# Stepwise transformation of a redox-active tetradentate ONNO ligand in the coordination sphere of tin(IV)

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## Content:

## General information about physical measurements

NMR spectra were recorded on Bruker Avance Neo 300 MHz and Bruker 400 MHz spectrometers.

Elemental analysis was performed with an Elementar Vario EL Cube elemental analyzer.

IR spectra were recorded on an FSM-1201 Fourier transform spectrometer in Nujol mulls (range 4000–400 $cm^{-1}$) in a KBr cell.

UV-vis-NIR spectra for solutions and solid samples as nujol mulls of complexes **5** and **8** were recorded in the range of 220–1400 nm on a Shimadzu UV-2600i spectrophotometer equipped with an ISR-2600Plus integrating sphere.

EPR spectra were registered on a Bruker MiniScope MS-5000 Magnettech spectrometer. Parameters of the recorded EPR spectra were determined by simulation of the spectra using the EasySpin program package.[1]

The magnetic susceptibility of complexes **5**-**7** was measured with a Quantum Design MPMSXL SQUID magnetometer (San Diego, California, USA) in the temperature range of 2-300 K with a magnetic field of up to 5 kOe. Diamagnetic corrections were made using the Pascal constants. The effective magnetic moment was calculated as $\mu_{eff}(T) = [(3k/N_A\mu_B^2)\chi T]^{1/2} \approx (8\chi T)^{1/2}$.

Cyclic voltammetry curves for **5** and **8** were recorded using a Smartstat PS-50 potentiostat. Measurements were performed in 2 mM solution (in $CH_2Cl_2$) of studied complexes. Supporting electrolyte was 0.2 M tetra-*n*-butyl ammonium perchlorate (TBAP). Experiments were performed in a standard three-electrode cell under argon atmosphere. A glassy carbon disc electrode (2 mm diameter) was used as a working electrode. The auxiliary electrode is a platinum wire. The reference electrode was Ag/AgCl/KCl(sat) electrode, and potentials were corrected to $Fc^+/Fc$ redox pair as a standard ($E_{1/2}$ = 0.51 V *vs* Ag/AgCl/KCl(sat)). All measurements were performed at room temperature.

Crystals suitable for SC XRD study were obtained directly from the reaction mixture for **1** (from a solution in diethyl ether) and **5** (from a solution in acetonitrile), and by recrystallization from a diethyl ether/acetonitrile mixture (in a volume ratio of 1:10) for **4** and from a solution in pentane for **8**.

The SC XRD data for **1**, **4**, **5**, and **8** were collected with *Rigaku OD Xcalibur E* diffractometer ($Mo_{K\alpha}$-radiation, $\omega$-scans technique, $\lambda = 0.71073$ Å, $T$ = 100.0(2) K) using

*CrysAlis*$^{Pro}$ software package.[2] The structures were solved *via* intrinsic phasing algorithm and refined by full-matrix least squares against $F^2$ using *SHELX*.[3,4] Implemented in *CrysAlis*$^{Pro}$ scaling algorithms were used to perform absorption corrections. All non-hydrogen atoms in **1**, **4**, **5**, and **8**were found from Fourier syntheses of electron density and refined anisotropically. Hydrogen atoms of secondary amines in **1** and **4** are found from Fourier syntheses of electron density and refined isotropically and freely. All other hydrogen atoms in all structures were placed in calculated positions and refined isotropically in the "riding" model with $U(H)_{iso} = 1.2U_{eq}$ of their parent atoms ($U(H)_{iso} = 1.5U_{eq}$ for methyl groups).

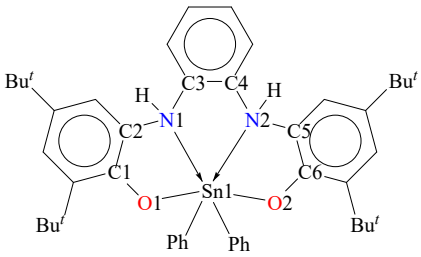
The crystallographic data and structures refinement details for all compounds are given in Table S1. CCDC 2390615 (**1**·2$Et_2O$), 2390616 (**4**·1.62$Et_2O$·1.38$CH_3CN$), 2390617 (**5**), and 2390618 (**8**) contain the supplementary crystallographic data for this paper. This data is provided free of charge by The Cambridge Crystallographic Data Centre: ccdc.cam.ac.uk/structures. The corresponding CIF are also available as ESI.

Density functional theory (DFT) calculations were performed using the Gaussian 09 software package.[5] The stationary points on the potential energy surfaces were located by full geometry optimization with calculation of the force constant. The geometry optimization was carried out on the PBE0/Jorge DZP-DKH full electronic basis for all elements[6] and was shown to give good results for tin(IV) complexes with redox-active ligands.[7]

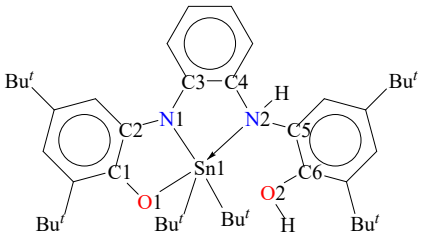
# SC XRD studies

**Table S1**. X-ray diffraction data collection and the structure refinement for complexes **1**·2$Et_2O$, **4**·1.62$Et_2O$·1.38$CH_3CN$, **5**, and **8**.

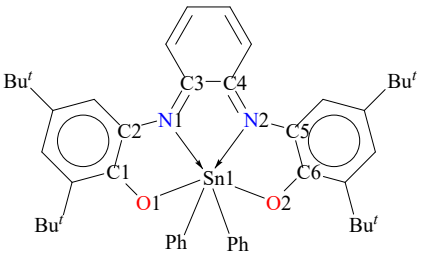
| | **1**·2$Et_2O$ | **4**·1.62$Et_2O$·1.38$CH_3CN$ | **5** | **8** |
|---|---|---|---|---|
| Formula | $C_{54}H_{76}N_2O_4Sn$ | $C_{48}H_{77}N_3O_3Sn$ | $C_{46}H_{54}N_2O_2Sn$ | $C_{46}H_{53}N_2O_2Sn$ |
| Formula weight | 935.85 | 862.81 | 785.60 | 784.59 |
| Crystal size, mm | 0.42×0.32×0.19 | 0.64×0.44×0.35 | 0.42×0.22×0.10 | 0.39×0.23×0.19 |
| Crystal system | Orthorhombic | Triclinic | Triclinic | Orthorhombic |
| Space group | $C222_1$ | P-1 | P-1 | Pbca |
| Unit cell dimentions | | | | |
| *a*, Å | 12.3983(2) | 13.0130(2) | 9.4959(3) | 28.6053(3) |
| *b*, Å | 15.2626(2) | 13.5064(2) | 12.4916(3) | 9.73400(10) |
| *c*, Å | 26.9230(4) | 14.5664(2) | 16.9054(5) | 29.2307(2) |
| α,deg | 90 | 72.5596(13) | 80.714(2) | 90 |
| β,deg | 90 | 84.7853(13) | 85.784(2) | 90 |
| γ, deg | 90 | 76.7192(13) | 89.996(2) | 90 |
| *V*, $Å^3$ | 5094.66(13) | 2376.49(7) | 1973.53(10) | 8139.11(13) |
| *Z* | 4 | 2 | 2 | 8 |
| $d_{calc}$, $g/cm^3$ | 1.220 | 1.206 | 1.322 | 1.281 |
| $\mu$, $mm^{-1}$ | 0.545 | 0.578 | 0.687 | 0.666 |
| $F_{000}$ | 1984 | 920 | 820 | 3272 |
| $\theta$ range, deg | 2.25-29.57 | 1.84-30.03 | 1.89-26.02 | 2.32-30.03 |
| *HKL* indices | -16 ≤ h ≤ 17<br>-19 ≤ k ≤ 21,<br>-37 ≤ l ≤ 24 | -18 ≤ h ≤ 18<br>-19 ≤ k ≤ 19,<br>-20 ≤ l ≤ 20 | -11 ≤ h ≤ 11<br>-15 ≤ k ≤ 15,<br>-20 ≤ l ≤ 20 | -40 ≤ h ≤ 40<br>-13 ≤ k ≤ 13,<br>-41 ≤ l ≤ 41 |
| Reflections collected | 15290 | 54645 | 35932 | 340306 |
| Independent reflections [$I > 2\sigma(I)$] | 6678 ($R_{int}$ = 0.0281) | 12178 ($R_{int}$ = 0.0377) | 6514 ($R_{int}$ = 0.0635) | 9636 ($R_{int}$ = 0.0957) |
| Data/restraints/ parameters | 7146 / 24 / 331 | 13875 / 841 / 751 | 7781 / 96 / 536 | 11913 / 48 / 505 |
| $R_1$; w$R_2$ [$I > 2\sigma(I)$] | 0.0282; 0.0558 | 0.0357; 0.0905 | 0.0354; 0.0682 | 0.0618; 0.1140 |
| $R_1$; w$R_2$ (all data) | 0.0328; 0.0575 | 0.0442; 0.0953 | 0.0509; 0.0735 | 0.0793; 0.1216 |
| $S(F^2)$ | 1.042 | 1.070 | 1.075 | 1.019 |
| $\Delta\rho_{max}/\Delta\rho_{min}$, $e/Å^3$ | 0.52 / -0.62 | 0.78 / -0.92 | 0.68 / -0.49 | 1.06 / -1.42 |



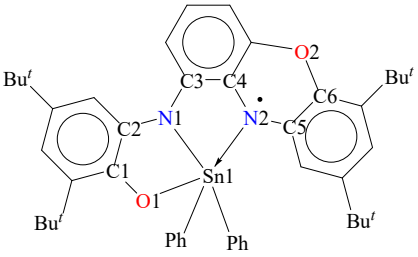

**1**·2Et$_2$O




**4**·1.62Et$_2$O·1.38CH$_3$CN




**5**




**8**

**Scheme S1**. Numbering of atoms in complexes **1**·2Et$_2$O, **4**·1.62Et$_2$O·1.38CH$_3$CN, **5**, and **8** to compare selected bond lengths.

