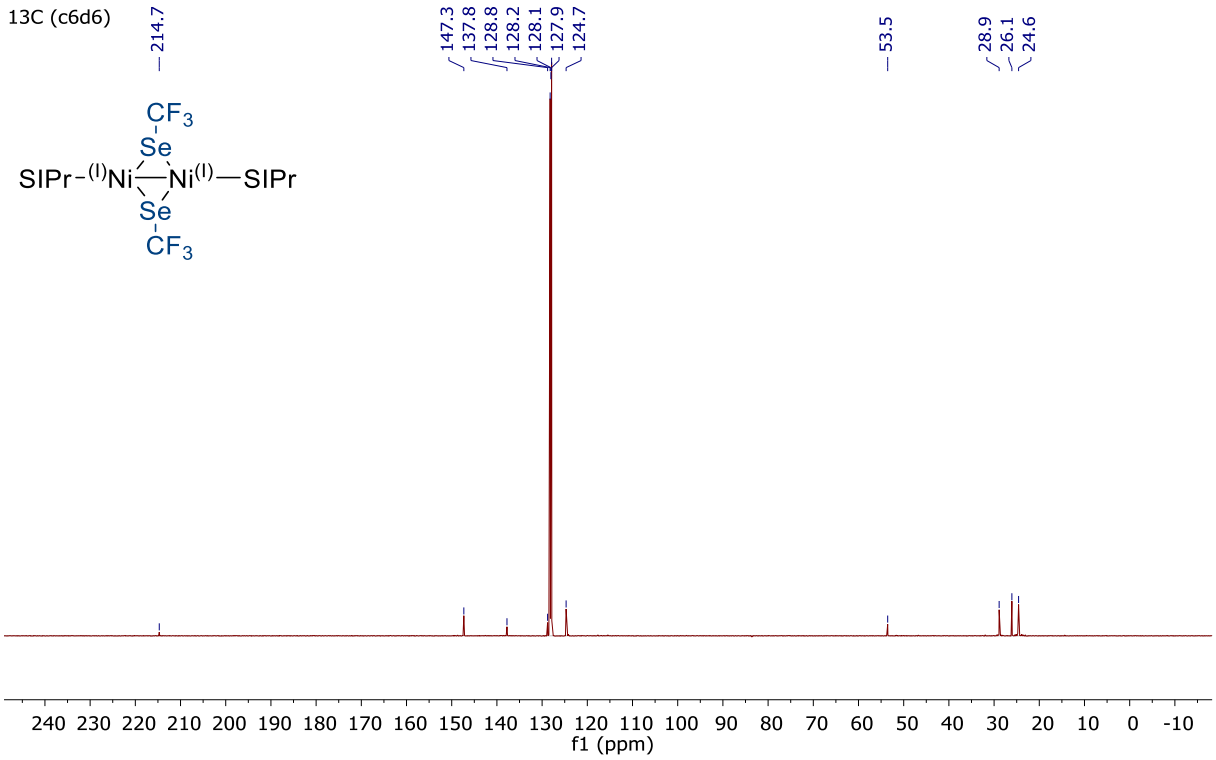
```
 Zero-point correction=                           0.698573 (Hartree/Particle)
  Thermal correction to Energy=                    0.737342
  Thermal correction to Enthalpy=                  0.738286
  Thermal correction to Gibbs Free Energy=         0.627202
  Sum of electronic and zero-point Energies=          -1574.211438
  Sum of electronic and thermal Energies=             -1574.172669
  Sum of electronic and thermal Enthalpies=           -1574.171725
  Sum of electronic and thermal Free Energies=        -1574.282809
 CPCM (Benzene) M06L/def2TZVP E = -3199.45039205
```

6. NMR Spectra

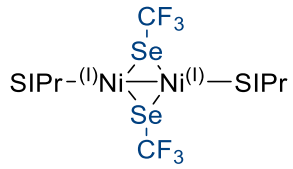




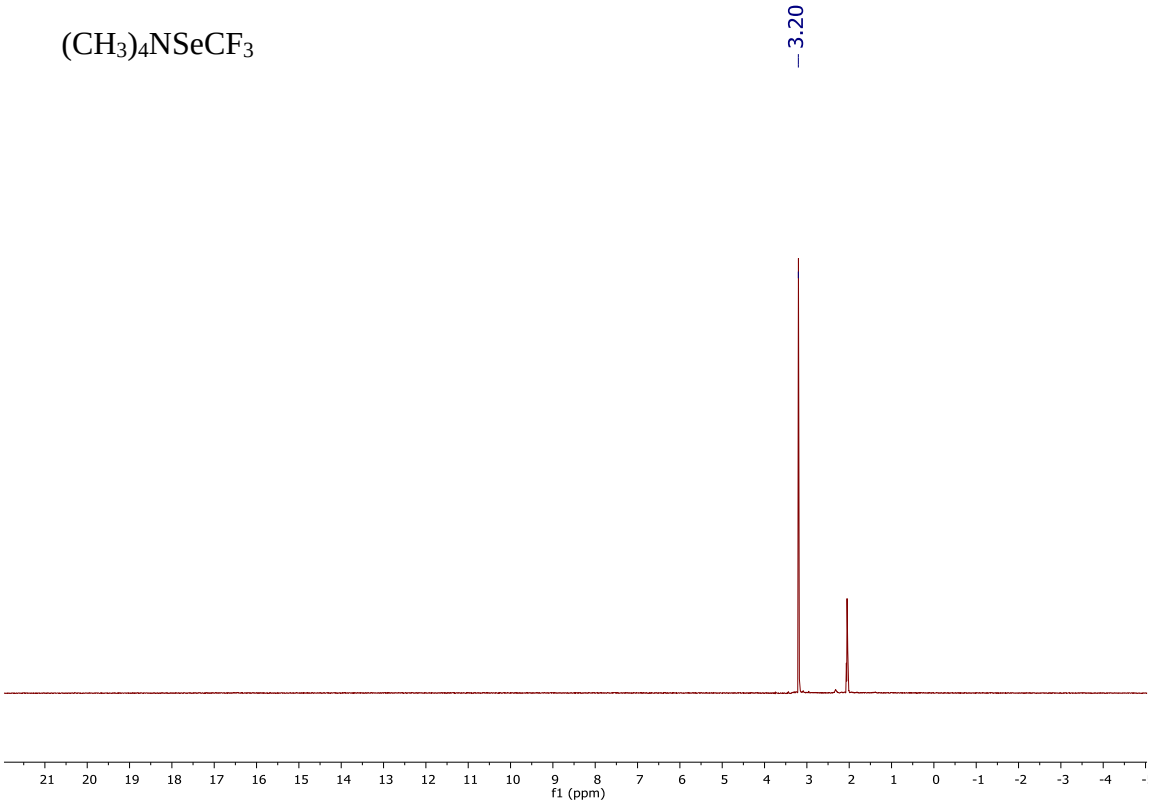

1H (c6d6)
CF3
Se
SIPr-(I)Ni—Ni(I)—SIPr
Se
CF3
7.29
7.28
7.27
7.21
7.20
3.52
3.51
3.50
3.49
3.48
3.47
3.46
3.32
1.65
1.64
1.15
1.14
4.05
7.94
8.00
7.56
23.54
23.94
f1 (ppm)


