SUPPORTING INFORMATION

Metal-mediated Reactions between Dialkylcyanamides and Acetamidoxime Generate Unusual (Nitrosoguanidinate)Nickel(II) Complexes

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Solid-state structures of nitrosoguanidinate complexes 1–3 and 5

The bond angles for compounds **1**–**3** and **5** are in the ranges 80.97(5)–81.56° for N(2)–Ni(1)–N(1) and 98.54(12)–99.03(5)° for N(1')–Ni(1)–N(2). The Ni(1)–N(1) and Ni(1)–N(2) bond lengths are within the 1.869(3)–1.877(2) Å, 1.841(3)–1.857(3) Å intervals, and these distances are comparable to those in complexes with the Ni–N(H)=C linkages (the Ni–N bond lengths is 1.822(3)–1.885(2) Å for bis{N-[1-(2-pyrrolyl)ethylidene]aminato}nickel(II);[1] $[Ni^{II}(^2L^{ISQ})_2]$, L^{ISQ} = *N,N*-coordinated *o*-diiminobenzosemiquinonate(1–) radical;[2] $[Ni(C_2H_5N_4S)_2]$;[3] $Ni(Hapt)_2$, apt = 4-amino-3-pyridinethiolate;[4] $[Ni(C_4H_{11}N_5)_2](CI)(OH)$;[5] $[Ni(C_4H_2N_4)_2]$.[6] The C(1)–N(3) bond length (1.391(2)–1.411(5) Å) is slightly longer than typical single C_{sp2}–N(2) bond (1.376(11) Å in imidazole,[7] indicating its single bond character. The C(1)–N(2) distances are 1.297(11)–1.319(4) Å, which is close to those distance for double C_{sp2}=N(2) bond (1.313(11) Å in imidazole.[7] The C(1)–N(4) bond lengths (1.331(3)–1.347(4) Å) lie in the range typical for similar C_{sp2}–N_{sp2} bonds (1.325(9) Å in amides, 1.334(8) and 1.347(10) Å in ureas),[7] involved into conjugation.

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[1] Birdsall, W. J., *Polyhedron* **1994,** *13*, 2055–2060.
[2] D. Herebian, E. B., F. Neese *J. Am. Chem. Soc.* **2003,** *125*, 9116–9128.
[3] Kabir, M. K.; Yamada, K.; Adachi, K.; Kondo, M.; Kawata, S., cis-Bis(amidinothioureato-[kappa]2N,N')nickel(II). *Acta Crystallographica Section E* **2002,** *58* (10), m580-m582.
[4] K. Matsumoto; M. Nishizawa; Hirao, Y., *Hererocycl.* **2014,** *88* (1).
[5] Lemoine, P., *Acta Cryst.* **1996,** *C52*, 1430–1436.
[6] Peng, S., *Acta Cryst.* **1984,** *C40*, 1541–1542.
[7] Allen, F. H.; Kennard, O.; Watson, D. G.; Brammer, L.; Orpen, A. G.; Taylor, R., Tables of bond lengths determined by X-ray and neutron diffraction. Part 1. Bond lengths in organic compounds. *Journal of the Chemical Society, Perkin Transactions 2* **1987,** (12), S1-S19.

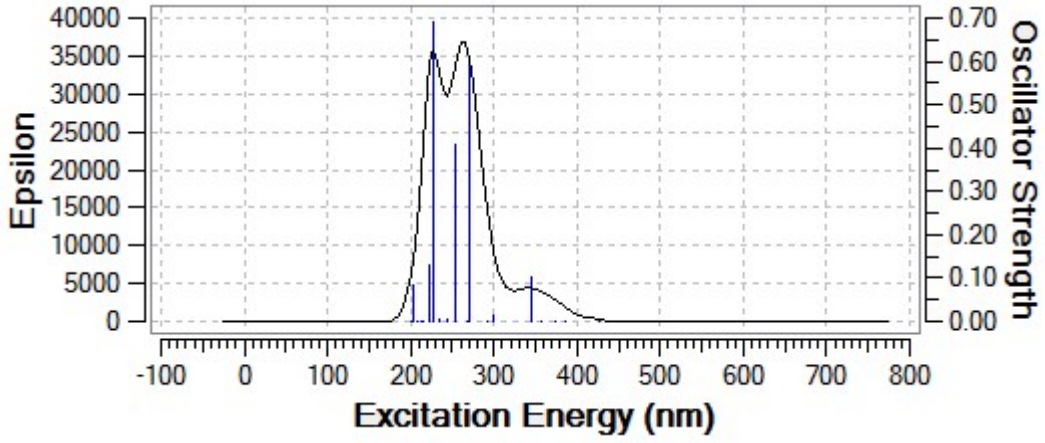
Theoretical discussions on the nature of the singlet excited electronic states of 1 and assignment of most significant transitions

To determine the nature of singlet excited electronic states of **1** and to assist in the assignment of significant transitions, theoretical TD-DFT calculations (CAM-B3LYP/6-311++G** level of theory) were carried out based on the equilibrium geometry of **1** in a dichloromethane solution. Theoretically calculated transition energies to the low-lying singlet excited electronic states of **1**, absorption wavelengths, oscillator strengths *f* and main contributing transitions are presented in **Table S1** and the corresponding theoretical UV-Vis absorption spectra is given in **Figure S1**.

Table S1. Theoretically calculated transition energies (in eV) to the low-lying singlet excited electronic states of **1**, absorption wavelengths (in nm), oscillator strengths *f* (only for $f \geq 0.10$), and main contributing transitions (CAM-B3LYP/6-311++G** level of theory).

State*	Transition energy	Wavelength	*f*	Main contributing transition
S7	3.59	345	0.10	HOMO → LUMO (88%)
S10	4.58	271	0.61	HOMO–4 → LUMO (24%)
S12	4.88	254	0.41	HOMO–1 → LUMO+2 (44%)
S20	5.48	226	0.69	HOMO–1 → LUMO+2 (46%)
S21	5.55	223	0.13	HOMO–8 → LUMO (36%)

* The excited states are labeled according to their vertical transition energies.



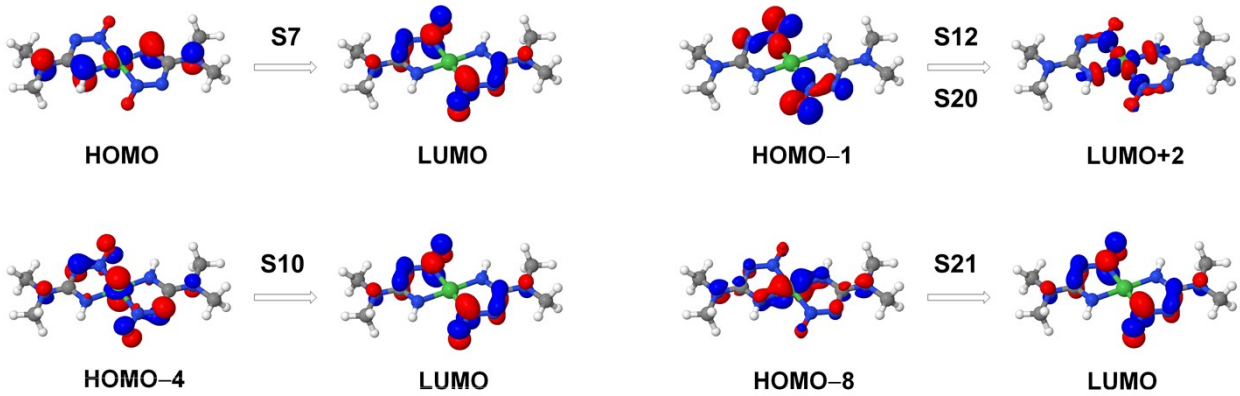
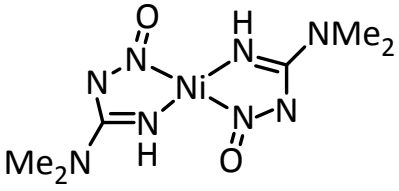


Figure S1. Theoretical UV-Vis absorption spectra of **1** and main contributing transitions of the bands.

For **1**, the electron density of the HOMO mainly includes contributions from the Ni center and N atoms of the NH and NMe_2 fragments, whereas the LUMO is located on the O=N–N–C–NMe_2 moieties. The theoretical absorption spectra of **1** determined by both metal-to-ligand charge transfer (^{1}MLCT) and intraligand charge transfer (^{1}LLCT) processes and characterized by three peaks with maxima centered at 226 (S20), 271 (S10), and 345 (S7) nm. The bands at 226 and 271 nm are by 6–7 times more intense than that at 345 nm. The overall shape of the theoretical spectra agrees well with the experimental one.

Spectra of 1–7

[Ni{NH=C(NMe$_2$)NN(O)}$_2$] (**1**, ZBM7)



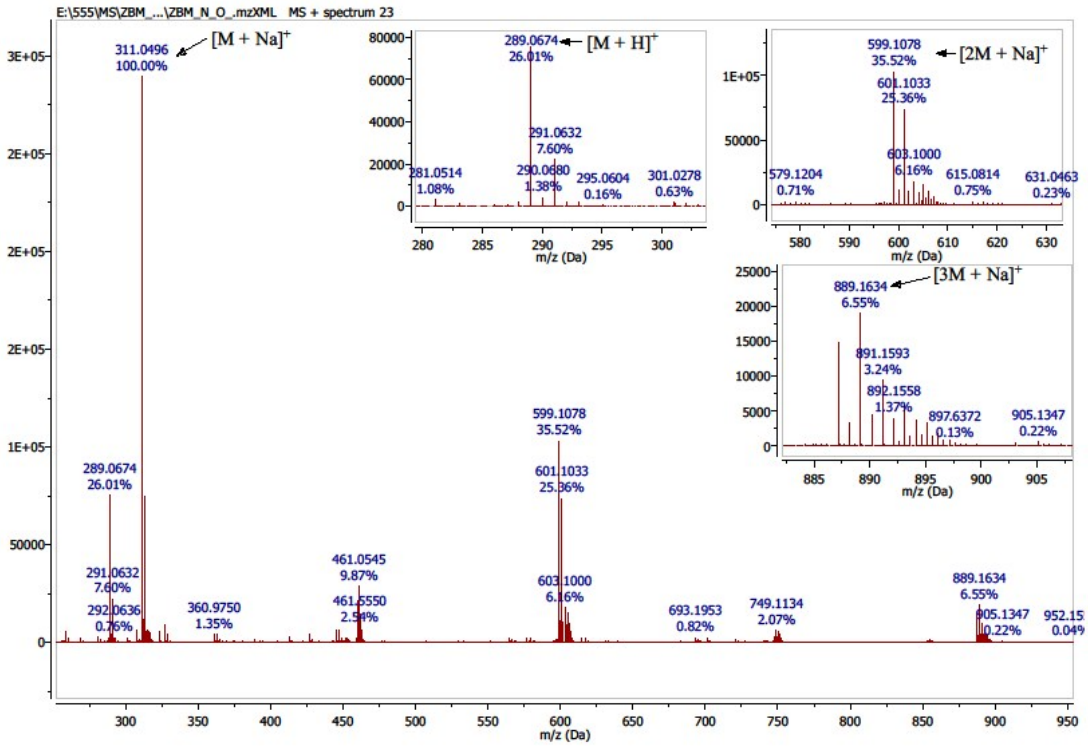


Figure S2. HRESI-MS of **1**.

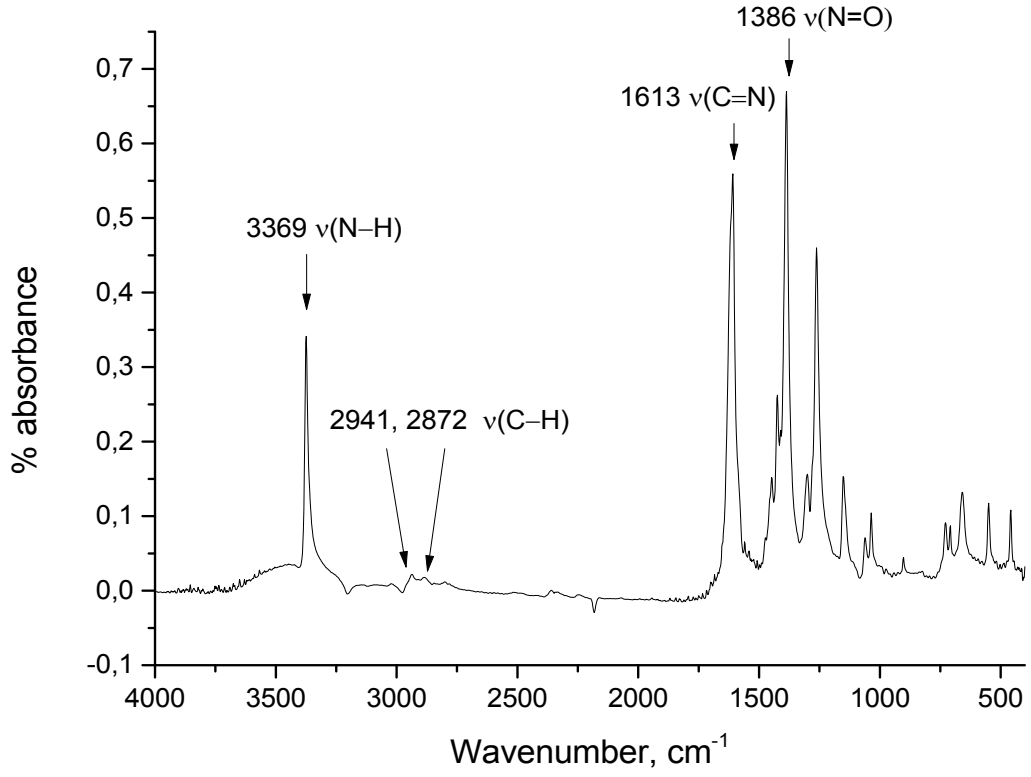


Figure S3. The FTIR spectrum of **1**.

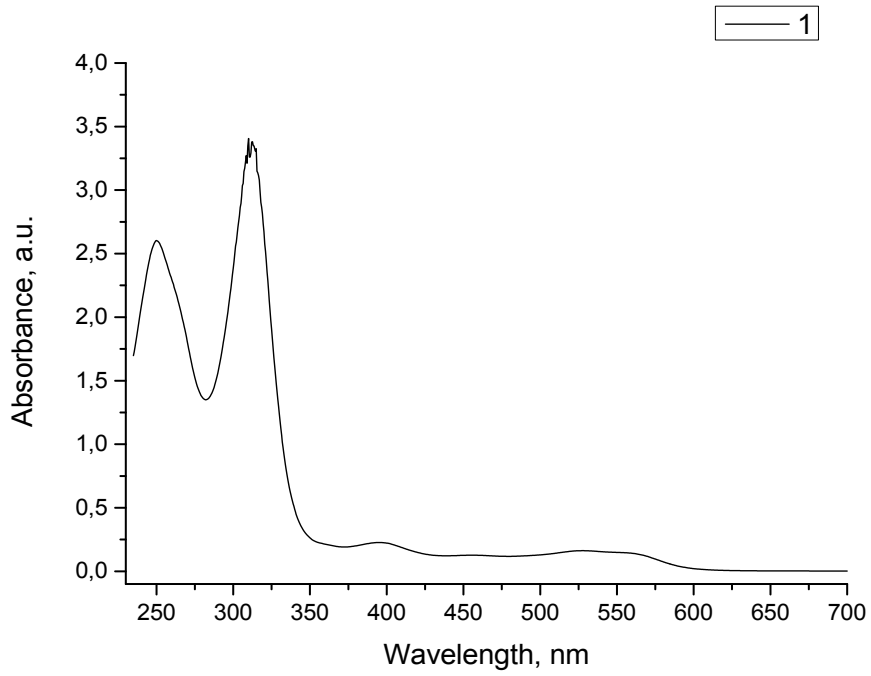


Figure S4. The UV-vis absorption spectrum of **1** in dichloromethane.

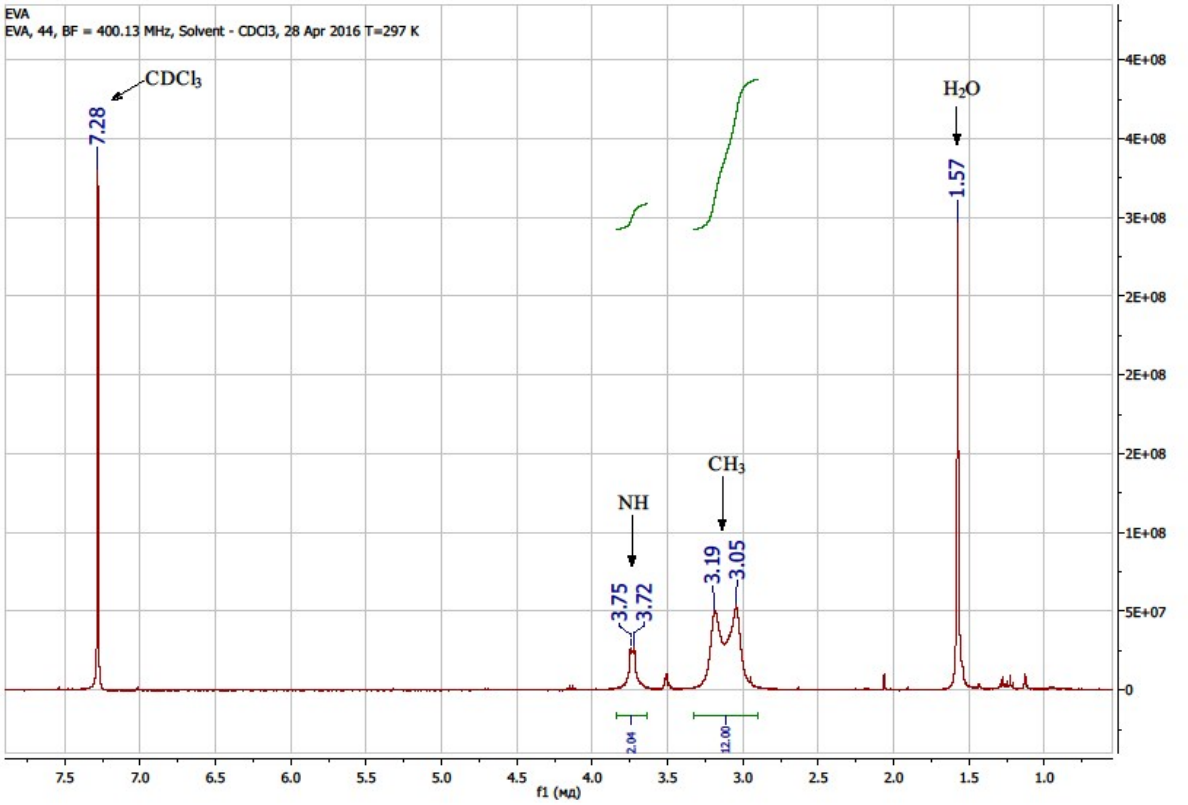


Figure S5. The ^{1}H NMR spectrum of **1**.