**Table S2**. Comparison of selected bond lengths (Å) of complexes **1**·2Et$_2$O, **4**, **5**, and **8** according to the numbering given in Scheme S1.

| **Bond** | **1**·2Et$_2$O | **4**·1.62Et$_2$O·1.38CH$_3$CN | **5** | **8** |
|---|---|---|---|---|
| Sn(1)-O(1) | 2.091(2) | 2.072(2) | 2.261(2) | 2.078(2) |
| Sn(1)-O(2) | 2.091(2) | - | 2.263(2) | - |
| Sn(1)-N(1) | 2.351(2) | 2.090(2) | 2.288(2) | 2.110(3) |
| Sn(1)-N(2) | 2.351(2) | 2.533(2) | 2.196(2) | 2.252(3) |
| O(1)-C(1) | 1.349(3) | 1.350(2) | 1.285(3) | 1.338(4) |
| N(1)-C(2) | 1.471(3) | 1.415(2) | 1.368(3) | 1.400(4) |
| O(2)-C(6) | 1.349(3) | 1.395(3) | 1.304(3) | 1.381(4) |
| N(2)-C(5) | 1.471(3) | 1.444(3) | 1.379(3) | 1.390(4) |
| N(1)-C(3) | 1.456(3) | 1.399(2) | 1.352(3) | 1.356(5) |
| N(2)-C(4) | 1.456(3) | 1.461(3) | 1.347(3) | 1.347(4) |

## NMR studies

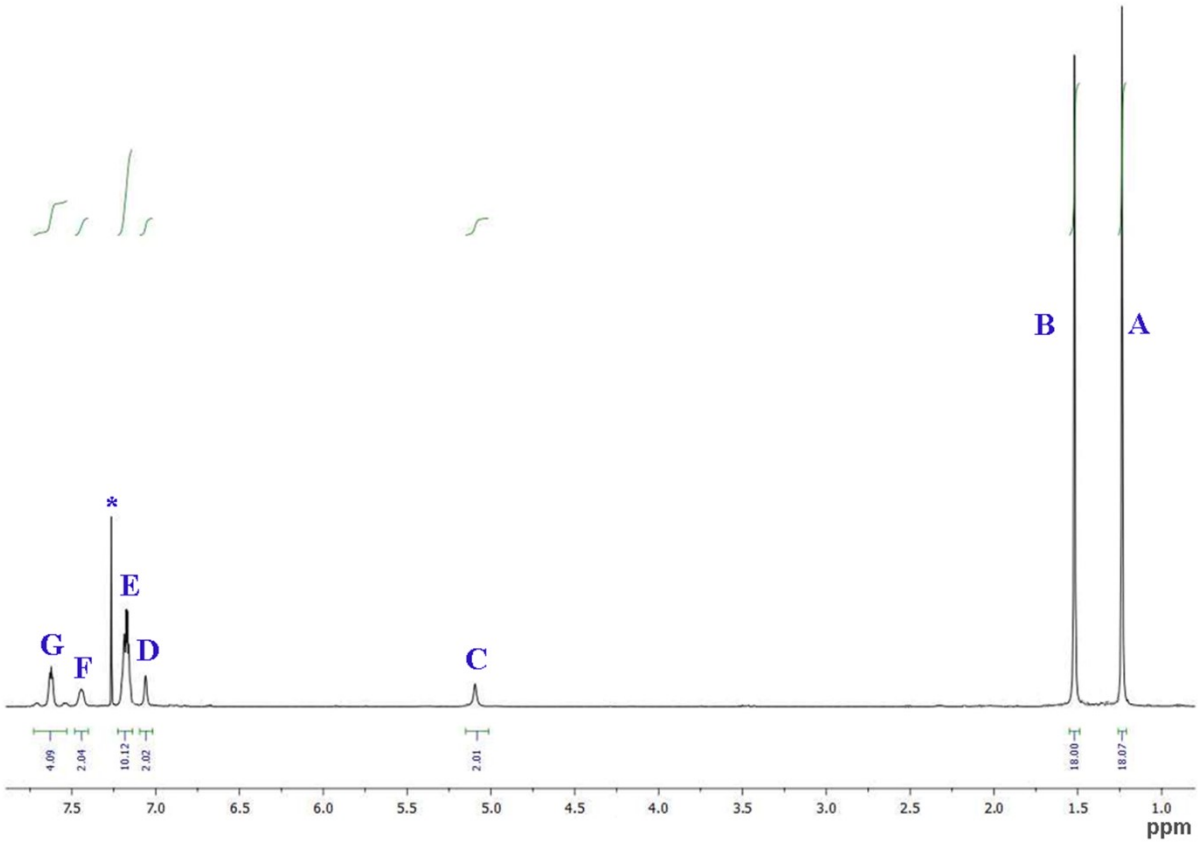



**Figure S1**. The $^{1}$H NMR spectrum of complex **1** in $CDCl_3$ at 298 K; * - solvent residual signal; δ/ppm: A – 1.24 (s, 18H, Bu$^t$), B – 1.52 (s, 18H, Bu$^t$), C – 5.09 (br.s, 2H, NH), D – 7.06 (s, 2H, C-$H_{O\text{-}Ph\text{-}N}$), E – 7.17 (m, 6H +2H + 2H, Sn-Ph + C-$H_{N\text{-}Ph\text{-}N}$ + C-$H_{O\text{-}Ph\text{-}N}$), F – 7.44 (m, 2H, C-$H_{N\text{-}Ph\text{-}N}$), G – 7.62 (m, 4H, $J_{SnH}$ = 32.8 Hz, Sn-Ph).