13C (c6d6)
CF3
Se
SIPr-(I)Ni—Ni(I)—SIPr
Se
CF3
214.7
147.3
137.8
128.8
128.2
128.1
127.9
124.7
53.5
28.9
26.1
24.6
f1 (ppm)

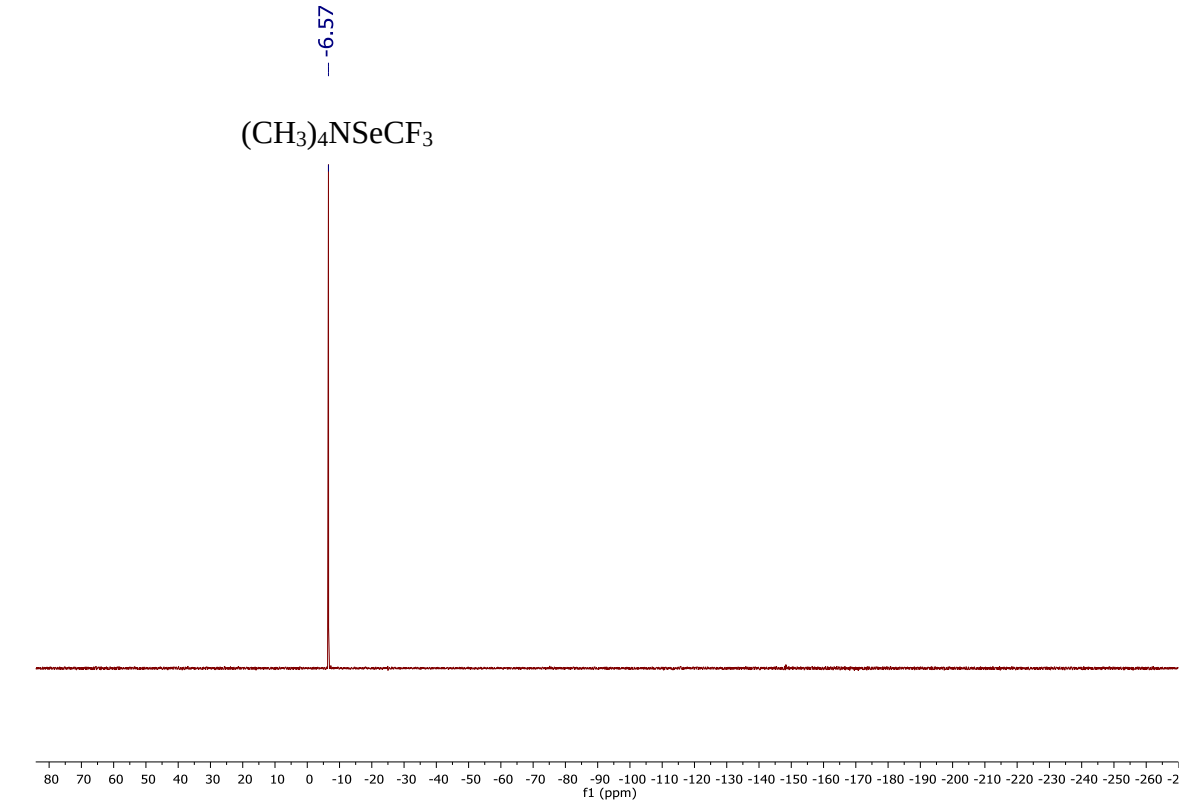
19F (c6d6)