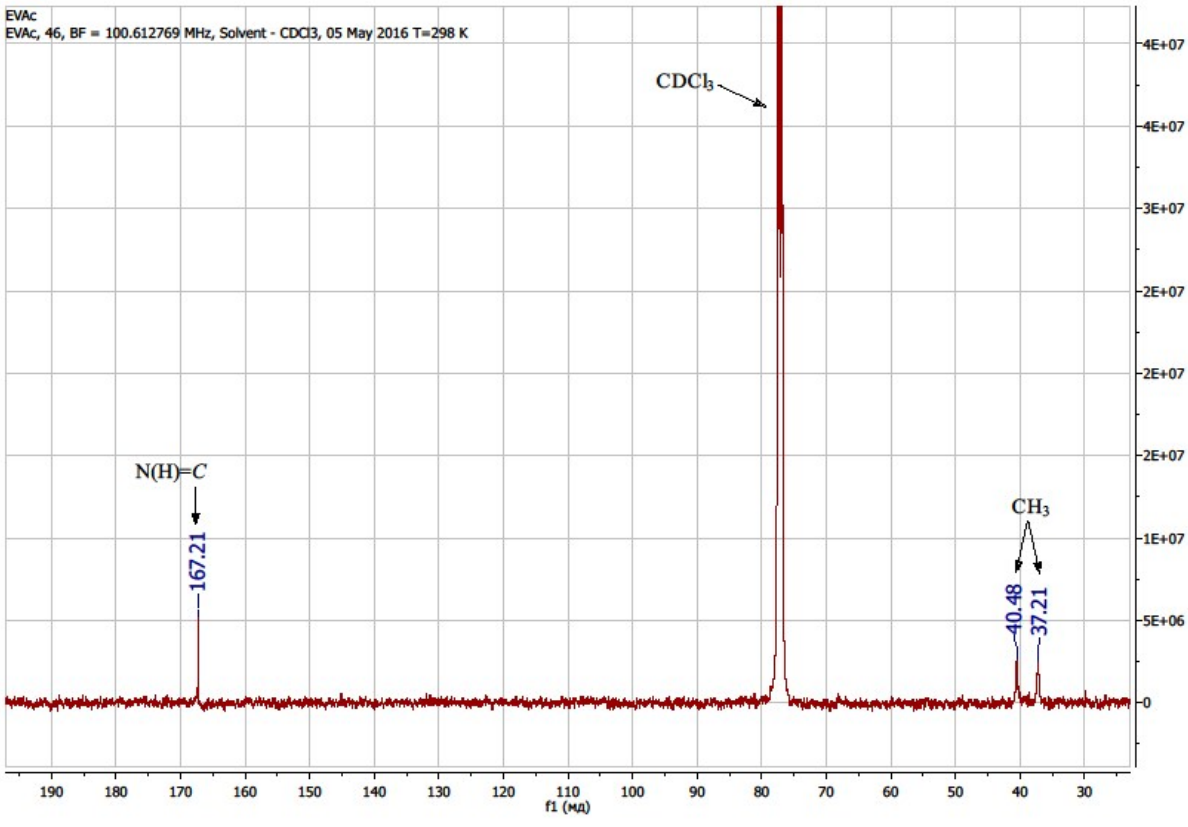


Figure S6. The ^{13}C{^{1}H} NMR spectrum of **1**.

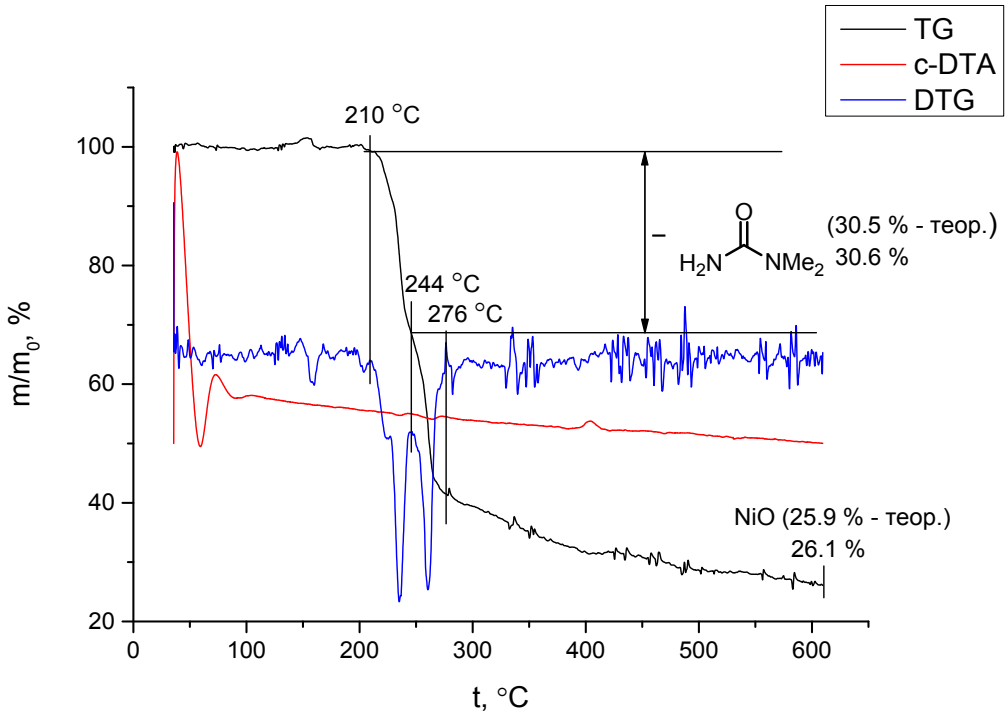
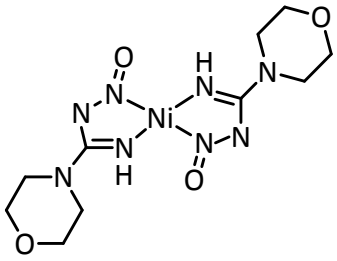


Figure S7. TG, dTG and c-DTA curves for **1**.

[Ni{NH=C(N(CH$_2$)$_4$O)NN(O)}$_2$] (**2**, ZBM28)



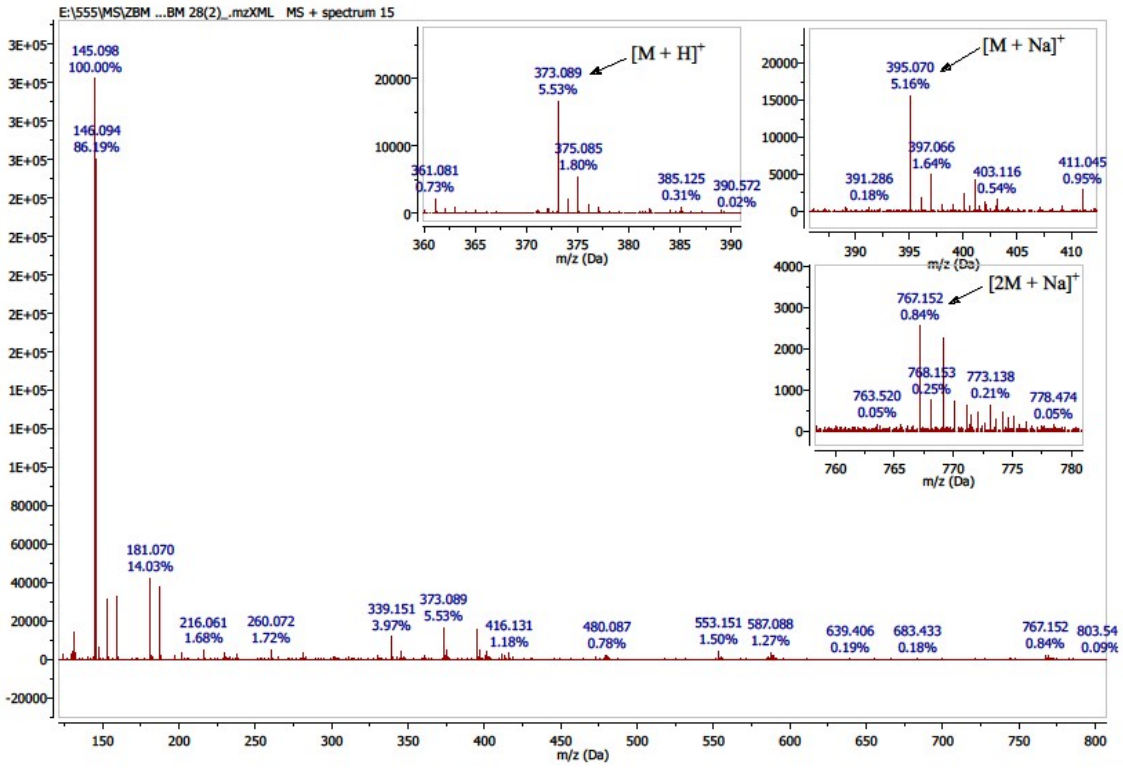


Figure S8. HRESI-MS of **2**.

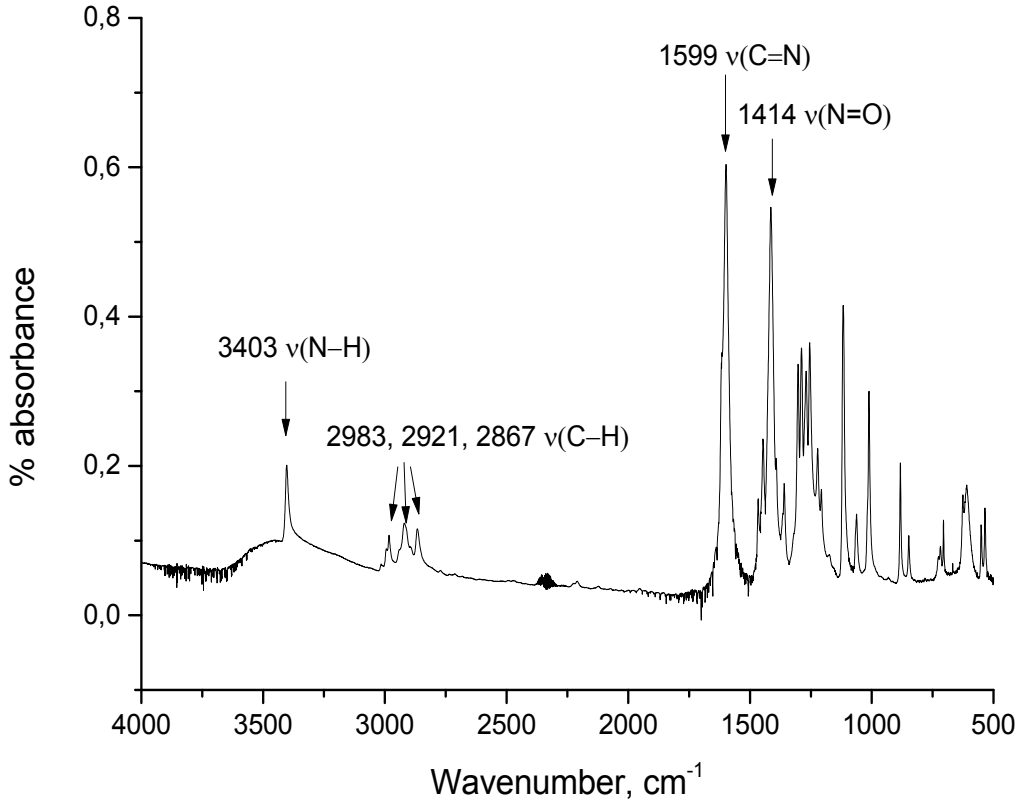


Figure S9. The FTIR spectrum of **2**.

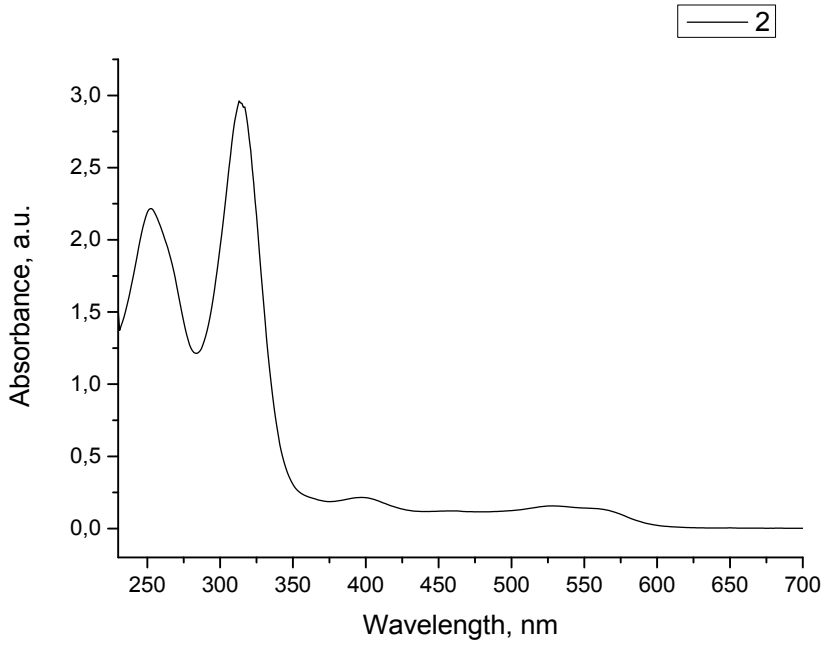


Figure S10. The UV-vis absorption spectrum of **1** in dichloromethane.

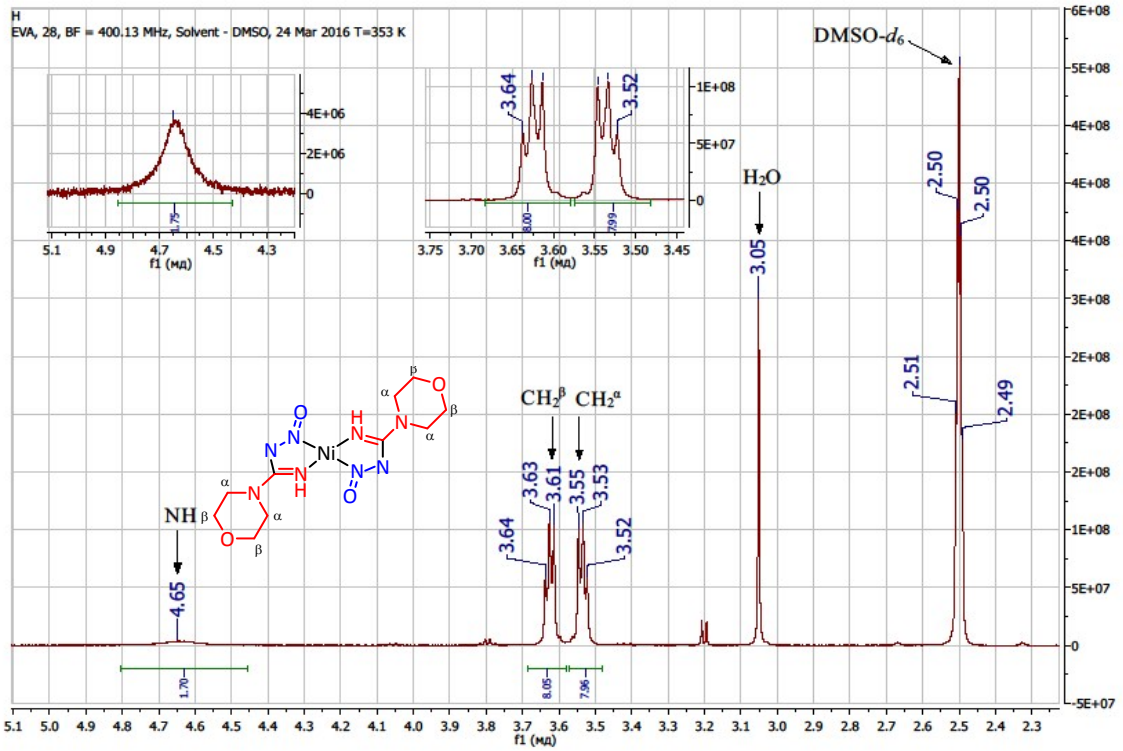


Figure S11. The ^{1}H NMR spectrum of **2**.

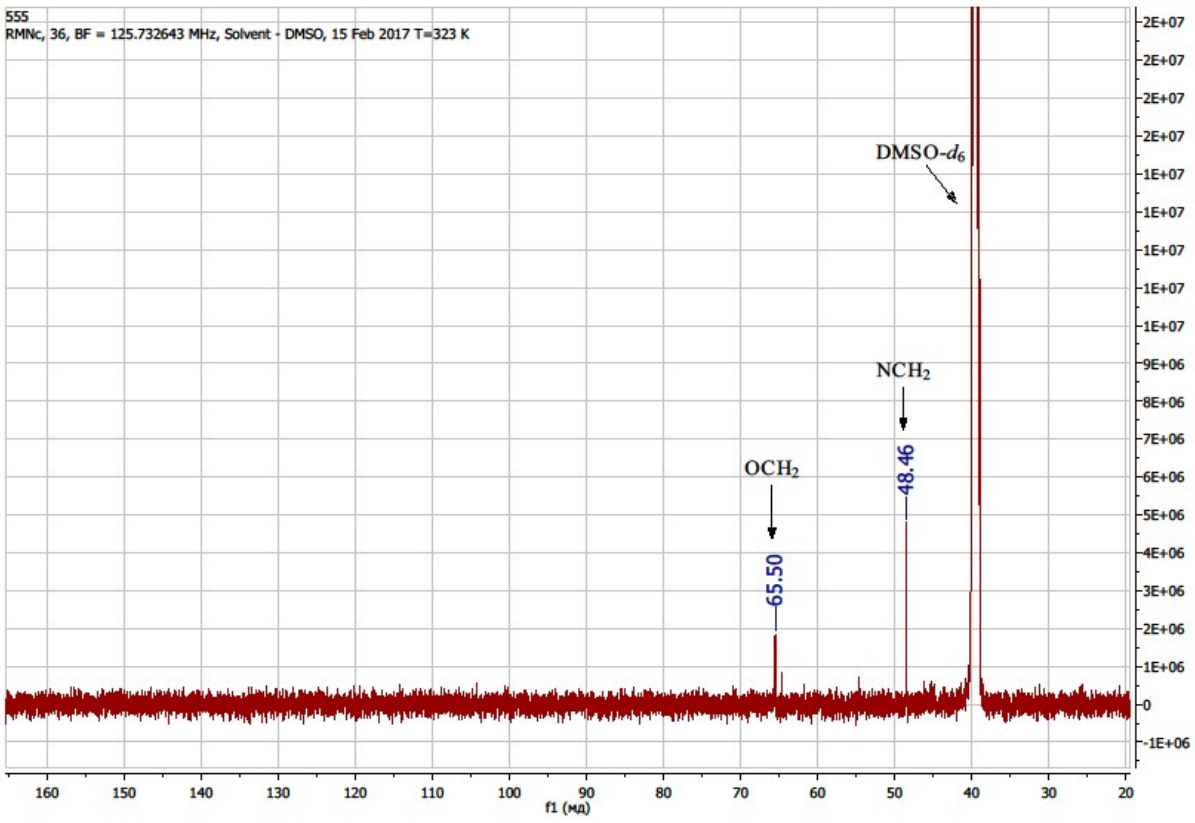


Figure S12. The $^{13}C\{^{1}H\}$ NMR spectrum of **2**.