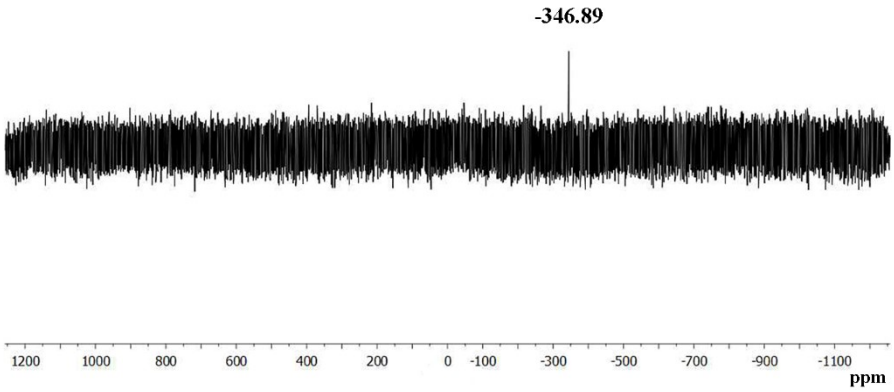



**Figure S2**. The $^{119}$Sn NMR spectrum of complex **1** in $CDCl_3$ at 298 K; δ/ppm: -346.89.

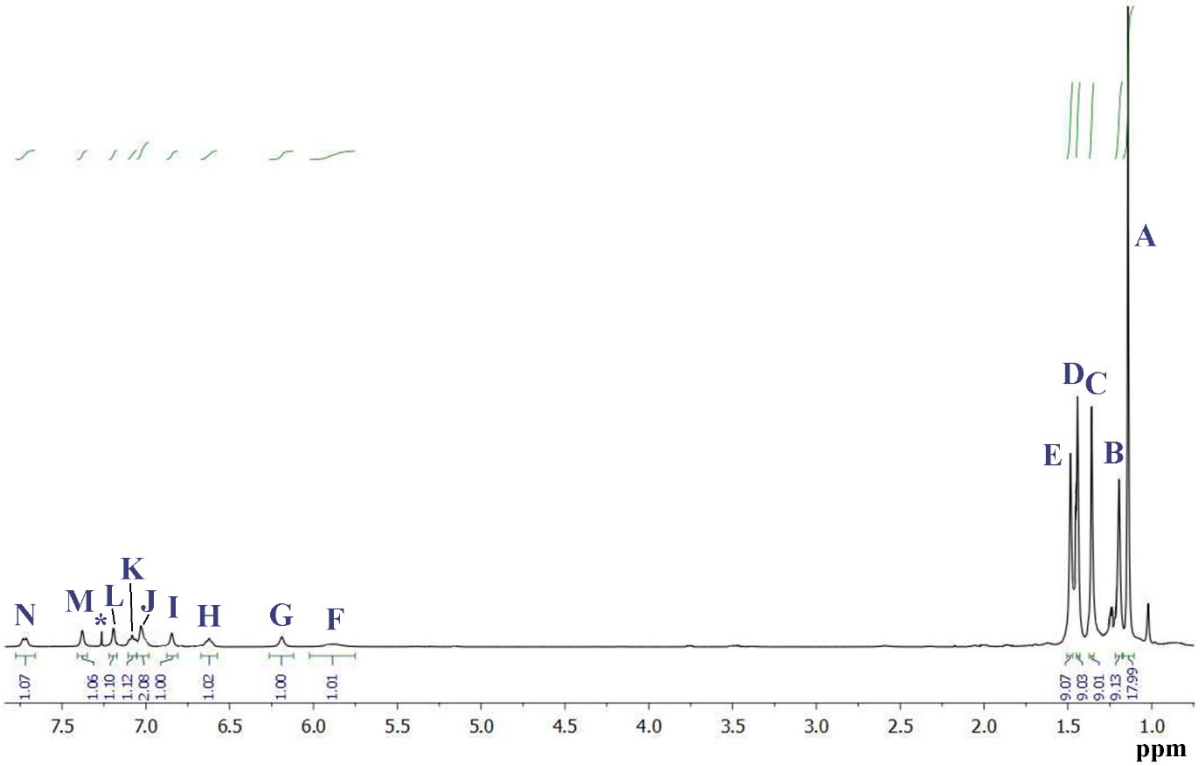



**Figure S3**. The $^{1}$H NMR spectrum of complex **4** in $CDCl_3$ at 298 K; * - solvent residual signal; δ/ppm: A – 1.14 (s, 18H, $J_{SnH}$ = 46.98 Hz, Sn-Bu$^t$), B – 1.20 (s, 9H, Bu$^t$), C - 1.36 (s, 9H, Bu$^t$), D - 1.44 (s, 9H, Bu$^t$), E - 1.48 (s, 9H, Bu$^t$), F - 5.86 (br.s, 1H, OH), G - 6.19 (br.s, 1H, NH), H - 6.62 (t, 1H, $J_{HH}$ = 6.9 Hz, C-$H_{N\text{-}Ph\text{-}N}$), I - 6.85 (s, 1H, C-$H_{O\text{-}Ph\text{-}N}$), J - 7.03 (m, 1H+1H, C-$H_{O\text{-}Ph\text{-}N}$ + C-$H_{N\text{-}Ph\text{-}N}$), K - 7.08 (t, 1H, $J_{HH}$ = 7.6 Hz, C-$H_{N\text{-}Ph\text{-}N}$), L - 7.19 (s, 1H, C-$H_{O\text{-}Ph\text{-}N}$), M - 7.38 (s, 1H, C-$H_{O\text{-}Ph\text{-}N}$), N - 7.72 (d, 1H, $J_{HH}$ = 7.7 Hz, C-$H_{N\text{-}Ph\text{-}N}$).

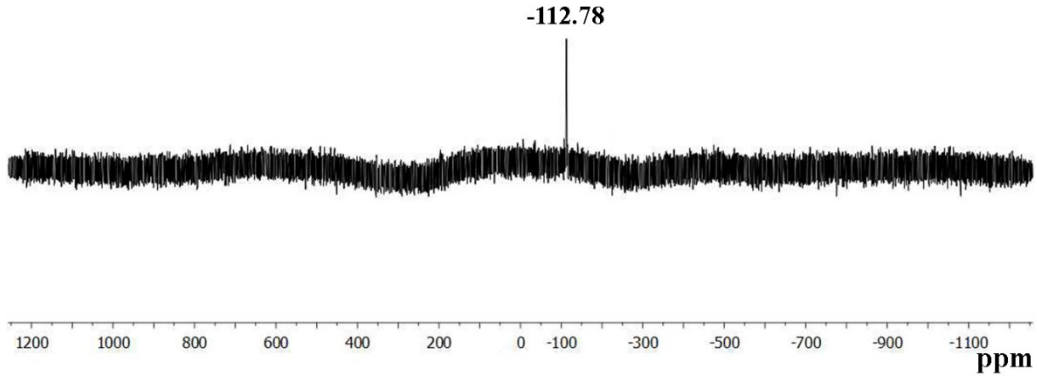



**Figure S4**. The $^{119}$Sn NMR spectrum of complex **4** in $CDCl_3$ at 298 K; δ/ppm: -112.78.

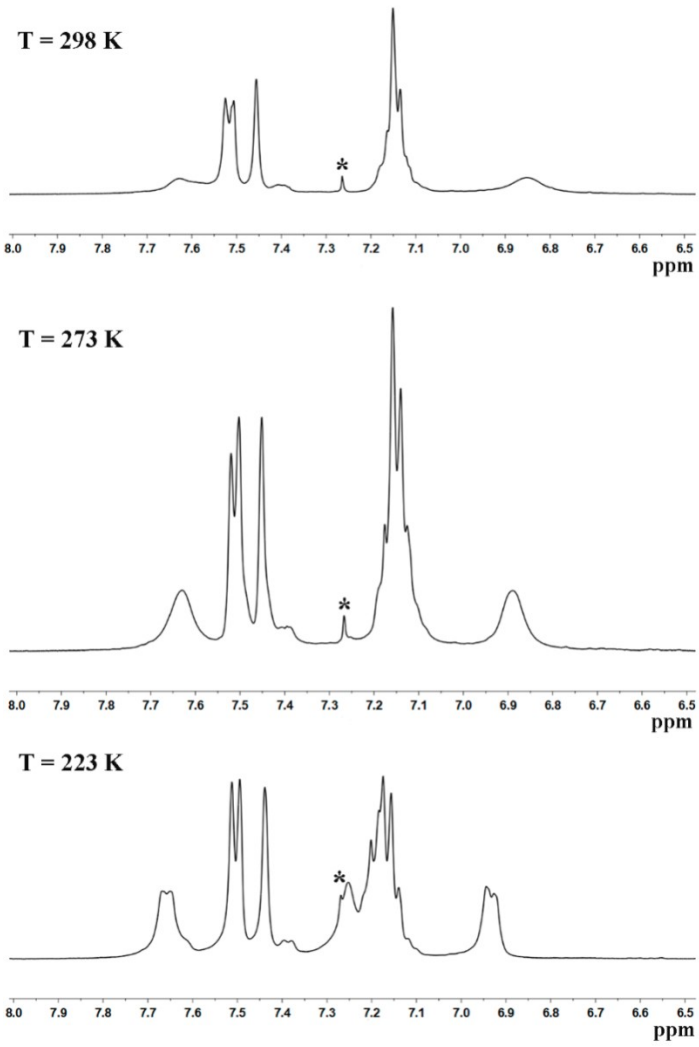



**Figure S5**. The weak-field region of the $^{1}H$ NMR spectrum of complex **5** at various temperatures in $CDCl_3$, * - solvent residual signal.

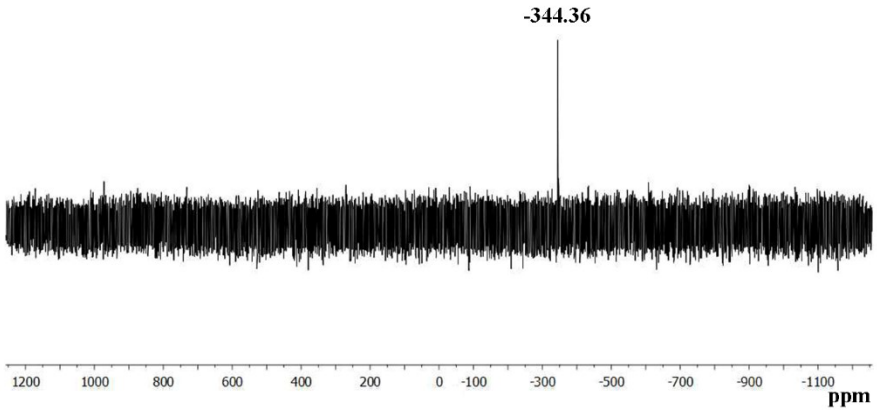



**Figure S6**. The $^{119}Sn$ NMR spectrum of complex **5** in $CDCl_3$ at 298 K; δ/ppm: -344.36.

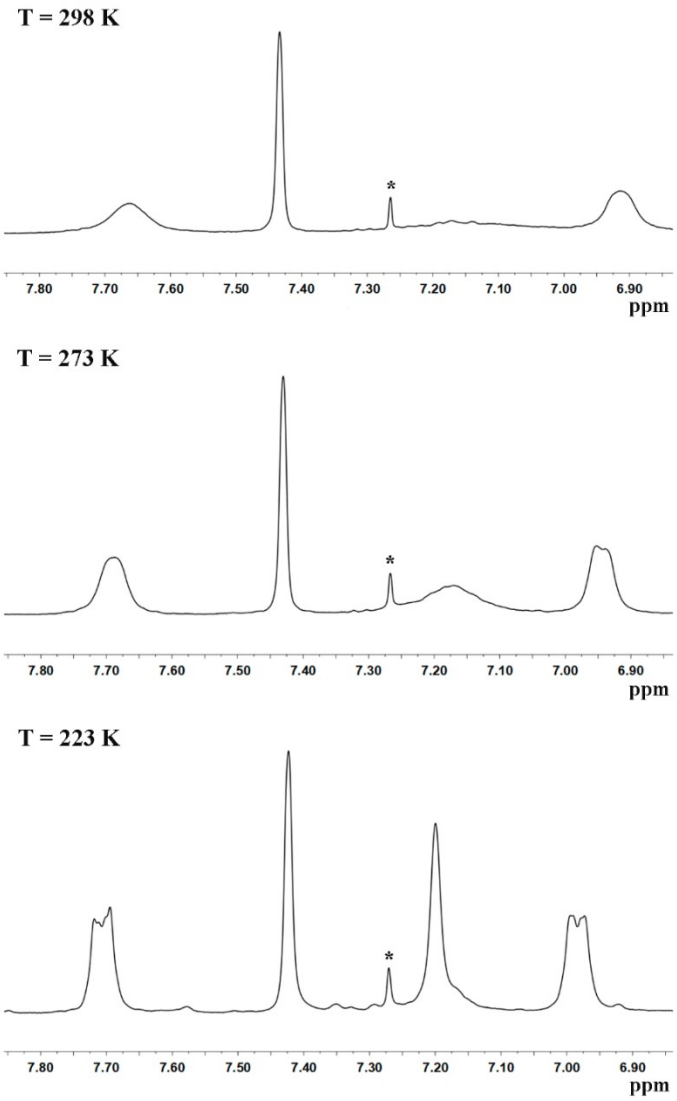



**Figure S7**. The weak-field region of the $^{1}$H NMR spectrum of complex **6** at various temperatures in $CDCl_3$, * - solvent residual signal.