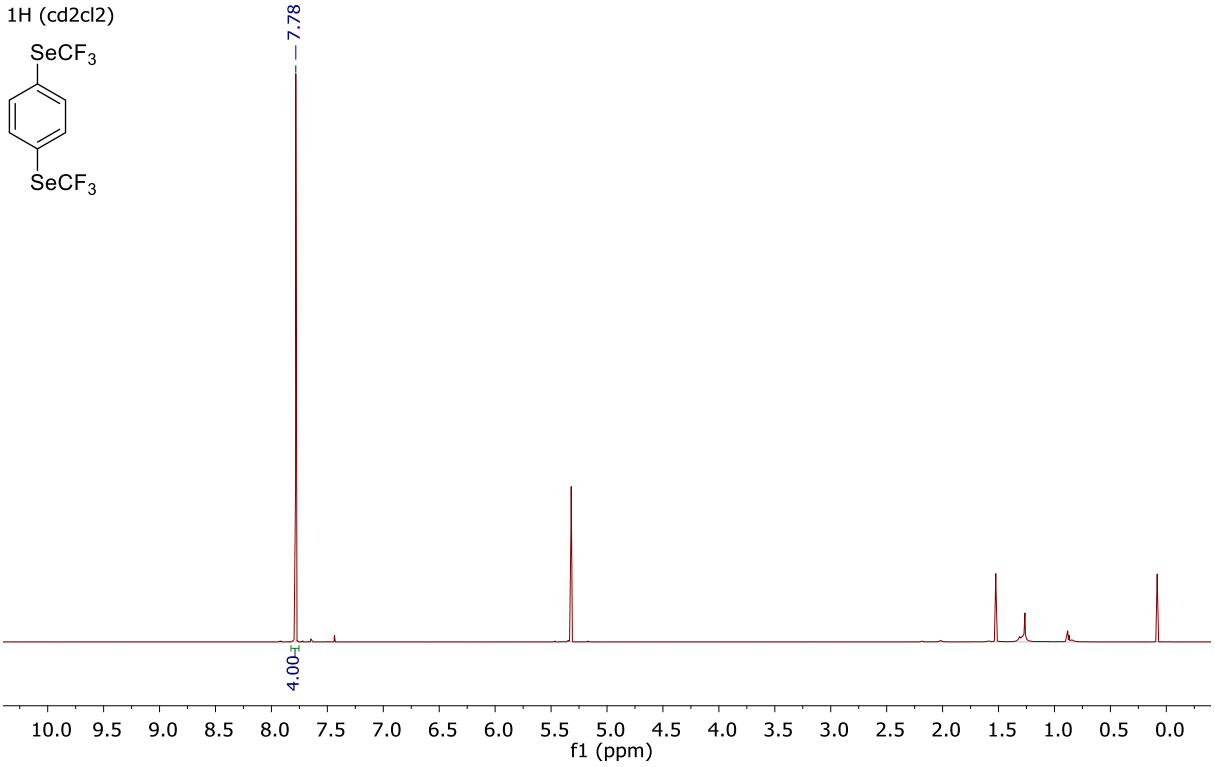


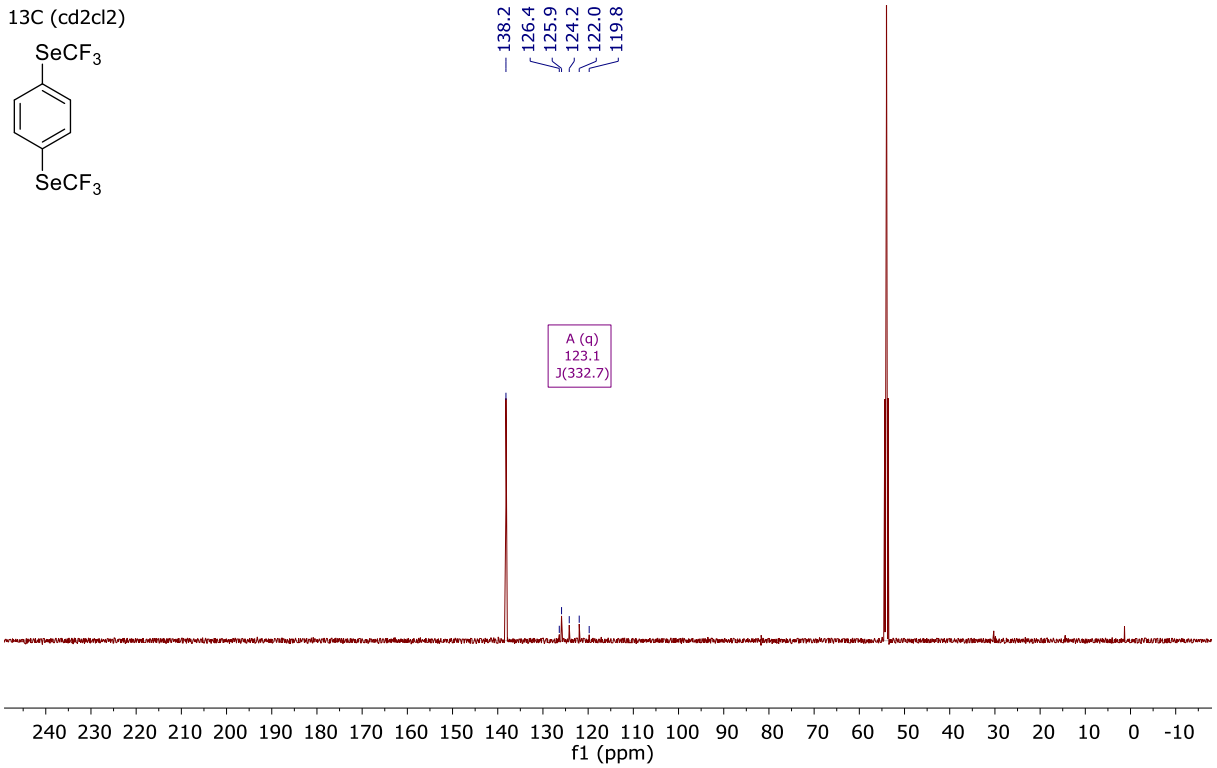
$(CH_3)_4NSeCF_3$

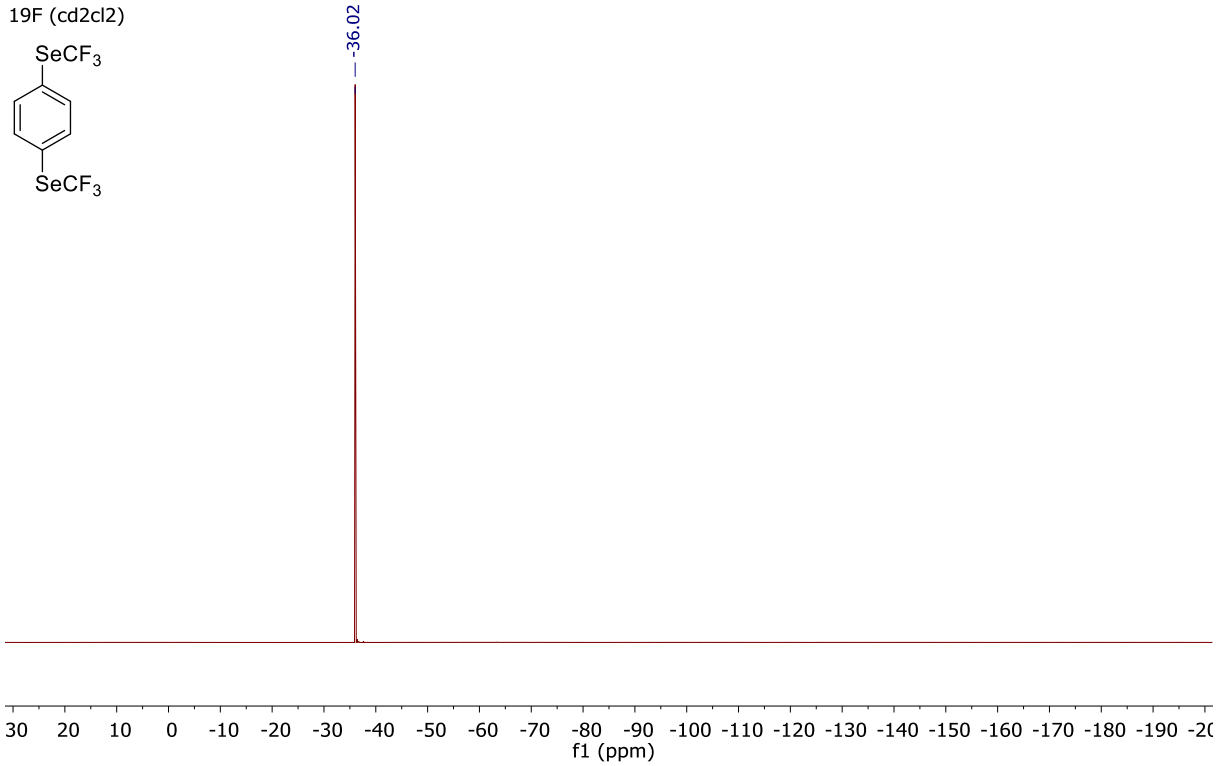


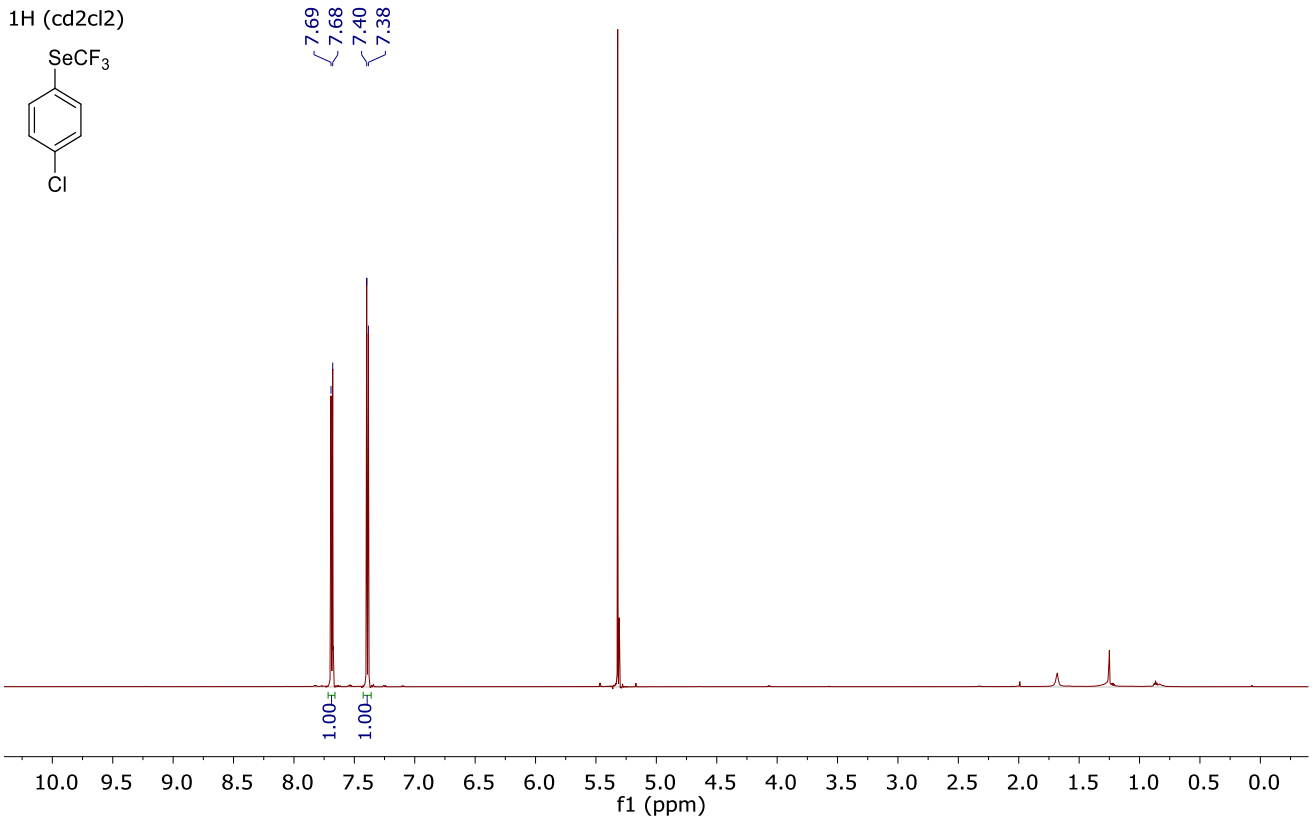
^{19}F-NMR [$(CD_3)_2CO$]