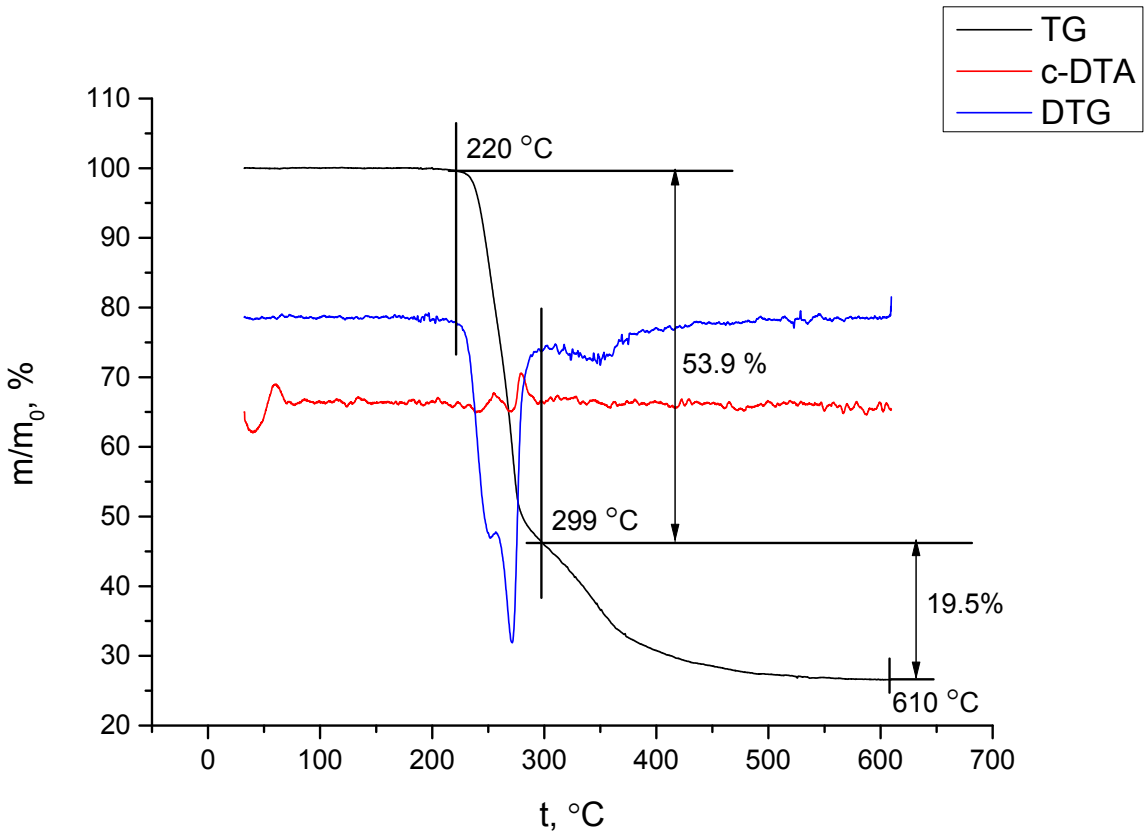
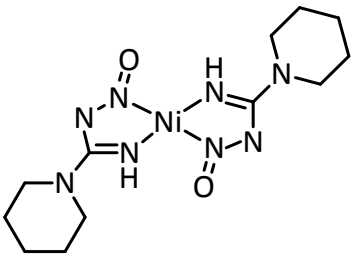


Figure S13. TG, dTG and c-DTA curves for **2**.

[Ni{NH=C(N(CH$_2$)$_5$)NN(O)}$_2$] (**3**, ZBM41)



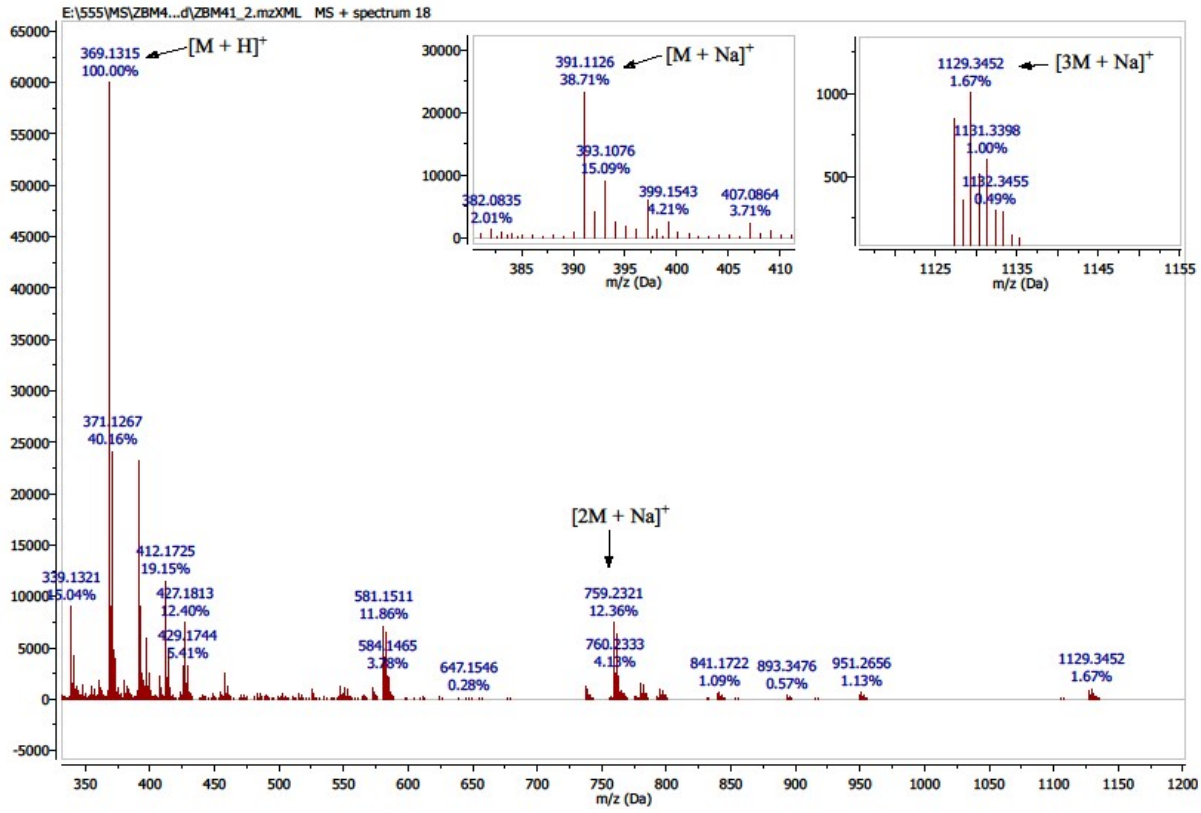


Figure S14. HRESI-MS of **3**.

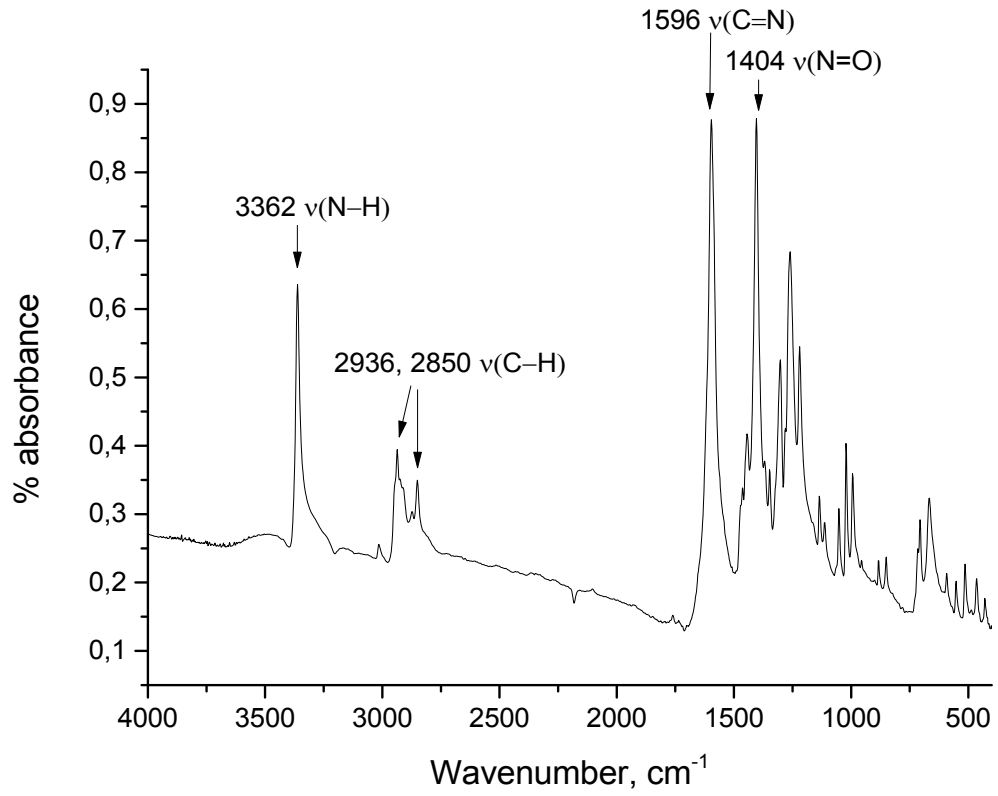


Figure S15. The FTIR spectrum of **3**.

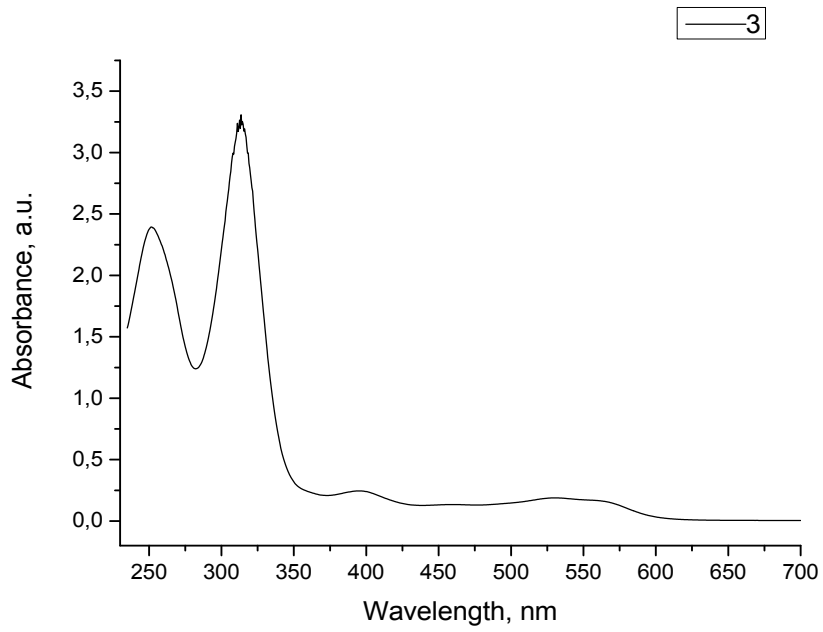


Figure S16. The UV-vis absorption spectrum of **3** in dichloromethane.

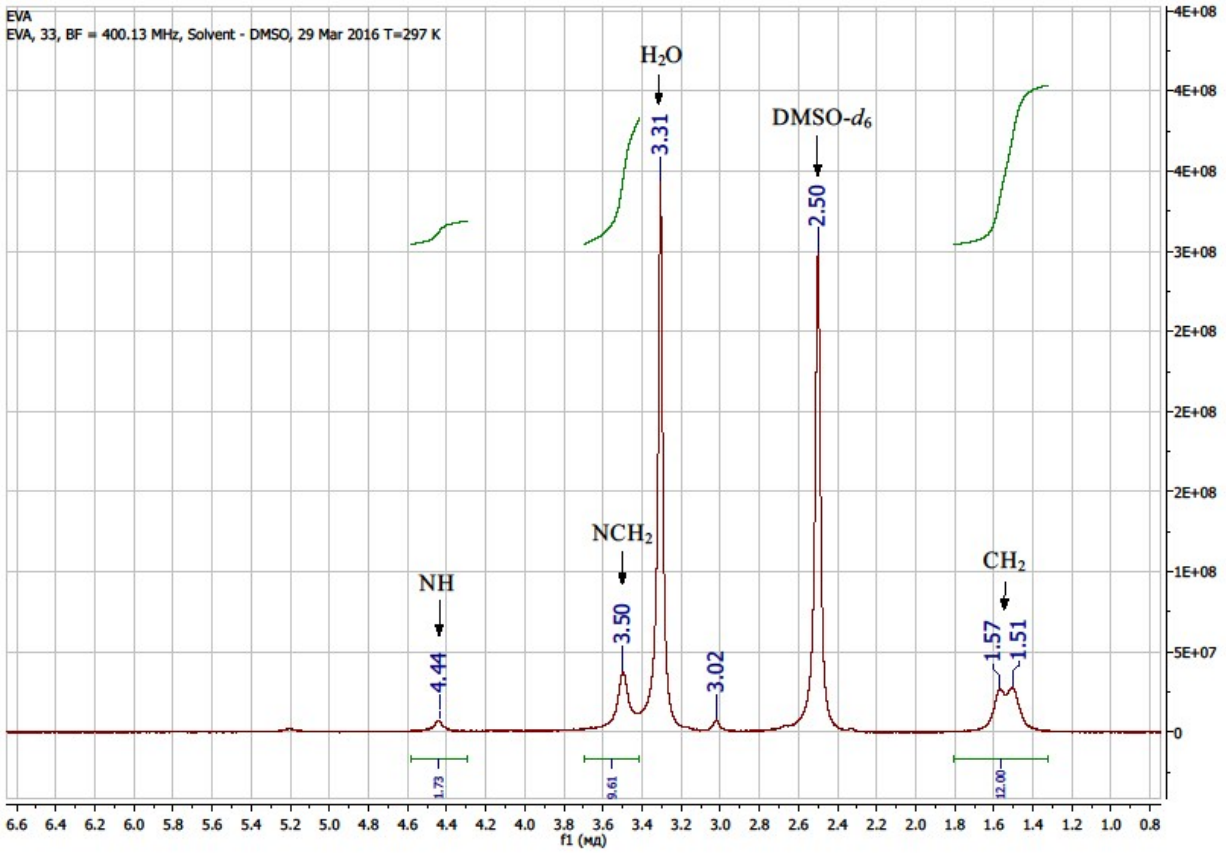


Figure S17. The ^{1}H NMR spectrum of **3**.

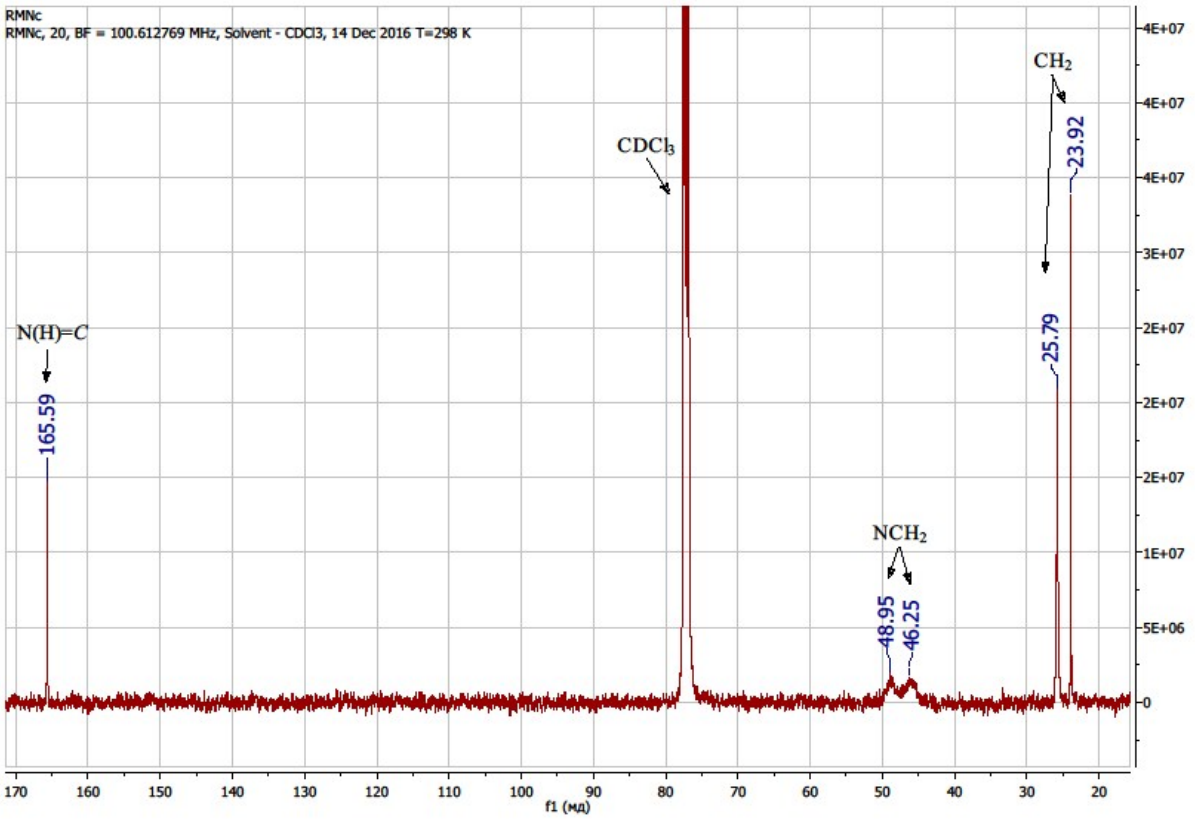


Figure S18. The ^{13}C{^{1}H} NMR spectrum of **3**.