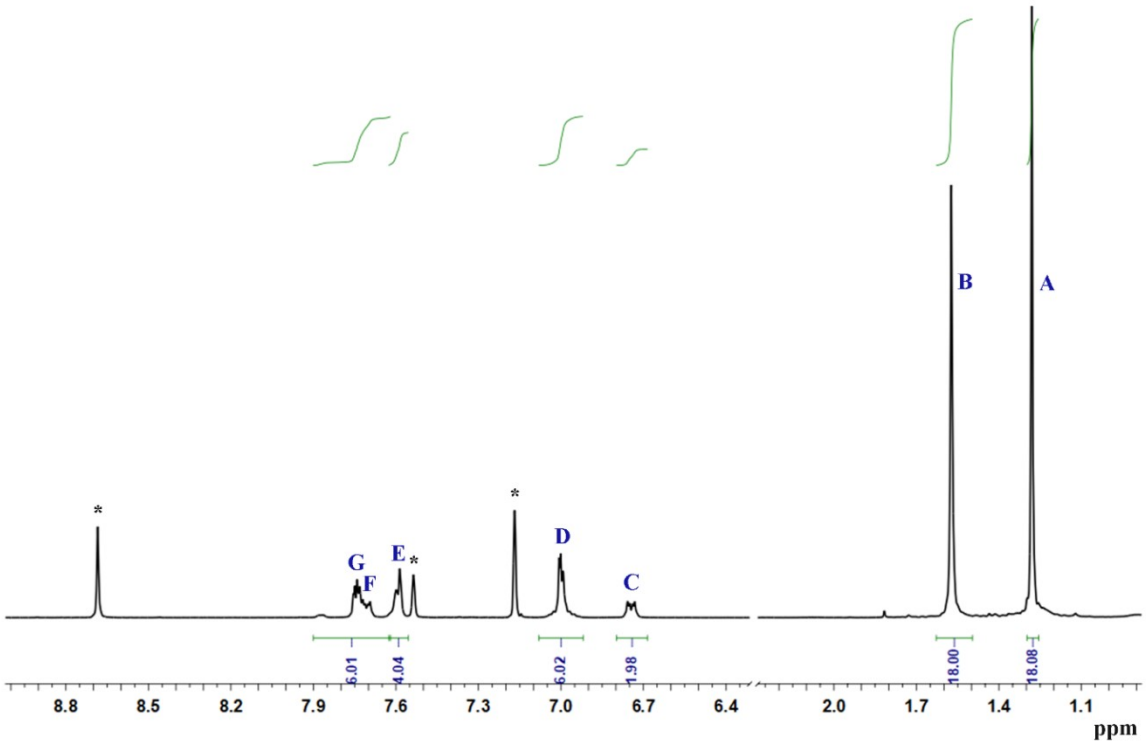



**Figure S8**. The $^{1}$H NMR spectrum of complex **5** in Pyridine-$d_5$ at 298 K; * - solvent residual signal; δ/ppm: A – 1.28 (s, 18H, Bu$^t$), B – 1.57 (s, 18H, Bu$^t$), C – 6.74 (m, 2H, $H_{phen}$), D – 6.99 (m, 6H, $J_{SnH}$ = 13.5 Hz, Sn-Ph), E – 7.59 (s + s, 2H +2H, $H_{arom}$), F – 7.71 (m, 2H, $H_{phen}$), G – 7.74 (m, 4H, $J_{SnH}$ = 47.8 Hz, Sn-Ph).

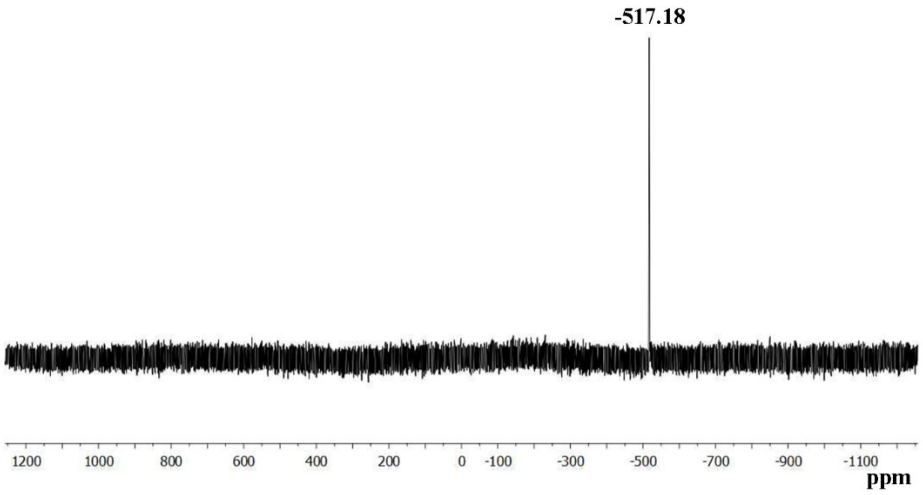



**Figure S9**. The $^{119}$Sn NMR spectrum of complex **5** in Pyridine-$d_5$ at 298 K; δ/ppm: -517.18.

## UV-vis spectroscopy investigations

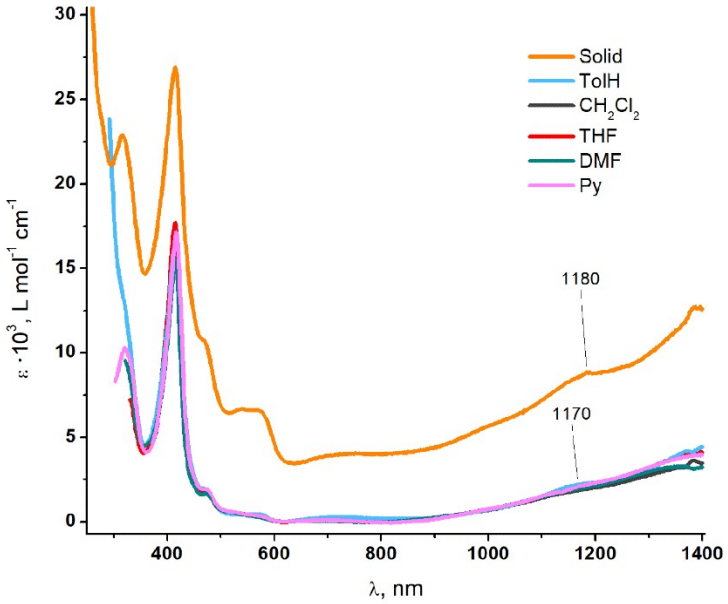



**Figure S10**. UV-vis spectra for complex **8** in different solvents and in solid.

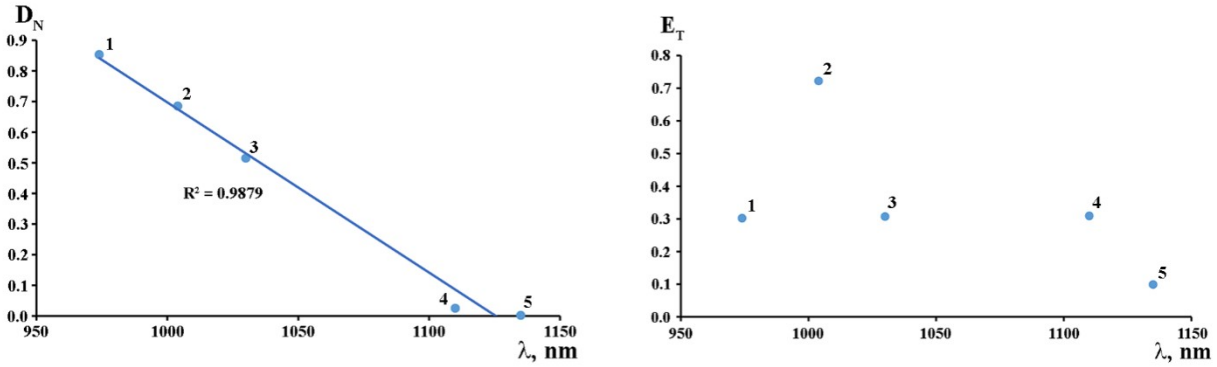



**Figure S11.** Dependences of the $\lambda_{max}$ value for complex **5** on the solvent donor number $D_N$ (on the left) and the empirical polarity parameter $E_T$ (on the right). Solvents: 1 – Py, 2 – DMF, 3 – THF, 4 – $CH_2Cl_2$, 5 – Toluene.

## Electrochemical investigations

**Table S3.** Redox potentials (V) of **5** and **8** in $CH_2Cl_2$ at 20 °C *vs* $Fc^+/Fc$, the energy of frontiers orbitals and HOMO-LUMO gap value (ΔE) calculated from the CV data

| | $E_{1/2}$(Red-2) | $E_{1/2}$(Red-1) | $E_{1/2}$(Ox-1) | $E_{1/2}$(Ox-2) | E(HOMO) | E(LUMO) | ΔE |
|---|---|---|---|---|---|---|---|
| **8** | | -0.81 | -0.13 | | -3.99 | -4.67 | **0.68** |
| **5** | -1.37 | -0.85 | 0.04 | 0.41 | -3.95 | -4.84 | **0.89** |

[a]for reversible process $E = E_{1/2} = (E^p_{red} + E^p_{ox})/2$;
[c]E(LUMO) = -(4.8 + E(ox1)), [d]E(HOMO) = -(4.8 + E(red1))[8] [DOI: 10.1002/adma.201004554];
[e]ΔE= E(ox1)-E(red1).