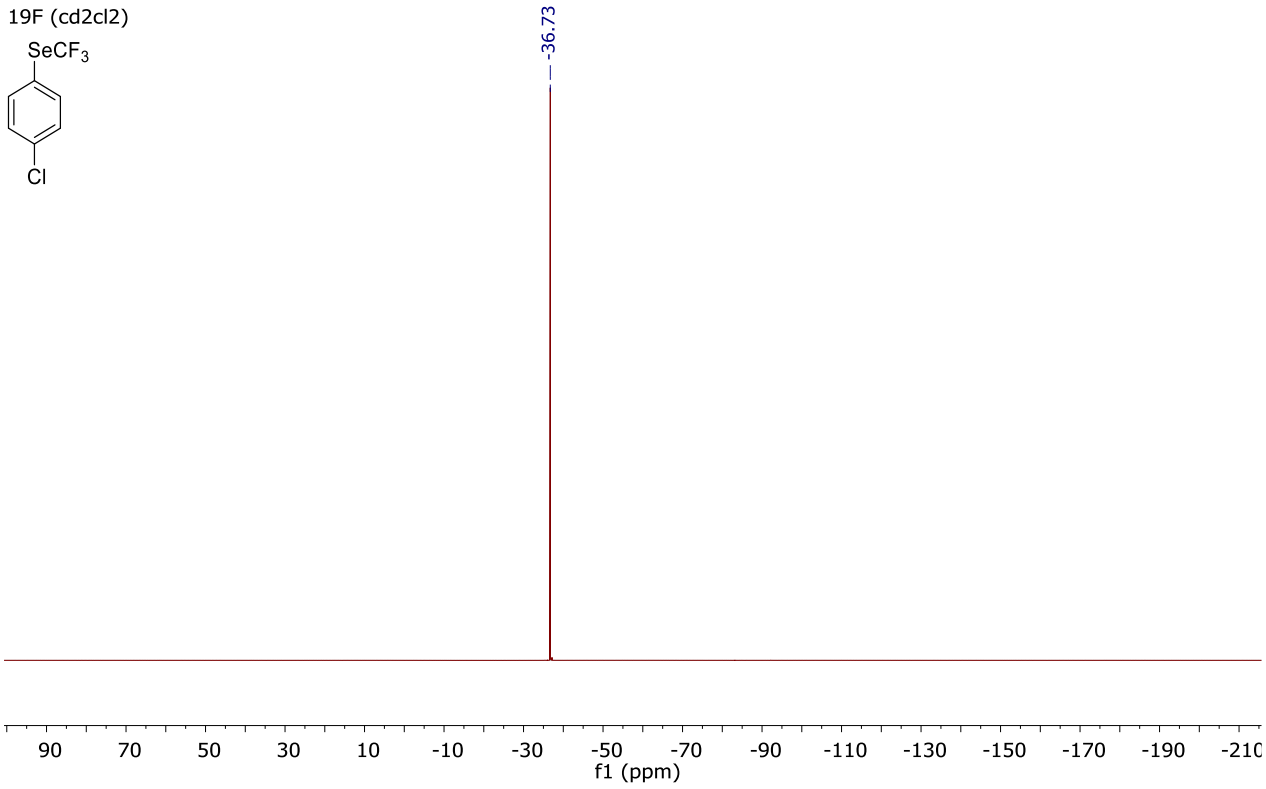




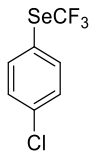

13C (cd2cl2)
SeCF3
SeCF3
138.2
126.4
125.9
124.2
122.0
119.8
A (q)
123.1
J(332.7)
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


19F (cd2cl2)
SeCF3
SeCF3
-36.02
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -20
f1 (ppm)

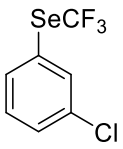

1H (cd2cl2)
SeCF3
Cl
7.69
7.68
7.40
7.38
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

