Electronic Supplementary Information

Nickel(II)-mediated Cyanamide–Pyrazole Coupling Highlights Distinct Reactivity of $NCNR_2$ and NCR Nitrile Ligands

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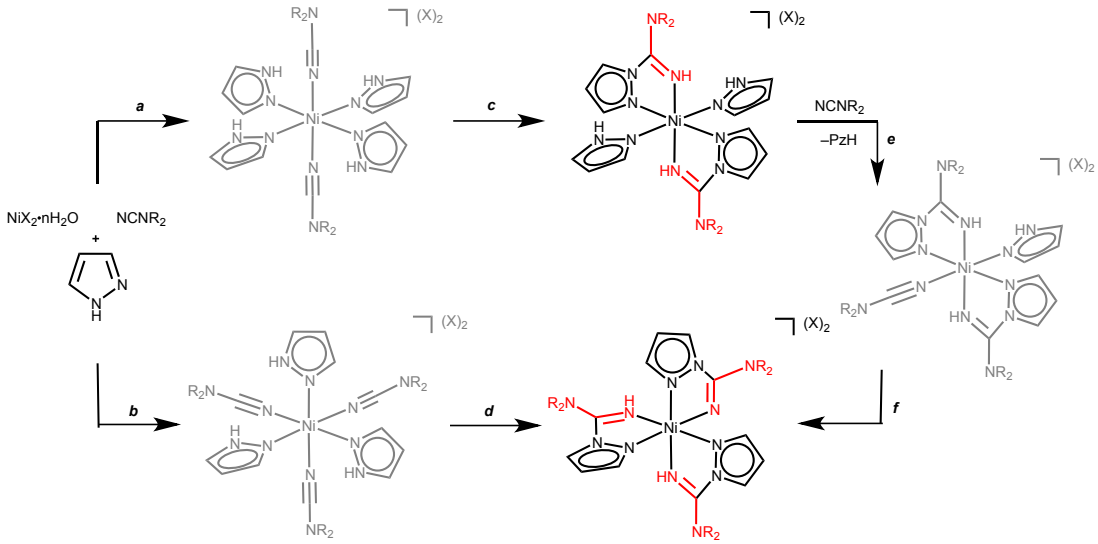
Table of contents

Scheme of possible reaction mechanism



Scheme S1. Possible reaction mechanism of formation of *bis*- and *tris*-chelate products; plausible intermediates are depictured in gray color.

Crystallographic data

Table S1. Crystallographic data and structure refinement for [**1**]Cl_2, [**1**–**2**]$(NO_3)_2$, and [**4**]$(NO_3)_2$.

Identification code	[**1**]Cl_2	[**1**]$(NO_3)_2$	[**2**]$(NO_3)_2$	[**4**]$(NO_3)_2$
Empirical formula	$C_{18}H_{28}Cl_2N_{12}Ni$	$C_{18}H_{28}N_{14}NiO_6$	$C_{22}H_{36}N_{14}NiO_6$	$C_{24}H_{36}N_{14}NiO_6$
Formula weight	542.13	595.25	651.36	675.38
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	triclinic	monoclinic
Space group	*C*2/*c*	$P2_1/n$	*P*-1	$P2_1/n$
a/Å	19.9358(11)	9.6235(7)	9.5039(7)	8.3309(4)
b/Å	9.2467(3)	8.0534(5)	9.5463(7)	9.7597(4)
c/Å	16.9617(10)	16.8565(12)	9.7514(8)	18.0944(11)
α/°	90	90	78.526(6)	90
β/°	126.983(8)	103.297(7)	61.114(8)	98.938(5)
γ/°	90	90	71.962(7)	90
Volume/Å^3	2497.7(3)	1271.39(16)	735.27(11)	1453.34(13)
Z	4	2	1	2
ρ_{calc}g/cm^3	1.442	1.555	1.471	1.543
μ/mm^{-1}	1.023	1.674	1.497	1.540
F(000)	1128.0	620.0	342.0	708.0
Crystal size/mm^3	0.11 × 0.08 × 0.05	0.13 × 0.09 × 0.06	0.12 × 0.1 × 0.08	0.1 × 0.07 × 0.06
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.094 to 54.998	9.738 to 139.972	9.762 to 124.954	9.896 to 134.974
Index ranges	-25 ≤ h ≤ 25, -11 ≤ k ≤ 12, -22 ≤ l ≤ 20	-11 ≤ h ≤ 11, -9 ≤ k ≤ 9, -19 ≤ l ≤ 20	-10 ≤ h ≤ 8, -10 ≤ k ≤ 10, -11 ≤ l ≤ 11	-9 ≤ h ≤ 9, -11 ≤ k ≤ 11, -21 ≤ l ≤ 14
Reflections collected	9275	6439	7422	5574
Independent reflections	2868 [R_{int} = 0.0305, R_{sigma} = 0.0329]	2399 [R_{int} = 0.0251, R_{sigma} = 0.0328]	2327 [R_{int} = 0.0422, R_{sigma} = 0.0394]	2612 [R_{int} = 0.0321, R_{sigma} = 0.0392]
Data/restraints/parameters	2868/0/152	2399/0/180	2327/0/198	2612/0/238
Goodness-of-fit on F^2	1.057	1.082	1.056	1.074
Final R indexes [I>=2σ (I)]	R_1 = 0.0302, wR_2 = 0.0688	R_1 = 0.0413, wR_2 = 0.0891	R_1 = 0.0551, wR_2 = 0.1447	R_1 = 0.0700, wR_2 = 0.1762
Final R indexes [all data]	R_1 = 0.0347, wR_2 = 0.0715	R_1 = 0.0505, wR_2 = 0.0932	R_1 = 0.0586, wR_2 = 0.1479	R_1 = 0.0849, wR_2 = 0.1860
Largest diff. peak/hole / e Å^{-3}	0.40/-0.41	0.33/-0.40	0.69/-0.55	0.76/-0.30
CCDC number	1966454	1966455	1966456	1966459

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

Table S2. Crystal data and structure refinement for [**1**]$(OTf)_2$, [**2**]$(OTf)_2$, [**3**]$(OTf)_2$, and [**9**]$(OTf)_2$.

Identification code	[**1**](OTf)$_2$	[**2**](OTf)$_2$	[**3**](OTf)$_2$	[**9**](OTf)$_2$
Empirical formula	$C_{20}H_{28}F_6N_{12}NiO_6S_2$	$C_{24}H_{36}F_6N_{12}NiO_6S_2$	$C_{30}H_{44}F_6N_{12}NiO_8S_2$	$C_{18}H_{32}N_8O_8F_6S_2Ni$
Formula weight	769.37	825.48	937.60	725.34
Temperature/K	100.01(10)	100.01(10)	100(2)	100(2)
Crystal system	monoclinic	triclinic	triclinic	triclinic
Space group	*Cc*	*P*-1	*P*-1	*P*-1
a/Å	25.009(2)	9.6380(6)	8.7256(4)	7.8741(5)
b/Å	9.6962(4)	10.2071(9)	10.0265(6)	9.1095(6)
c/Å	17.1351(17)	10.3141(9)	12.2050(7)	11.9118(7)
α/°	90	101.057(8)	82.723(5)	102.589(6)
β/°	131.427(16)	101.885(6)	72.312(5)	108.164(6)
γ/°	90	111.644(7)	84.509(4)	96.805(5)
Volume/Å^3	3115.5(7)	882.01(13)	1007.26(10)	776.15(9)
Z	4	1	1	1
ρ_{calc}g/cm^3	1.640	1.554	1.546	1.552
μ/mm^{-1}	0.850	0.756	0.676	2.982
F(000)	1576.0	426.0	486.0	374.0
Crystal size/mm^3	0.12 × 0.1 × 0.08	0.14 × 0.1 × 0.08	0.12 × 0.08 × 0.06	0.28 × 0.22 × 0.16
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.342 to 54.998	6.444 to 54.998	5.676 to 61.944	8.114 to 139.988
Index ranges	-32 ≤ h ≤ 32, -12 ≤ k ≤ 12, -22 ≤ l ≤ 22	-12 ≤ h ≤ 12, -13 ≤ k ≤ 13, -13 ≤ l ≤ 13	-11 ≤ h ≤ 12, -12 ≤ k ≤ 13, -15 ≤ l ≤ 16	-9 ≤ h ≤ 9, -11 ≤ k ≤ 11, -14 ≤ l ≤ 14
Reflections collected	14306	15571	10085	5217
Independent reflections	7034 [R_{int} = 0.0331, R_{sigma} = 0.0479]	4053 [R_{int} = 0.0590, R_{sigma} = 0.0477]	5621 [R_{int} = 0.0204, R_{sigma} = 0.0410]	2842 [R_{int} = 0.0280, R_{sigma} = 0.0352]
Data/restraints/parameters	7034/2/437	4053/0/234	5621/0/270	2842/2/208
Goodness-of-fit on F^2	1.033	1.068	1.028	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0310, wR_2 = 0.0684	R_1 = 0.0545, wR_2 = 0.1352	R_1 = 0.0347, wR_2 = 0.0741	R_1 = 0.0354, wR_2 = 0.0881
Final R indexes [all data]	R_1 = 0.0341, wR_2 = 0.0710	R_1 = 0.0685, wR_2 = 0.1487	R_1 = 0.0462, wR_2 = 0.0808	R_1 = 0.0410, wR_2 = 0.0928
Largest diff. peak/hole / e Å^{-3}	0.44/-0.32	1.13/-0.99	0.56/-0.48	0.44/-0.43
Flack parameter	0.606(11)			
CCDC number	1965150	1966457	1966458	1962312

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma[w(F_o^2)^2]]^{1/2}$.

View of the molecular structures

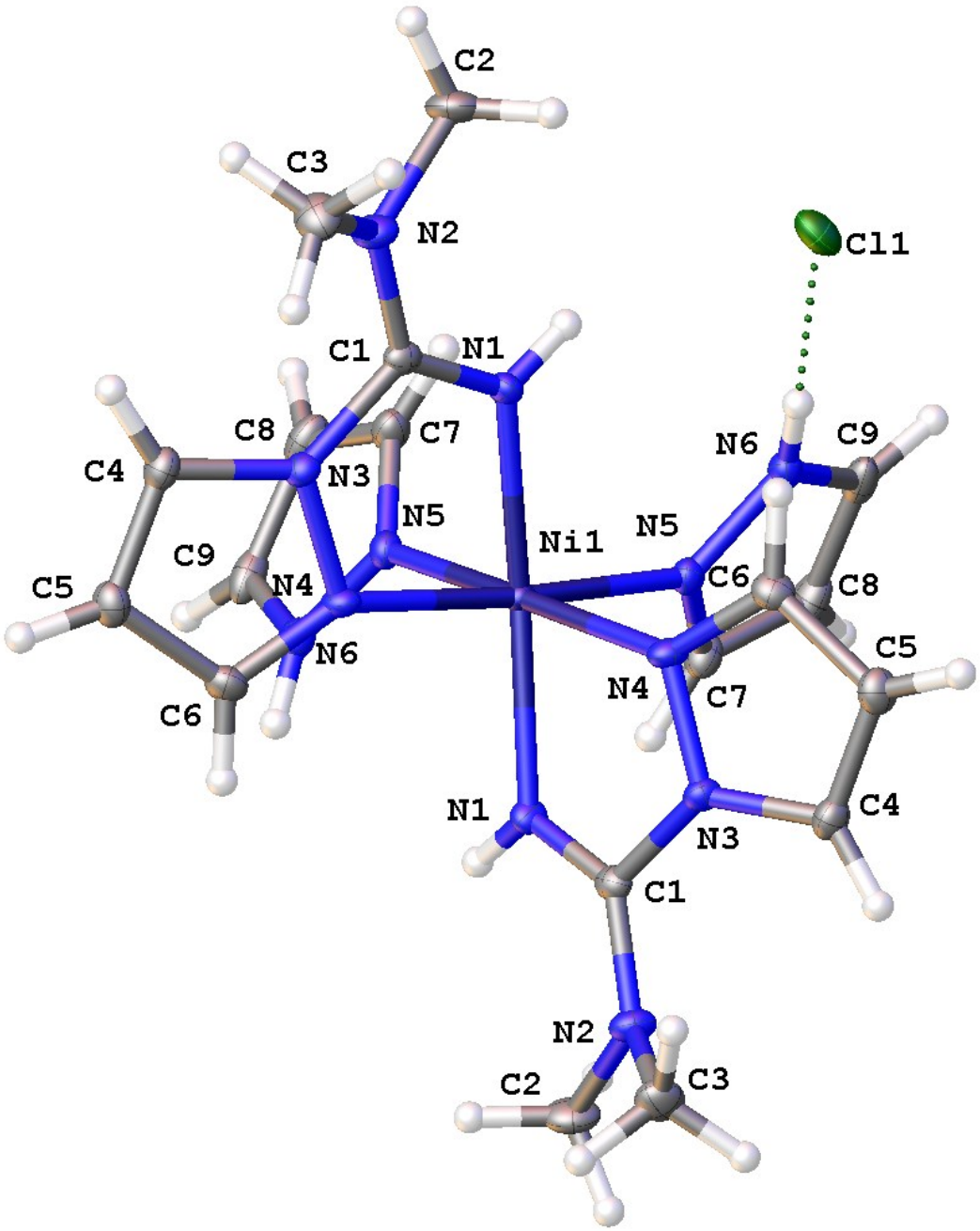


Figure S1. View of the molecular structure of *cis*$_{(PzH)}$-[**1**]Cl_2 , only one cation and one anion are depictured.

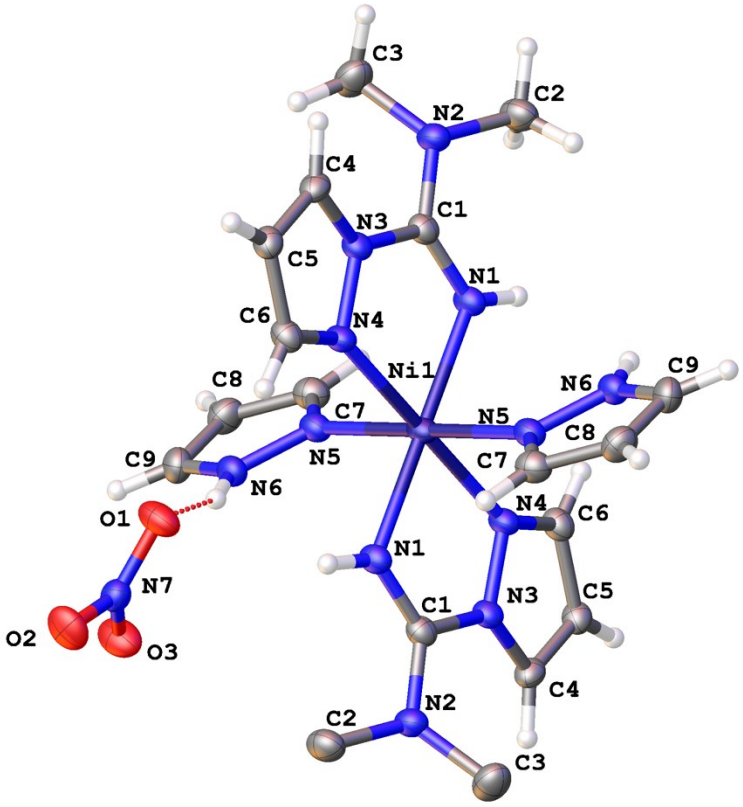


Figure S2. View of the molecular structure of *trans*-[**1**]$(NO_3)_2$, only one cation and one anion are depictured, H atoms at one of the NMe_2 groups are omitted for simplicity.