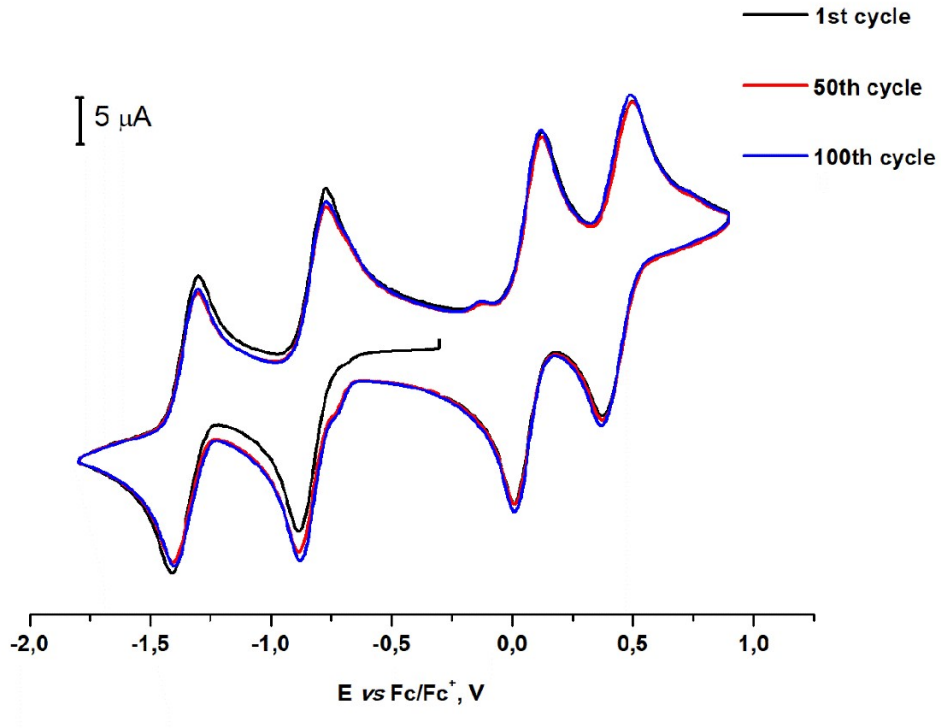


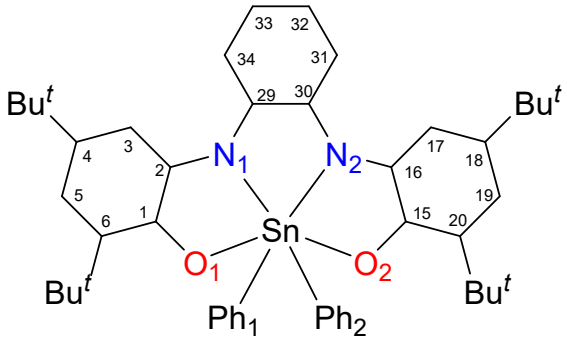

**Figure S12**. The 1st, 50th and 100th cycles of voltammogram of compound **5** in dichloromethane solution under argon atmosphere at 293 K.

## Magnetochemical studies

**Table S4.** The best fit values for the analysis of the $\mu_{eff}(T)$ dependencies for the complexes **5-7** using the equation $\chi = C/(T-\theta) + \chi_0$ (where C is the Curie constant, θ – Weiss temperature, and $\chi_0$ – temperature independent part of magnetic susceptibility), and the fraction of the high-spin paramagnetic state $\omega = C_{exp} / C_{teor} = C/0.75$.

| Complex | C, K·cm³/mol | θ, K | $\chi_0$, cm³/mol | $C_{exp}/C_{teor}$, % |
|---|---|---|---|---|
| **5** | 0.0065±0.0003 | –1.56±0.04 | $2.1\cdot10^{-5}\pm0.2\cdot10^{-5}$ | 0.87 |
| **6** | 0.0189±0.0015 | –4.5±0.6 | $4.4\cdot10^{-5}\pm0.6\cdot10^{-5}$ | 2.5 |
| **7** | 0.0224±0.0007 | –1.00±0.01 | $2.5\cdot10^{-4}\pm0.7\cdot10^{-4}$ | 3.0 |

## DFT investigations




**Scheme S2**. Numbering of atoms in complex **5** to compare the values of selected bond lengths and angles obtained from X-ray diffraction experiment and DFT calculations.

**Table S5.** The values of selected bond lengths (Å) and angles (°) for complex **5** obtained from X-ray diffraction experiment and DFT calculations.

| Bond | X-ray | **5**(OSS) | **5**(CSS) | **5**(T) | **5**$^+$ | **5**$^-$ | **5·Py**(OSS) | **5·Py**(CSS) | **5·Py**(T) |
|---|---|---|---|---|---|---|---|---|---|
| C1-01* | 1.295 | 1.277 | 1.284 | 1.274 | 1.346 | 1.300 | 1.285 | 1.291 | 1.280 |
| C2-N1* | 1.374 | 1.356 | 1.367 | 1.353 | 1.348 | 1.382 | 1.356 | 1.368 | 1.348 |
| C1-C2* | 1.442 | 1.462 | 1.452 | 1.466 | 1.481 | 1.442 | 1.456 | 1.447 | 1.464 |
| C2-C3* | 1.404 | 1.416 | 1.416 | 1.415 | 1.414 | 1.407 | 1.418 | 1.416 | 1.419 |
| C3-C4* | 1.372 | 1.379 | 1.377 | 1.380 | 1.378 | 1.390 | 1.378 | 1.379 | 1.377 |
| C4-C5* | 1.413 | 1.428 | 1.424 | 1.428 | 1.440 | 1.409 | 1.424 | 1.419 | 1.427 |
| C5-C6* | 1.373 | 1.377 | 1.381 | 1.377 | 1.369 | 1.392 | 1.381 | 1.383 | 1.379 |
| C6-C1* | 1.434 | 1.443 | 1.440 | 1.444 | 1.453 | 1.429 | 1.440 | 1.438 | 1.442 |
| C29-N1* | 1.355 | 1.372 | 1.338 | 1.386 | 1.360 | 1.352 | 1.356 | 1.327 | 1.381 |
| C29-C30 | 1.455 | 1.440 | 1.465 | 1.430 | 1.446 | 1.437 | 1.451 | 1.474 | 1.433 |
| C30-C31* | 1.422 | 1.411 | 1.429 | 1.403 | 1.418 | 1.418 | 1.419 | 1.436 | 1.406 |
| C31-C32* | 1.358 | 1.386 | 1.369 | 1.392 | 1.376 | 1.383 | 1.380 | 1.365 | 1.392 |
| C32-C33 | 1.416 | 1.402 | 1.422 | 1.396 | 1.413 | 1.407 | 1.409 | 1.427 | 1.396 |
| Sn-Ph* | 2.134 | 2.060 | 2.065 | 2.059 | 2.047 | 2.080 | 2.085 | 2.091 | 2.077 |
| Sn-O* | 2.272 | 2.226 | 2.273 | 2.355 | 2.346 | 2.282 | 2.298 | 2.262 | 2.340 |
| Sn-N1,2* | 2.243 | 2.184 | 2.219 | 2.169 | 2.212 | 2.175 | 2.282 | 2.319 | 2.244 |
| Sn-N3 | - | - | - | - | - | - | 2.552 | 2.494 | 2.641 |
| Angle | | | | | | | | | |
| O1-Sn-O2 | 147.4 | 143.7 | 143.2 | 144.2 | 149.9 | 141.2 | 148.7 | 149.2 | 148.6 |
| N1-Sn-N2 | 71.3 | 74.1 | 73.4 | 74.2 | 73.6 | 74.1 | 71.2 | 70.4 | 71.8 |
| Ph-Sn-Ph | 146.6 | 148 | 154.2 | 145.5 | 149.5 | 150.4 | 171.1 | 174.6 | 167.2 |

* Values are an average of two fragments of the molecule.

**Atomic coordinates in the optimized structures**

## 5_CSS

Charge = 0, S = 0, E =-8.008172744586289E+03

| | | | |
|---|---|---|---|
| Sn | -0.008854017 | -0.807139146 | 0.394866957 |
| O | 2.158023250 | -1.512552427 | 0.298082280 |
| O | -2.155375808 | -1.516594828 | 0.253779361 |
| N | 1.320413184 | 0.967181444 | 0.513974013 |
| N | -1.332011786 | 0.966160968 | 0.527928154 |
| C | 3.020690436 | -0.601614201 | 0.034744519 |
| C | 2.624330490 | 0.792133282 | 0.144255147 |
| C | 3.530319443 | 1.824832214 | -0.198541526 |
| C | 4.820779433 | 1.533380277 | -0.585310086 |
| C | 5.215450578 | 0.165284473 | -0.612651515 |
| C | 4.380194510 | -0.898062709 | -0.337112128 |
| C | 5.825204271 | 2.606871832 | -1.005433445 |
| C | 5.226626140 | 4.013045323 | -0.944873850 |
| C | 6.288044601 | 2.342153501 | -2.447286013 |
| C | 7.040482843 | 2.558936586 | -0.064675257 |
| C | 4.850401230 | -2.351139714 | -0.428280131 |
| C | 6.327928161 | -2.451301754 | -0.815716913 |
| C | 4.028286723 | -3.088739005 | -1.498538141 |
| C | 4.672284344 | -3.041173136 | 0.934809258 |
| C | -3.027287958 | -0.600443121 | 0.021563071 |
| C | -2.642290300 | 0.789742327 | 0.176929118 |
| C | -3.562086477 | 1.824457753 | -0.117878643 |
| C | -4.852339707 | 1.535833284 | -0.509437946 |
| C | -5.228127342 | 0.167158463 | -0.602754461 |
| C | -4.377845968 | -0.896920707 | -0.374416450 |
| C | -5.870443740 | 2.616464382 | -0.875618037 |
| C | -5.297492367 | 4.026286904 | -0.722336613 |
| C | -6.311932297 | 2.431928374 | -2.336563029 |
| C | -7.095446631 | 2.492656173 | 0.045169978 |
| C | -4.825275958 | -2.348855404 | -0.558077158 |
| C | -3.985066468 | -3.001396490 | -1.668822024 |
| C | -4.646215083 | -3.126622767 | 0.756399319 |
| C | -6.298943430 | -2.447902076 | -0.960789893 |
| C | 0.728597055 | 2.067004901 | 0.993141266 |
| C | -0.736974942 | 2.060730325 | 1.013551738 |
| C | -1.408467876 | 3.184878017 | 1.587252971 |
| C | -0.708017024 | 4.246858782 | 2.092236776 |
| C | 0.714132111 | 4.255625979 | 2.066404719 |
| C | 1.407952712 | 3.199495332 | 1.540223491 |
| C | 0.009354940 | -1.171963657 | -1.635663318 |
| C | -0.021174568 | -0.100115775 | -2.534397230 |
| C | 0.043741746 | -2.474367860 | -2.151747182 |
| C | -0.016485382 | -0.320032672 | -3.914133517 |
| C | 0.048115468 | -2.700145080 | -3.527333709 |