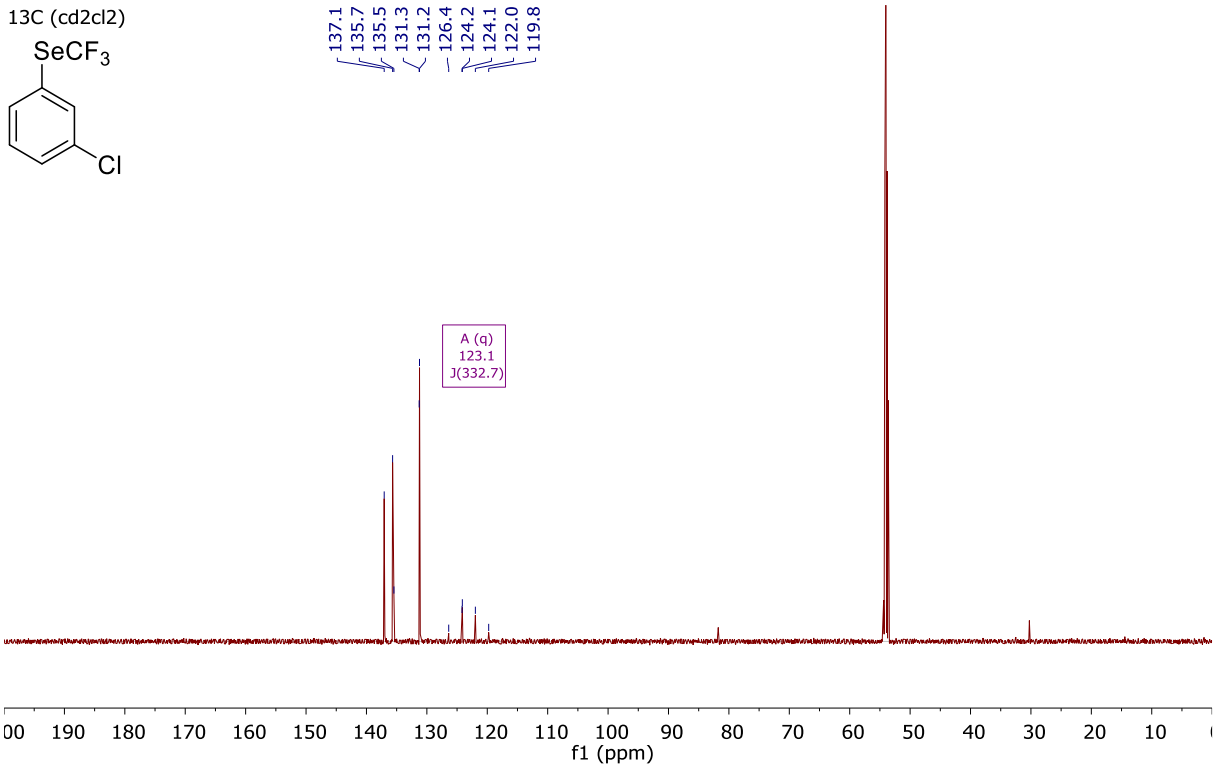

19F (cd2cl2)
SeCF3
Cl
-36.73
90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

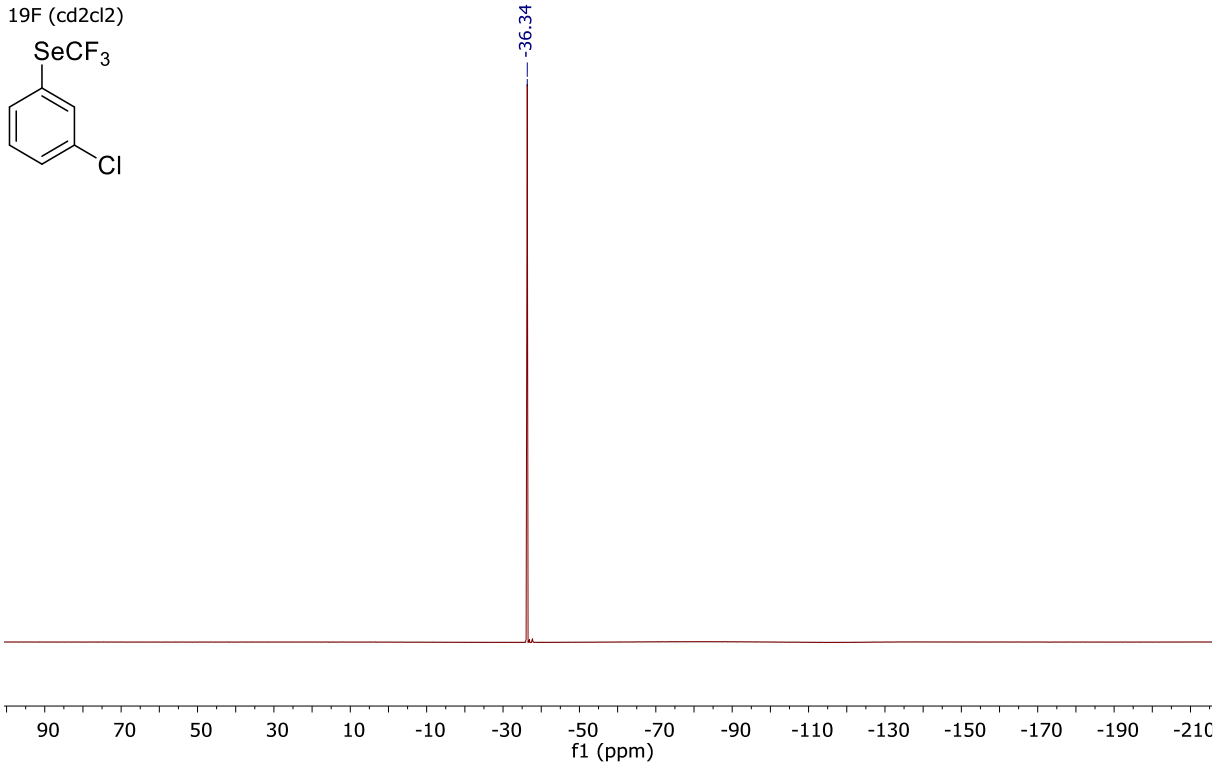
13C (cd2cl2)



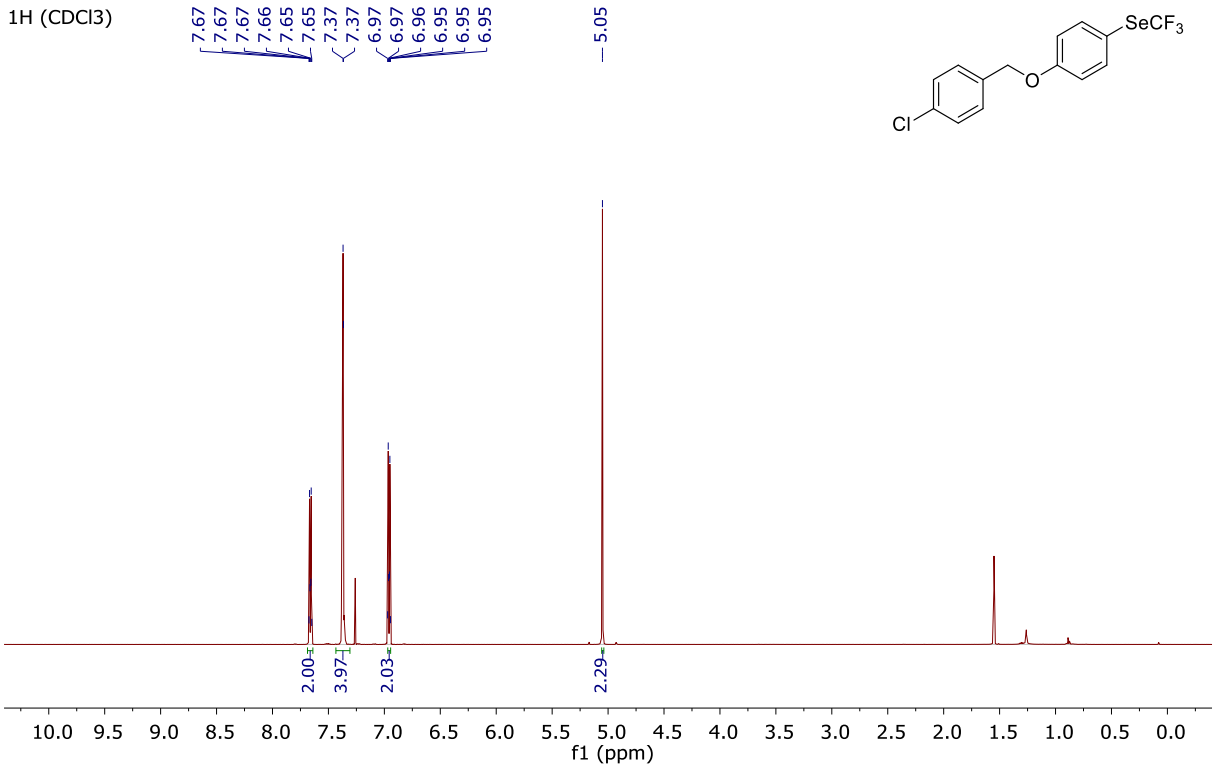
1H (cd2cl2)