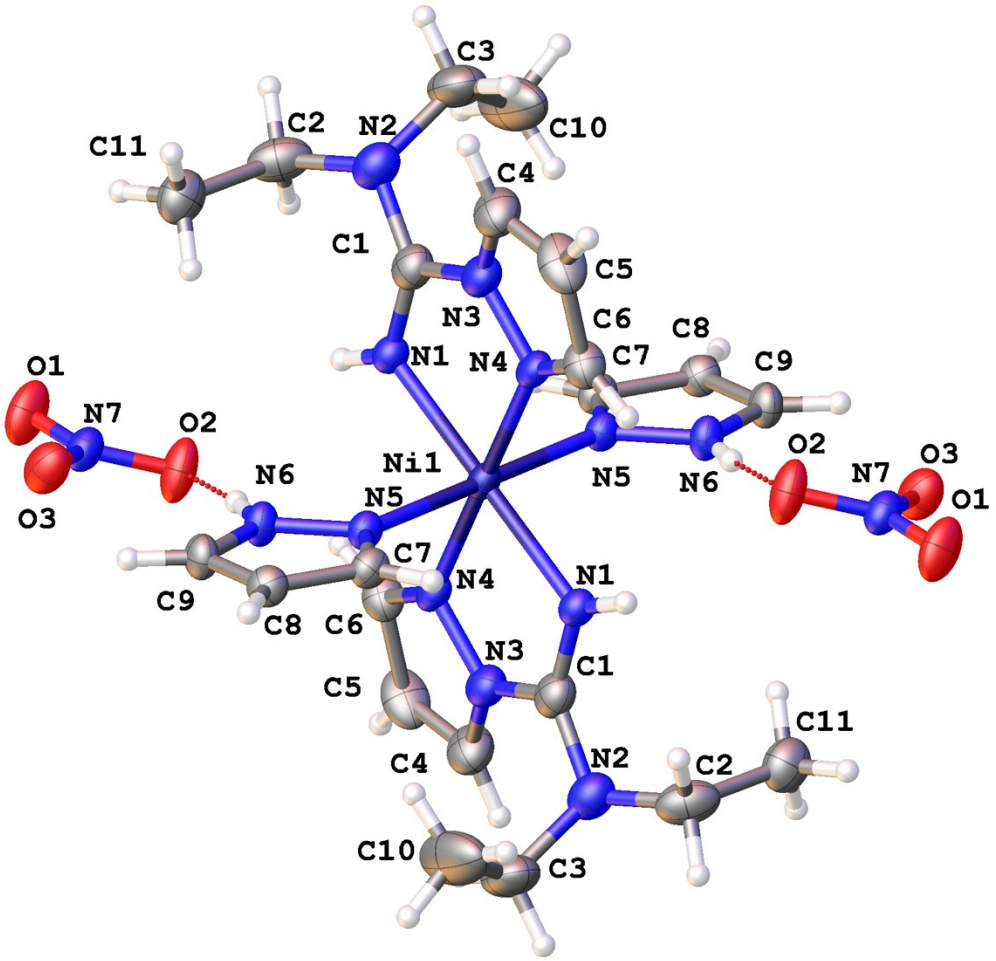


Figure S3. View of the molecular structure of *trans*-[**2**]$(NO_3)_2$.

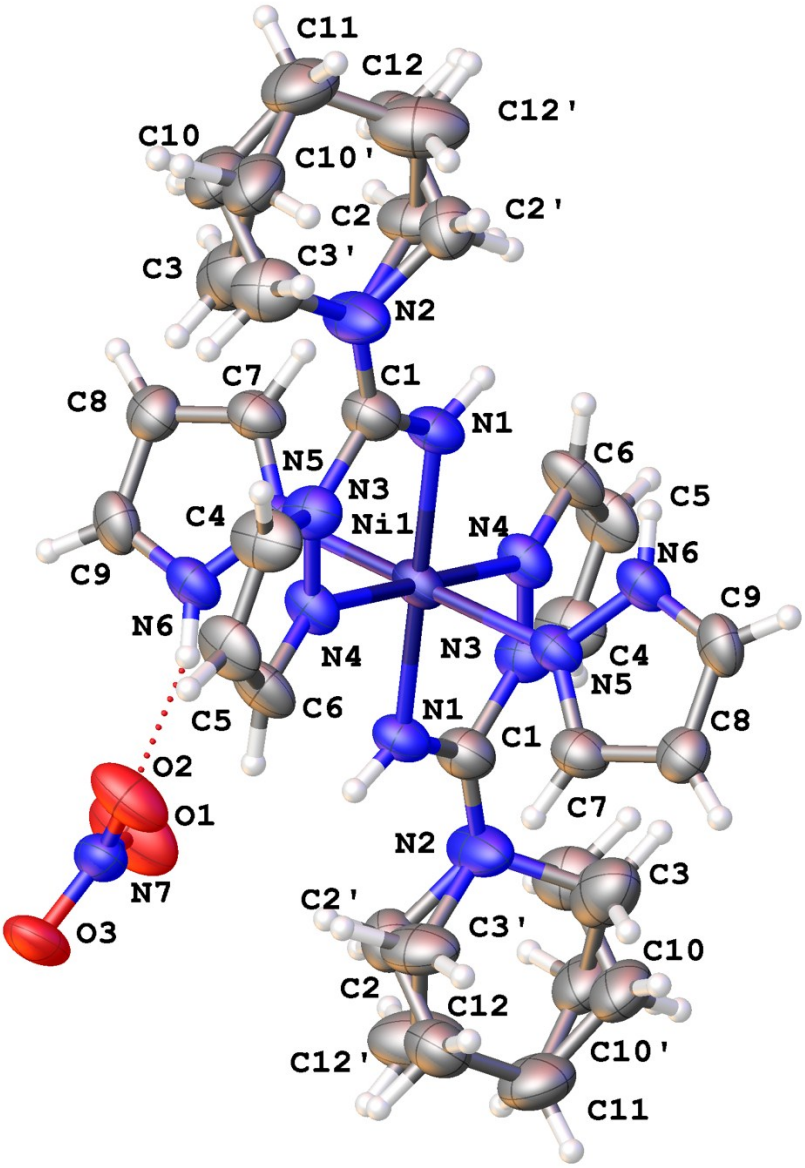


Figure S4. View of the molecular structure of *trans*-[**4**]$(NO_3)_2$, only one cation and one anion are depictured.

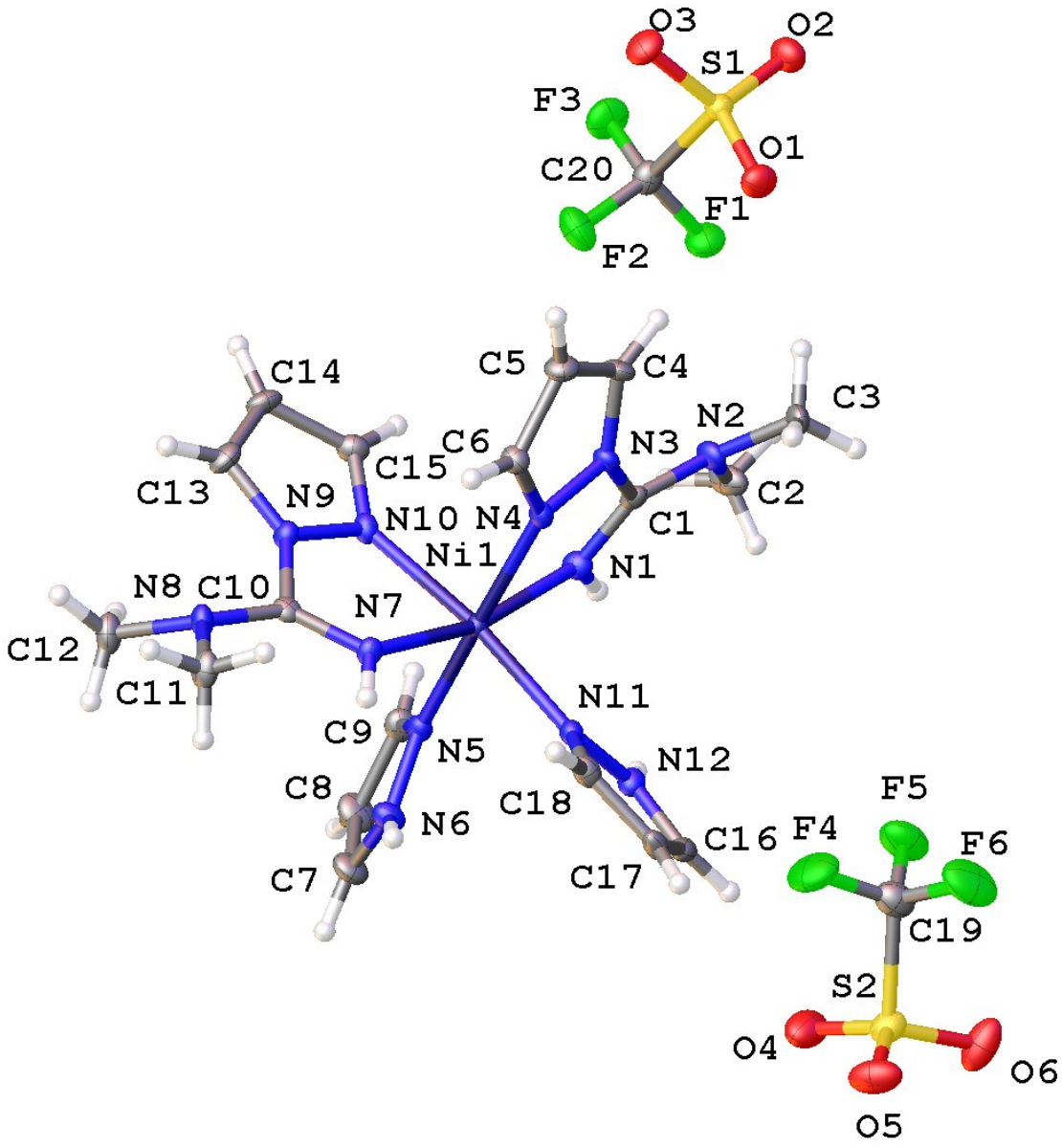


Figure S5. View of the molecular structure of *cis*$_{(PzH)}$-[**1**](OTf)$_2$.

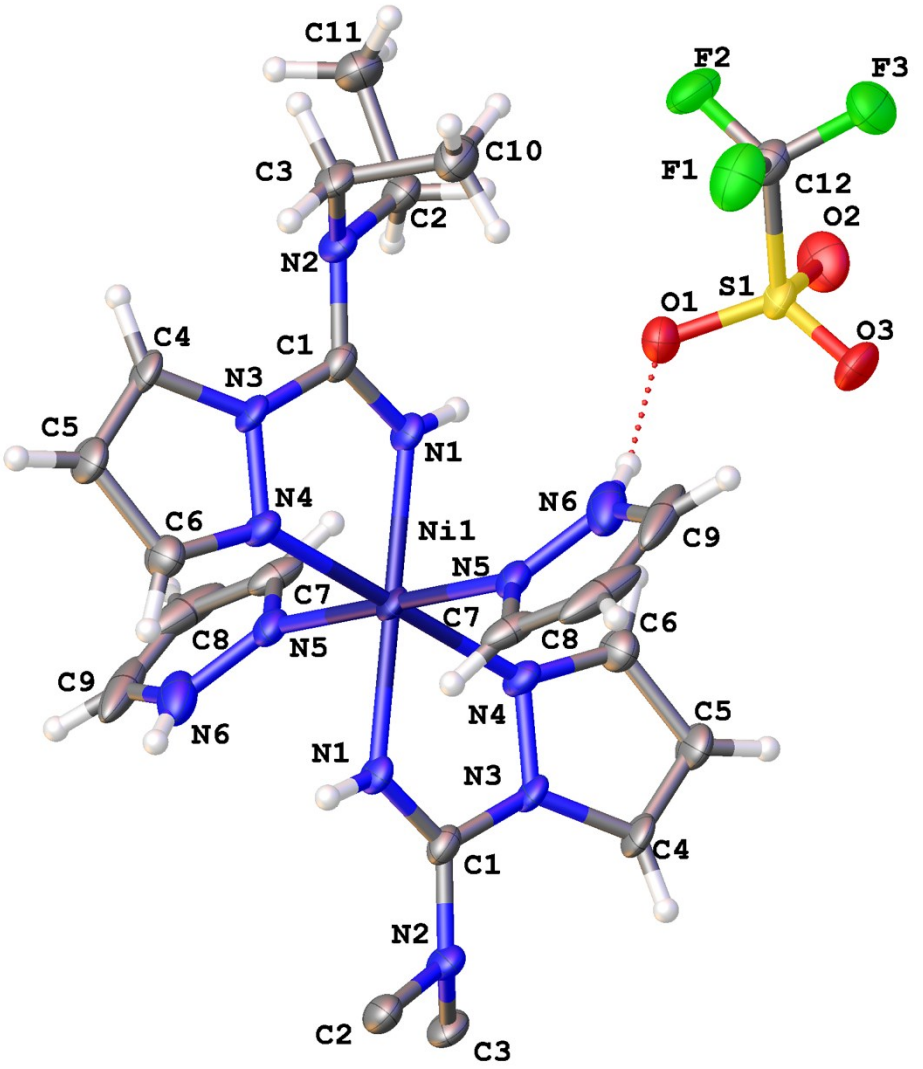


Figure S6. View of the molecular structure of *trans*-[**2**](OTf)$_2$, only one cation and one anion are depictured, the fragment of one of the NEt$_2$ groups is omitted for simplicity.

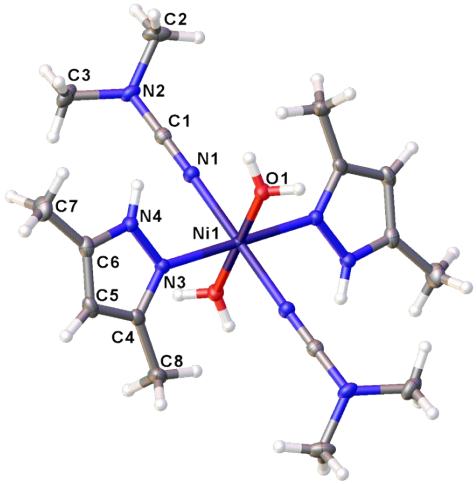


Fig. S7. View of the molecular structure of [**9**](OTf)$_2$, where anions were omitted for simplicity.

The structure of [**9**](OTf)$_2$ (**Fig. S7**) is composed by the *trans*-[Ni(PzH)$_2$(NCNMe$_2$)$_2$(H$_2$O)$_2$]$^{2+}$ cations and the OTf$^-$ anions. The Ni–N$_{Pz}$ (2.0853(17) Å) distance is close to those found for the *bis*- and *tris*-chelate products. The Ni–N$_{nitrile}$ (2.0657 (17) Å) and Ni–O (2.0964(15) Å) distances are similar or slightly longer than those found for the previously characterized complexes [Ni(NCNR$_2$)$_4$(H$_2$O)$_2$]$^{2+}$ (2.027(3)–2.057(2) and 2.044(6)–2.096(8) Å, correspondingly).[1] The C≡N distance (1.149(3) Å) is coherent with a typical CN triple bond of cyanamide ligands.[1]

1. E. V. Andrusenko, N. A. Bokach, G. L. Starova and V. Y. Kukushkin, *Inorg. Chim. Acta*, 2014, **423**, 307-312.

Table S3. Crystallographic data and structure refinement for [**8**]Br_2.

Identification code	[**8**]Br_2
Empirical formula	$NiN_{12}C_{18}Br_2H_{30}$
Formula weight	633.07
Temperature/K	100(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	12.1459(10)
b/Å	12.2077(11)
c/Å	12.2693(9)
α/°	102.359(7)
β/°	106.094(7)
γ/°	119.553(9)
Volume/Å^3	1380.1(2)
Z	2
ρ_{calc}g/cm^3	1.523
μ/mm^{-1}	4.648
F(000)	640.0
Crystal size/mm^3	0.14 × 0.12 × 0.06
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.264 to 139.978
Index ranges	-13 ≤ h ≤ 14, -14 ≤ k ≤ 14, -14 ≤ l ≤ 14
Reflections collected	11250
Independent reflections	5160 [R_{int} = 0.0523, R_{sigma} = 0.0584]
Data/restraints/parameters	5160/0/314
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0713, wR_2 = 0.1919
Final R indexes [all data]	R_1 = 0.0788, wR_2 = 0.2018
Largest diff. peak/hole / e Å^{-3}	2.67/-0.81
CCDC number	1962791

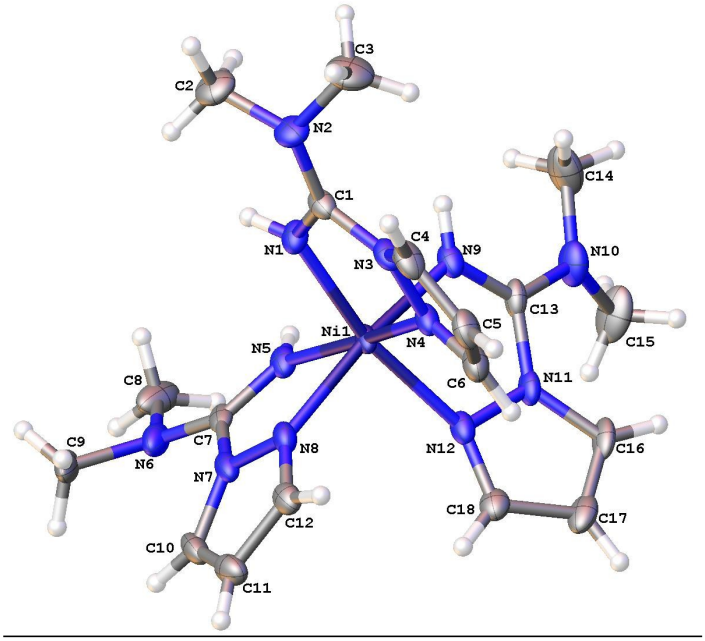


Fig. S8. View of the molecular structure of [**8**]Br_2, where anions were omitted for simplicity.