| | | | |
|---|---|---|---|
| C | 0.017858520 | -1.620705006 | -4.412087123 |
| C | 0.005792567 | -1.363679462 | 2.385518243 |
| C | 1.171179649 | -1.199775038 | 3.148571907 |
| C | -1.135397281 | -1.873574773 | 3.020099165 |
| C | 1.190847104 | -1.513014039 | 4.507282109 |
| C | -1.117049722 | -2.195677175 | 4.378138624 |
| C | 0.045376247 | -2.014536844 | 5.125242553 |
| H | 3.169754862 | 2.853237958 | -0.224228954 |
| H | 6.247181058 | -0.056282913 | -0.897943411 |
| H | 4.361363113 | 4.122629496 | -1.621980503 |
| H | 5.983555165 | 4.754580090 | -1.253850640 |
| H | 4.901796856 | 4.280105089 | 0.076364503 |
| H | 5.434903664 | 2.369448543 | -3.147986595 |
| H | 6.773958541 | 1.356864427 | -2.549658966 |
| H | 7.018455258 | 3.108731073 | -2.764336217 |
| H | 7.543434861 | 1.577120338 | -0.090647941 |
| H | 6.740140834 | 2.755188652 | 0.979914898 |
| H | 7.784493884 | 3.322158751 | -0.357341325 |
| H | 6.532013252 | -2.008656939 | -1.806918607 |
| H | 6.618372016 | -3.514882872 | -0.866489433 |
| H | 6.988068048 | -1.965168798 | -0.075195463 |
| H | 4.181169570 | -2.633658689 | -2.493691005 |
| H | 2.953393716 | -3.056183571 | -1.266249623 |
| H | 4.345427480 | -4.146229748 | -1.555816540 |
| H | 5.016973671 | -4.089651657 | 0.874358611 |
| H | 3.617393041 | -3.039453421 | 1.248817471 |
| H | 5.271709285 | -2.533500258 | 1.712396236 |
| H | -3.214506371 | 2.857212174 | -0.103764724 |
| H | -6.255066063 | -0.055470753 | -0.904126376 |
| H | -4.985594032 | 4.233972564 | 0.316585670 |
| H | -6.065314373 | 4.772280788 | -0.991344640 |
| H | -4.429590825 | 4.193608146 | -1.384037451 |
| H | -5.451951533 | 2.522657014 | -3.023514877 |
| H | -7.056672915 | 3.199947721 | -2.614709778 |
| H | -6.772727304 | 1.443663487 | -2.505245622 |
| H | -6.810384721 | 2.629077718 | 1.103500863 |
| H | -7.583193112 | 1.507160661 | -0.046615821 |
| H | -7.847802427 | 3.261209126 | -0.209736048 |
| H | -2.910785761 | -2.955245953 | -1.435174653 |
| H | -4.150219591 | -2.491527909 | -2.634972626 |
| H | -4.274979721 | -4.061378896 | -1.790196685 |
| H | -5.236006823 | -2.666484702 | 1.569884321 |
| H | -3.589210833 | -3.153901357 | 1.060376103 |
| H | -4.997668830 | -4.166983477 | 0.630623512 |
| H | -6.971461990 | -2.023210001 | -0.194087158 |
| H | -6.570058556 | -3.510605352 | -1.084107972 |
| H | -6.505202222 | -1.944145443 | -1.921757340 |
| H | -2.492613939 | 3.144614704 | 1.700487859 |

| | | | |
|---|---|---|---|
| H | -1.245804886 | 5.072904087 | 2.569495307 |
| H | 1.259028597 | 5.088675881 | 2.522910935 |
| H | 2.496164665 | 3.172020778 | 1.612977452 |
| H | -0.048903382 | 0.932149127 | -2.164427597 |
| H | 0.069141319 | -3.337275255 | -1.475814418 |
| H | -0.040007084 | 0.533283379 | -4.601377889 |
| H | 0.075754606 | -3.726448767 | -3.910533847 |
| H | 0.021407482 | -1.795724455 | -5.494046525 |
| H | 2.085309385 | -0.827211357 | 2.676336787 |
| H | -2.051564763 | -2.018160126 | 2.441625467 |
| H | 2.112167994 | -1.371377033 | 5.083755448 |
| H | -2.021098383 | -2.595289402 | 4.851936501 |
| H | 0.060904336 | -2.267654229 | 6.191671370 |

## 5_OSS

Charge = 0, S = 0, E =-8.008179428660118E+03

| | | | |
|---|---|---|---|
| Sn | -0.011401583 | -0.830438349 | 0.403189218 |
| O | 2.212585161 | -1.528018579 | 0.226971380 |
| O | -2.207494423 | -1.526479144 | 0.176582087 |
| N | 1.307073441 | 0.895486198 | 0.632827864 |
| N | -1.324255355 | 0.897209294 | 0.647017095 |
| C | 3.037492232 | -0.584389815 | -0.005738407 |
| C | 2.588840609 | 0.792388965 | 0.201561077 |
| C | 3.454275122 | 1.871576113 | -0.100062745 |
| C | 4.738616077 | 1.642661946 | -0.546040308 |
| C | 5.182610637 | 0.291718467 | -0.676617588 |
| C | 4.396204873 | -0.812876766 | -0.436936287 |
| C | 5.693546824 | 2.773367314 | -0.928289652 |
| C | 5.070905643 | 4.154467133 | -0.718415716 |
| C | 6.073550118 | 2.635427252 | -2.411890881 |
| C | 6.963181001 | 2.681457164 | -0.065921769 |
| C | 4.907889158 | -2.241569686 | -0.626160627 |
| C | 6.375708527 | -2.268784203 | -1.059165012 |
| C | 4.077209461 | -2.942742230 | -1.714228015 |
| C | 4.791534426 | -3.013563641 | 0.699371590 |
| C | -3.045452423 | -0.580682409 | -0.017496208 |
| C | -2.611523231 | 0.791265029 | 0.236424632 |
| C | -3.494794557 | 1.869937362 | -0.014540133 |
| C | -4.780007734 | 1.643095289 | -0.457304672 |
| C | -5.202793595 | 0.293598672 | -0.648056156 |
| C | -4.397599578 | -0.809069822 | -0.462946683 |
| C | -5.754654043 | 2.775989351 | -0.778615968 |
| C | -5.150336006 | 4.154869546 | -0.508488133 |
| C | -6.147280172 | 2.703504207 | -2.263415345 |
| C | -7.014246976 | 2.625092479 | 0.090024352 |
| C | -4.886070095 | -2.232126179 | -0.740248136 |
| C | -4.040598291 | -2.848088872 | -1.867821489 |
| C | -4.763078454 | -3.087667236 | 0.531643908 |

| | | | |
|---|---|---|---|
| C | -6.352241527 | -2.257280270 | -1.179874550 |
| C | 0.714091068 | 1.988620717 | 1.212760259 |
| C | -0.725587941 | 1.983539065 | 1.232264796 |
| C | -1.398614374 | 3.018644891 | 1.914465733 |
| C | -0.696532073 | 4.039116854 | 2.535828331 |
| C | 0.705675261 | 4.046435375 | 2.512795309 |
| C | 1.398136844 | 3.030683313 | 1.872737689 |
| C | 0.007248058 | -1.126551898 | -1.635255306 |
| C | -0.003403101 | -0.025376570 | -2.498430946 |
| C | 0.023990920 | -2.411708691 | -2.193951501 |
| C | 0.003018441 | -0.199847812 | -3.884399259 |
| C | 0.031063547 | -2.592680208 | -3.576250531 |
| C | 0.020133003 | -1.484233199 | -4.424700602 |
| C | 0.013782785 | -1.657640451 | 2.290130747 |
| C | 1.138839246 | -1.471058273 | 3.106331508 |
| C | -1.069697269 | -2.379852797 | 2.807682824 |
| C | 1.175322340 | -1.974510528 | 4.405973750 |
| C | -1.033356075 | -2.893111040 | 4.105276525 |
| C | 0.087990724 | -2.689873262 | 4.907643127 |
| H | 3.067030186 | 2.888311725 | -0.030426937 |
| H | 6.210587075 | 0.128128046 | -1.009563403 |
| H | 4.168978740 | 4.299387943 | -1.338231625 |
| H | 5.795904521 | 4.936368794 | -1.003421290 |
| H | 4.796203616 | 4.327356802 | 0.337022165 |
| H | 5.179543542 | 2.706033949 | -3.056395946 |
| H | 6.565263628 | 1.670876984 | -2.624493561 |
| H | 6.772812766 | 3.439500985 | -2.705200617 |
| H | 7.491380542 | 1.722731750 | -0.204339531 |
| H | 6.721292069 | 2.780535803 | 1.007179883 |
| H | 7.666867201 | 3.490095506 | -0.334604704 |
| H | 6.535076342 | -1.765107264 | -2.029107925 |
| H | 6.699716454 | -3.317197862 | -1.177106810 |
| H | 7.040232595 | -1.801086465 | -0.310825506 |
| H | 4.181705564 | -2.423243824 | -2.683748893 |
| H | 3.009717554 | -2.965199089 | -1.448696904 |
| H | 4.429531176 | -3.982261960 | -1.845955007 |
| H | 5.167534838 | -4.044804081 | 0.568407434 |
| H | 3.747060062 | -3.065097117 | 1.042661646 |
| H | 5.397615719 | -2.531766166 | 1.488149270 |
| H | -3.119950927 | 2.887896956 | 0.089918363 |
| H | -6.228420719 | 0.128989173 | -0.987415436 |
| H | -4.867661362 | 4.280694984 | 0.551482456 |
| H | -5.889743099 | 4.938419510 | -0.748529638 |
| H | -4.257019266 | 4.343860586 | -1.128979896 |
| H | -5.260745082 | 2.817585725 | -2.912034180 |
| H | -6.860399327 | 3.510667218 | -2.511466376 |
| H | -6.628108559 | 1.743545112 | -2.517814624 |
| H | -6.763230425 | 2.677159028 | 1.164318998 |