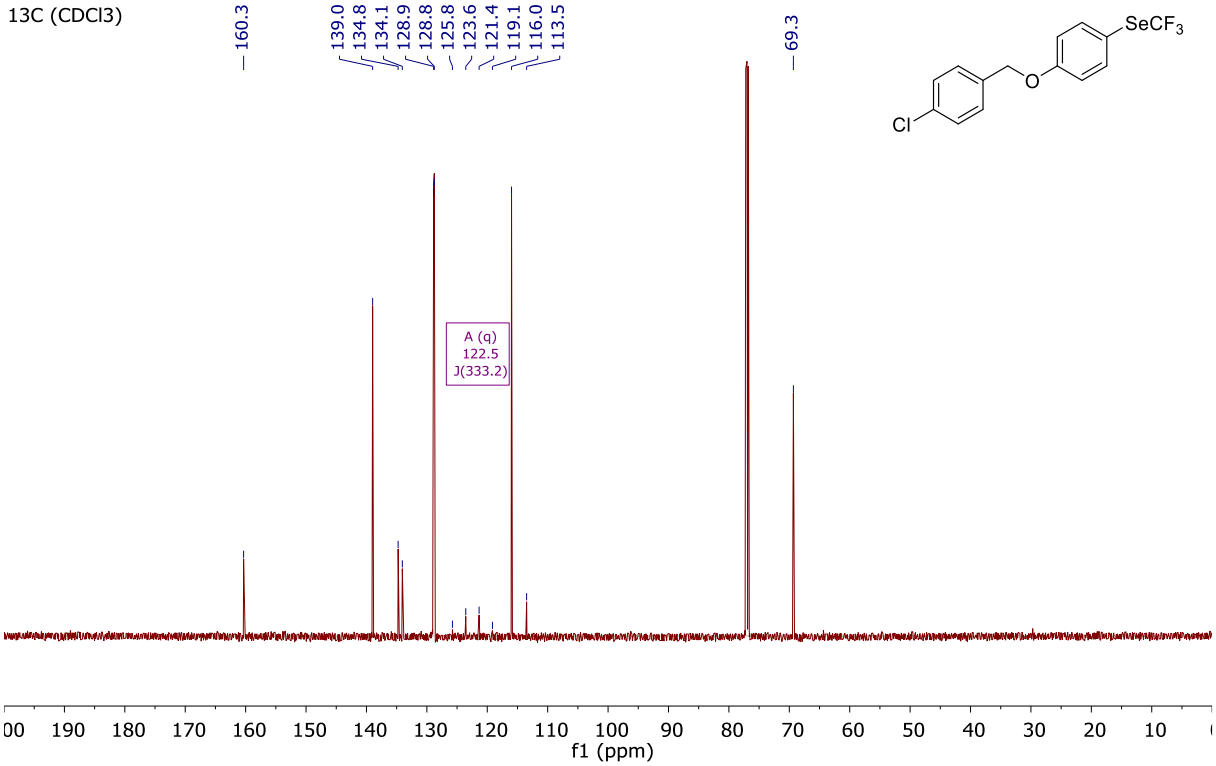

13C (cd2cl2)
SeCF3
Cl
137.1
135.7
135.5
131.3
131.2
126.4
124.2
124.1
122.0
119.8
A (q)
123.1
J(332.7)
f1 (ppm)


19F (cd2cl2)
SeCF3
Cl
-36.34
f1 (ppm)

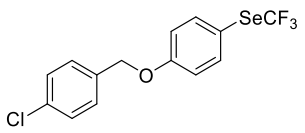
1H (CDCl3)



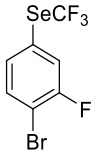
13C (CDCl3)



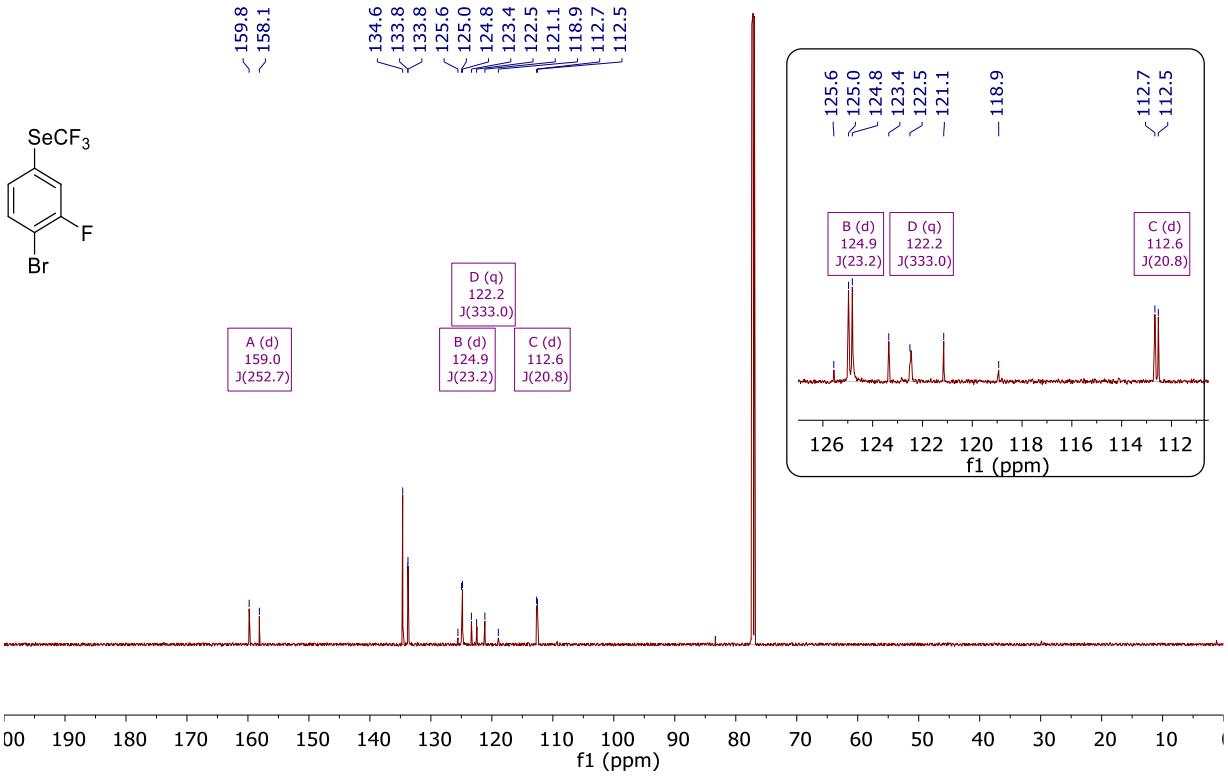
19F (CDCl3)



