**Supplementary Information**

IR and Raman spectroscopic analysis, DFT modeling and magnetic properties of a nickel(II) complex, [Ni(succ)(H2O)4]n

DARIUSZ BIEŃKO\*, MAGDALENA MALIK-GAJEWSKA, PAULINA WALENCIK, MICHALINA KAJ, WIKTOR ZIERKIEWICZ, GHULAM MURTAZA, TOBIAS RUFFER and SAEED AHMAD\*

***Abbreviations***

**1** = [Ni(succ)(H2O)4]n

**2** = [Ni(succ)(H2O)4]

**3** = [Ni(succ)(H2O)4]2

Figure S1. The FT-IR (on the top) and Raman (on the bottom) spectra of succinic acid in the 3600-500 cm-1 range.

Figure S2. The FT-IR (on the top) and Raman (on the bottom) spectra of succinic acid in the 600-100 cm-1 range.

Figure S3. The FT-IR (on the top) and Raman (on the bottom) spectra of **1** in the 600-100 cm-1 range.

Table S1. The theoretical (unscaled) frequencies, ν (cm-1), IR intensities, IIR (km mol-1), Raman scattering activities, SR (Å4 amu-1) and vibrational assignments for monomer of **1**. The calculations were made for unit in gas phase, only selected bands are presented.

Table S2. The theoretical (unscaled) frequencies, ν (cm-1), IR intensities, IIR (km mol-1), Raman scattering activities, SR (Å4 amu‑1) and vibrational assignments for monomer of **1**. The calculations were made for unit in a solvent (H2O) medium, only selected bands are presented.

Table S3. The theoretical (unscaled) frequencies, ν (cm-1), IR intensities, IIR (km mol-1), Raman scattering activities, SR (Å4 amu-1), and vibrational assignments for dimer of **1** (figure S4). The calculations were made for unit in gas phase, only selected bands are presented.

Table S4. Energy values of the izo-complexes calculated at the B3LYP-D3/Def2TZVP level theory (Hartree unit).



Figure S1. The FT-IR (on the top) and Raman (on the bottom) spectra of succinic acid in the 3600-500 cm-1 range.



Figure S2. The FT-IR (on the top) and Raman (on the bottom) spectra of succinic acid in the 600-100 cm‑1 range.



Figure S3. The FT-IR (on the top) and Raman (on the bottom) spectra of **1** in the 600-100 cm-1 range.

Table S1. The theoretical (unscaled) frequencies, ν (cm-1), IR intensities, IIR (km mol-1), Raman scattering activities, SR (Å4 amu-1) and vibrational assignments for monomer of **1**. The calculations were made for unit in gas phase, only selected bands are presented.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| No. | Calcd. |  |  |  |  |
|  | **har** | **IIR** | **SR** | **PED[%]** | **Assignmentsa** |
| 1 | 3424 | 1284 |  | O5-H (29),O6-H (15), O8-H (28),O7-H (16) | O-H (88) |
| 2 | 3084 | 9 | 57 | C4-H (83), C2’-H (16) | C-H (99) |
| 3 | 1630 | 112 |  | scissO-H (51) |  sciss H-O-H (51) |
| 4 | 1566 | 895 |  | asC1asC3 | asC |
| 5 | 1444 | 476 |  | sC1sC3 | sC |
| 6 | 1412 | 406 |  | C3’-C4’ (9),C1-C2 (9),C4’-H (7),C2’’-H (7) | C-H (32) |
| 7 | 1336 | 14 |  | C2-H (23),C3’=O (21) | C-H (23), C=O (21)  |
| 8 | 1268 | 13 |  | C4-H (30), C2-H (36) | C-H (66) |
| 9 | 1193 | 13 |  | twist C4’-H (25), twist C2-H (22), twistC2’’-H (25), twistC4-H (22) |  twistC-H (99) |
| 10 | 1083 | 63 |  | C4’-C2 (69), C4-C2’ (31) | C4-C2 (100) |
| 11 | 1048 | 30 |  | C4-H (10),  O6-H (10), C2-H (10) | C-H (20) |
| 12 | 966 | 50 |  | C1-C2 (15), C3-C4 (14) | C-C (29) |
| 13 | 909 | 0 |  | C1’’-C2’’ (17), C3’-C4’ (16) | C-C (23) |
| 14 | 811 | 246 | 0 | ρr CH2 (59) | ρr CH2 (59) |
| 15 | 670 | 76 |  |  Nicoord (75),  C3’-O (10),  C1’-O (10) |  Nicoord (75),  C-O (20) |

a Abbreviations are under table 1 (see paper).