Spectral information

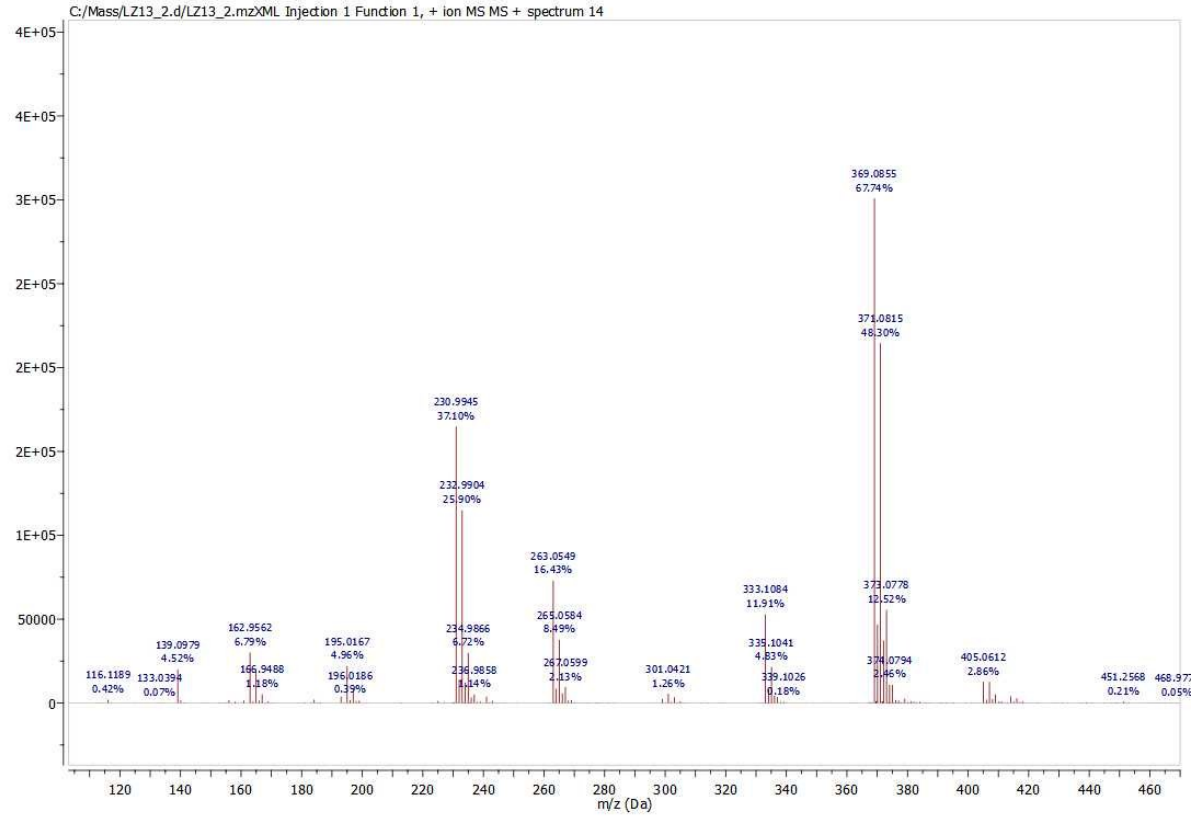


Figure S9. HR MS(ESI)$^+$ spectrum of [**1**]Cl_2

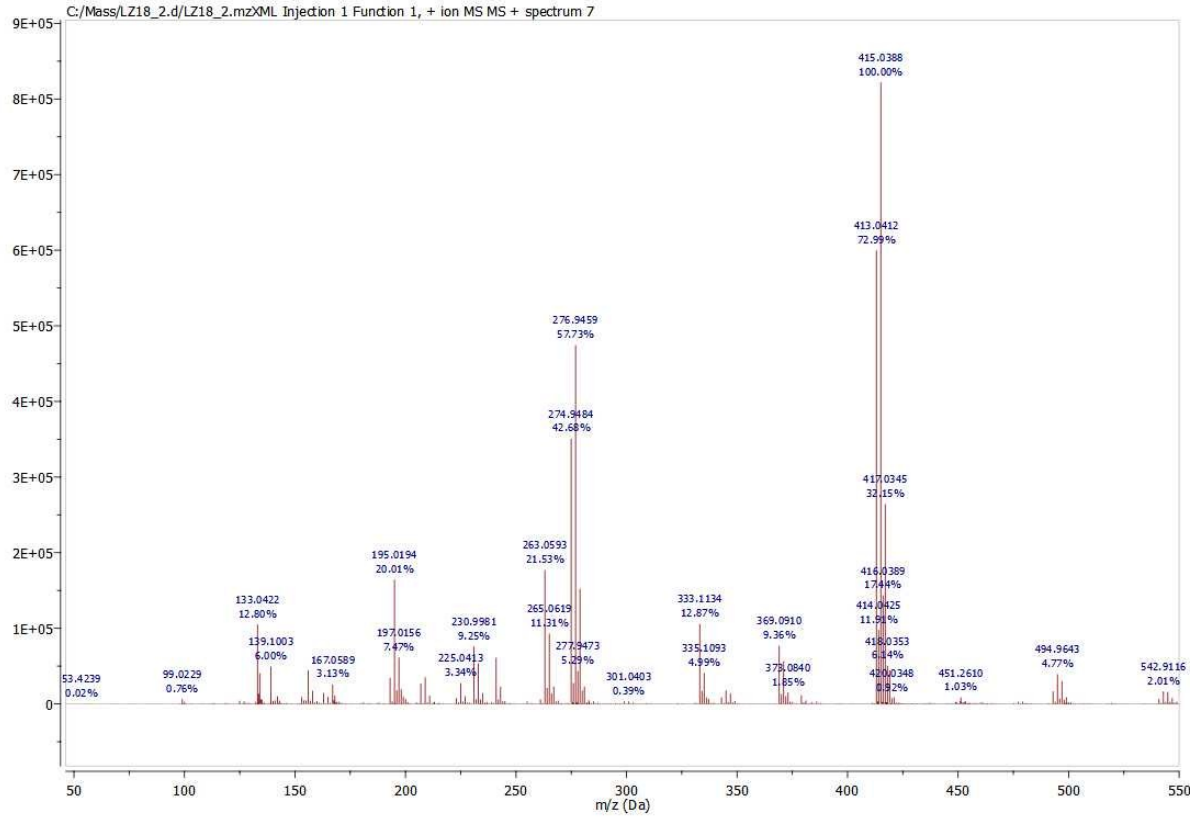


Figure S10. HR MS(ESI)$^+$ spectrum of [**1**]Br_2

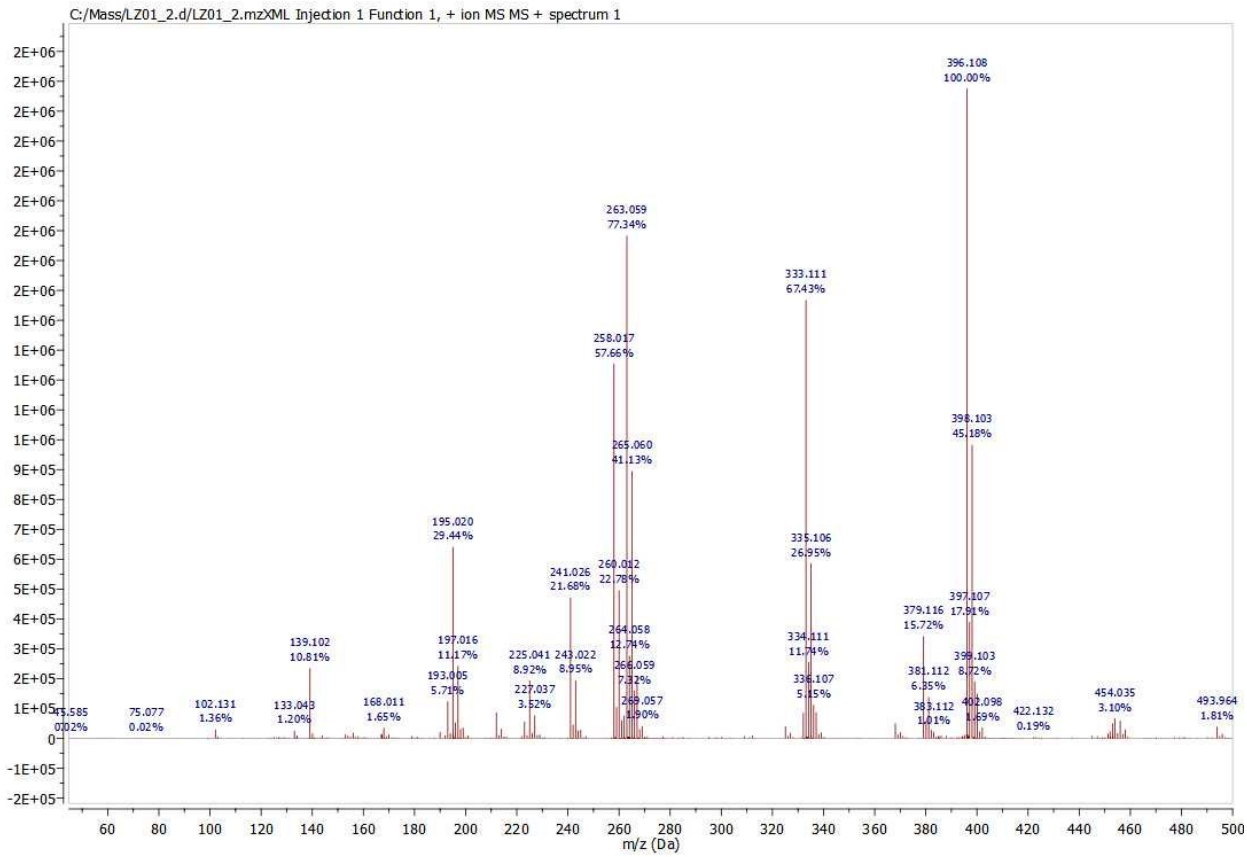


Figure S11. HR MS(ESI)$^+$ spectrum of [**1**]$(NO_3)_2$

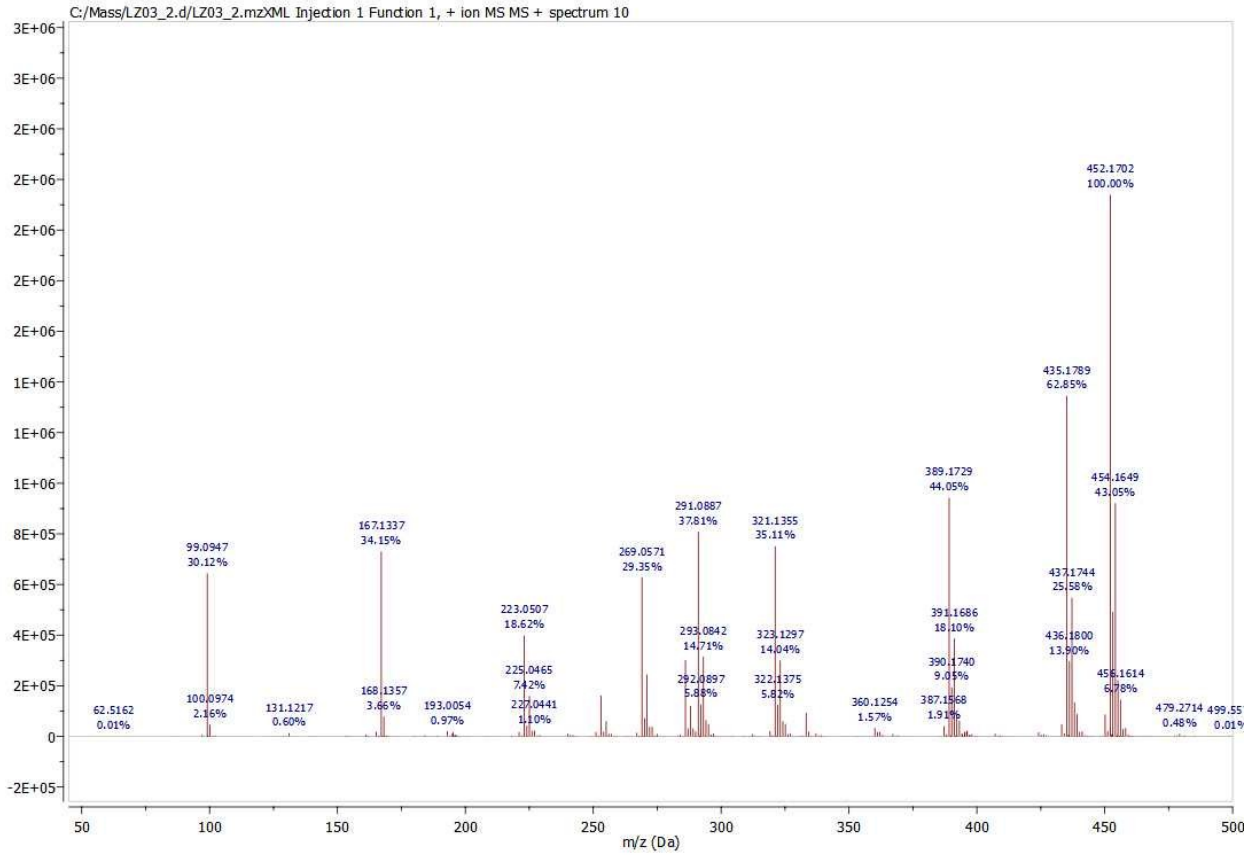


Figure S12. HR MS(ESI)$^+$ spectrum of [**2**]$(NO_3)_2$

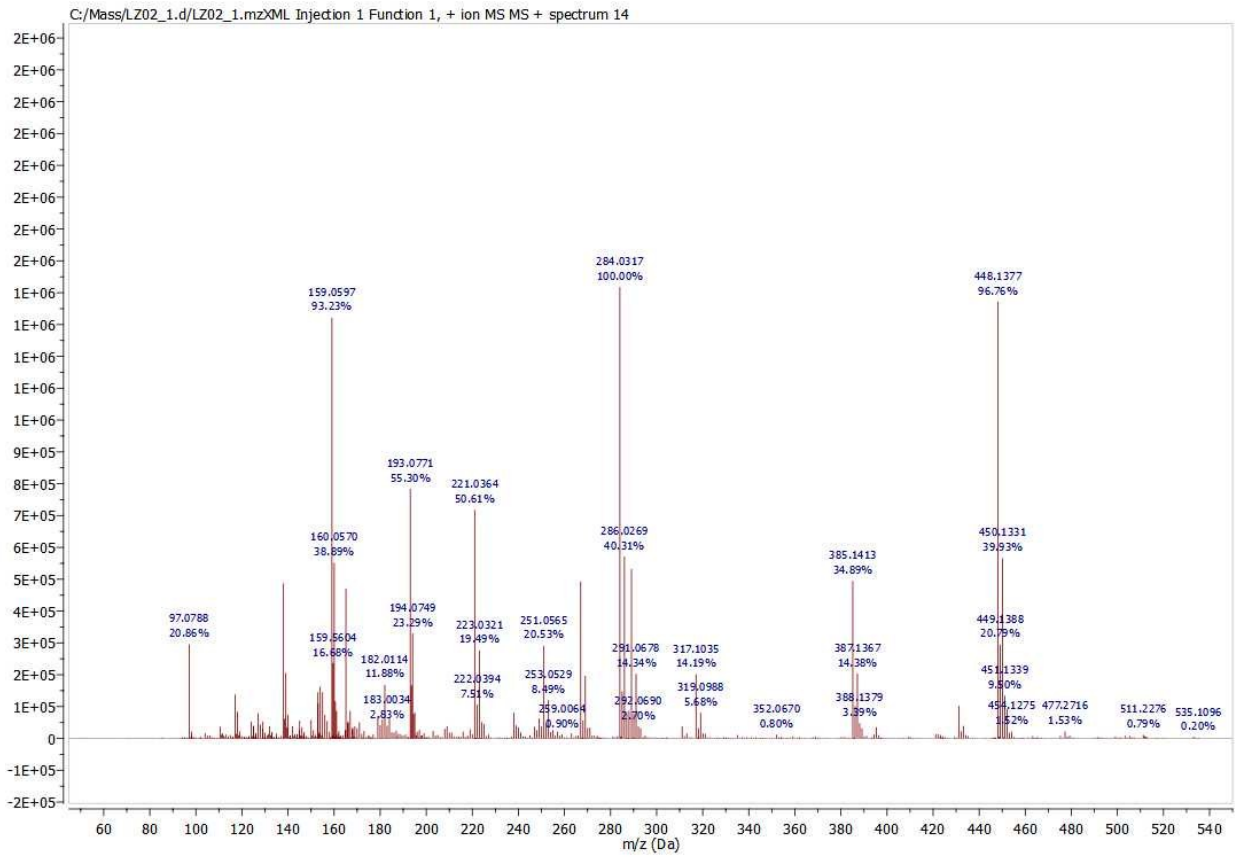


Figure S13. HR MS(ESI)$^+$ spectrum of [**3**]$(NO_3)_2$

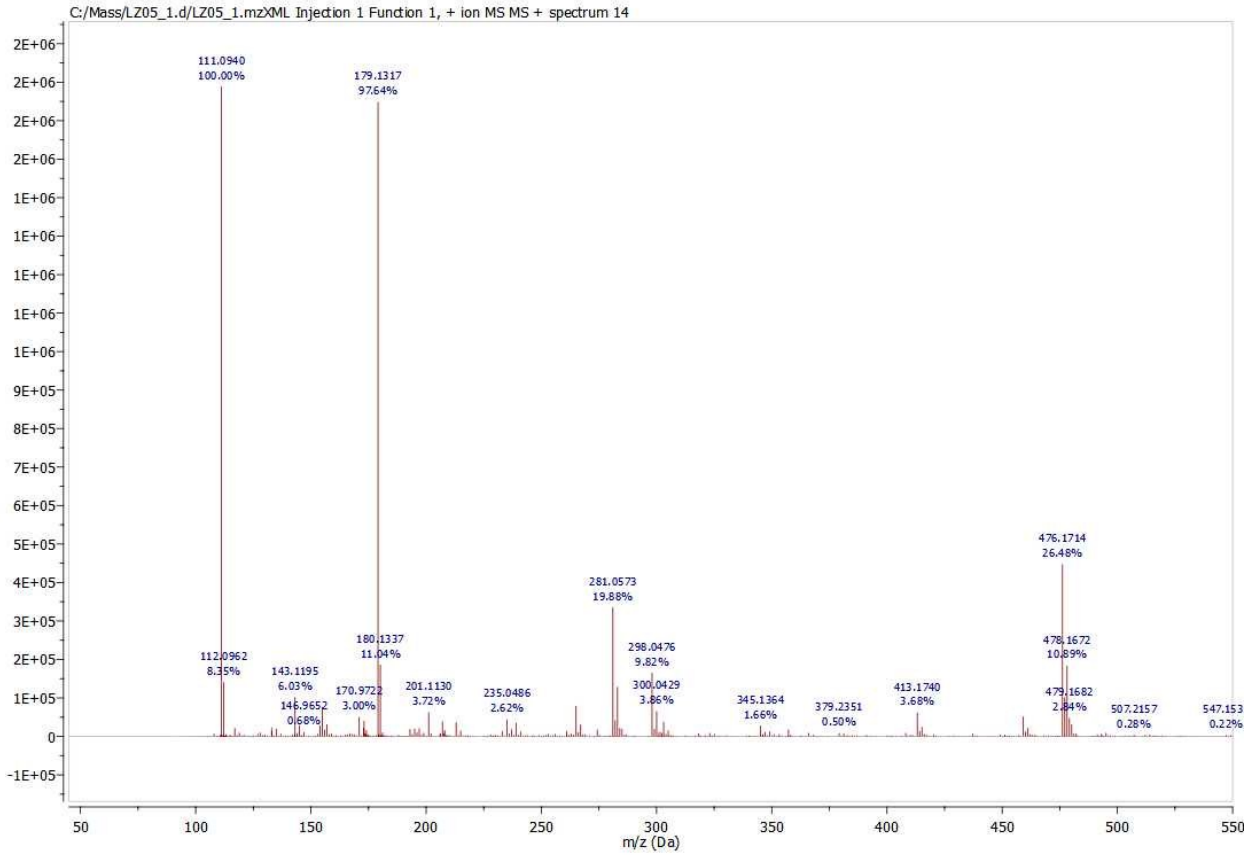