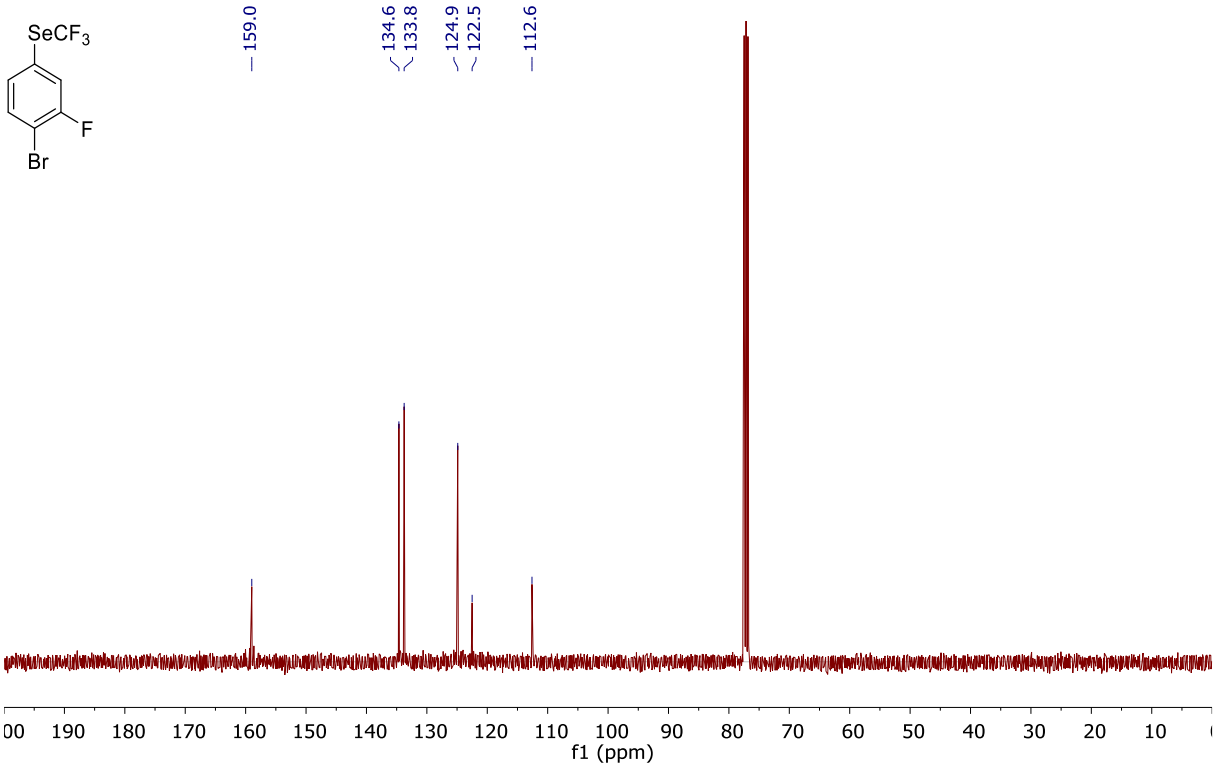
1H (CDCl3)