| | | | |
|---|---|---|---|
| H | -7.530033447 | 1.666053173 | -0.088028859 |
| H | -7.732287479 | 3.434726701 | -0.134012526 |
| H | -2.972295070 | -2.863768638 | -1.604524068 |
| H | -4.156440615 | -2.271663001 | -2.803162682 |
| H | -4.370485928 | -3.884769752 | -2.064469650 |
| H | -5.366822948 | -2.661894423 | 1.353386452 |
| H | -3.716698681 | -3.155795187 | 0.864268254 |
| H | -5.132140384 | -4.110659951 | 0.334696025 |
| H | -7.027199012 | -1.848819946 | -0.406679967 |
| H | -6.657675280 | -3.301562728 | -1.364966146 |
| H | -6.517134322 | -1.696676110 | -2.116954032 |
| H | -2.485136522 | 2.974536660 | 2.008896265 |
| H | -1.242396524 | 4.820245001 | 3.075256680 |
| H | 1.260696802 | 4.834005112 | 3.033277213 |
| H | 2.487869643 | 2.998982924 | 1.929886212 |
| H | -0.016409968 | 0.994433871 | -2.094215238 |
| H | 0.033846954 | -3.296712141 | -1.546506683 |
| H | -0.005386938 | 0.675540770 | -4.543700527 |
| H | 0.045399010 | -3.605941809 | -3.993389574 |
| H | 0.025388957 | -1.623615312 | -5.511863552 |
| H | 2.008080887 | -0.927669281 | 2.721524925 |
| H | -1.958138800 | -2.535706181 | 2.189930548 |
| H | 2.062877356 | -1.810958499 | 5.027749530 |
| H | -1.891084079 | -3.457564001 | 4.488810384 |
| H | 0.116521341 | -3.091123240 | 5.927284997 |

## 5_T

Charge = 0, S = 1, E = -8.008176706732738E+03 a.u.

| | | | |
|---|---|---|---|
| Sn | -0.009635348 | -0.856011400 | 0.417668762 |
| O | 2.243874977 | -1.539910451 | 0.194632559 |
| O | -2.237144541 | -1.534676391 | 0.147646065 |
| N | 1.302062053 | 0.848053824 | 0.699377443 |
| N | -1.314736689 | 0.853207941 | 0.705143634 |
| C | 3.046180846 | -0.576959012 | -0.025893195 |
| C | 2.571059979 | 0.785807000 | 0.233631354 |
| C | 3.409074664 | 1.890110112 | -0.049151971 |
| C | 4.688893588 | 1.699500197 | -0.527746555 |
| C | 5.157905013 | 0.362806128 | -0.714911309 |
| C | 4.400117837 | -0.764631364 | -0.493205712 |
| C | 5.616187090 | 2.861079126 | -0.883672125 |
| C | 4.972852952 | 4.222082391 | -0.612915659 |
| C | 5.972766352 | 2.784134574 | -2.377614060 |
| C | 6.902052244 | 2.761241059 | -0.046424830 |
| C | 4.933933547 | -2.175749392 | -0.741979598 |
| C | 6.392743431 | -2.159247295 | -1.205051597 |
| C | 4.093351569 | -2.853408443 | -1.837426109 |
| C | 4.858276451 | -2.996195398 | 0.557127725 |
| C | -3.051422362 | -0.570477559 | -0.037934258 |
| C | -2.588026211 | 0.788150075 | 0.256581703 |

| | | | |
|---|---|---|---|
| C | -3.441486093 | 1.891639344 | 0.014152921 |
| C | -4.723321918 | 1.702576908 | -0.456834067 |
| C | -5.176143186 | 0.367424081 | -0.686327027 |
| C | -4.402349918 | -0.757835093 | -0.509529282 |
| C | -5.668221565 | 2.864174236 | -0.762809168 |
| C | -5.036103116 | 4.222760574 | -0.455744979 |
| C | -6.046294526 | 2.833033224 | -2.252934958 |
| C | -6.940311071 | 2.722038058 | 0.089233407 |
| C | -4.920292294 | -2.163304609 | -0.819562037 |
| C | -4.072302972 | -2.781066711 | -1.944316309 |
| C | -4.837246969 | -3.042267120 | 0.439596063 |
| C | -6.379586338 | -2.144446203 | -1.281786214 |
| C | 0.711174688 | 1.930239480 | 1.331387341 |
| C | -0.718811224 | 1.928018941 | 1.343737598 |
| C | -1.395090392 | 2.917780558 | 2.073592756 |
| C | -0.692603747 | 3.909043779 | 2.752991953 |
| C | 0.702829002 | 3.912779204 | 2.738488496 |
| C | 1.396875471 | 2.923004247 | 2.047989626 |
| C | 0.006970113 | -1.123794509 | -1.623491770 |
| C | 0.008103761 | -0.011647453 | -2.472544971 |
| C | 0.011169226 | -2.401888600 | -2.198330311 |
| C | 0.013793379 | -0.168452375 | -3.860462260 |
| C | 0.017790760 | -2.565541740 | -3.582909152 |
| C | 0.018652817 | -1.446287015 | -4.416968402 |
| C | 0.011794275 | -1.791382730 | 2.250642916 |
| C | 1.149787595 | -1.685931733 | 3.063283775 |
| C | -1.088998052 | -2.508207882 | 2.738286424 |
| C | 1.182659266 | -2.263805301 | 4.331772622 |
| C | -1.056926894 | -3.094706156 | 4.004388041 |
| C | 0.077998280 | -2.972356153 | 4.804250058 |
| H | 3.006405502 | 2.896078830 | 0.071890711 |
| H | 6.181473119 | 0.233042492 | -1.074534331 |
| H | 4.058745118 | 4.373845018 | -1.212866306 |
| H | 5.679784194 | 5.026600114 | -0.879681748 |
| H | 4.711942712 | 4.350872026 | 0.452171688 |
| H | 5.066448262 | 2.859936892 | -3.004039159 |
| H | 6.480482077 | 1.838814326 | -2.634377873 |
| H | 6.650289183 | 3.612977199 | -2.652224465 |
| H | 7.446183936 | 1.819009243 | -0.229267124 |
| H | 6.677093862 | 2.815653048 | 1.033500143 |
| H | 7.585134081 | 3.593162872 | -0.296319909 |
| H | 6.521150989 | -1.622952110 | -2.161964144 |
| H | 6.735877200 | -3.196469873 | -1.361765481 |
| H | 7.062831215 | -1.700171702 | -0.456379367 |
| H | 4.160382811 | -2.292291335 | -2.786812618 |
| H | 3.033612394 | -2.914376890 | -1.547746990 |
| H | 4.467817160 | -3.877305887 | -2.020426169 |
| H | 5.247570796 | -4.015480761 | 0.380242248 |
| H | 3.822144831 | -3.077505149 | 0.919339942 |
| H | 5.473566836 | -2.533527458 | 1.350184522 |
| H | -3.047440833 | 2.897531961 | 0.158804268 |
| H | -6.199766141 | 0.236806112 | -1.045344347 |

| | | | |
|---|---|---|---|
| H | -4.761887911 | 4.318923828 | 0.609446453 |
| H | -5.755350493 | 5.027699385 | -0.685827484 |
| H | -4.132036109 | 4.405011012 | -1.062458183 |
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| H | -6.736044261 | 3.663459667 | -2.489742417 |
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| N | 1.292639507 | 1.350110352 | 0.420575983 |
| N | -1.379639326 | 1.314236590 | 0.390966355 |
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| C | 0.620348298 | 4.598629723 | 2.004631948 |
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| H | -0.953735870 | -5.511473019 | -2.049449361 |
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| N | 1.374378156 | -1.272275412 | 0.463750150 |
| N | -0.094164694 | 3.081644019 | -0.020914694 |
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| C | 4.236288911 | 2.501894586 | -1.959901791 |
| C | 4.533591712 | 2.893258744 | 0.510752363 |
| C | 6.423259919 | 2.081987078 | -0.866829546 |
| C | -0.658346510 | -2.406060126 | 0.988300495 |
| C | 0.791826243 | -2.361418606 | 1.026470801 |
| C | 1.475912072 | -3.398288466 | 1.712941352 |
| C | 0.795364883 | -4.454812238 | 2.283216628 |
| C | -0.610367443 | -4.516282393 | 2.212357011 |
| C | -1.318717192 | -3.508538799 | 1.590437338 |
| C | -0.168860434 | 0.459863862 | -1.853263294 |
| C | 0.709635100 | -0.322184279 | -2.615816076 |
| C | -1.164615263 | 1.173388837 | -2.532042931 |
| C | 0.600248881 | -0.388004592 | -4.005944669 |
| C | -1.277198570 | 1.116885322 | -3.922113828 |
| C | -0.393618696 | 0.334899209 | -4.664619015 |
| C | 0.115229137 | 0.945244110 | 2.266321295 |
| C | -0.952485419 | 0.627300422 | 3.115894196 |
| C | 1.265139663 | 1.509691811 | 2.834406730 |
| C | -0.874820069 | 0.857045069 | 4.490822813 |
| C | 1.347455867 | 1.745056976 | 4.207701063 |
| C | 0.277386277 | 1.418251692 | 5.040384367 |
| C | 0.543744964 | 3.705506276 | -1.013949076 |