Figure S14. HR MS(ESI)$^+$ spectrum of [**4**]$(NO_3)_2$

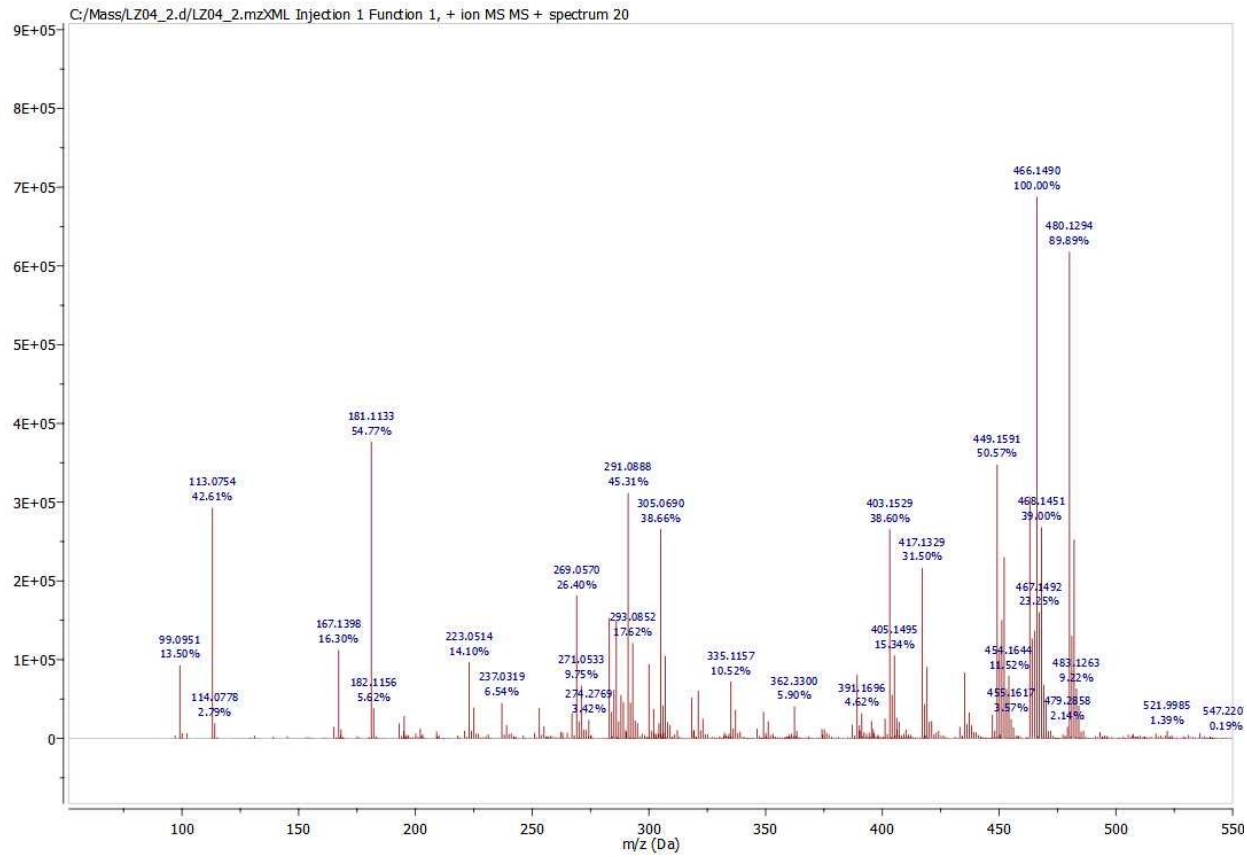


Figure S15. HR MS(ESI)$^+$ spectrum of [**5**]$(NO_3)_2$

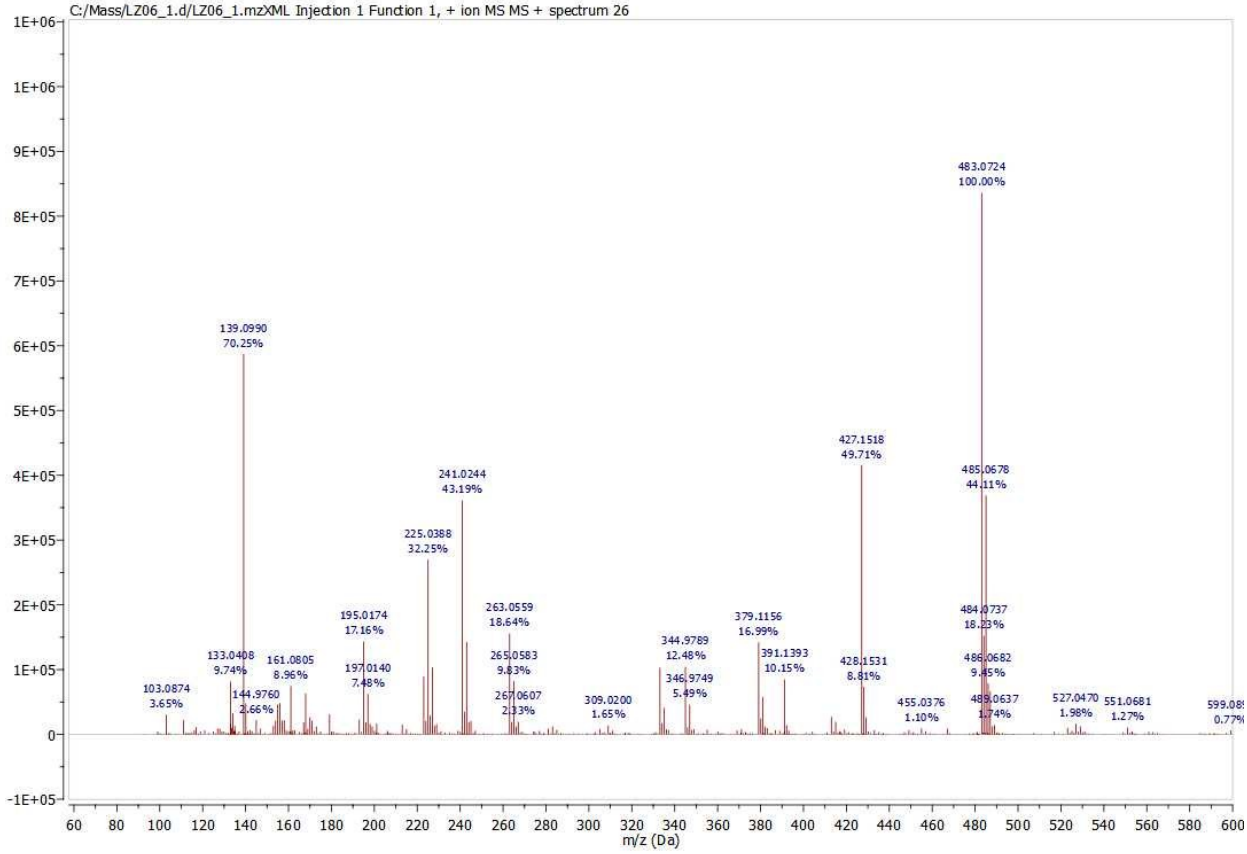


Figure S16. HR MS(ESI)$^+$ spectrum of [**1**]$(OTf)_2$

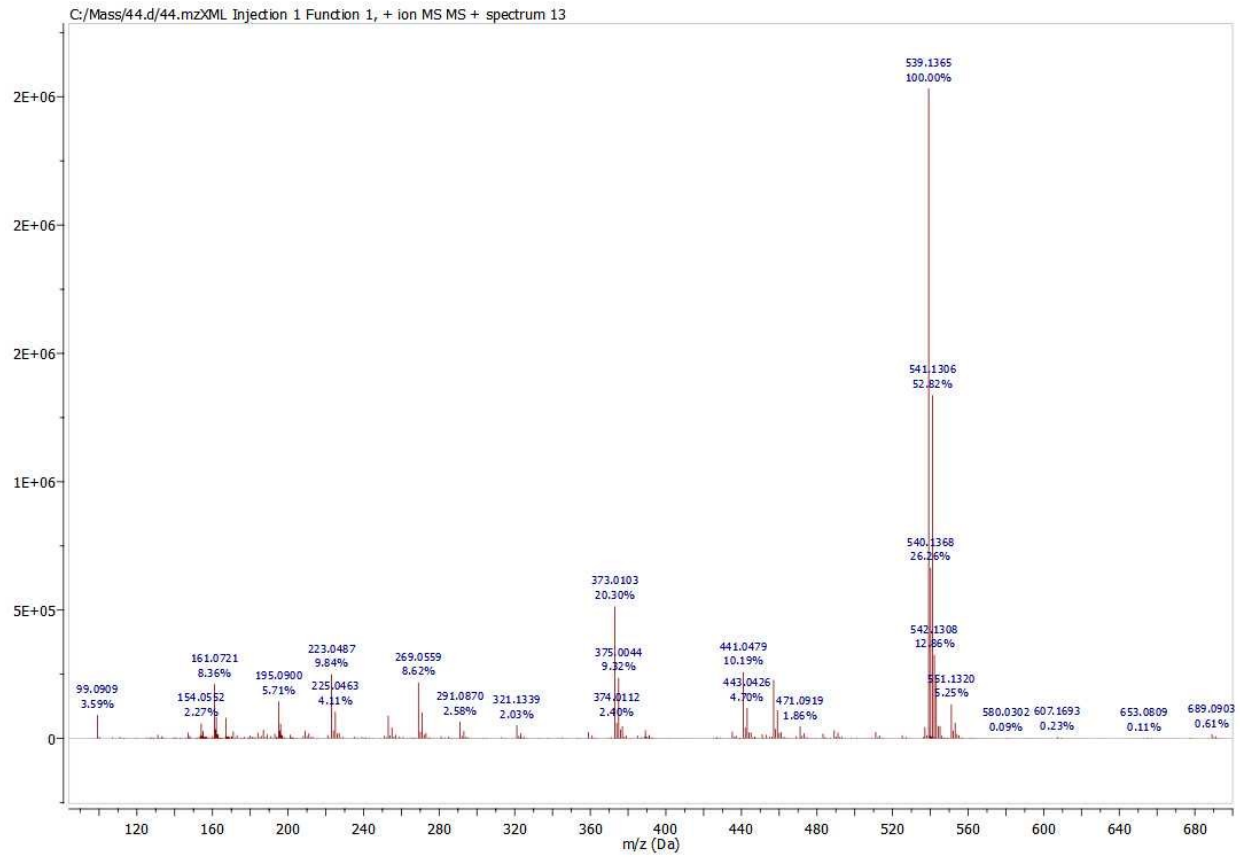


Figure S17. HR MS(ESI)$^+$ spectrum of [**2**](OTf)$_2$

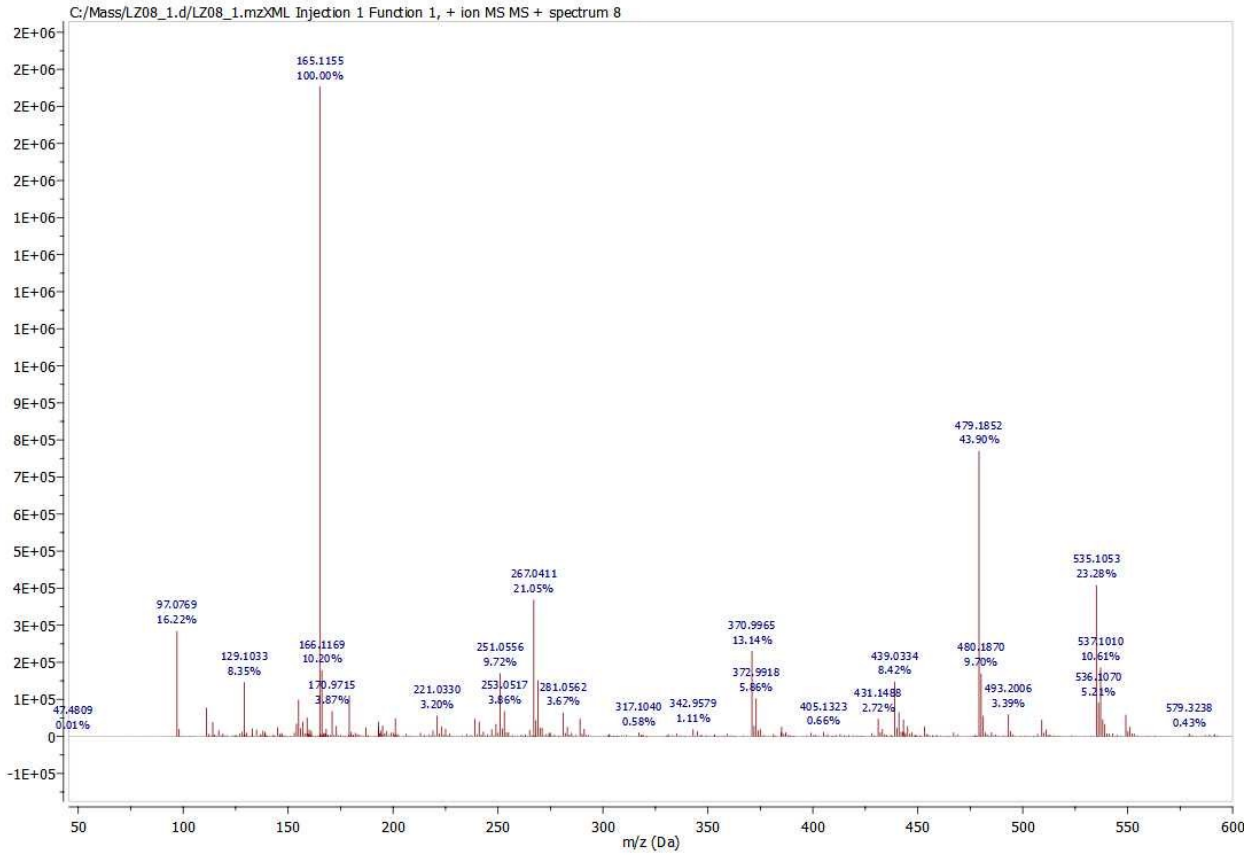


Figure S18. HR MS(ESI)$^+$ spectrum of [**3**](OTf)$_2$

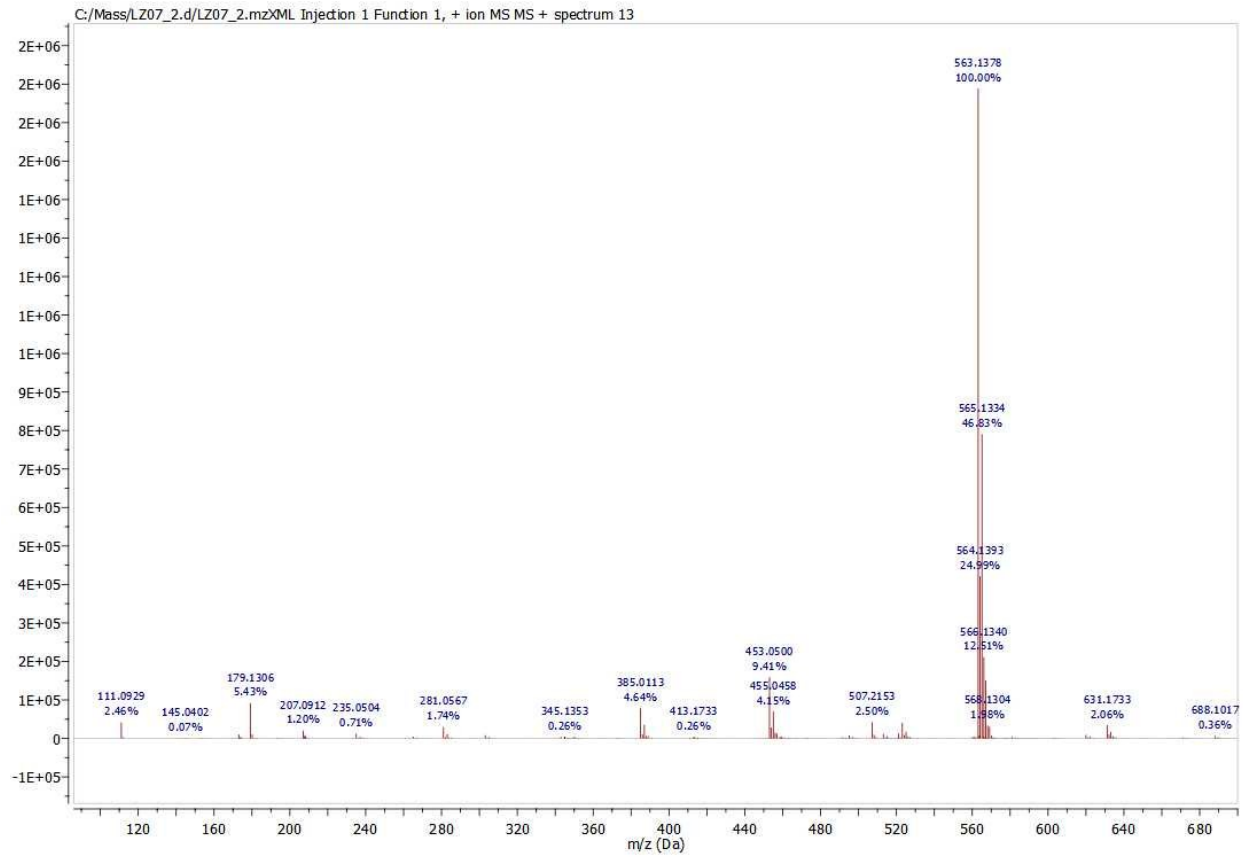