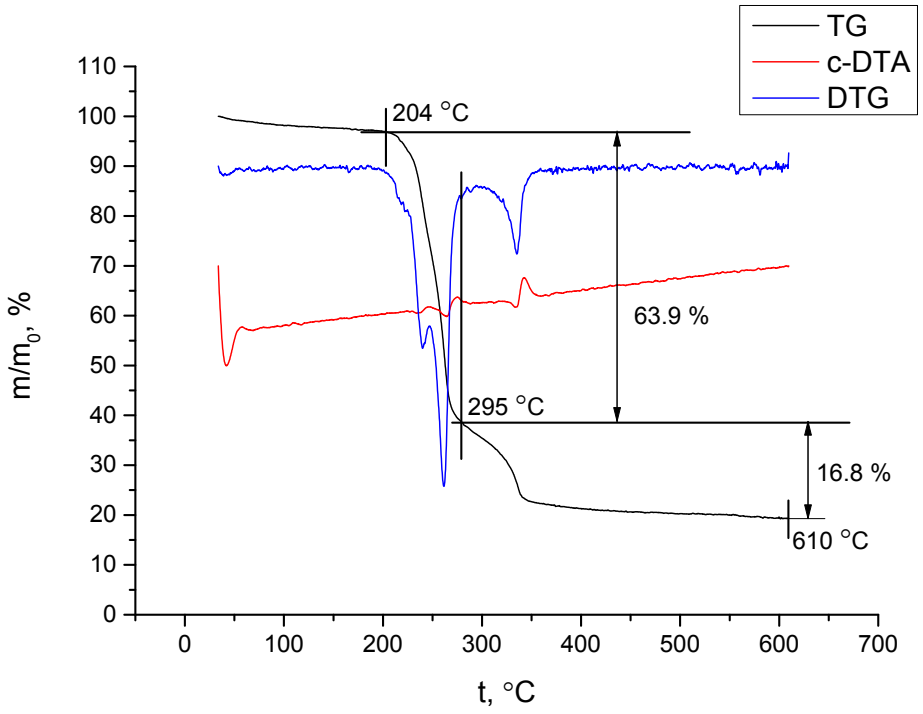
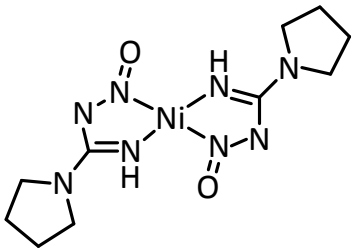


Figure S19. TG, dTG and c-DTA curves for **3**.

[Ni{NH=C(N(CH$_2$)$_4$)NN(O)}$_2$] (**4**, ZBM63)



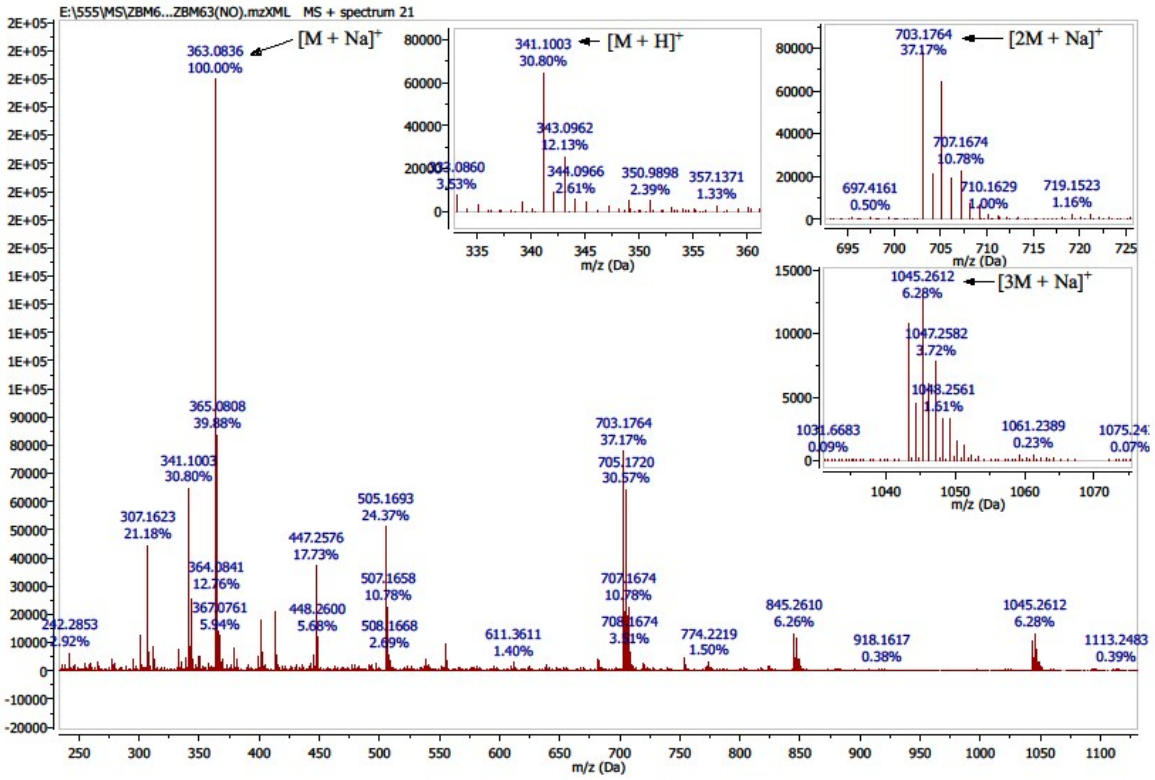


Figure S20. HRESI-MS of **4**.

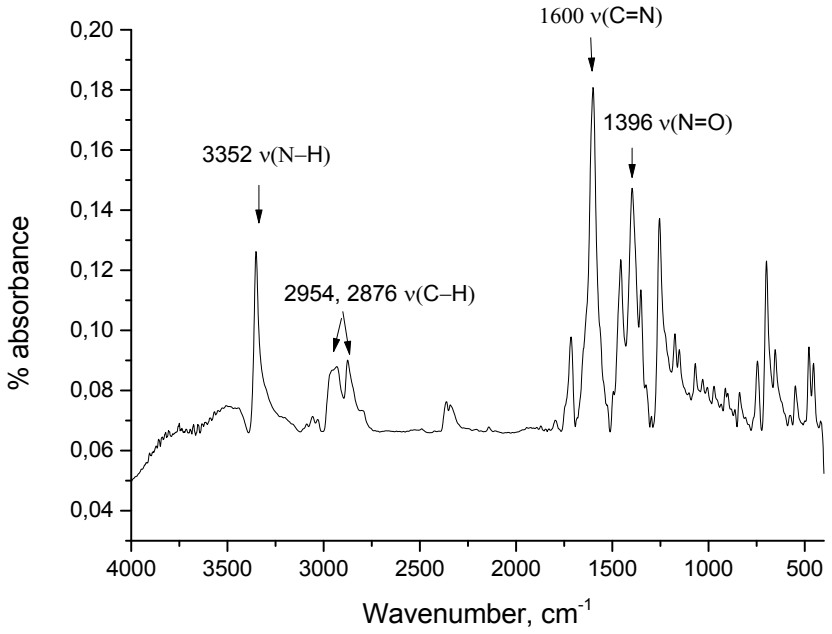


Figure S21. The FTIR spectrum of **4**.

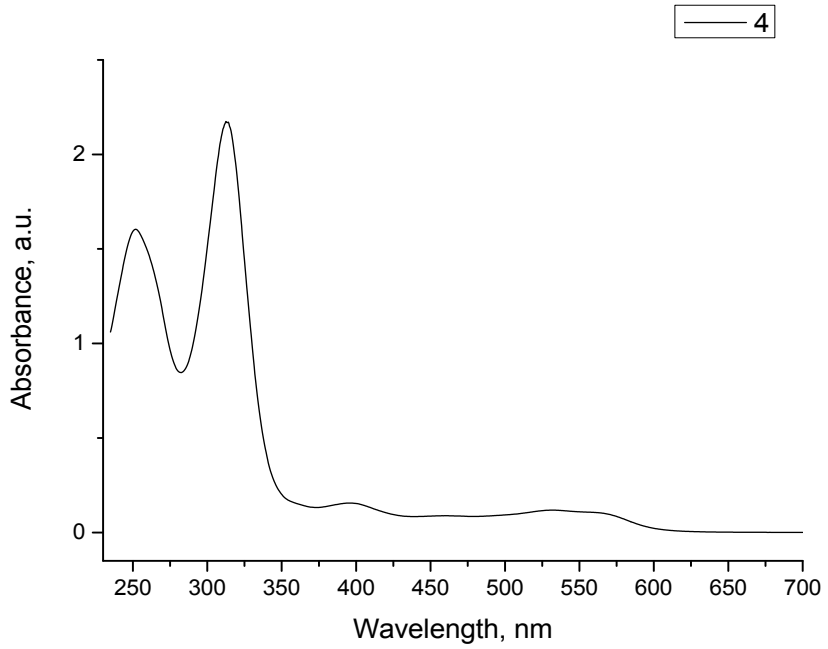


Figure S22. The UV-vis absorption spectrum of **4** in dichloromethane.

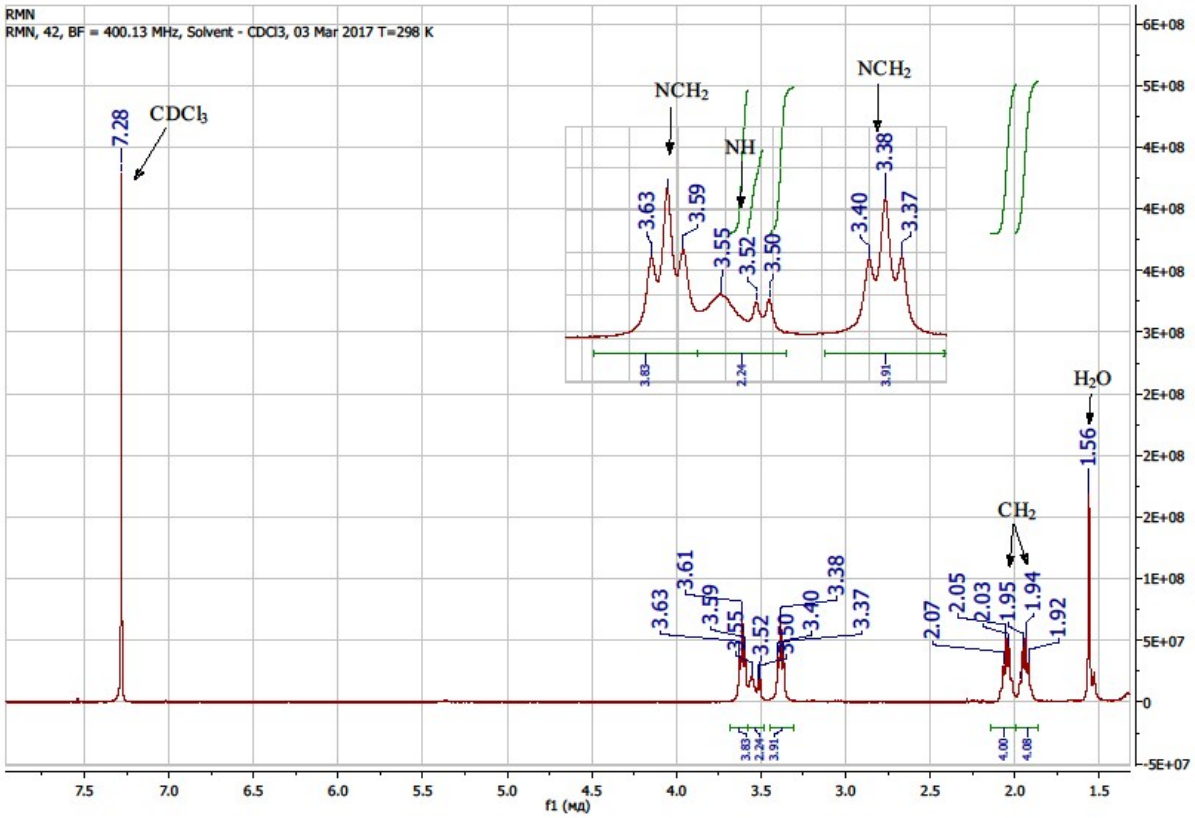


Figure S23. The ^{1}H NMR spectrum of **4**.

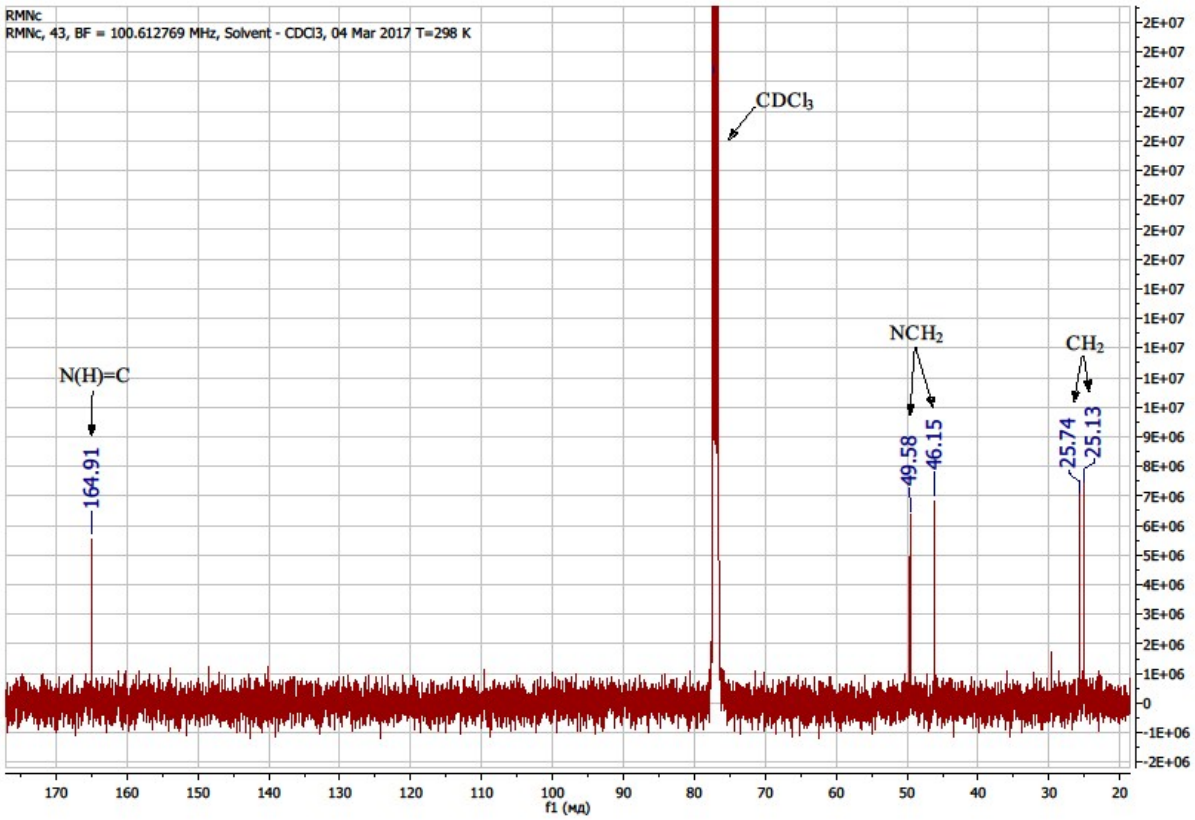


Figure S24. The $^{13}C\{^{1}H\}$ NMR spectrum of **4**.

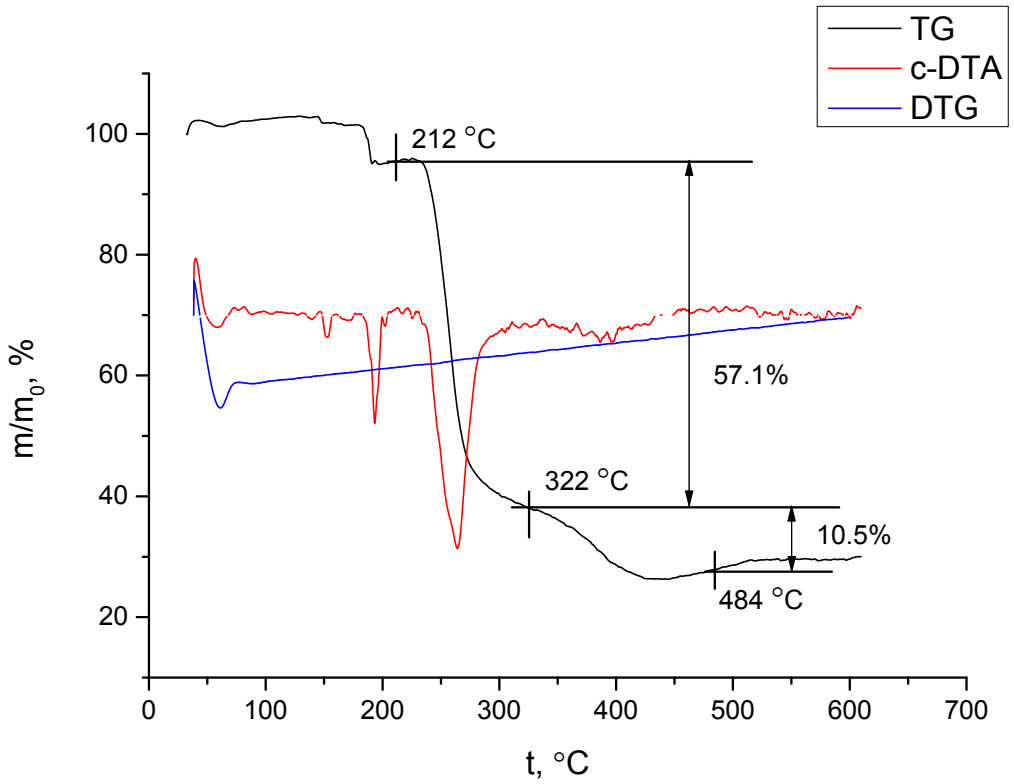
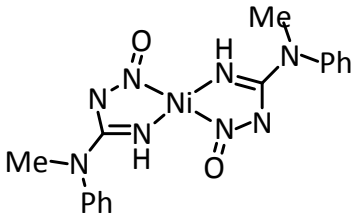


Figure S25. TG, dTG and c-DTA curves for **4**.