Table S2. The theoretical (unscaled) frequencies, ν (cm-1), IR intensities, IIR (km mol-1), Raman scattering activities, SR (Å4 amu‑1) and vibrational assignments for monomer of **1**. The calculations were made for unit in a solvent (H2O) medium, only selected bands are presented.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| No. | Calcd. |  |  |  |  |
|  | **har** | **IIR** | **SR** | **PED[%]** | **Assignmentsa** |
| 1 | 3743 | 68 |  | O6-H (73), O7-H (30) | O-H (100) |
| 2 | 3100 | 17 |  | C4’-H (52),C2-H (52) | C-H (104) |
| 3 | 1639 | 64 |  | scissH-O5-H (36) | scissH-O-H (36) |
| 4 | 1572 | 923 |  | asC1 | asC |
| 5 | 1427 | 531 |  | sC1 | sC |
| 6 | 1403 | 437 |  | C3’-C4’ (16),C3’=O (17),C4’-H (20) | C-C (36) |
| 7 | 1314 | 1 |  | C2-H (26),C4’-H (24) | C-H (50) |
| 8 | 1267 | 6 |  | C3’-H (22), C2-H (24) | C-H (46) |
| 9 | 1194 | 2 |  | twist C4’-H (29), twist C2-H (25) | twist C-H (54) |
| 10 | 1090 | 75 |  | C4’-C2 (59), C3’-O4’ (14) | C-C (59) |
| 11 | 1066 | 190 |  | O-H…O (20), C4-C2’’ (35) | C-C (35), O-H…O (20) |
| 12 | 1053 | 126  |  | O5-H(47) | O-H(47) |
| 13 | 937 | 31 |  | C1-C2 (40), C3-C4 (36) | C-C (76) |
| 14 | 894 | 31 |  | C1’’-C2’’ (35), C3’-C4’ (48), C3’-O4’ (10), C1’’-O1’’(20) | C-C (83), C-O (30) |
| 15 | 676 | 261 |  |  Nicoord(66), O8-H…O5 (35) |  Nicoord(66), O8-H…O5 (35) |

a Abbreviations are under table 1 (see paper).

Table S3. The theoretical (unscaled) frequencies, ν (cm-1), IR intensities, IIR (km mol-1), Raman scattering activities, SR (Å4 amu-1), and vibrational assignments for dimer of **1** (figure S4). The calculations were made for unit in gas phase, only selected bands are presented.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| No. | Calcd. |  |  |  |  |
|  | **har** | **IIR** | **SR** | **PED[%]** | **Assignmentsa** |
| **1** | 34313400 | 6541505 |  | O7-H (11),O8-H (34)O5-H (37),O6-H (11) | O-H (93) |
| **2** | 310831073104 | 8138 |  | C2-H (81),C4’-H (18)C2’’-H (39),C4-H (60)C2’-H (26),C4’’-H (74) | C-H (100) |
| **4** | 1627 | 12 |  | scissH-O-H (22) | scissH-O-H (22) |
| **5** | 1566 | 653 |  | asC1 | asC |
| **6** | 1449144314411436 | 480181123 |  | sC1sC3sC1’’sC3’’sC3 | sC |
| **7** | 14131412 | 183339 |  | C3’-C4’ (18),C2’-C1’ (18) | C-C (36) |
| **8** | 13371335 | 74 |  | C2-H (30),C3’=O (23)C4’’-H (27), C1’=O (26) | C-H (57),C=O (49) |
| **9** | 12691268 | 36 |  | C4’’-H (25),C2-H (28), C4’-H (11) | C-H (64) |
| **10** | 11931192 | 84 |  | twist C4’-H (24), twist C2-H (25), twistC2’-H (25), twistC4’’-H (25) | twistC-H (99) |
| **11** | 108610841082 | 36341 |  | C4’’-C2’ (68), C4’-C2 (69),C4’’-C2’ (73) | C-C (73) |
| **12** | 10521048 | 1214 |  | rockC4-H (10),rockC2’’-H (10)rockC4’’-H (20), rockC2’-H (20) | C-H (60) |
| **13** | 966964961 | 1031811 |  | C3’’-C4’’ (20) C1-C2 (23)C2’’-C1’’ (13) | C-C (56) |
| **14** | 913909904 | 33757 |  | C1’-C2’ (29)C3’-C4’ (26)O-H-O (34) | C-C (55)O-H-O (34) |
| **15** | 809 | 66 | 5 | ρr CH2 (59) | ρr CH2 |
| **16** | 682 | 187 |  |  Nicoord (94),  O6-H (8) |  Nicoord (94),  O-H (8) |

a Abbreviations are under table 1 (see paper).

Table S4. Energy values of the izo-complexes calculated at the B3LYP-D3/Def2TZVP level theory (Hartree unit).

|  |  |  |
| --- | --- | --- |
|  | In the gas phase | In water solvent |
| A | -4997.9675 | -4998.0112 |
| B | -4997.9625 | -4998.0125 |
| C | -4997.8328 | -4998.0106 |
| D | -4997.9578 | -4997.9328 |