Figure S19. HR MS(ESI)$^+$ spectrum of [**4**](OTf)$_2$

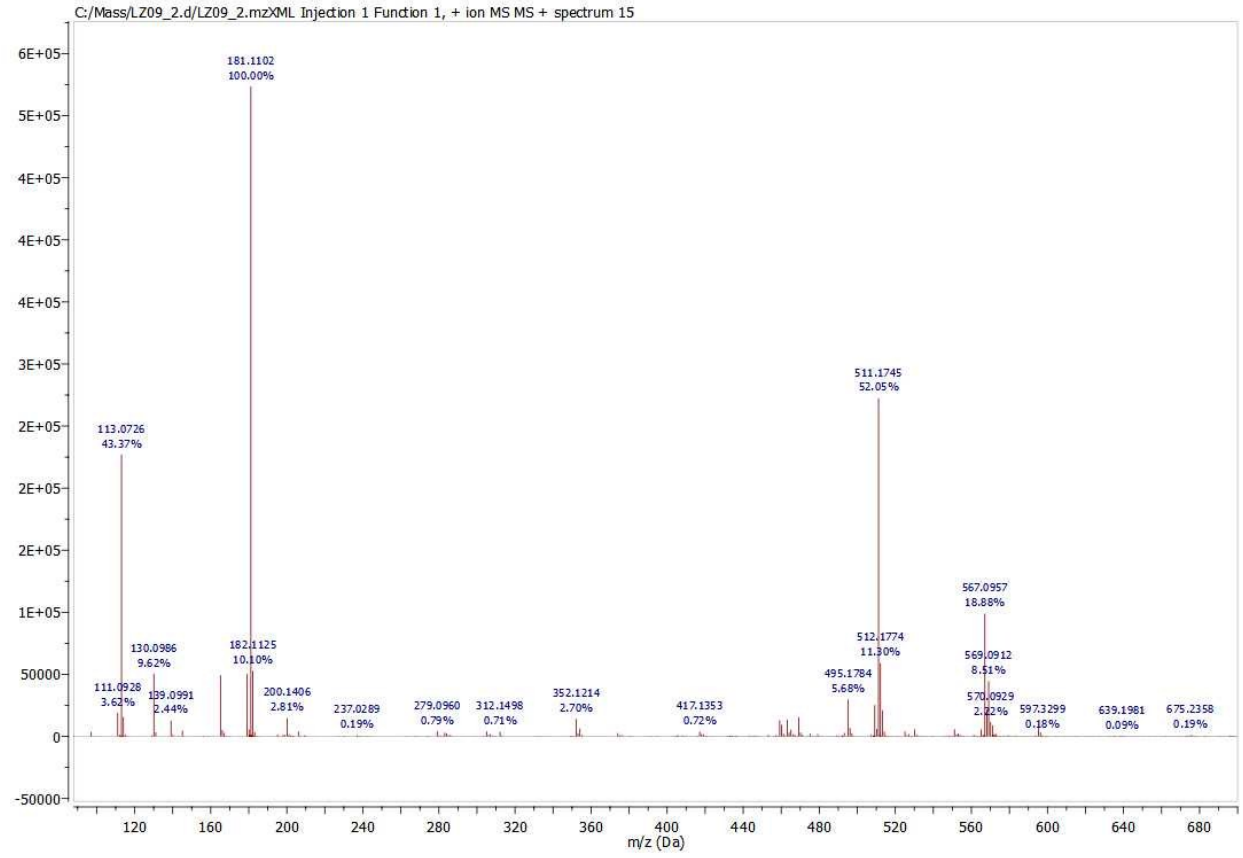


Figure S20. HR MS(ESI)$^+$ spectrum of [**5**](OTf)$_2$

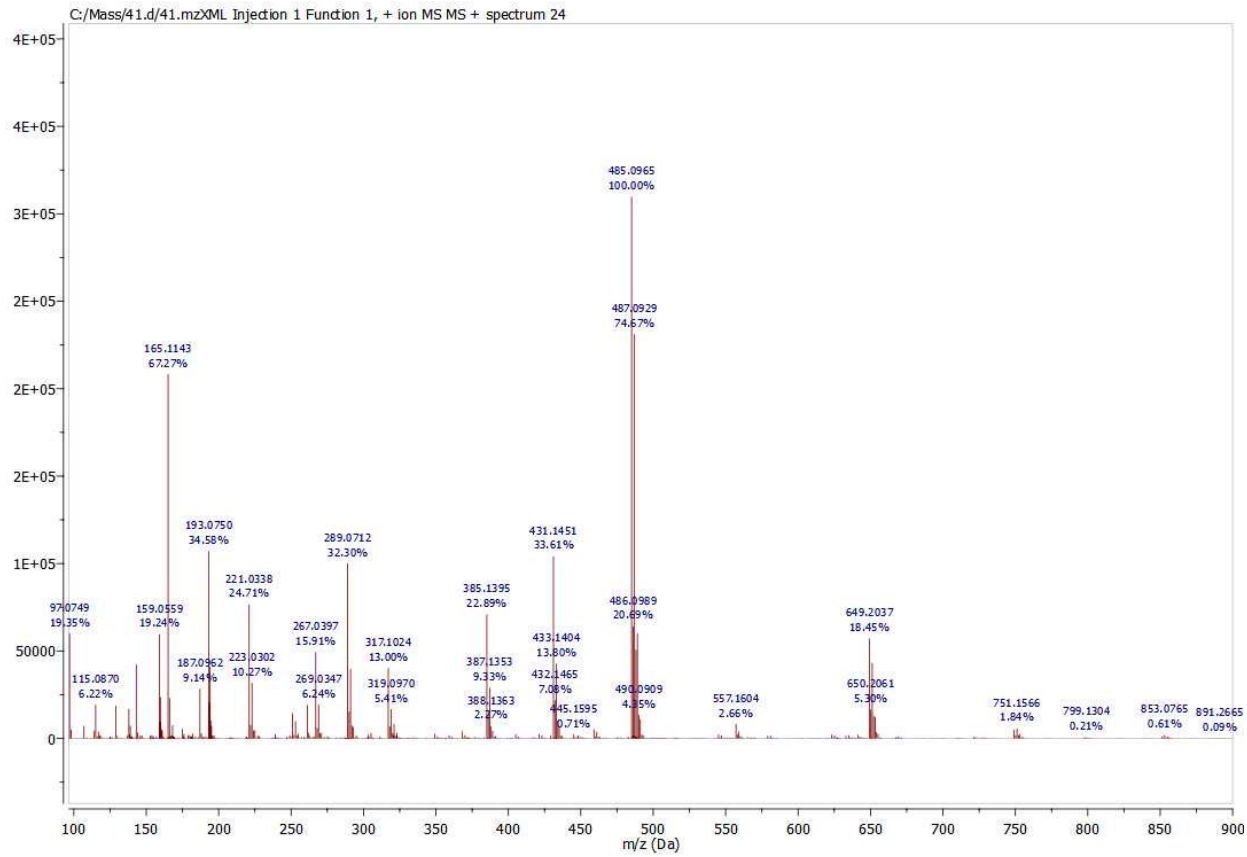


Figure S21. HR MS(ESI)$^+$ spectrum of [**6**]$(ClO_4)_2$

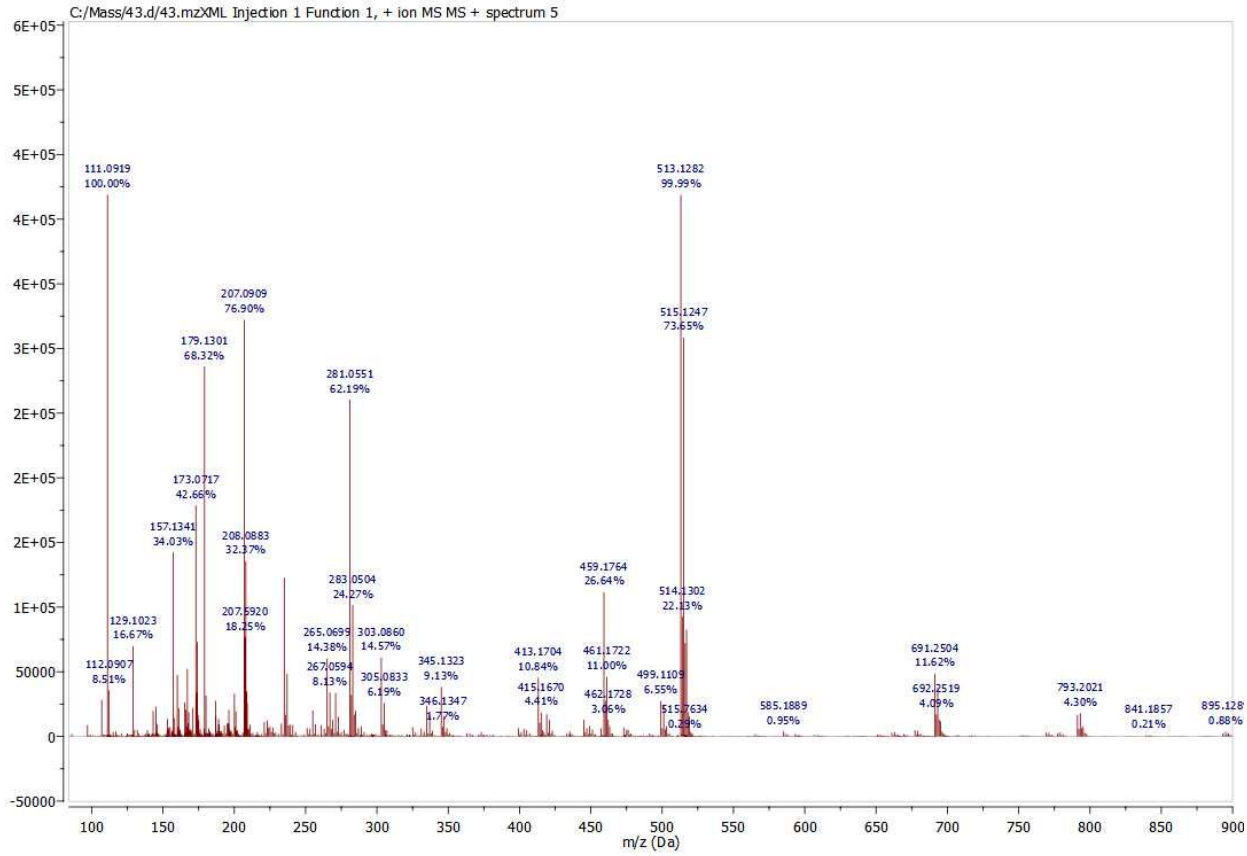


Figure S22. HR MS(ESI)$^+$ spectrum of [**7**]$(ClO_4)_2$

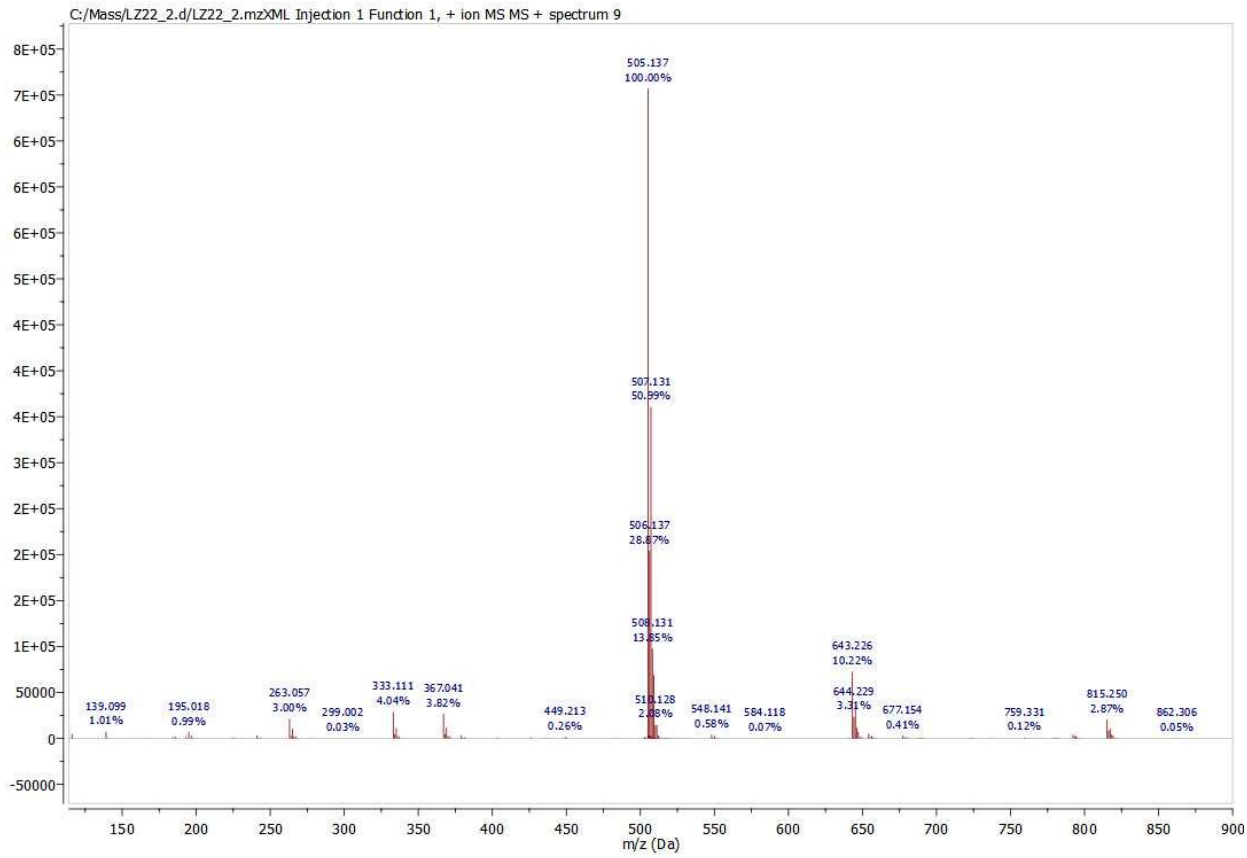


Figure S23. HR MS(ESI)$^+$ spectrum of [**8**](OTs)$_2$

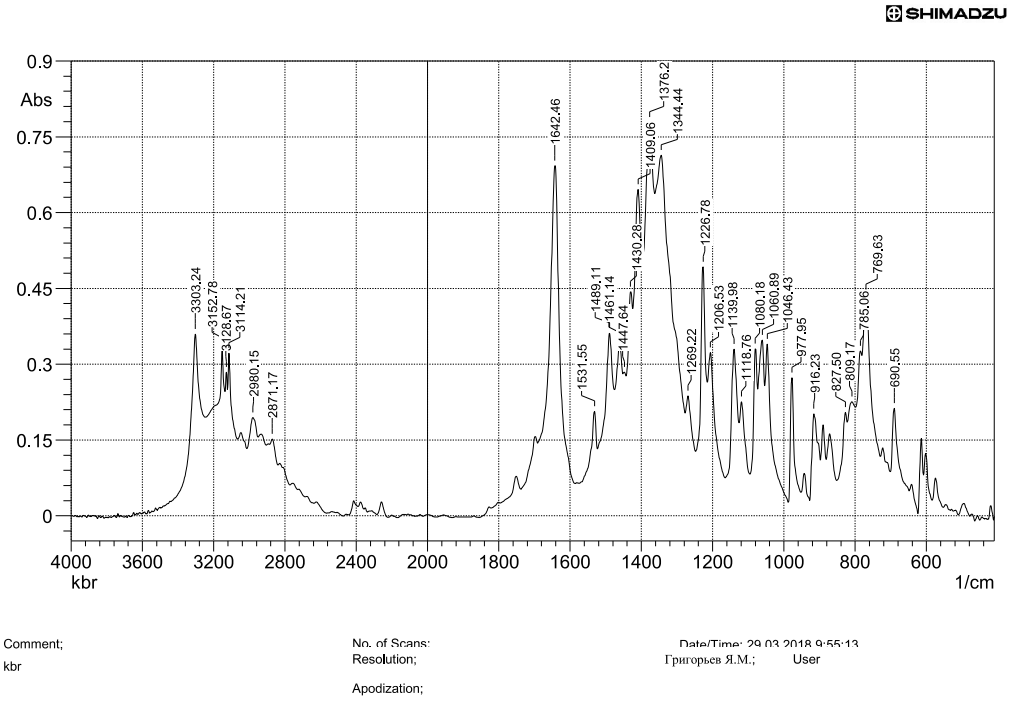


Figure S24. IR spectrum of [**1**](NO$_3$)$_2$ in KBr pellet.