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| C | -0.181697663 | 5.853662471 | -0.242840503 |
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| H | -6.318455888 | -0.534237898 | -0.630854212 |
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| H | -5.773104072 | -5.275831962 | -1.368739789 |
| H | -4.665504260 | -4.820983442 | -0.052385080 |
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| H | -6.959808713 | -3.598268210 | -2.732768397 |
| H | -7.477234999 | -2.287927756 | 0.050627894 |
| H | -6.559589948 | -3.473267077 | 1.015764524 |
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| H | -6.810432030 | 1.492455185 | -1.311682437 |
| H | -6.946305432 | 2.851687119 | -0.171918156 |
| H | -7.128446654 | 1.185393159 | 0.423052867 |
| H | -4.518884839 | 2.382402797 | -2.054161028 |
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| H | 4.565134883 | 1.912899945 | -2.834792479 |
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| H | 3.443844610 | 2.935733426 | 0.652430478 |
| H | 4.904265770 | 3.919152028 | 0.332928402 |
| H | 6.976854517 | 1.728664595 | 0.021372267 |
| H | 6.703422283 | 3.136626509 | -1.033229400 |
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| H | 2.257206773 | 2.189120986 | 4.628605884 |
| H | 0.341143784 | 1.601621451 | 6.119233778 |
| H | 1.082162548 | 3.057308417 | -1.713325302 |
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| H | 1.070103884 | 5.553139060 | -1.997740065 |
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| N | 1.263893239 | 1.272663981 | 0.556063396 |
| N | -1.366876619 | 1.211825140 | 0.576570834 |
| N | 0.101248102 | -3.179860507 | 0.025059228 |
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| C | 4.670088549 | 2.142022010 | -0.587524089 |
| C | 5.204165667 | 0.817736412 | -0.564893708 |
| C | 4.477656772 | -0.313844568 | -0.258470133 |
| C | 5.570991966 | 3.295111761 | -1.029279293 |
| C | 4.842478706 | 4.639958990 | -1.004091631 |
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| C | -3.574914840 | 2.175606842 | 0.038799398 |
| C | -4.873877957 | 1.945626166 | -0.356453251 |
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| C | -5.887221040 | 3.071584597 | -0.562449401 |
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| H | 0.038275773 | -1.657436591 | -5.512331557 |
| H | 1.930445828 | -0.775791892 | 2.769541379 |
| H | -1.914396194 | -2.645051600 | 2.113805983 |
| H | 1.958582621 | -1.647027071 | 5.075225915 |
| H | -1.861049306 | -3.544788853 | 4.412614834 |

| | | | |
|---|---|---|---|
| H | 0.068243801 | -3.043768967 | 5.913239680 |

**8**

Charge = 0, S = 1/2, E =-8.007597811891716E+03

| | | | |
|---|---|---|---|
| Sn | -0.397024354 | -0.798773854 | 0.336306530 |
| O | 2.968478072 | 2.908611345 | 0.282545174 |
| O | -2.410424505 | -1.366244183 | 0.534926527 |
| N | 1.230549457 | 0.718136083 | 0.073214157 |
| N | -1.404109414 | 1.030312835 | 0.228732919 |
| C | 4.848931530 | 1.534164518 | -0.225501760 |
| C | 5.316959475 | 0.247887770 | -0.534649751 |
| C | 4.487120885 | -0.872345398 | -0.658895675 |
| C | 3.120197365 | -0.688992747 | -0.459716551 |
| C | 2.591387852 | 0.566503295 | -0.140687575 |
| C | 3.467307964 | 1.670238489 | -0.034218779 |
| C | 1.621349862 | 3.080907034 | 0.406359088 |
| C | 0.757729649 | 1.964728570 | 0.289408217 |
| C | -0.667142521 | 2.156269986 | 0.403011571 |
| C | 1.136969478 | 4.343309861 | 0.671788988 |
| C | -0.249649461 | 4.507645432 | 0.845985201 |
| C | -1.137002937 | 3.455199817 | 0.713844202 |
| C | -2.778580113 | 0.916891624 | 0.048480140 |
| C | -3.273389527 | -0.413338587 | 0.223508305 |
| C | -4.657458464 | -0.670281225 | 0.048005585 |
| C | -5.470837234 | 0.400755109 | -0.313978507 |
| C | -4.998255619 | 1.707657242 | -0.541327132 |
| C | -3.642322787 | 1.946934753 | -0.361162642 |
| C | -5.213585345 | -2.085797504 | 0.229092010 |
| C | -4.929241497 | -2.577276806 | 1.657322209 |
| C | -6.727516834 | -2.144270521 | 0.009437927 |
| C | -4.550607004 | -3.027925580 | -0.789732056 |
| C | -5.975547232 | 2.800056771 | -0.985261377 |
| C | -6.633993063 | 2.393918450 | -2.313173696 |
| C | -7.062932341 | 2.978360939 | 0.086310506 |
| C | -5.282875782 | 4.148818991 | -1.189626911 |
| C | 5.020575595 | -2.263513486 | -1.012279437 |
| C | 6.544427486 | -2.282064689 | -1.147994981 |
| C | 4.622476699 | -3.257344936 | 0.090098765 |
| C | 4.407818837 | -2.712392691 | -2.348788759 |
| C | 5.811423067 | 2.724190576 | -0.097180079 |
| C | 5.454339868 | 3.806280441 | -1.130522442 |
| C | 5.745783127 | 3.302525201 | 1.326746748 |
| C | 7.263619849 | 2.308271472 | -0.354756836 |
| C | -0.052498205 | -1.870202131 | -1.389341860 |
| C | 0.065781671 | -3.266716819 | -1.337599782 |
| C | 0.025911884 | -1.240544589 | -2.638316888 |
| C | 0.266092578 | -4.013546231 | -2.499610985 |

| | | | |
|---|---|---|---|
| C | 0.226945106 | -1.981531393 | -3.802938269 |
| C | 0.347560522 | -3.369500302 | -3.734108878 |
| C | 0.165963713 | -1.452639857 | 2.213287321 |
| C | -0.745778736 | -2.194369620 | 2.980107960 |
| C | 1.434283683 | -1.195311767 | 2.753112907 |
| C | -0.398954338 | -2.664485703 | 4.247069521 |
| C | 1.783390211 | -1.662919296 | 4.020380000 |
| C | 0.866884654 | -2.400753690 | 4.768766437 |
| H | 6.387956970 | 0.119653645 | -0.686948276 |
| H | 2.424590622 | -1.526520124 | -0.562690822 |
| H | 1.833937492 | 5.180543777 | 0.767125815 |
| H | -0.636073731 | 5.498787212 | 1.104912878 |
| H | -2.197738664 | 3.615134803 | 0.904696554 |
| H | -6.538724013 | 0.210320747 | -0.447771446 |
| H | -3.227692738 | 2.929243442 | -0.582993400 |
| H | -5.328365996 | -3.598927237 | 1.796616362 |
| H | -3.847383438 | -2.595120430 | 1.857007593 |
| H | -5.411248330 | -1.918942165 | 2.402388668 |
| H | -7.075315565 | -3.181971257 | 0.154387523 |
| H | -7.277847309 | -1.508776604 | 0.725752950 |
| H | -7.013028862 | -1.841091355 | -1.013280799 |
| H | -4.919122331 | -4.061206453 | -0.649981917 |
| H | -4.794010843 | -2.718243423 | -1.822161838 |
| H | -3.455625757 | -3.025541303 | -0.676759757 |
| H | -7.350186209 | 3.168346123 | -2.644440877 |
| H | -5.876353221 | 2.264970703 | -3.106465109 |
| H | -7.187589937 | 1.443802629 | -2.221952545 |
| H | -7.782288220 | 3.760876282 | -0.217950969 |
| H | -7.631670669 | 2.047566316 | 0.252179268 |
| H | -6.618983215 | 3.276602977 | 1.052733397 |
| H | -6.023267272 | 4.903937669 | -1.506632987 |
| H | -4.813915925 | 4.516882893 | -0.259897686 |
| H | -4.505233087 | 4.100078227 | -1.972053998 |
| H | 6.881897258 | -3.303720284 | -1.393729787 |
| H | 6.896317973 | -1.616602946 | -1.955618800 |
| H | 7.047077291 | -1.984416986 | -0.210912107 |
| H | 4.998526833 | -4.268171856 | -0.150828642 |
| H | 5.045626836 | -2.958756261 | 1.065748110 |
| H | 3.527633795 | -3.328705552 | 0.206737636 |
| H | 4.773786694 | -3.719703048 | -2.619155587 |
| H | 3.306021401 | -2.756667269 | -2.305527244 |
| H | 4.684275976 | -2.018743211 | -3.162761864 |
| H | 6.163395683 | 4.650044908 | -1.049956677 |
| H | 5.523725325 | 3.403818331 | -2.156789415 |
| H | 4.437719913 | 4.201470720 | -0.985076319 |
| H | 6.453451809 | 4.145963768 | 1.422495614 |
| H | 4.740492312 | 3.671361791 | 1.579915786 |
| H | 6.029905166 | 2.537883185 | 2.071603478 |

| | | | |
|---|---|---|---|
| H | 7.914579463 | 3.193379070 | -0.251330604 |
| H | 7.617438341 | 1.553757845 | 0.369208633 |
| H | 7.410237719 | 1.909077492 | -1.373490520 |
| H | -0.006762507 | -3.793547352 | -0.377459630 |
| H | -0.059325934 | -0.149504793 | -2.713716211 |
| H | 0.356550005 | -5.103880477 | -2.439107007 |
| H | 0.287393627 | -1.470776074 | -4.770532238 |
| H | 0.504627048 | -3.952758625 | -4.648402601 |
| H | -1.747350214 | -2.391548609 | 2.584370940 |
| H | 2.170561973 | -0.616740944 | 2.185603947 |
| H | -1.127585710 | -3.238453520 | 4.830684012 |
| H | 2.778717789 | -1.446221498 | 4.424286929 |
| H | 1.139571574 | -2.768336395 | 5.764679994 |

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