[Ni{NH=C(N(CH$_3$)Ph)NN(O)}$_2$] (**5**, ZBM70)



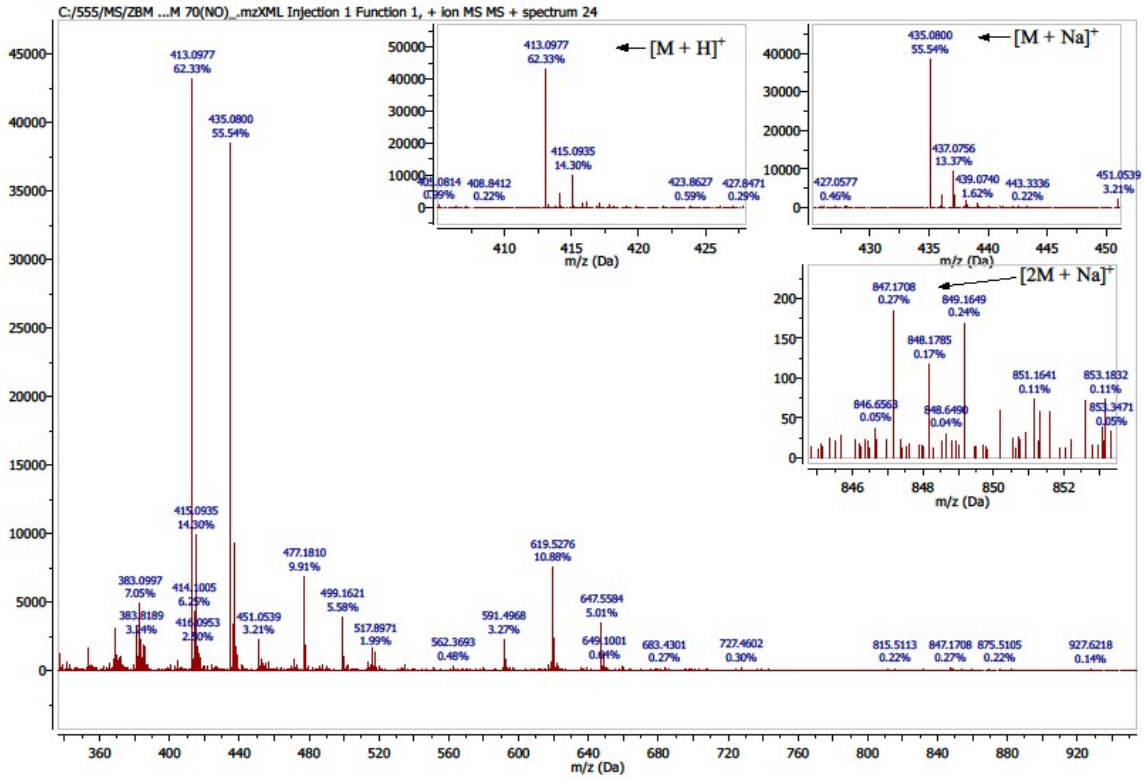


Figure S26. HRESI-MS of **5**.

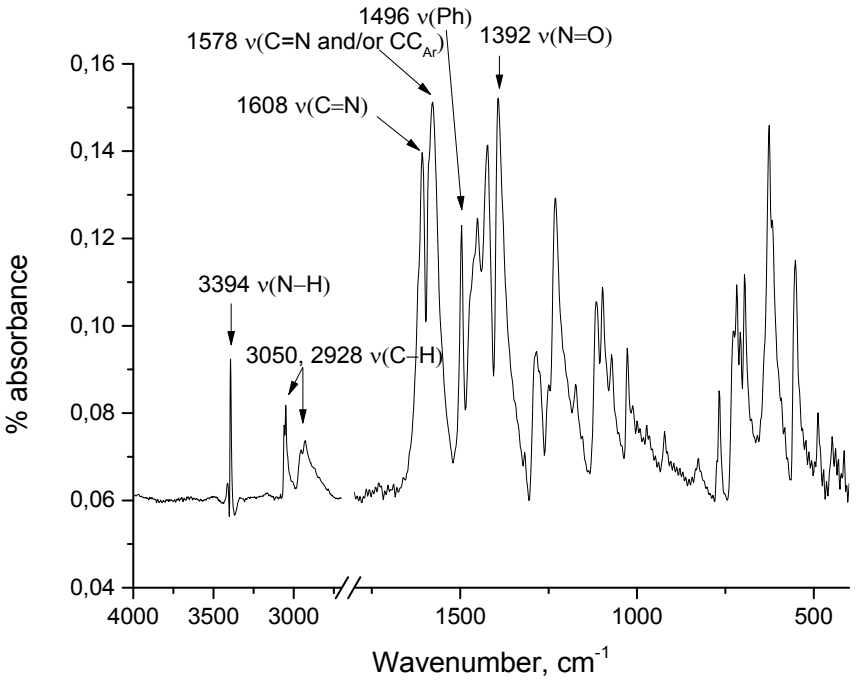


Figure S27. The FTIR spectrum of **5**.

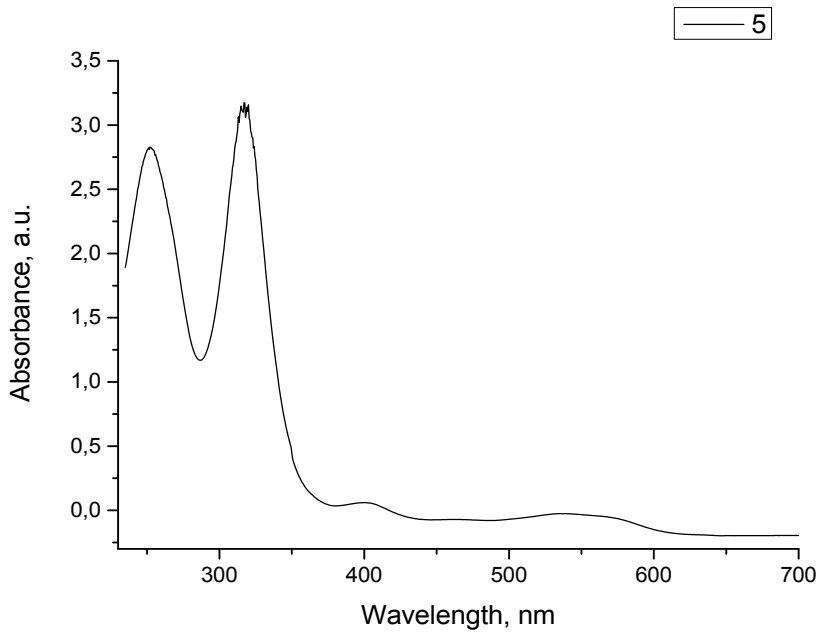


Figure S28. The UV-vis absorption spectrum of **5** in dichloromethane.

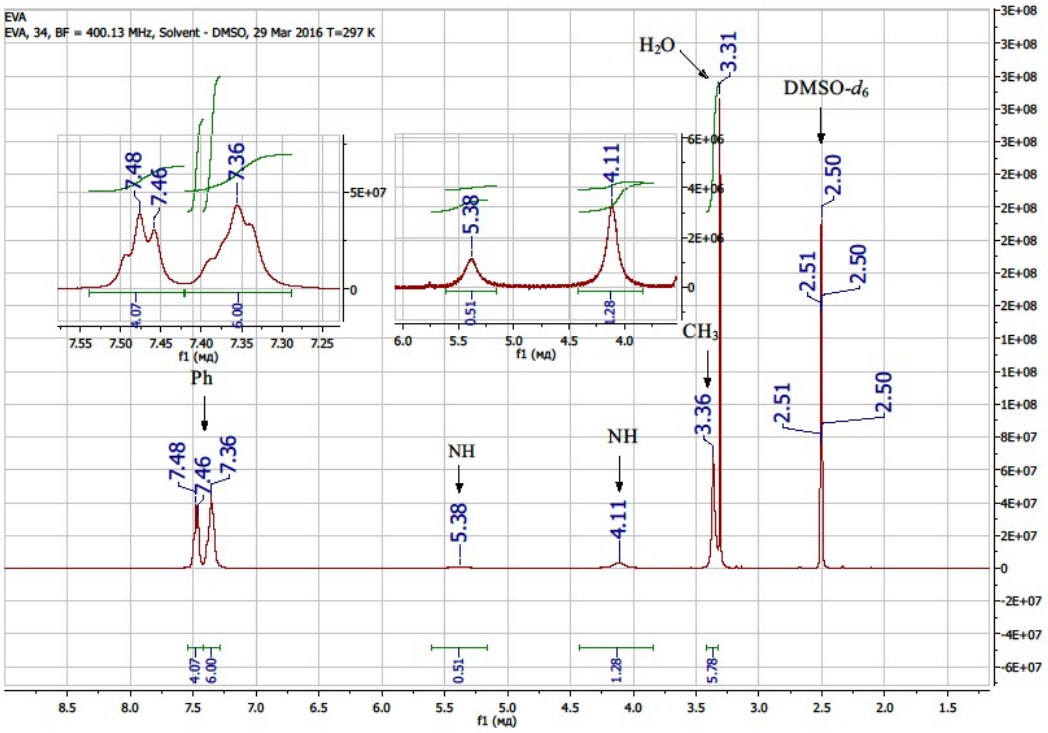


Figure S29. The ^{1}H NMR spectrum of **5**.

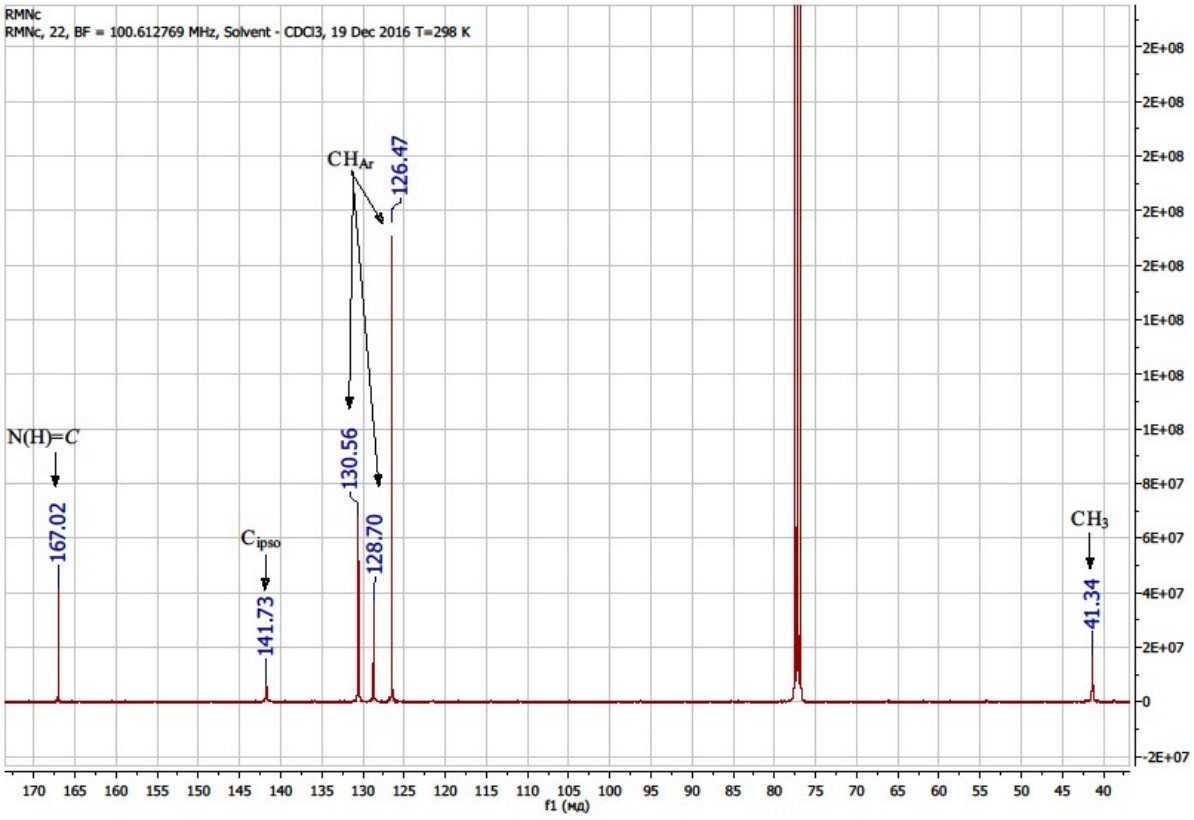


Figure S30. The ^{13}C{^{1}H} NMR spectrum of **5**.

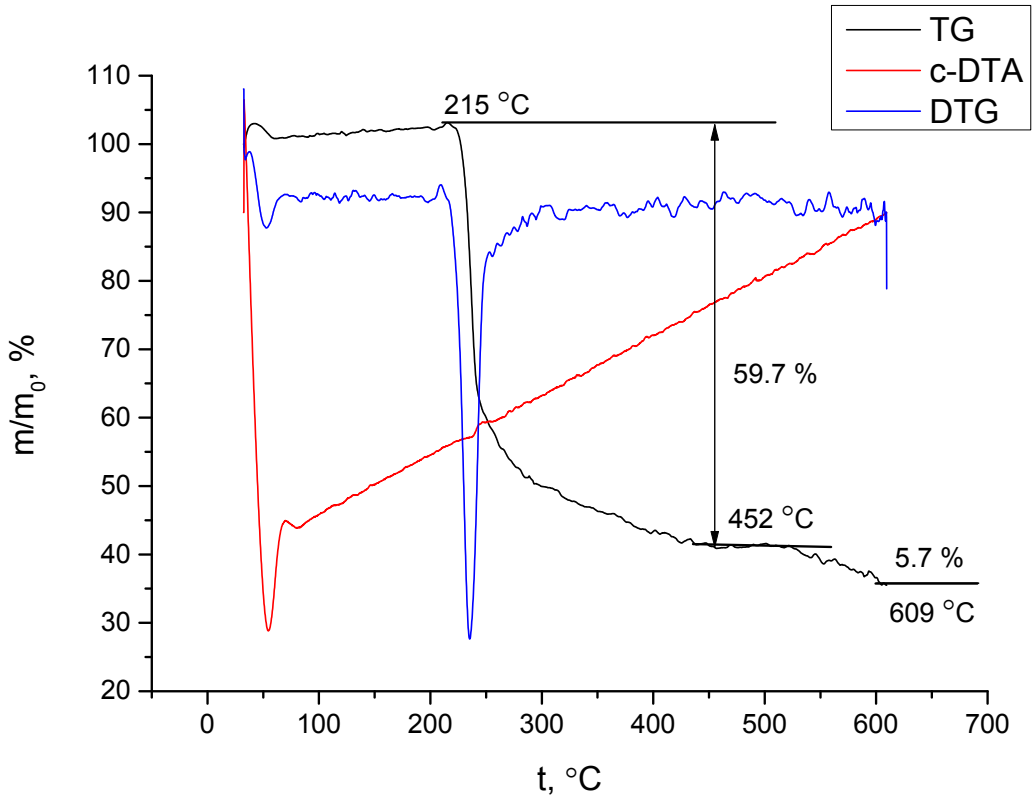
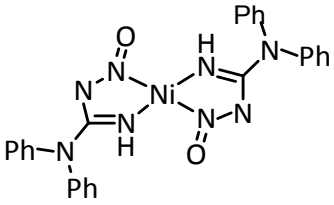


Figure S31. TG, dTG and c-DTA curves for the thermal decomposition of **5**.

[Ni{NH=C(NPh$_2$)NN(O)}$_2$] (**6**, ZBM75)



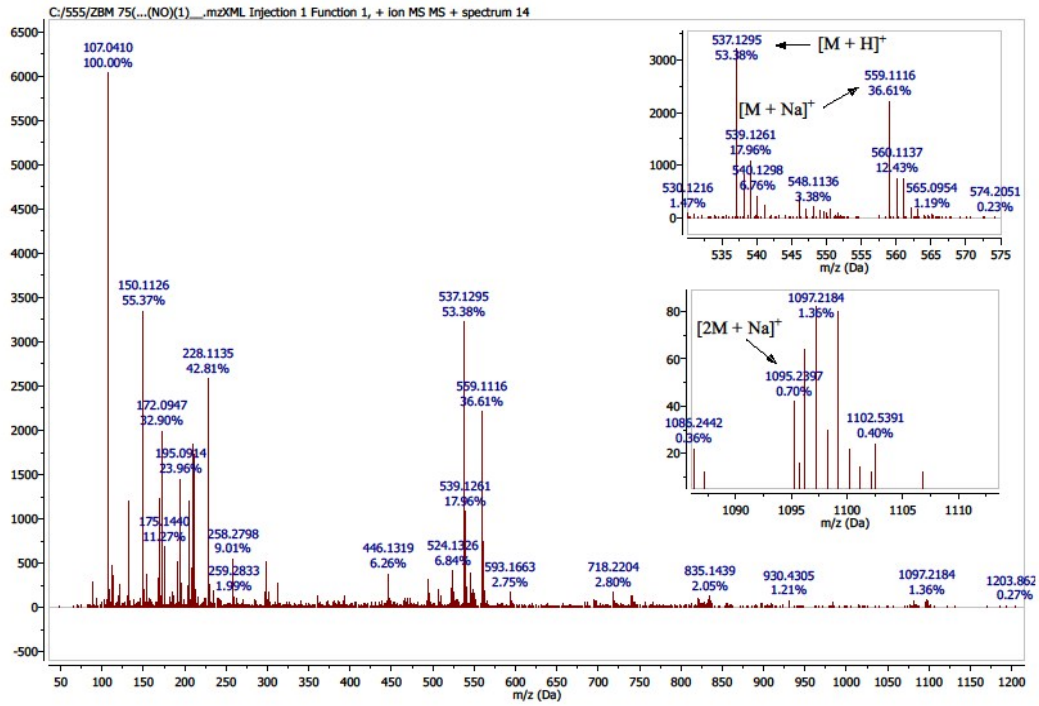


Figure S32. HRESI-MS of **6**.

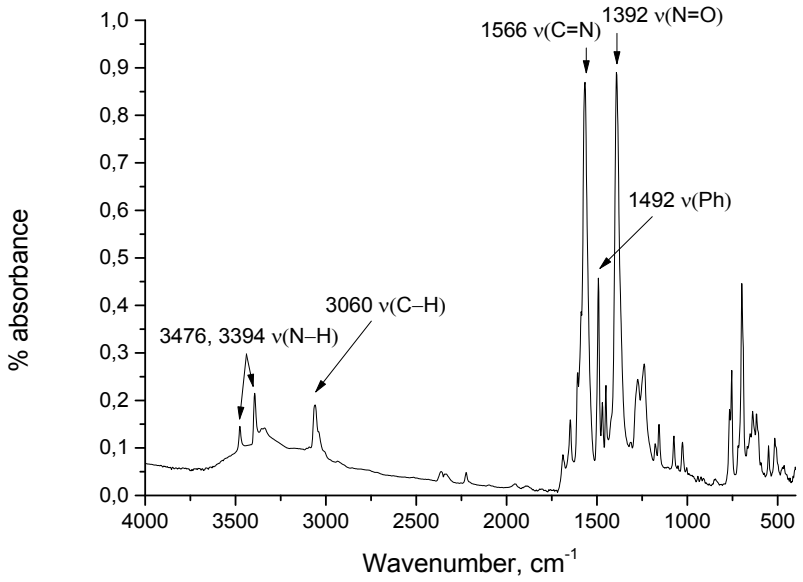


Figure S33. The FTIR spectrum of **6**.