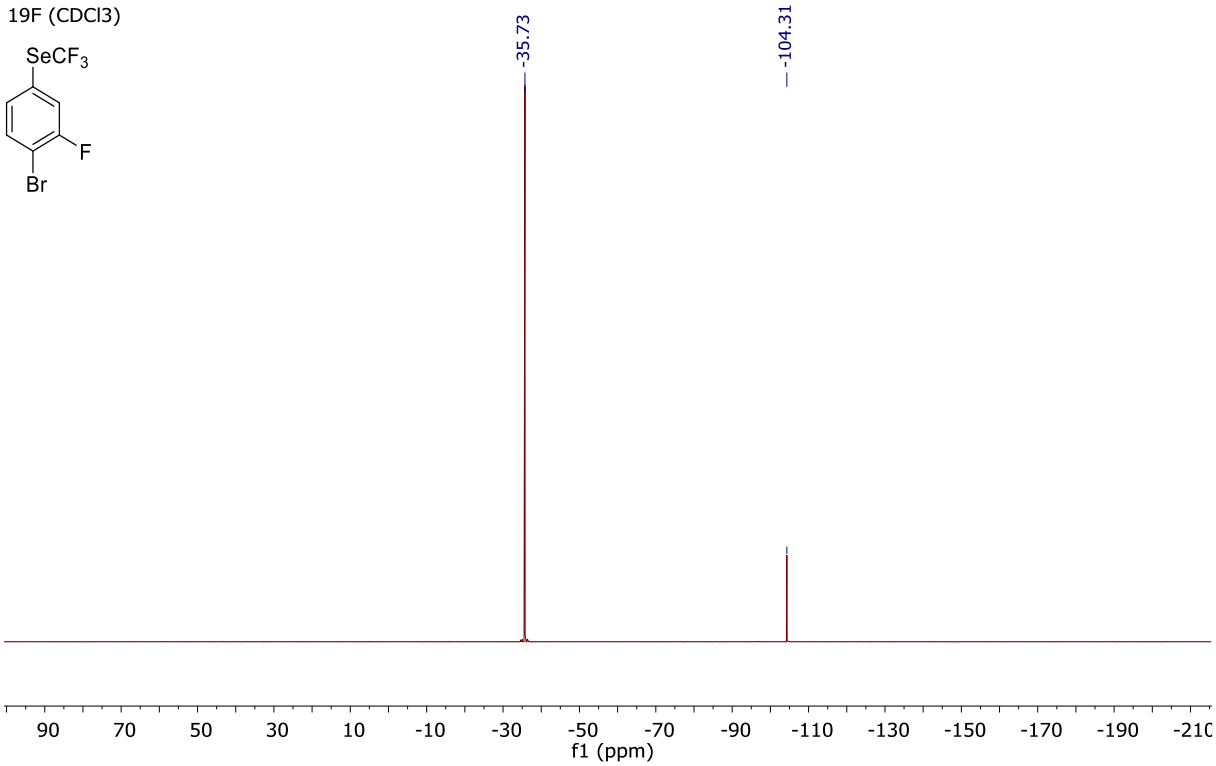


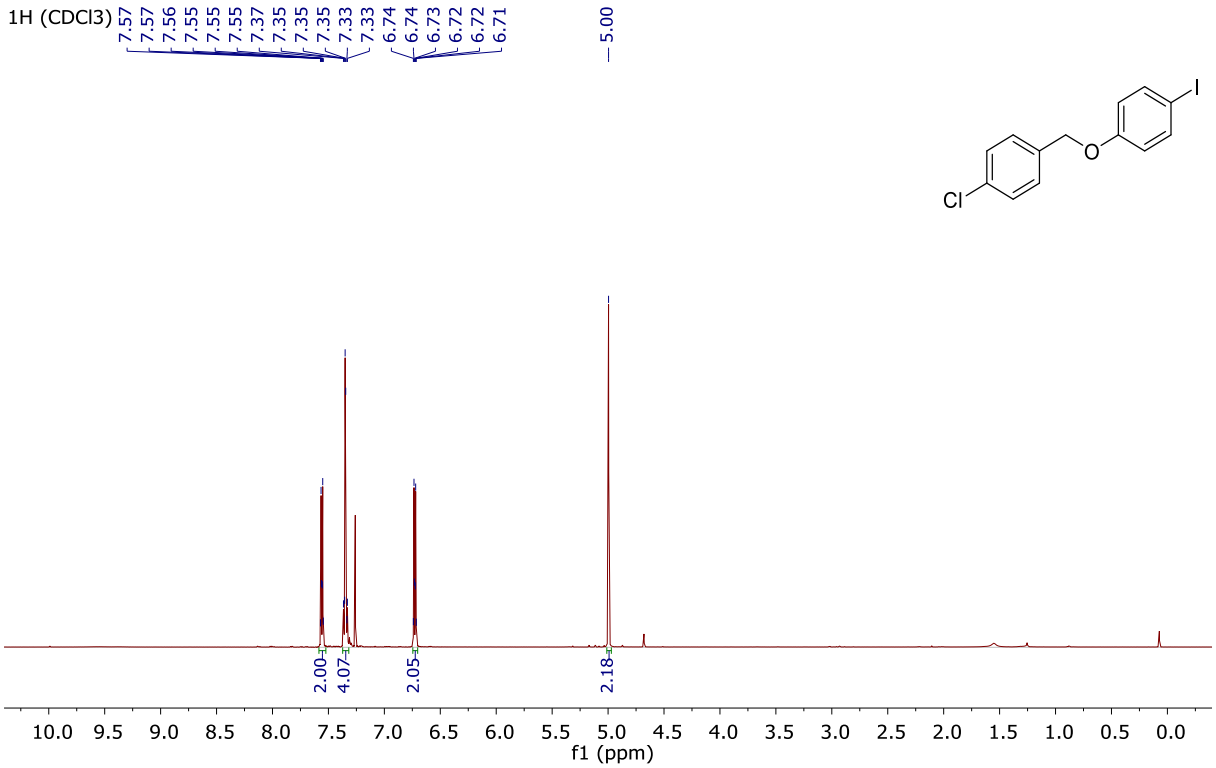
$^{13}C\{^{1}H\}$ ($CDCl_3$)

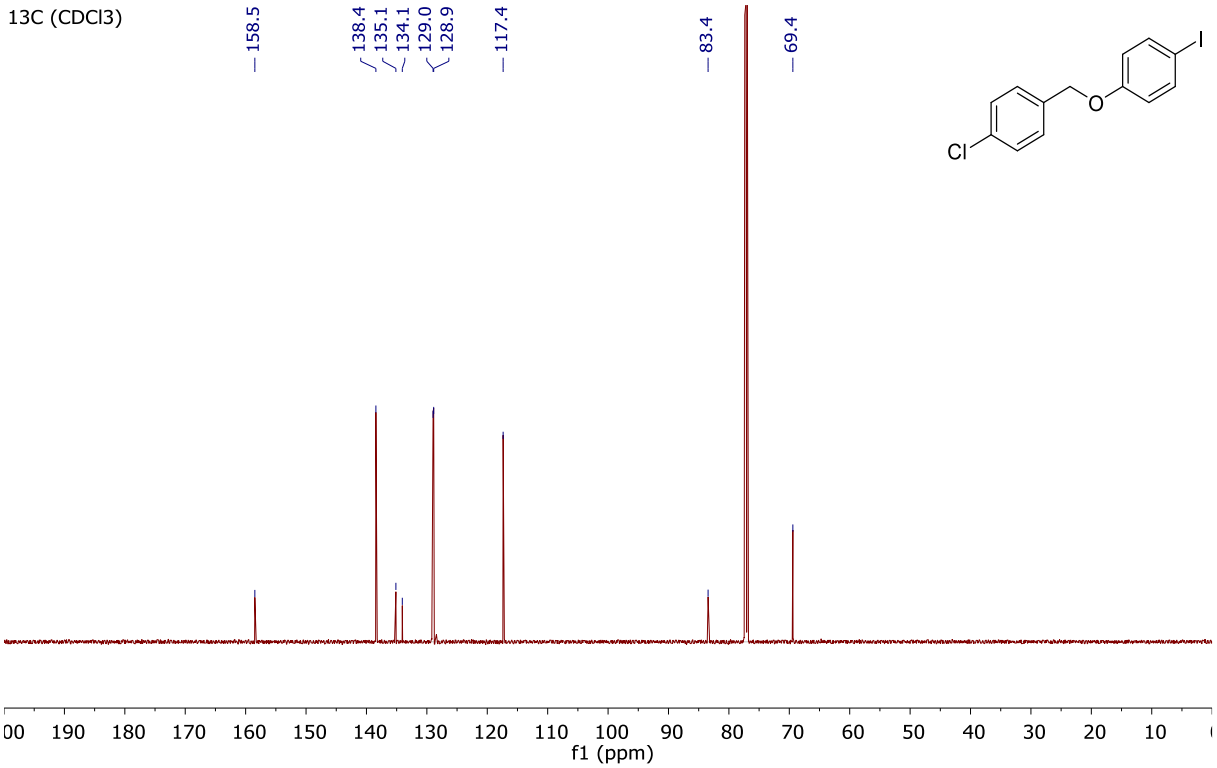


$^{13}C\ \{^{1}H,^{19}F\}$ ($CDCl_3$)




19F (CDCl3)
SeCF3
F
Br
-35.73
-104.31
90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)


1H (CDCl3)
7.57 7.57 7.56 7.55 7.55 7.55 7.37 7.35 7.35 7.35 7.33 7.33
6.74 6.74 6.73 6.72 6.72 6.71
5.00
I
O
Cl
2.00 4.07 2.05 2.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


13C (CDCl3)
158.5
138.4
135.1
134.1
129.0
128.9
117.4
83.4
69.4
Cl
O
I
f1 (ppm)

7. References

[1] J. Ebels, S. Spirk, R. Pietschnig (2006) 10th International Electronic Conference on Synthetic Organic Chemistry (ECSOC-10), https://www.usc.es/congresos/ecsoc/10/SST/d002/d002.pdf.

[2] A. Crochet, Katharina M. Fromm, *Z. Anorg. Allg. Chem.* **2010**, *636*, 1484-1496.

[3] W. Tyrra, D. Naumann, Y. L. Yagupolskii, *Journal of Fluorine Chemistry* **2003**, *123*, 183-187.

[4] C. Chen, L. Ouyang, Q. Lin, Y. Liu, C. Hou, Y. Yuan, Z. Weng, *Chem. Eur. J.* **2014**, *20*, 657-661.

[5] M. Aufiero, T. Sperger, A. S. K. Tsang, F. Schoenebeck, *Angew. Chem. Int. Ed.* **2015**, *54*, 10322-10326.

[6] Q. Lefebvre, R. Pluta, M. Rueping, *Chem. Commun.* **2015**, *51*, 4394-4397.

[7] M. Aufiero, T. Scattolin, F. Proutière, F. Schoenebeck, *Organometallics* **2015**, *34*, 5191-5195.

[8] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[9] C. J. Cramer, Essentials of Computational Chemistry: Theories and Models; 2nd ed.; Wiley: New York, USA, 2004.

[10] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.

[11] (a) D. P. Hruszkewycz, D. Balcells, L. M. Guard, N. Hazari, M. Tilset, *J. Am. Chem. Soc.* **2014**, *136*, 7300-7316; (b) D. Rappoport, N. R. M. Crawford, F. Furche, K. Burke, in *Encyclopedia of Inorganic Chemistry*, John Wiley & Sons, Ltd, **2006**.