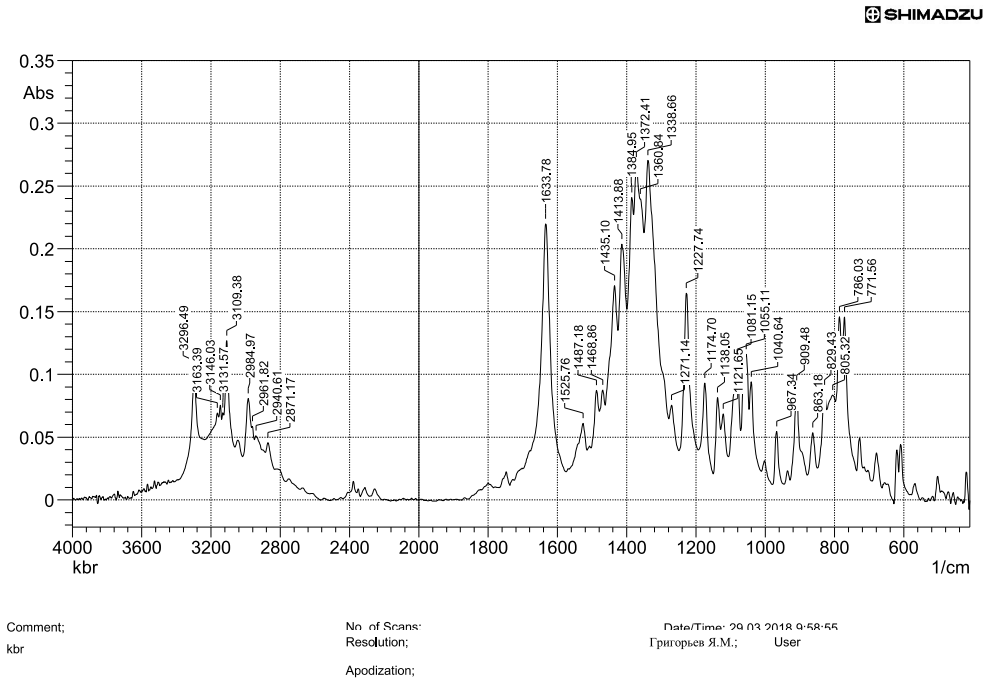


Figure S25. IR spectrum of [**2**]$(NO_3)_2$ in KBr pellet.

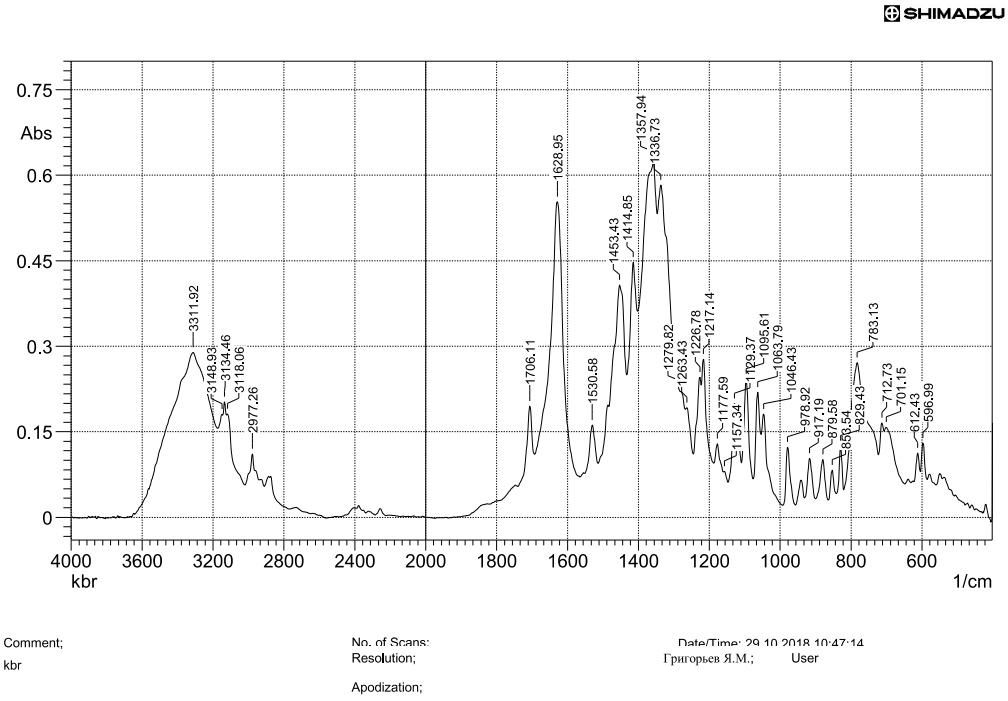


Figure S26. IR spectrum of [**3**]$(NO_3)_2$ in KBr pellet.

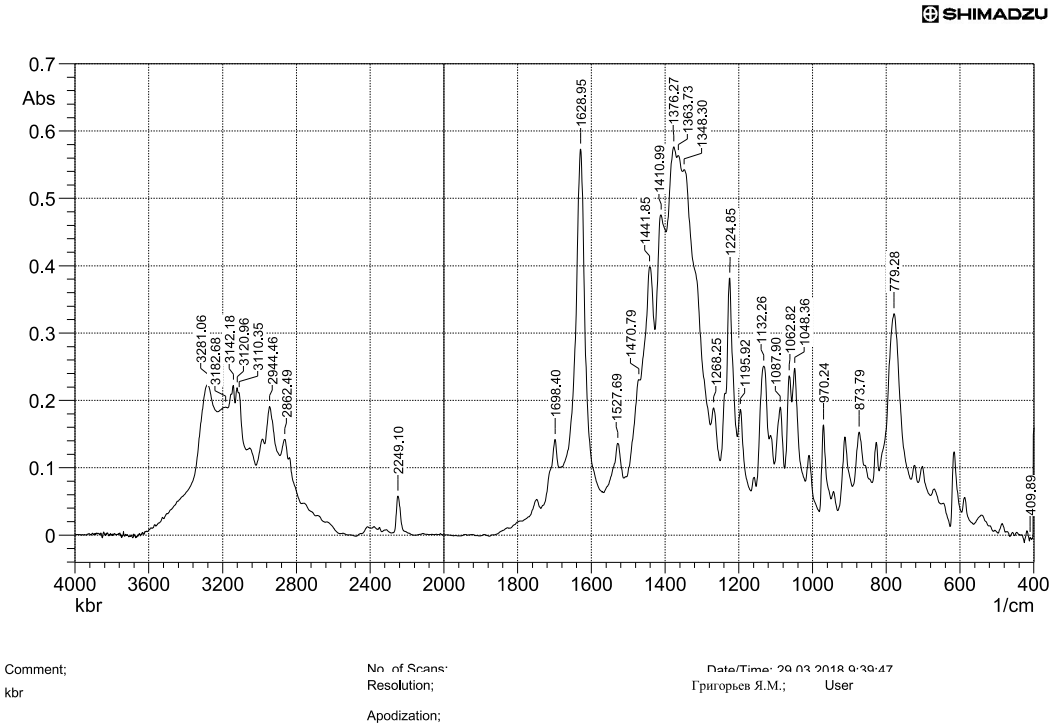


Figure S27. IR spectrum of [**4**]$(NO_3)_2$ in KBr pellet.

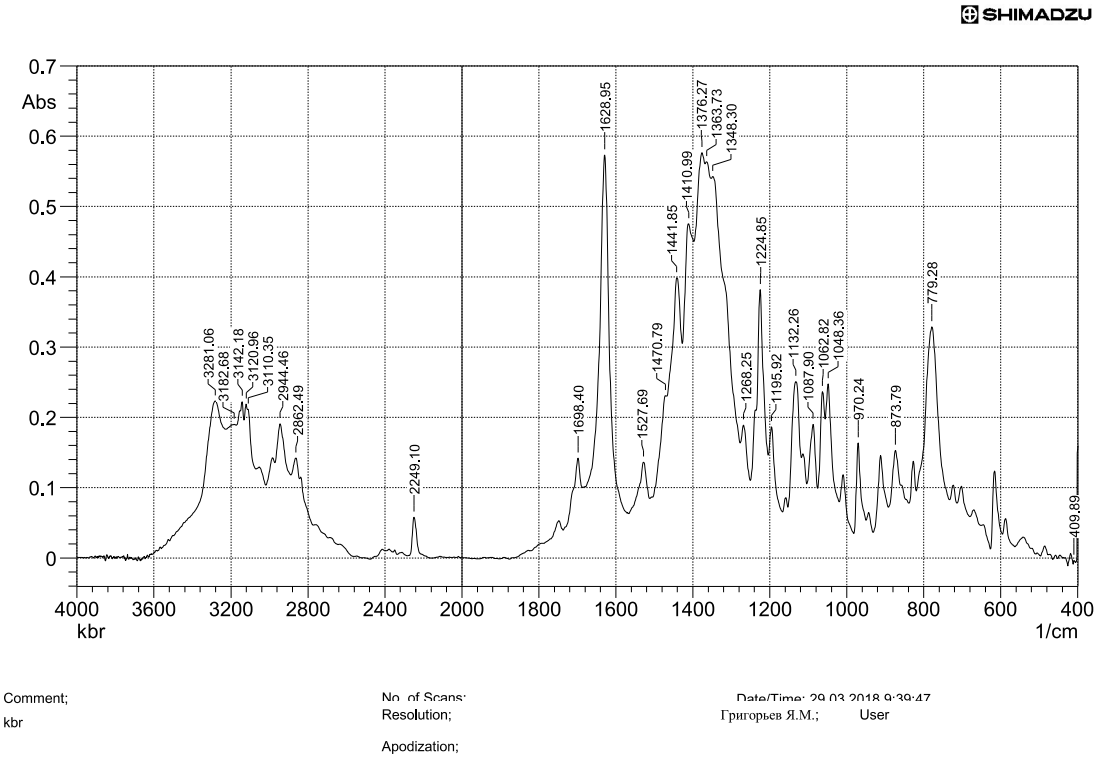


Figure S28. IR spectrum of [**5**]$(NO_3)_2$ in KBr pellet.

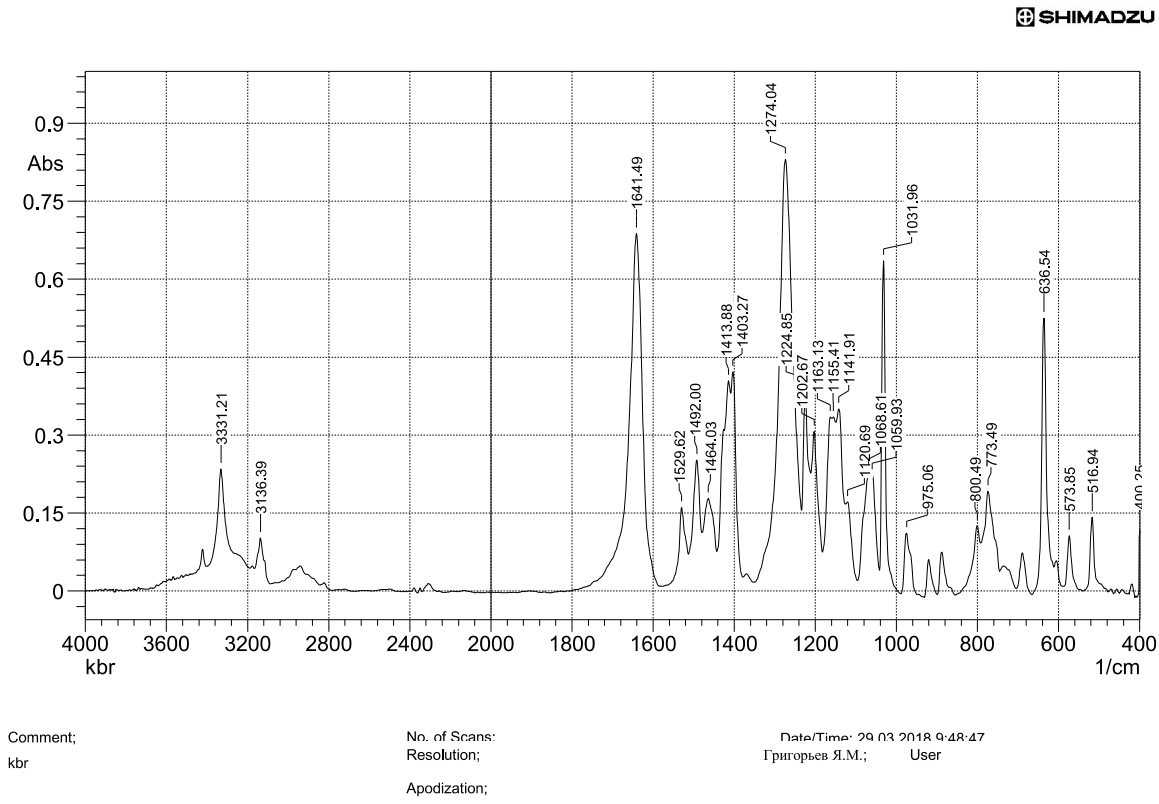


Figure S29. IR spectrum of [**1**](OTf)$_2$ in KBr pellet.