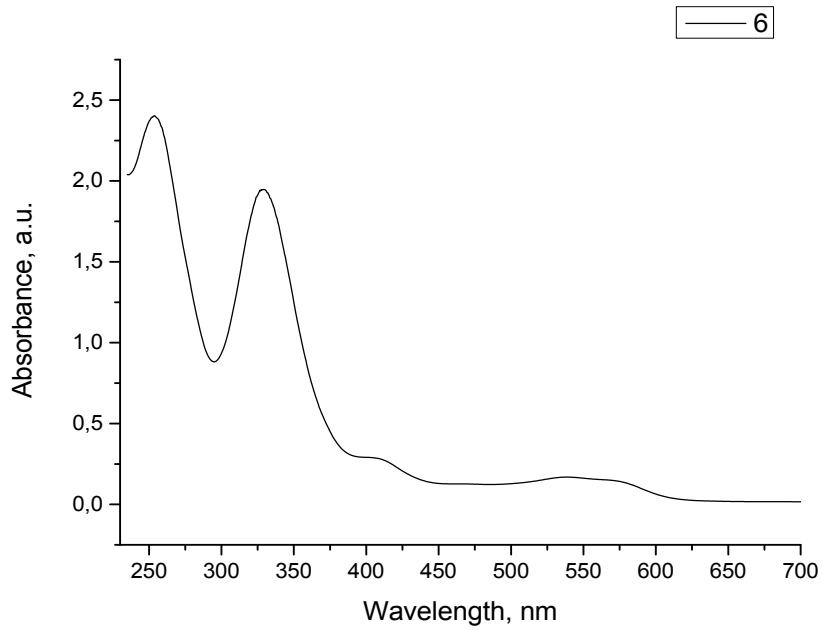


Figure S34. The UV-vis absorption spectrum of **6** in dichloromethane.

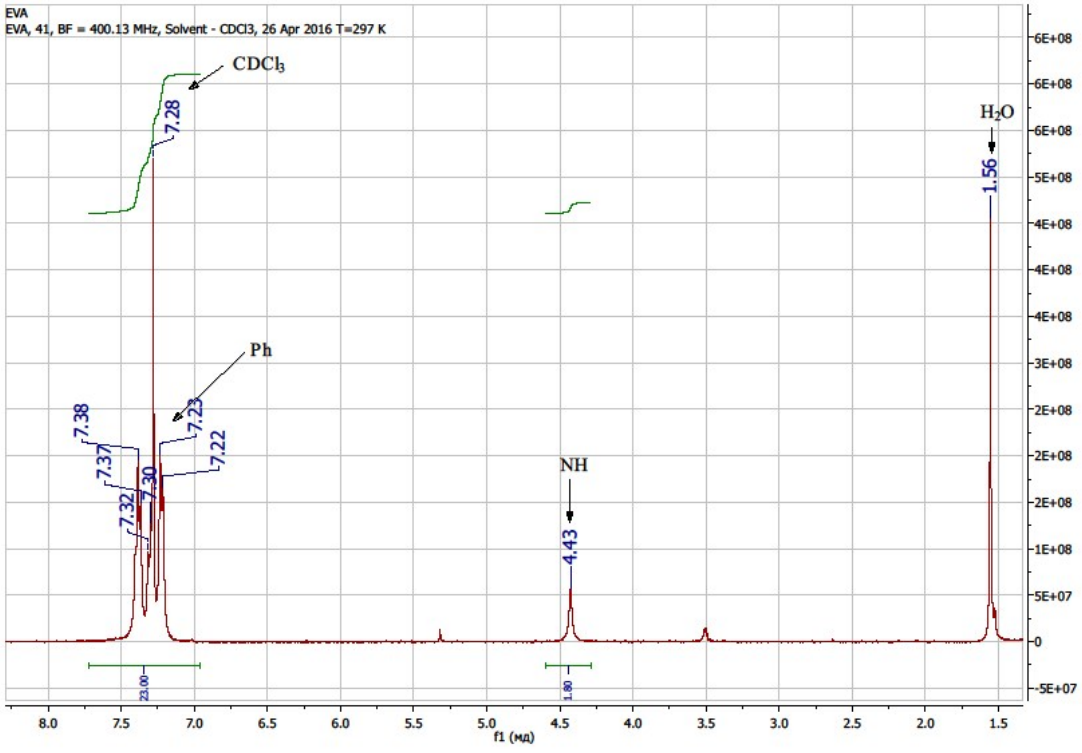


Figure S35. The ^{1}H NMR spectrum of **6**.

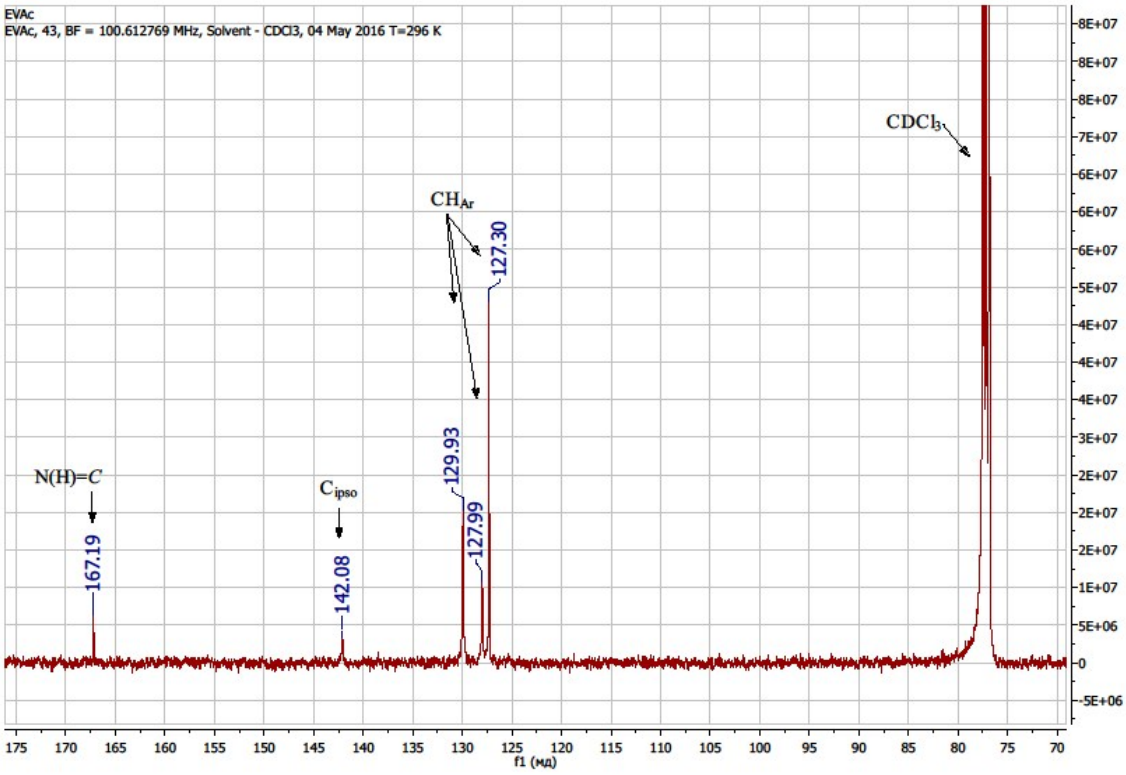


Figure S36. The $^{13}C\{^{1}H\}$ NMR spectrum of **6**.

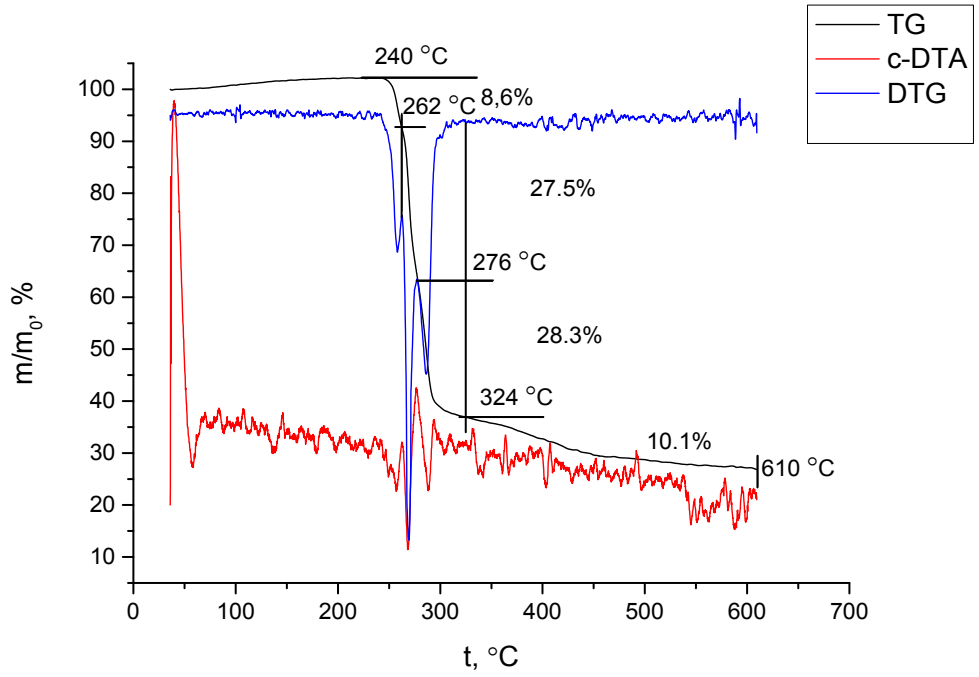
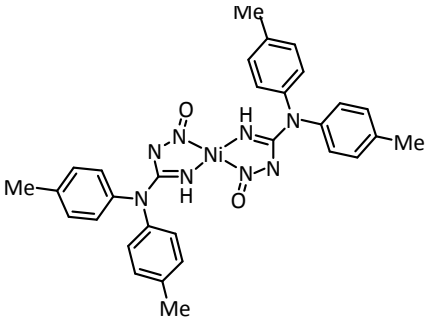


Figure S37. TG, dTG and c-DTA curves for the thermal decomposition of **6**.

[Ni{NH=C(N(*p*-Tol)$_2$)NN(O)}$_2$] (**7**, ZBM107)



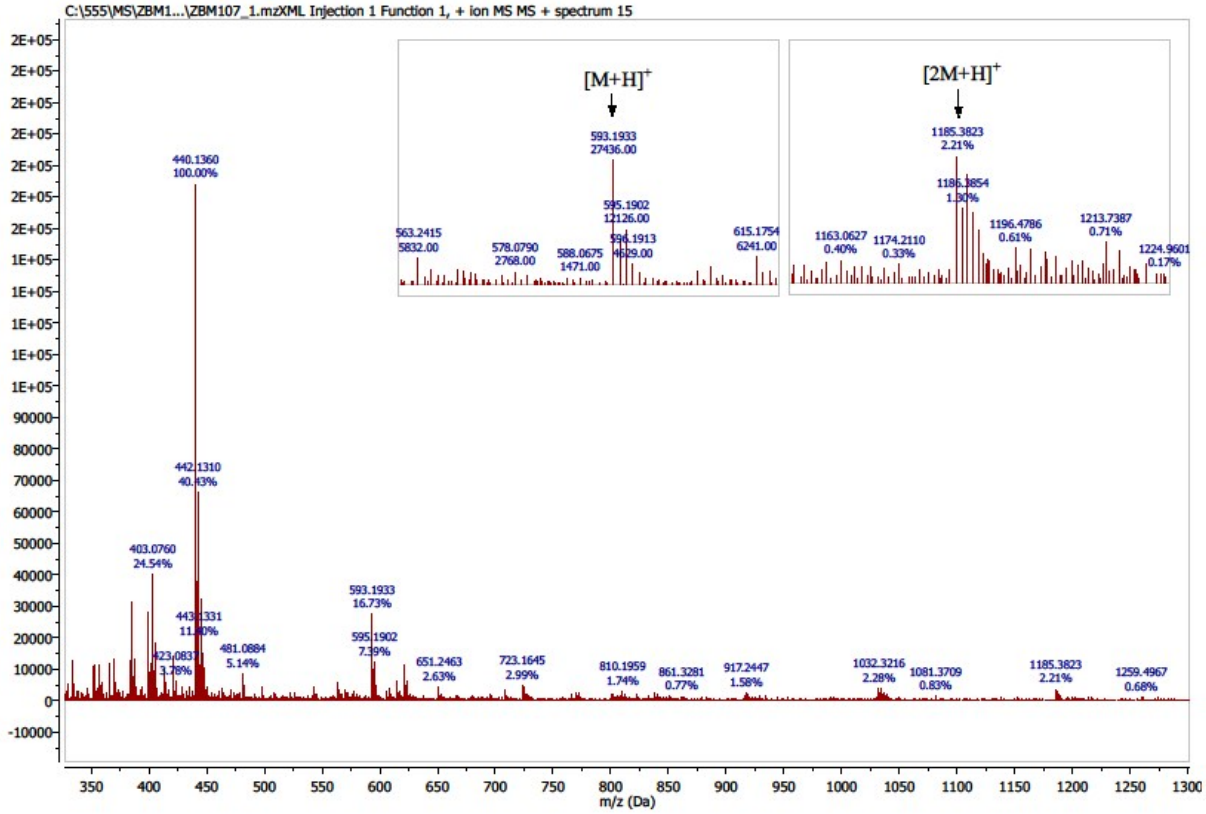


Figure S38. HRESI-MS of **7**.

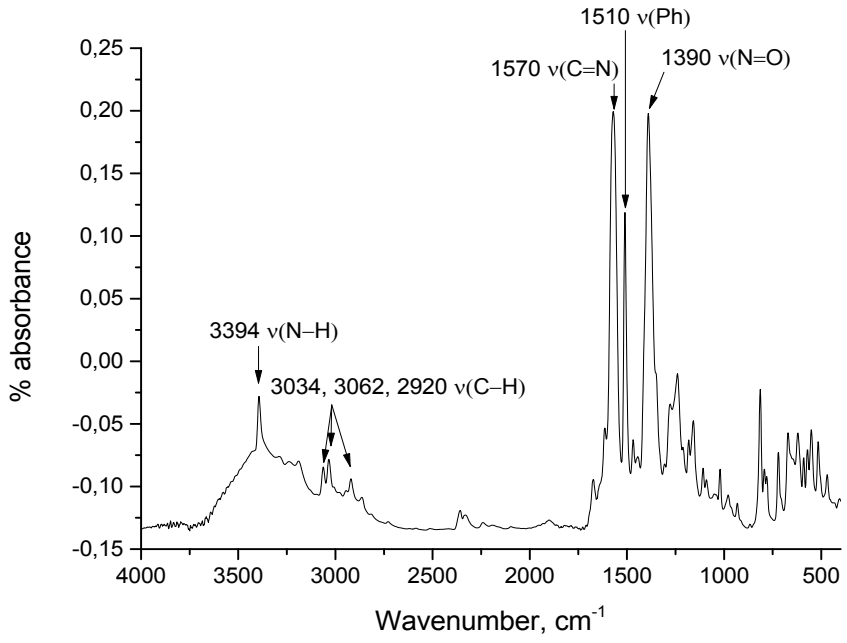


Figure S39. The FTIR spectrum of **7**.

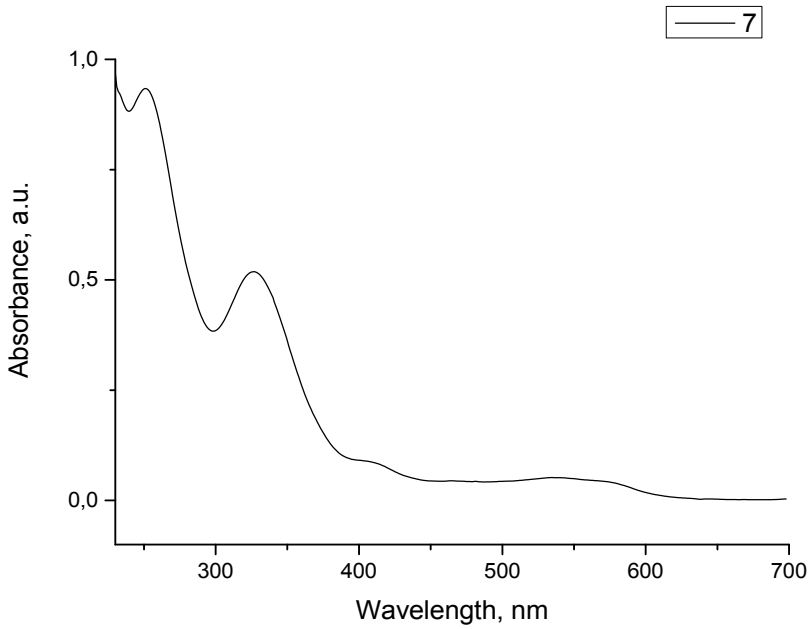


Figure S40. The UV-vis absorption spectrum of **7** in dichloromethane.

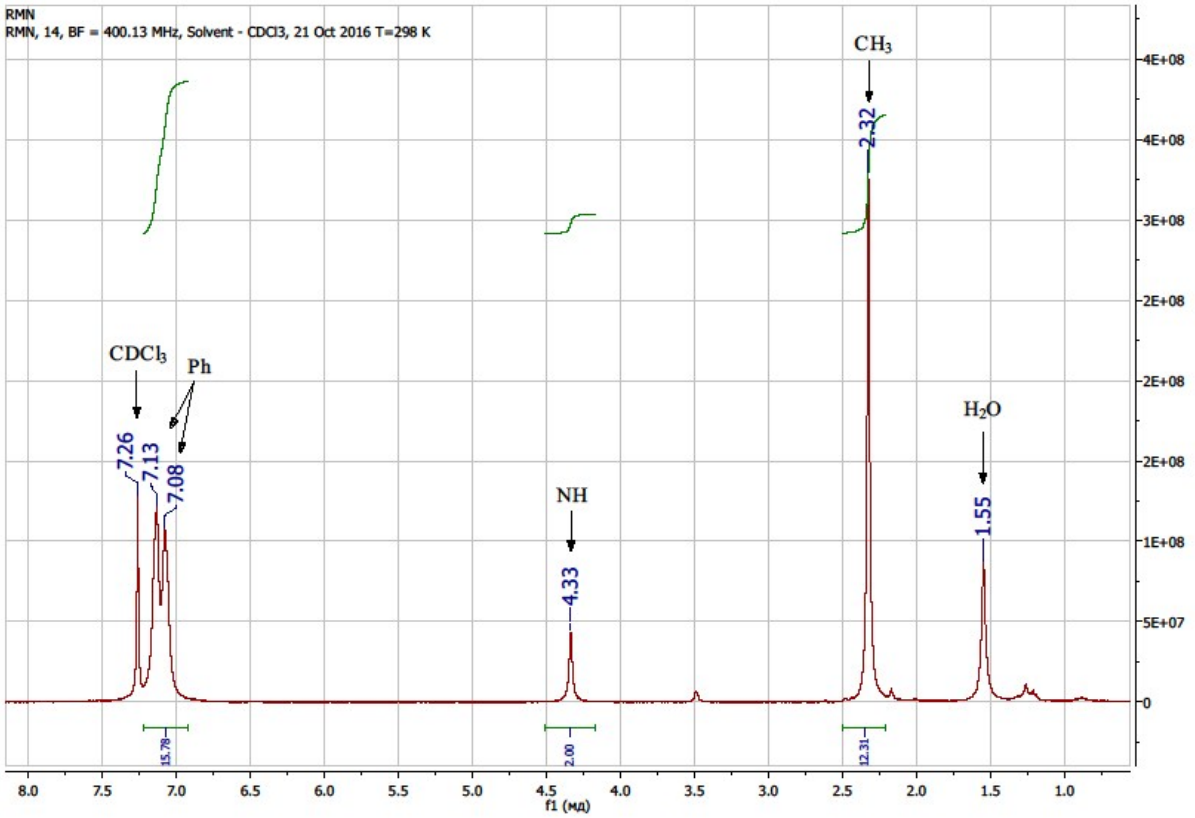


Figure S41. The ^{1}H NMR spectrum of **7**.

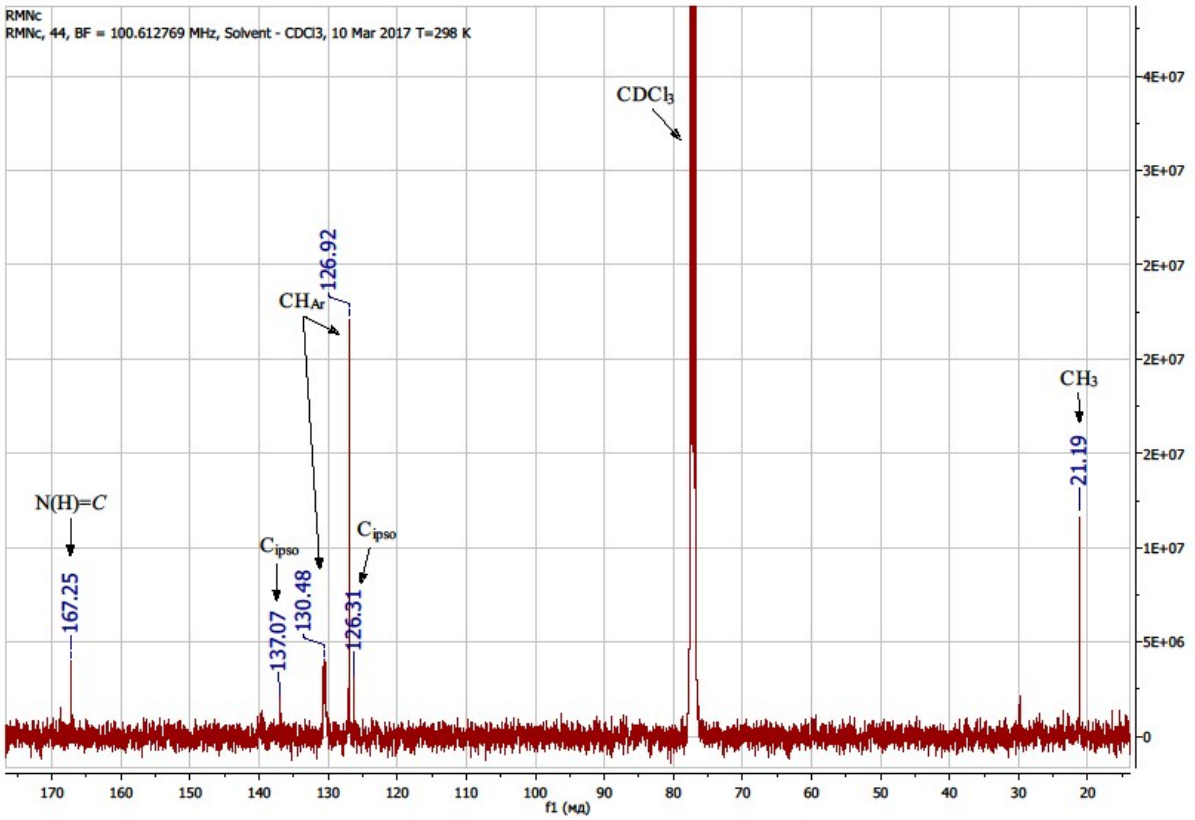


Figure S42. The $^{13}C\{^{1}H\}$ NMR spectrum of **7**.

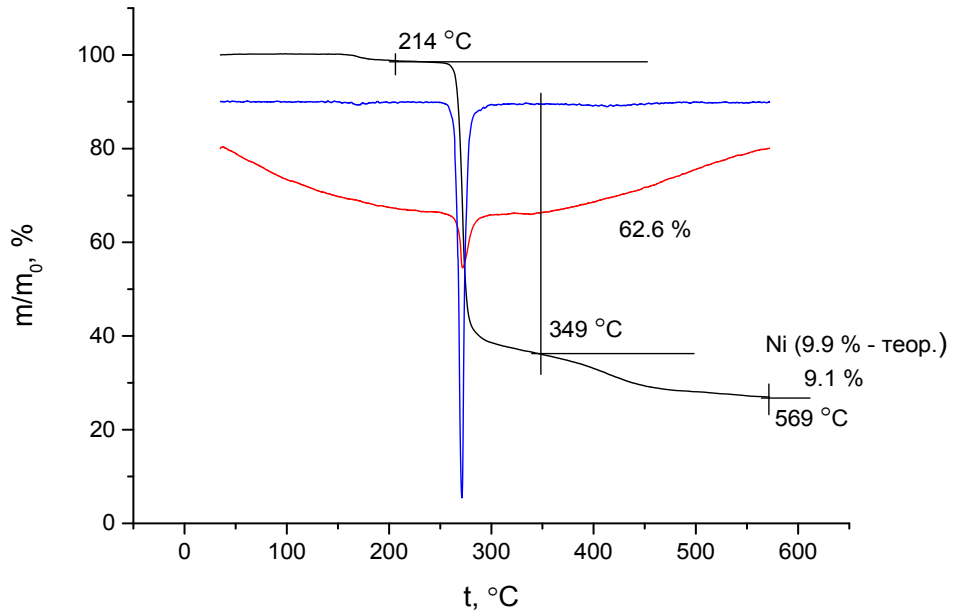


Figure S43. TG, dTG and c-DTA curves for the thermal decomposition of **7**.

Molecular structure of [Ni{NH=C(NH$_2$)NN(O)}$_2$], 1, and 3–5

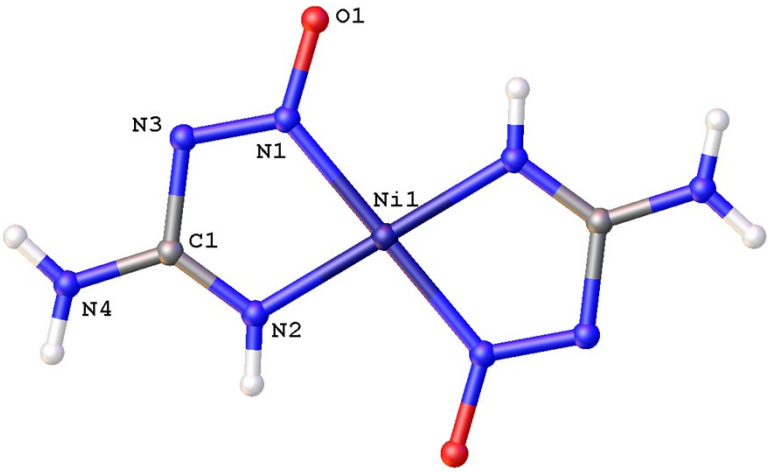


Figure S44. Molecular structure of [Ni{NH=C(NH$_2$)NN(O)}$_2$] (ngH) with the atomic numbering scheme. No atomic displacement parameters (ADP).[8]

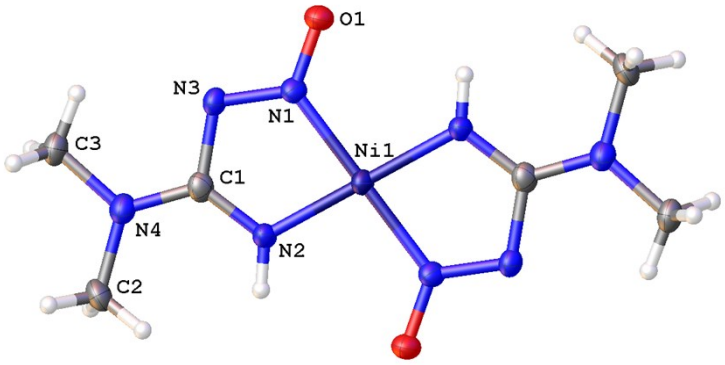


Figure S45. Molecular structure of **1** with the atomic numbering scheme. ADP ellipsoids are drawn at the 50% probability level.

[8] Murmann, R. K.; Glaser, R.; Barnes, C. L., Structure of the nitrosoguanidine complexes of nickel(II) and copper(II) by X-ray crystallography and computational analysis. *Journal of Coordination Chemistry* **2005,** *58* (3), 279-294.

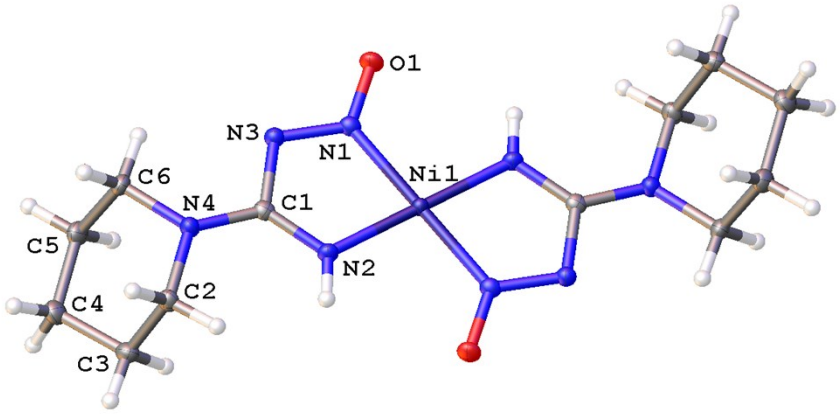


Figure S46. Molecular structure of **3** with the atomic numbering scheme. ADP ellipsoids are drawn at the 50% probability level.

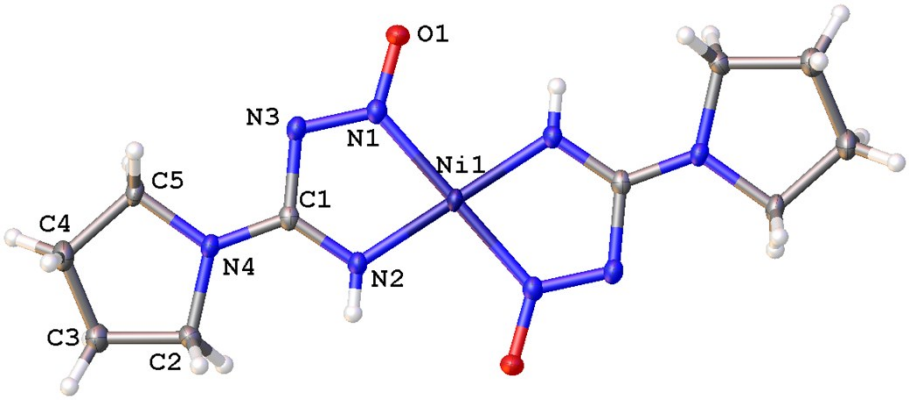


Figure S47. Molecular structure of **4** with the atomic numbering scheme. ADP ellipsoids are drawn at the 50% probability level.

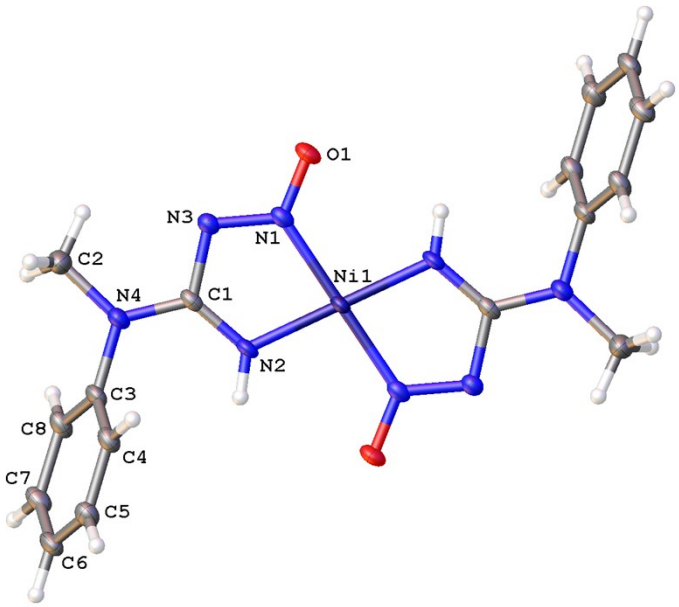


Figure S48. Molecular structure of **5** with the atomic numbering scheme. ADP ellipsoids are drawn at the 50% probability level.

Crystal data and structure refinement for 1 and 3–5

Table S2. Crystal data and structure refinement for 1, 3–5.

Identification code	**1**	**3**	**4**	**5**
Empirical formula	$C_6H_{14}N_8NiO_2$	$C_{12}H_{22}N_8NiO_2$	$C_{10}H_{18}N_8NiO_2$	$C_{16}H_{18}N_8NiO_2$
Formula weight	288.96	369.08	341.03	413.09
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	$P2_1/n$	P-1	P-1
a/Å	5.4378(10)	6.5790(3)	6.7068(10)	6.5902(4)
b/Å	6.6766(12)	14.3346(7)	6.7518(12)	11.1021(7)
c/Å	15.437(2)	8.3734(4)	7.8797(10)	12.3601(8)
α/°	90	90	75.399(13)	90.489(5)
β/°	96.885(16)	91.976(5)	81.175(12)	95.586(5)
γ/°	90	90	81.118(14)	101.506(5)
Volume/Å^3	556.40(17)	789.21(7)	338.70(9)	881.59(10)
Z	2	2	1	2
ρ_{calc}g/cm^3	1.725	1.553	1.672	1.556
μ/mm^{-1}	2.624	1.253	2.262	1.861
F(000)	300.0	388.0	178.0	428.0
Crystal size/mm^3	0.2 × 0.15 × 0.15	0.1 × 0.1 × 0.1	0.2 × 0.1 × 0.1	0.15 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	11.548 to 144.984	5.636 to 54.998	11.69 to 151.846	7.19 to 139.988
Index ranges	$-6 \le h \le 6$, $-7 \le k \le 8$, $-19 \le l \le 17$	$-8 \le h \le 8$, $-18 \le k \le 18$, $-10 \le l \le 10$	$-8 \le h \le 8$, $-8 \le k \le 8$, $-9 \le l \le 9$	$-8 \le h \le 5$, $-13 \le k \le 13$, $-15 \le l \le 15$
Reflections collected	2788	13141	2391	6966
Independent reflections	1105 [R_{int} = 0.0542, R_{sigma} = 0.0550]	1820 [R_{int} = 0.0353, R_{sigma} = 0.0179]	1368 [R_{int} = 0.0377, R_{sigma} = 0.0464]	3301 [R_{int} = 0.0723, R_{sigma} = 0.0547]

Data/restraints/parameters	1105/0/81	1820/0/106	1368/0/101	3301/0/249
Goodness-of-fit on F^2	1.073	1.068	1.080	1.092
Final R indexes [I>=2σ (I)]	R_1 = 0.0497, wR_2 = 0.1244	R_1 = 0.0229, wR_2 = 0.0576	R_1 = 0.0376, wR_2 = 0.0923	R_1 = 0.0607, wR_2 = 0.1503
Final R indexes [all data]	R_1 = 0.0640, wR_2 = 0.1380	R_1 = 0.0253, wR_2 = 0.0591	R_1 = 0.0445, wR_2 = 0.0991	R_1 = 0.0799, wR_2 = 0.1605
Largest diff. peak/hole / e $Å^{-3}$	0.51/-0.56	0.40/-0.24	0.62/-0.37	1.24/-0.60
CCDC number	1530063	1530062	1530060	1530064

Cartesian atomic coordinates of model structures

Table S3. Cartesian atomic coordinates of model structures.

Atom	X	Y	Z
5-100			
Ni	5.387071	-0.352562	12.296351
O	5.255363	-2.135535	10.183469
N	5.160411	1.284238	11.478644
N	5.200828	-0.944953	10.533054
N	4.996221	-0.055978	9.578858
N	4.743415	2.257273	9.375968
C	4.969013	1.209062	10.192446
C	4.780427	3.597706	9.902252
C	4.838043	6.182564	10.888419
C	5.971010	4.120572	10.371972
C	3.655582	5.654575	10.407632
C	3.617475	4.352426	9.912089
C	4.407784	2.098591	7.966806
C	5.990765	5.417947	10.882271
O	5.518780	1.430411	14.409233
N	5.613732	-1.989361	13.114059
N	5.573315	0.239829	14.059648
N	5.777922	-0.649146	15.013845
N	6.030728	-2.962397	15.216735
C	5.805130	-1.914186	14.400257
C	5.993715	-4.302829	14.690451
C	5.936099	-6.887687	13.704283
C	4.803133	-4.825696	14.220730
C	7.118561	-6.359699	14.185071
C	7.156668	-5.057549	14.680614

C	6.366359	-2.803715	16.625897
C	4.783377	-6.123071	13.710432
H	5.179250	2.029146	11.906557
H	4.858960	7.052173	11.216732
H	6.749574	3.613193	10.348609
H	2.881544	6.171151	10.413780
H	2.820852	3.992759	9.593613
H	5.125683	2.437175	7.426996
H	3.603647	2.586066	7.773753
H	4.273116	1.168533	7.773753
H	6.782959	5.770557	11.219191
H	5.594893	-2.734270	12.686146
H	5.915183	-7.757296	13.375971
H	4.024568	-4.318317	14.244093
H	7.892599	-6.876275	14.178923
H	7.953291	-4.697883	14.999089
H	5.648460	-3.142298	17.165706
H	7.170496	-3.291189	16.818949
H	6.501027	-1.873657	16.818949
H	3.991184	-6.475681	13.373512
Ni	2.091971	-0.352562	12.296351
O	1.750630	2.316103	11.664811
N	2.014014	-1.191150	10.658477
N	1.789725	1.157759	11.222880
N	1.620542	0.992253	9.937911
N	1.598698	-0.758287	8.386112
C	1.738758	-0.378077	9.657554
C	1.816772	-2.132535	8.014762
C	1.044693	0.134697	7.367974

C	0.996396	-4.313032	7.457737
C	0.751595	-2.992862	7.818020
C	2.290244	-4.770282	7.317559
C	3.124810	-2.583152	7.870894
C	3.356387	-3.906027	7.529056
O	2.433313	-3.021227	12.927892
N	2.169929	0.486027	13.934225
N	2.394218	-1.862883	13.369823
N	2.563401	-1.697377	14.654791
N	2.585245	0.053163	16.206591
C	2.445185	-0.327047	14.935148
C	2.367170	1.427412	16.577941
C	3.139250	-0.839821	17.224729
C	3.187547	3.607909	17.134965
C	3.432348	2.287738	16.774682
C	1.893699	4.065159	17.275144
C	1.059132	1.878028	16.721808
C	0.827555	3.200903	17.063647
H	2.144229	-2.034610	10.556418
H	0.149707	-0.138794	7.155247
H	1.587866	0.093181	6.577318
H	1.034423	1.034591	7.702434
H	0.283250	-4.890792	7.308951
H	-0.121272	-2.690265	7.926228
H	2.448127	-5.656749	7.083928
H	3.838096	-2.000547	8.002465
H	4.228537	-4.215751	7.441752
H	2.039714	1.329486	14.036285
H	4.034236	-0.566330	17.437456