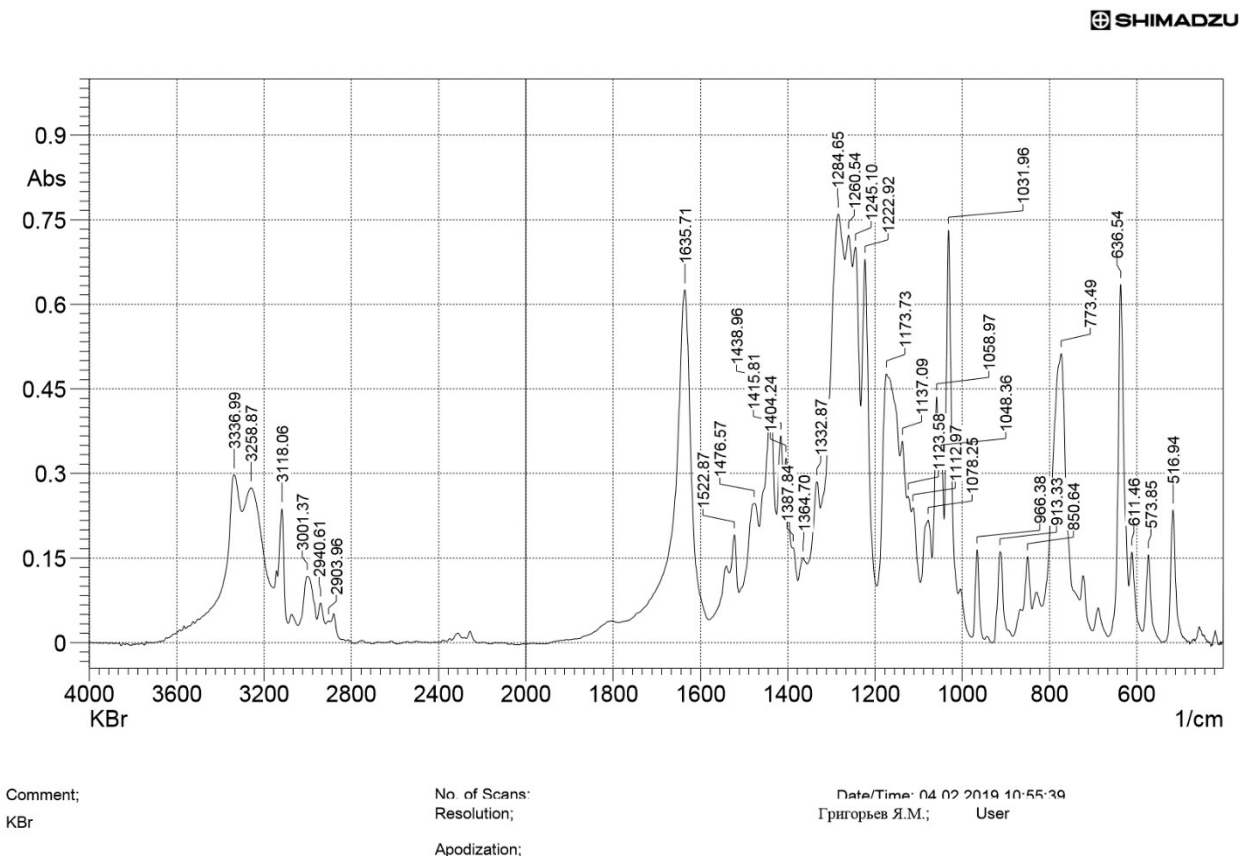


Figure S30. IR spectrum of [**2**](OTf)$_2$ in KBr pellet.

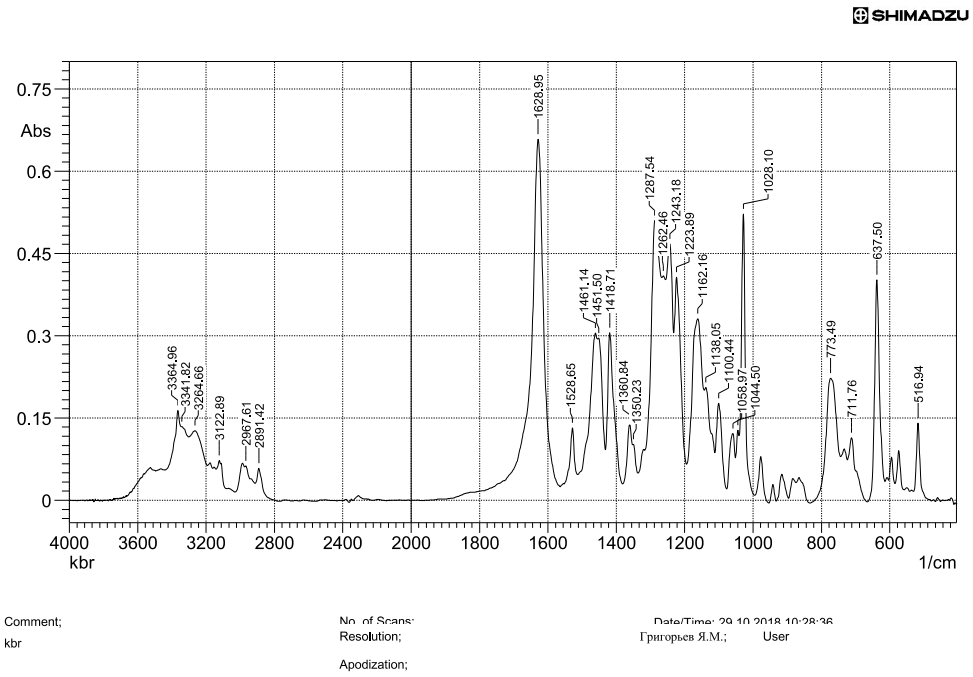


Figure S31. IR spectrum of [**3**](OTf)$_2$ in KBr pellet.

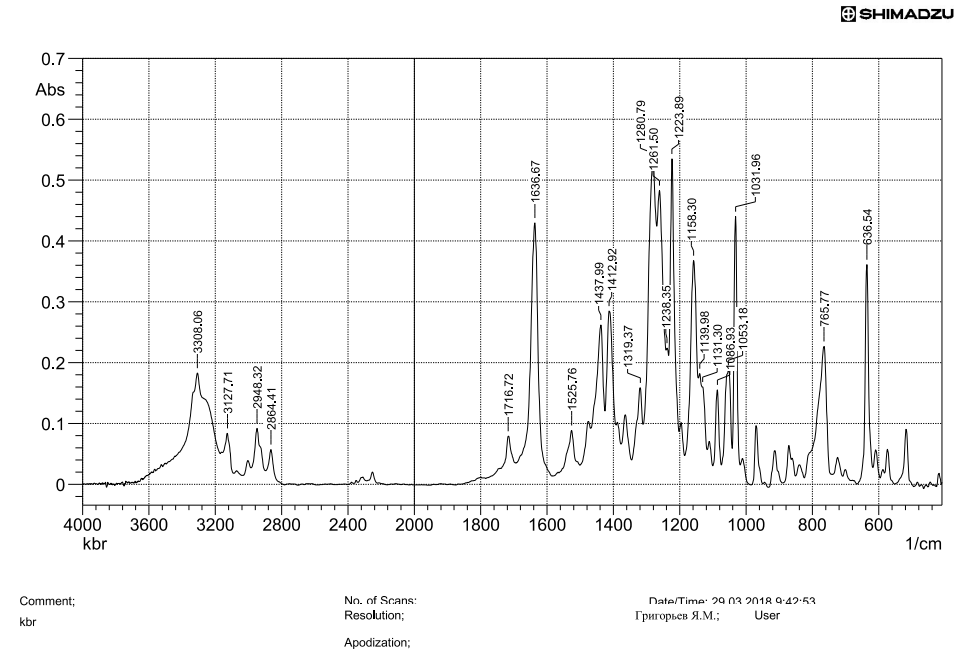


Figure S32. IR spectrum of [**4**](OTf)$_2$ in KBr pellet.

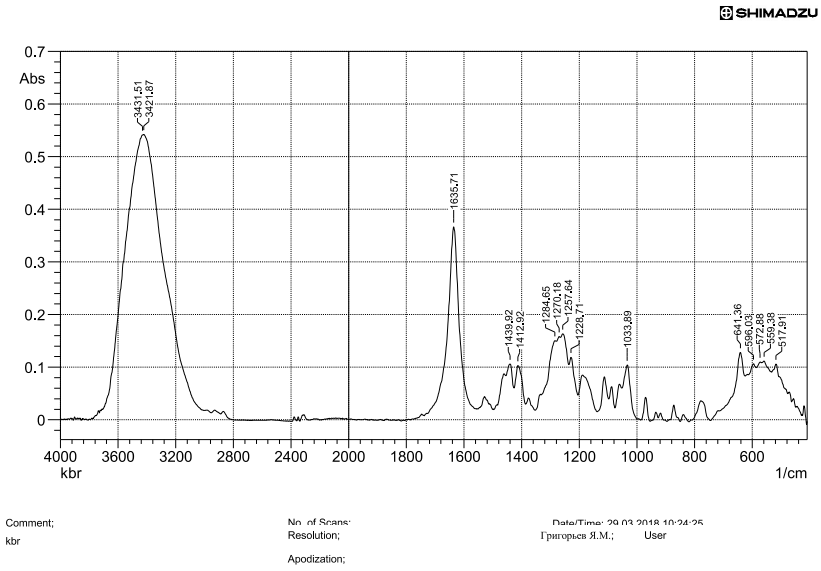


Figure S33. IR spectrum of [**5**](OTf)$_2$ in KBr pellet.

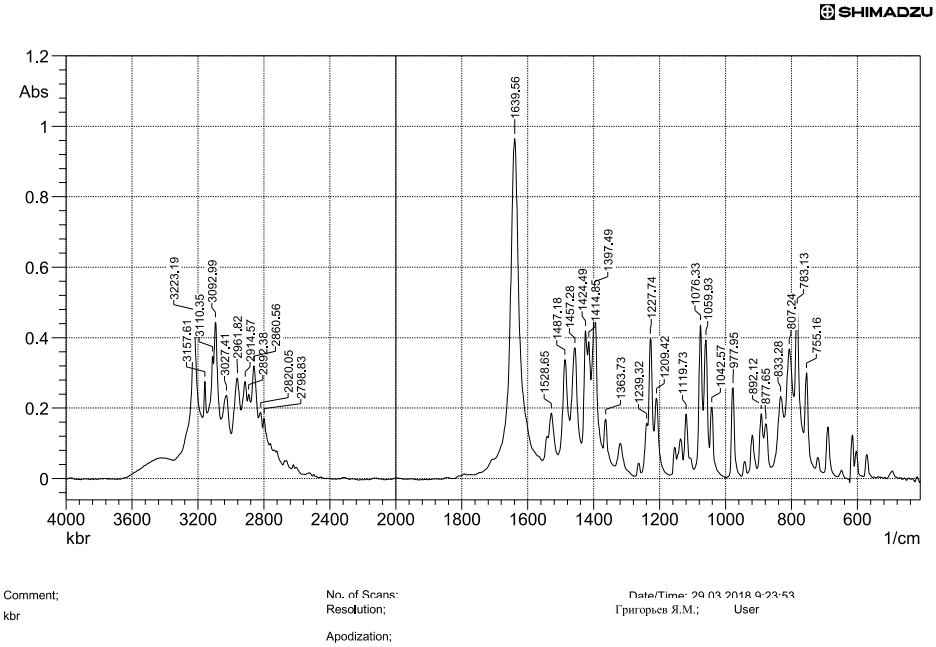


Figure S34. IR spectrum of [**1**](Cl)$_2$ in KBr pellet.

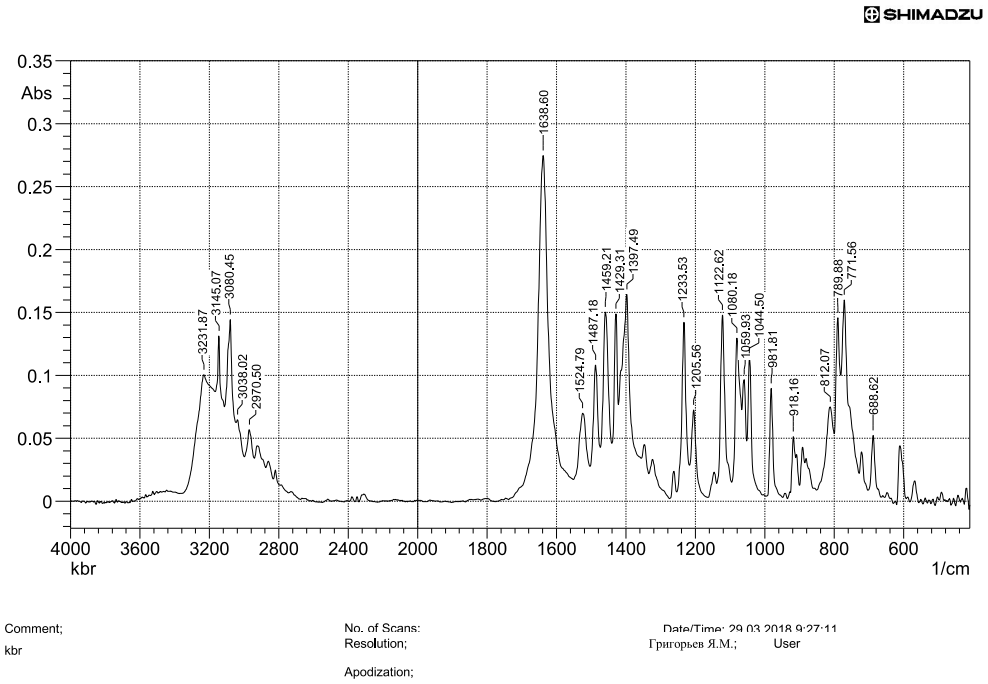


Figure S35. IR spectrum of [**1**](Br)$_2$ in KBr pellet.

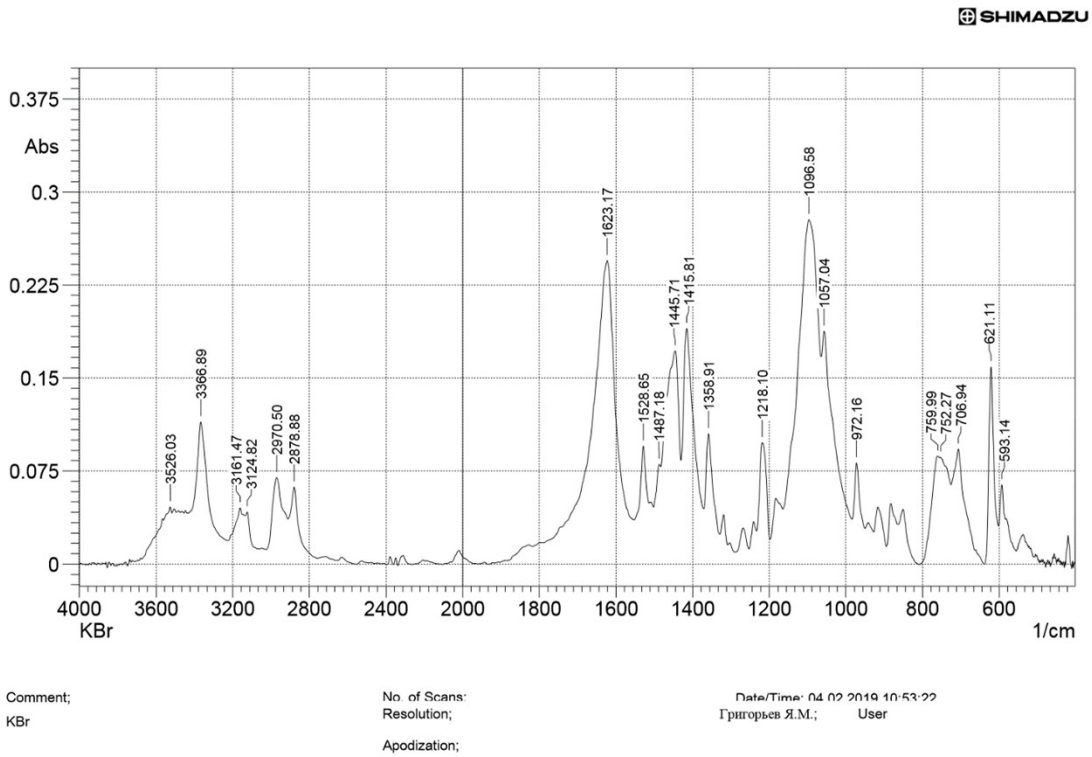


Figure S36. IR spectrum of [**6**](ClO$_4$)$_2$ in KBr pellet.