H	2.596076	-0.798304	18.015384
H	3.149520	-1.739714	16.890268
H	3.900693	4.185669	17.283751
H	4.305214	1.985141	16.666474
H	1.735816	4.951625	17.508775
H	0.345847	1.295423	16.590237
H	-0.044595	3.510627	17.150951
Ni	-1.203129	-0.352562	12.296351
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N	-1.429789	1.284238	11.478644
N	-1.389372	-0.944953	10.533054
N	-1.593979	-0.055978	9.578858
N	-1.846785	2.257273	9.375968
C	-1.621187	1.209062	10.192446
C	-1.809773	3.597706	9.902252
C	-1.752157	6.182564	10.888419
C	-0.619190	4.120572	10.371972
C	-2.934618	5.654575	10.407632
C	-2.972725	4.352426	9.912089
C	-2.182416	2.098591	7.966806
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H	-2.317084	1.168533	7.773753
H	0.192759	5.770557	11.219191
H	-0.995307	-2.734270	12.686146
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C	-5.545507	0.134697	7.367974
C	-5.593804	-4.313032	7.457737
C	-5.838605	-2.992862	7.818020
C	-4.299956	-4.770282	7.317559
C	-3.465390	-2.583152	7.870894
C	-3.233813	-3.906027	7.529056
O	-4.156887	-3.021227	12.927892
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C	-3.157852	2.287738	16.774682
C	-4.696501	4.065159	17.275144
C	-5.531068	1.878028	16.721808
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H	-6.440493	-0.138794	7.155247
H	-5.002334	0.093181	6.577318
H	-5.555777	1.034591	7.702434
H	-6.306950	-4.890792	7.308951
H	-6.711472	-2.690265	7.926228
H	-4.142073	-5.656749	7.083928
H	-2.752104	-2.000547	8.002465

H	-2.361663	-4.215751	7.441752
H	-4.550486	1.329486	14.036285
H	-2.555964	-0.566330	17.437456
H	-3.994124	-0.798304	18.015384
H	-3.440680	-1.739714	16.890268
H	-2.689507	4.185669	17.283751
H	-2.284986	1.985141	16.666474
H	-4.854384	4.951625	17.508775
H	-6.244353	1.295423	16.590237
H	-6.634795	3.510627	17.150951
5-RT			
Ni	9.668991	5.117347	12.395428
O	9.537232	3.363021	10.265894
N	9.118555	7.756673	9.491179
N	9.490796	4.548156	10.620403
N	9.475382	6.762464	11.586007
N	9.314545	5.450499	9.680829
C	9.305222	6.702469	10.295643
C	9.156433	9.095918	10.015506
C	10.358456	9.612486	10.474137
C	8.007339	9.861628	10.040297
C	10.391408	10.909765	10.969954
C	8.068348	11.171620	10.515042
C	9.257290	11.688113	10.976152
C	8.801947	7.612488	8.079340
O	9.800750	6.871672	14.524963
N	10.219427	2.478020	15.299677
N	9.847185	5.686538	14.170454
N	9.862600	3.472230	13.204850

N	10.023436	4.784195	15.110027
C	10.032760	3.532224	14.495214
C	10.181548	1.138775	14.775350
C	8.979526	0.622207	14.316720
C	11.330643	0.373065	14.750560
C	8.946574	-0.675071	13.820902
C	11.269634	-0.936926	14.275815
C	10.080692	-1.453420	13.814705
C	10.536035	2.622205	16.711516
H	9.496388	7.503748	12.021086
H	11.131863	9.098161	10.451825
H	7.200538	9.507081	9.744046
H	11.189144	11.255618	11.299672
H	7.302536	11.698584	10.518760
H	9.294215	12.561453	11.292235
H	9.602791	7.717062	7.559972
H	8.165064	8.284508	7.823994
H	8.429693	6.742060	7.921918
H	9.841593	2.730945	12.769770
H	8.206119	1.136533	14.339031
H	12.137444	0.727612	15.046810
H	8.148838	-1.020925	13.491184
H	12.035446	-1.463890	14.272096
H	10.043766	-2.326760	13.498621
H	9.735191	2.517631	17.230885
H	11.172917	1.950186	16.966862
H	10.908289	3.492634	16.868938
Ni	6.313841	5.117347	12.395428
O	6.021323	7.784314	11.747147

N	6.245989	4.289038	10.765429
N	6.054457	6.627734	11.319505
N	5.882513	4.716895	8.479712
N	5.905540	6.459217	10.022943
C	6.009513	5.094308	9.767597
C	6.090928	3.346707	8.107850
C	5.427339	5.639567	7.448413
C	7.372292	2.877450	7.938032
C	5.019753	2.495954	7.916960
C	6.530853	0.723267	7.382717
C	5.253473	1.183964	7.545097
C	7.576869	1.573946	7.576086
O	6.606359	2.450379	13.043709
N	6.381693	5.945655	14.025427
N	6.573225	3.606959	13.471351
N	6.745168	5.517799	16.311144
N	6.722142	3.775477	14.767913
C	6.618169	5.140386	15.023259
C	6.536754	6.887986	16.683007
C	7.200343	4.595126	17.342444
C	5.255390	7.357244	16.852824
C	7.607929	7.738740	16.873896
C	6.096829	9.511426	17.408139
C	7.374208	9.050729	17.245759
C	5.050813	8.660747	17.214771
H	6.361089	3.443248	10.665026
H	4.652080	5.277119	7.013333
H	6.125729	5.768810	6.802611
H	5.203679	6.482882	7.850025

H	8.097878	3.444532	8.068184
H	4.149498	2.803091	8.037196
H	6.684312	-0.162231	7.142246
H	4.534641	0.610630	7.403789
H	8.445572	1.263329	7.462048
H	6.266592	6.791446	14.125830
H	7.975602	4.957574	17.777523
H	6.501953	4.465884	17.988245
H	7.424003	3.751812	16.940832
H	4.529804	6.790162	16.722672
H	8.478184	7.431603	16.753661
H	5.943370	10.396924	17.648611
H	8.093041	9.624064	17.387067
H	4.182109	8.971365	17.328809
Ni	13.024141	5.117347	12.395428
O	12.731623	7.784314	11.747147
N	12.956289	4.289038	10.765429
N	12.764757	6.627734	11.319505
N	12.592813	4.716895	8.479712
N	12.615840	6.459217	10.022943
C	12.719813	5.094308	9.767597
C	12.801228	3.346707	8.107850
C	12.137639	5.639567	7.448413
C	14.082592	2.877450	7.938032
C	11.730053	2.495954	7.916960
C	13.241153	0.723267	7.382717
C	11.963773	1.183964	7.545097
C	14.287169	1.573946	7.576086
O	13.316659	2.450379	13.043709

N	13.091993	5.945655	14.025427
N	13.283525	3.606959	13.471351
N	13.455468	5.517799	16.311144
N	13.432442	3.775477	14.767913
C	13.328469	5.140386	15.023259
C	13.247054	6.887986	16.683007
C	13.910643	4.595126	17.342444
C	11.965690	7.357244	16.852824
C	14.318229	7.738740	16.873896
C	12.807129	9.511426	17.408139
C	14.084508	9.050729	17.245759
C	11.761113	8.660747	17.214771
H	13.071389	3.443248	10.665026
H	11.362380	5.277119	7.013333
H	12.836029	5.768810	6.802611
H	11.913979	6.482882	7.850025
H	14.808178	3.444532	8.068184
H	10.859798	2.803091	8.037196
H	13.394612	-0.162231	7.142246
H	11.244941	0.610630	7.403789
H	15.155872	1.263329	7.462048
H	12.976892	6.791446	14.125830
H	14.685902	4.957574	17.777523
H	13.212253	4.465884	17.988245
H	14.134303	3.751812	16.940832
H	11.240104	6.790162	16.722672
H	15.188484	7.431603	16.753661
H	12.653670	10.396924	17.648611
H	14.803341	9.624064	17.387067

H	10.892409	8.971365	17.328809
Ni	16.379291	5.117347	12.395428
O	16.247532	3.363021	10.265894
N	15.828855	7.756673	9.491179
N	16.201096	4.548156	10.620403
N	16.185682	6.762464	11.586007
N	16.024845	5.450499	9.680829
C	16.015522	6.702469	10.295643
C	15.866733	9.095918	10.015506
C	17.068756	9.612486	10.474137
C	14.717639	9.861628	10.040297
C	17.101708	10.909765	10.969954
C	14.778648	11.171620	10.515042
C	15.967590	11.688113	10.976152
C	15.512247	7.612488	8.079340
O	16.511050	6.871672	14.524963
N	16.929727	2.478020	15.299677
N	16.557485	5.686538	14.170454
N	16.572900	3.472230	13.204850
N	16.733736	4.784195	15.110027
C	16.743060	3.532224	14.495214
C	16.891848	1.138775	14.775350
C	15.689826	0.622207	14.316720
C	18.040943	0.373065	14.750560
C	15.656874	-0.675071	13.820902
C	17.979934	-0.936926	14.275815
C	16.790992	-1.453420	13.814705
C	17.246335	2.622205	16.711516
H	16.206688	7.503748	12.021086

H	17.842163	9.098161	10.451825
H	13.910838	9.507081	9.744046
H	17.899444	11.255618	11.299672
H	14.012836	11.698584	10.518760
H	16.004515	12.561453	11.292235
H	16.313091	7.717062	7.559972
H	14.875364	8.284508	7.823994
H	15.139993	6.742060	7.921918
H	16.551893	2.730945	12.769770
H	14.916419	1.136533	14.339031
H	18.847744	0.727612	15.046810
H	14.859138	-1.020925	13.491184
H	18.745746	-1.463890	14.272096
H	16.754066	-2.326760	13.498621
H	16.445491	2.517631	17.230885
H	17.883217	1.950186	16.966862
H	17.618589	3.492634	16.868938
1 (equilibrium geometry in dichloromethane solution)			
Ni	0.000000	0.000000	0.000000
O	0.636678	2.492035	1.032596
N	0.926565	1.297113	1.027607
N	1.909865	0.896355	1.759332
N	1.231773	-1.115315	0.821362
H	1.336168	-2.111609	0.688324
N	3.067358	-1.056772	2.277199
C	2.069044	-0.479115	1.608616
C	4.016007	-0.319505	3.104008
H	3.762659	0.734691	3.111311
H	5.025615	-0.442982	2.705551

H	3.989142	-0.702592	4.126140
C	3.271444	-2.492322	2.150517
H	2.391608	-3.048137	2.484348
H	4.113345	-2.778928	2.775884
H	3.497298	-2.769167	1.117141
O	-0.636678	-2.492035	-1.032596
N	-0.926565	-1.297113	-1.027607
N	-1.909865	-0.896355	-1.759332
N	-1.231773	1.115315	-0.821362
H	-1.336168	2.111609	-0.688324
N	-3.067358	1.056772	-2.277199
C	-2.069044	0.479115	-1.608616
C	-4.016007	0.319505	-3.104008
H	-3.762659	-0.734691	-3.111311
H	-5.025615	0.442982	-2.705551
H	-3.989142	0.702592	-4.126140
C	-3.271444	2.492322	-2.150517
H	-2.391608	3.048137	-2.484348
H	-4.113345	2.778928	-2.775884
H	-3.497298	2.769167	-1.117141
1 (equilibrium geometry in gas phase)			
Ni	0.000001	0.000045	-0.021444
O	0.584064	2.702667	-0.015421
N	1.056696	1.581969	-0.016513
N	2.351268	1.440445	-0.010620
N	1.676025	-0.782746	-0.019232
H	1.865823	-1.777062	-0.005610
N	3.960552	-0.231677	-0.018002
C	2.652834	0.092901	-0.013700

C	5.017894	0.756541	0.091977
H	4.594549	1.756386	0.025722
H	5.743407	0.620190	-0.717977
H	5.542255	0.654043	1.050526
C	4.343957	-1.625308	0.003990
H	4.035265	-2.122026	0.933677
H	5.430562	-1.694089	-0.070323
H	3.915439	-2.172762	-0.843938
O	-0.583957	-2.702622	-0.014778
N	-1.056617	-1.581947	-0.016006
N	-2.351208	-1.440460	-0.009987
N	-1.676084	0.782784	-0.018608
H	-1.866003	1.777080	-0.005224
N	-3.960537	0.231632	-0.016888
C	-2.652824	-0.092939	-0.012990
C	-5.018066	-0.756667	0.090296
H	-4.594379	-1.756487	0.025907
H	-5.545301	-0.653654	1.047189
H	-5.741210	-0.620951	-0.721907
C	-4.343929	1.625288	0.004482
H	-3.916975	2.172054	-0.844710
H	-5.430674	1.693975	-0.067788
H	-4.033510	2.122777	0.933154
3 (equilibrium geometry in gas phase)			
Ni	-0.000077	-0.000011	0.000206
O	0.398958	2.731248	0.154708
N	0.931652	1.656415	-0.048581
N	1.688892	-0.637129	-0.403736
H	1.938287	-1.611180	-0.516977

N	3.890683	0.123332	-0.831455
N	2.205722	1.622381	-0.314967
C	2.589917	0.309435	-0.513578
C	4.886485	1.168833	-0.588592
H	4.399487	2.141884	-0.644166
H	5.625577	1.109816	-1.400939
C	4.478121	-1.207627	-0.861297
H	5.240538	-1.209361	-1.653655
H	3.733735	-1.950808	-1.158347
C	5.118742	-1.529471	0.481154
H	5.579404	-2.524680	0.447673
H	4.332665	-1.568910	1.250197
C	5.554282	0.936048	0.757927
H	4.799435	1.074265	1.546892
H	6.327181	1.696625	0.925314
C	6.149766	-0.464623	0.838237
H	6.996254	-0.537310	0.136389
H	6.564207	-0.651610	1.836176
O	-0.398688	-2.731315	-0.153345
N	-0.931679	-1.656425	0.048939
N	-1.689321	0.637181	0.402938
H	-1.938243	1.610798	0.520856
N	-3.890856	-0.123316	0.832073
N	-2.206084	-1.622299	0.313851
C	-2.590217	-0.309457	0.513180
C	-4.886939	-1.168697	0.588848
H	-4.400197	-2.141835	0.645023
H	-5.626322	-1.109234	1.400896
C	-4.478233	1.207733	0.861069

H	-5.241034	1.209751	1.653091
H	-3.734006	1.950915	1.158648
C	-5.118000	1.529347	-0.481756
H	-5.578509	2.524632	-0.448755
H	-4.331519	1.568507	-1.250406
C	-5.554027	-0.936160	-0.758005
H	-4.798905	-1.074939	-1.546590
H	-6.327139	-1.696533	-0.925350
C	-6.149062	0.464637	-0.839060
H	-6.995899	0.537692	-0.137619
H	-6.563061	0.651366	-1.837212
4 (equilibrium geometry in gas phase)			
Ni	0.000000	0.000000	0.000000
O	-1.351420	-2.315238	0.692427
N	-2.317518	-0.506470	1.410245
N	-3.030338	1.607049	1.976644
N	-1.048873	1.330431	0.745195
C	-4.228023	1.073082	2.631398
H	-3.961978	0.627795	3.600442
H	-4.680842	0.287457	2.022834
N	-1.351053	-1.101511	0.769750
C	-2.105232	0.857034	1.363028
C	-2.949438	3.059260	2.059878
H	-3.108806	3.509204	1.067171
H	-1.961333	3.378878	2.415470
C	-5.092219	2.312079	2.796605
H	-5.651698	2.503945	1.871495
H	-5.817718	2.213538	3.609081
C	-4.069126	3.416795	3.027972

H	-4.461871	4.423553	2.860676
H	-3.696090	3.372796	4.059290
H	-0.890825	2.329365	0.687198
O	1.351420	2.315238	-0.692427
N	2.317518	0.506470	-1.410245
N	3.030338	-1.607049	-1.976644
N	1.048873	-1.330431	-0.745195
C	4.228023	-1.073082	-2.631398
H	3.961978	-0.627795	-3.600442
H	4.680842	-0.287457	-2.022834
N	1.351053	1.101511	-0.769750
C	2.105232	-0.857034	-1.363028
C	2.949438	-3.059260	-2.059878
H	3.108806	-3.509204	-1.067171
H	1.961333	-3.378878	-2.415470
C	5.092219	-2.312079	-2.796605
H	5.651698	-2.503945	-1.871495
H	5.817718	-2.213538	-3.609081
C	4.069126	-3.416795	-3.027972
H	4.461871	-4.423553	-2.860676
H	3.696090	-3.372796	-4.059290
H	0.890825	-2.329365	-0.687198
5 (equilibrium geometry in gas phase)			
Ni	0.000000	0.000000	0.000000
O	-0.664844	2.610219	-0.638482
N	-0.100407	-0.858196	-1.637867
N	-0.500589	1.489189	-1.076627
N	-0.666601	1.278951	-2.353109
N	-0.576193	-0.440723	-3.906080

C	-0.433681	-0.054185	-2.616441
C	-0.322399	-1.796073	-4.276519
C	-0.978780	0.462560	-4.974199
C	-1.141002	-3.958744	-4.927670
C	-1.386783	-2.647288	-4.546735
C	0.164938	-4.419263	-5.032369
C	0.985921	-2.252785	-4.386095
C	1.227253	-3.567271	-4.759855
O	0.664844	-2.610219	0.638482
N	0.100407	0.858196	1.637867
N	0.500589	-1.489189	1.076627
N	0.666601	-1.278951	2.353109
N	0.576193	0.440723	3.906080
C	0.433681	0.054185	2.616441
C	0.322399	1.796073	4.276519
C	0.978780	-0.462560	4.974199
C	1.141002	3.958744	4.927670
C	1.386783	2.647288	4.546735
C	-0.164938	4.419263	5.032369
C	-0.985921	2.252785	4.386095
C	-1.227253	3.567271	4.759855
H	0.061255	-1.841645	-1.825231
H	-1.919300	0.124831	-5.424740
H	-0.209364	0.482496	-5.754375
H	-1.114612	1.464087	-4.570750
H	-1.973471	-4.626517	-5.135445
H	-2.404508	-2.275096	-4.446089
H	0.356102	-5.448894	-5.324833
H	1.805869	-1.571440	-4.166786

H	2.250001	-3.927535	-4.838347
H	-0.061255	1.841645	1.825231
H	1.919300	-0.124831	5.424740
H	0.209364	-0.482496	5.754375
H	1.114612	-1.464087	4.570750
H	1.973471	4.626517	5.135445
H	2.404508	2.275096	4.446089
H	-0.356102	5.448894	5.324833
H	-1.805869	1.571440	4.166786
H	-2.250001	3.927535	4.838347