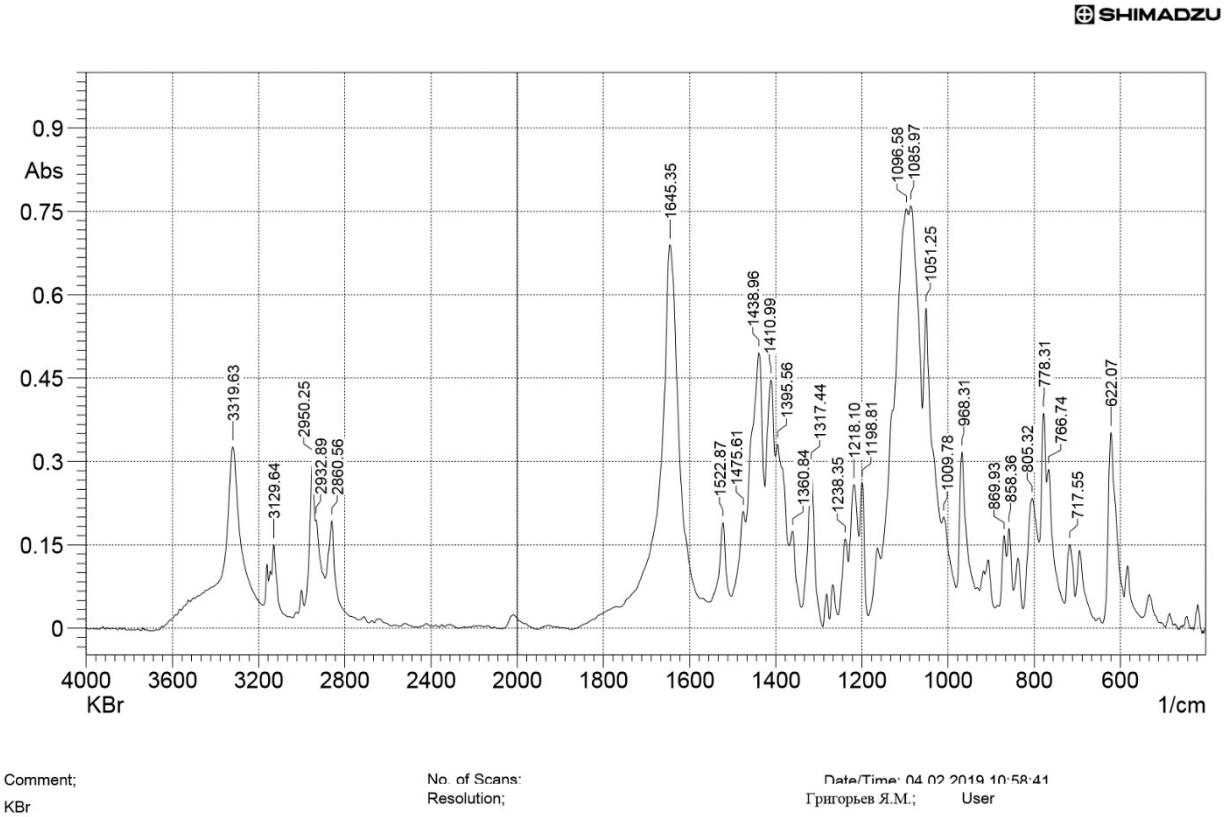


Figure S37. IR spectrum of [**7**]$(ClO_4)_2$ in KBr pellet.

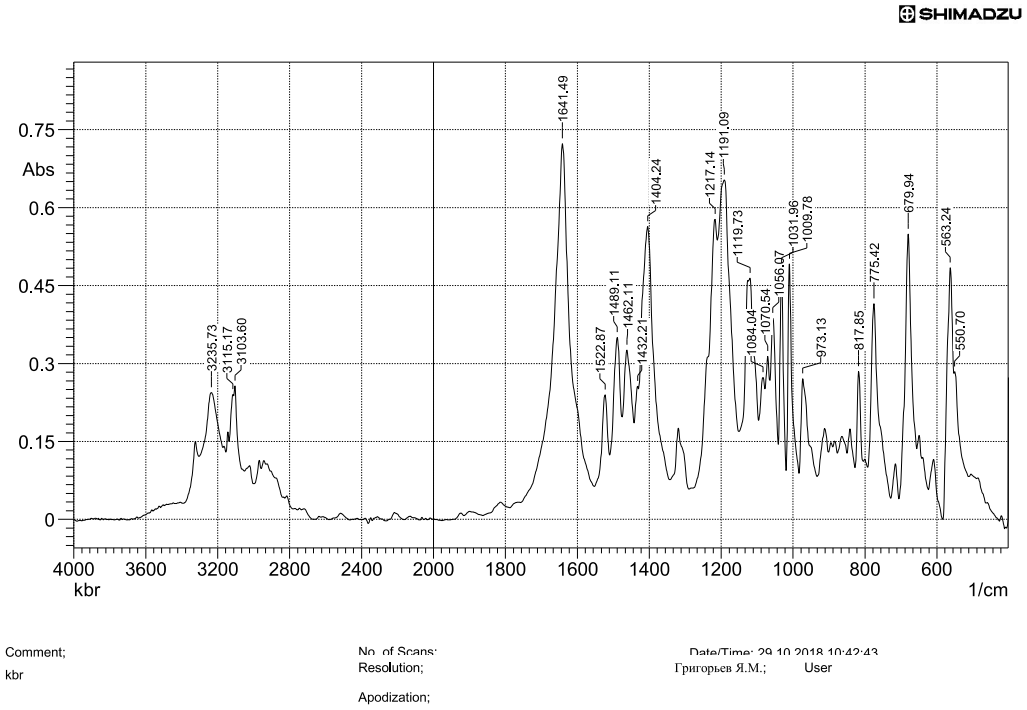


Figure S38. IR spectrum of [**8**]$(OTs)_2$ in KBr pellet.

Computational details

Taking into account very shallow potential energy surface near the equilibrium geometry of complex **V•••**BH^+ (B is a base) toward the proton transfer to **V**, the energy of deprotonation of PzH in *trans*-**I** was calculated using the following procedure. First, structure of the molecular complex *trans*-**I•••**B bearing a base B in the second coordination sphere and bound with *trans*-**I** via a hydrogen bond was fully optimized. Dimethylcyanamide $NCNMe_2$ or water trimer $(H_2O)_3$ were used as a base in these calculations. Second, in the equilibrium geometry of *trans*-**I•••**B, a proton of the NH group in one of the PzH ligands (the nearest to B) was transferred to the nucleophilic atom of B (the amino N atom of $NCNMe_2$ or the O atom of $(H_2O)_3$), and the corresponding H–O/N distance was fixed to 1 Å. Thus, initial geometry of complex **V•••**BH^+ was constructed. Third, partial geometry optimization with the fixed H–O/N distance and relaxed all other internal coordinates was done. The deprotonation energy was calculated as a difference between total energies of **V•••**BH^+ and *trans*-**I•••**B calculated at the SMD-M06/6-311+G*//gas-M06/6-31G* level. Since, the entropic term of the *trans*-**I•••**B → **V•••**BH^+ transformation is close to zero, thus found deprotonation energy should be close to the Gibbs free energy of deprotonation. The same procedure was applied for calculations of the deprotonation energies in complexes *cis*-**I**, **IX** and $\mathbf{IX_N}$.

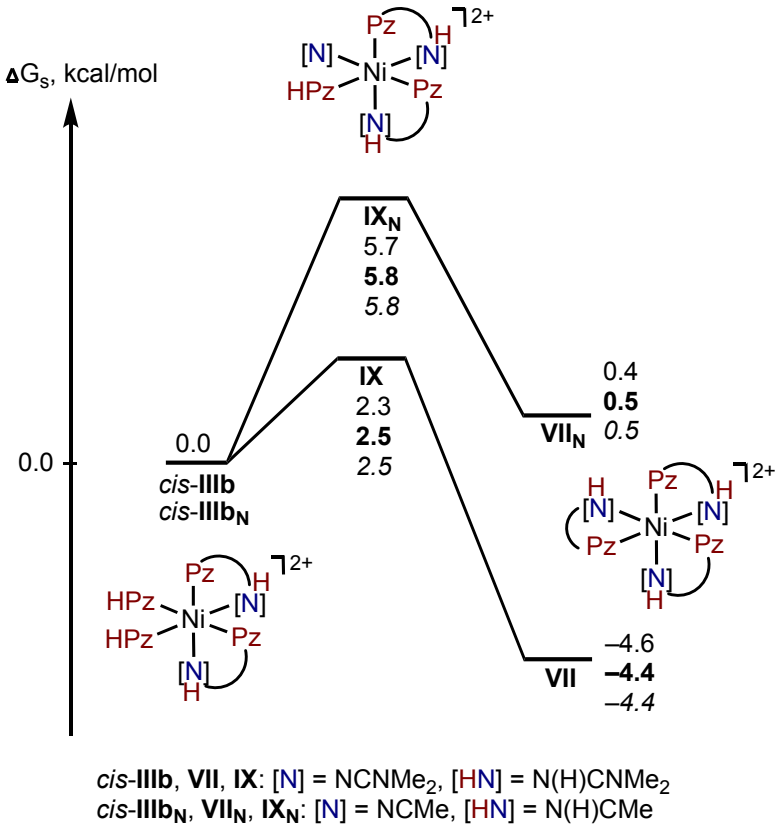


Figure S39. Energy profile of the *tris*-chelate product formation from the *bis*-chelate products (Gibbs free energies are indicated relative to ***cis*-IIIb** and ***cis*-IIIbN** calculated using the M06 (plain text), CAM-B3LYP (bold) and wB97XD (italic) functionals).

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Table S4. Cartesian atomic coordinates (in Å) of the calculated structures.

$[Ni(H_2O)_6]^{2+}$

Ni	-0.022042	0.182498	-0.655387
O	1.235239	1.809282	-0.469411
O	-0.014021	0.260696	-2.718282
O	-0.030051	0.104284	1.407507
O	1.538776	-1.159192	-0.816770
O	-1.279325	-1.444284	-0.841349
O	-1.582854	1.524197	-0.493995
H	0.577058	0.656090	1.928156
H	-0.303340	-0.639527	1.968580
H	0.259258	1.004512	-3.279354
H	-0.621144	-0.291101	-3.238924
H	0.881685	2.713872	-0.499711
H	2.178442	1.856292	-0.695031
H	2.160953	-1.422413	-0.119326
H	1.975026	-1.313608	-1.671191
H	-2.019111	1.678593	0.360426
H	-2.205029	1.787428	-1.191438
H	-2.222534	-1.491290	-0.615755
H	-0.925777	-2.348877	-0.811047

$[Ni(PzH)_3(NCNMe_2)_2(H_2O)]^{2+}$, isomer 1

Ni	0.032376	-0.232285	-0.327086
N	2.130329	-0.006691	-0.195454
N	1.063709	-2.885780	0.670640
N	0.220768	-2.290619	-0.193986
C	0.962668	-4.229906	0.628532
H	1.565738	-4.863536	1.266418
C	0.009057	-4.532384	-0.321351
H	-0.326378	-5.515077	-0.623025
H	1.632589	-2.308162	1.277556
C	-0.423860	-3.290657	-0.799210
H	-1.179457	-3.069913	-1.545478
N	-2.008487	-0.428496	-0.717564
N	0.365899	2.452896	-1.655212
N	0.511866	0.779315	2.487314
H	1.208928	1.372359	2.054098
N	-0.194756	-0.069942	1.716202
N	-0.167205	1.811782	-0.598024
C	-1.024741	-0.697710	2.550294
H	-1.700470	-1.452203	2.162213
C	0.026378	3.757940	-1.672419
H	0.360926	4.419801	-2.461221
C	-0.757149	3.985681	-0.559361
H	-1.196273	4.923978	-0.249203
C	-0.852204	-0.246799	3.864049
H	-1.377347	-0.569901	4.752342
H	0.853752	1.902647	-2.353757
C	-0.850557	2.740050	0.073179
H	-1.379946	2.465400	0.980052

C	0.143932	0.704449	3.783113
H	0.610718	1.320988	4.540831
C	3.271829	0.175537	-0.391399
N	4.538029	0.380331	-0.598180
C	5.085485	1.740142	-0.665192
C	5.481639	-0.736586	-0.724941
H	5.597713	1.877909	-1.624150
H	5.800220	1.890555	0.152167
H	4.278482	2.472382	-0.579445
H	6.215808	-0.691897	0.087729
H	6.000664	-0.665361	-1.687412
H	4.944836	-1.687113	-0.676333
C	-3.171328	-0.302188	-0.644436
N	-4.459987	-0.156600	-0.582183
C	-5.347722	-1.292443	-0.311013
C	-5.082407	1.144172	-0.852883
H	-5.696098	1.437650	0.006236
H	-5.716239	1.071650	-1.744333
H	-4.309012	1.898792	-1.018847
H	-5.998780	-1.465157	-1.175833
H	-5.963180	-1.070101	0.567931
H	-4.756607	-2.191113	-0.118900
O	0.315388	-0.323389	-2.485844
H	-0.556926	-0.478958	-2.884391
H	0.859206	-1.090514	-2.726733

$[Ni(PzH)_3(NCNMe_2)_2(H_2O)]^{2+}$, isomer 2

Ni	0.012211	-0.321154	-0.374111
N	1.713574	0.829111	-0.700789
N	0.521088	-3.280184	-0.775201
N	-1.227704	1.353120	-0.346231
N	1.119913	-2.080268	-0.631250
C	1.404653	-4.251759	-1.073729
H	1.089676	-5.277031	-1.222204
C	2.651970	-3.661294	-1.128744
H	3.595509	-4.143698	-1.344396
H	-0.485453	-3.336627	-0.657817
C	2.420646	-2.310439	-0.851335
H	3.122417	-1.485158	-0.802535
O	-0.365125	-0.440590	-2.478401
N	1.360557	-1.006569	2.237174
N	-2.295773	-1.531271	1.149623
H	-1.740128	-1.265791	1.955829
N	-1.744560	-1.428655	-0.075735
N	0.413223	-0.234642	1.668259
C	-2.701956	-1.815956	-0.926252
H	-2.502817	-1.807069	-1.992307
C	1.676723	-0.583241	3.476584
H	2.411801	-1.100113	4.080743
C	0.898972	0.528437	3.734363
H	0.883253	1.120454	4.639269

C	-3.864951	-2.180924	-0.238174
H	-4.793266	-2.550219	-0.652450
H	1.738878	-1.784656	1.707308
C	0.135128	0.706774	2.575730
H	-0.599576	1.469256	2.342402
C	-3.564530	-1.981765	1.095146
H	-4.148668	-2.138078	1.993412
C	2.537858	1.659040	-0.657884
N	3.462932	2.570314	-0.596838
C	3.961141	3.041833	0.699202
C	4.078433	3.124792	-1.806698
H	3.829799	4.127885	0.766539
H	5.025894	2.799318	0.796366
H	3.403888	2.560891	1.507859
H	5.150577	2.896508	-1.811988
H	3.939265	4.211760	-1.821324
H	3.614012	2.690778	-2.695338
C	-2.114884	2.116503	-0.382267
N	-3.110198	2.951407	-0.415454
C	-4.492398	2.460527	-0.434809
C	-2.899709	4.400461	-0.491001
H	-4.498375	1.368702	-0.369837
H	-4.980977	2.770771	-1.365880
H	-5.039656	2.877740	0.418223
H	-3.395438	4.884916	0.357864
H	-3.322950	4.785956	-1.425855
H	-1.830800	4.624346	-0.458878
H	0.427543	-0.740178	-2.951746
H	-0.569261	0.441877	-2.826617

$[Ni(PzH)_3(NCNMe_2)_2(H_2O)]^{2+}$, isomer 3

Ni	-0.202689	-0.135864	-0.509566
N	1.900783	-0.360184	-0.555484
N	-0.980852	2.757227	-0.510096
N	0.004980	1.905216	-0.847295
C	-0.653729	4.037724	-0.771769
H	-1.337921	4.850635	-0.564177
C	0.616873	4.026774	-1.310132
H	1.194483	4.878344	-1.642441
H	-1.838598	2.378128	-0.123705
C	0.981085	2.676497	-1.332550
H	1.906336	2.225344	-1.675084
N	-0.228334	0.102240	1.538156
N	0.542648	-2.961029	0.178568
N	-2.917445	0.139953	-1.812840
H	-2.356971	0.181084	-2.658276
N	-2.277338	0.050767	-0.629094
N	-0.410644	-2.188411	-0.375983
C	-3.243292	-0.061922	0.287503
H	-2.977412	-0.160735	1.333623
C	0.161335	-4.251799	0.254710

H	0.810741	-5.011129	0.671592
C	-1.109641	-4.328612	-0.277088
H	-1.724773	-5.212000	-0.379293
C	-4.507315	-0.044629	-0.312159
H	-5.472788	-0.114606	0.169886
H	1.411313	-2.523120	0.462517
C	-1.421324	-3.017051	-0.651055
H	-2.331937	-2.630684	-1.097318
C	-4.255608	0.082217	-1.664091
H	-4.922444	0.138960	-2.515304
C	3.055786	-0.187006	-0.658604
N	4.332499	0.027810	-0.768981
C	4.982640	1.084792	0.015457
C	5.190860	-0.838657	-1.585728
H	5.564125	1.723528	-0.658664
H	5.652576	0.639364	0.760185
H	4.225942	1.690525	0.521309
H	5.906058	-1.363133	-0.941474
H	5.737936	-0.225487	-2.310377
H	4.582346	-1.571158	-2.121556
C	-0.178093	0.202317	2.702274
N	-0.128320	0.313220	3.997105
C	0.302487	1.559477	4.637840
C	-0.546252	-0.788340	4.870197
H	-1.400066	-0.471261	5.480360
H	0.284597	-1.066991	5.528484
H	-0.834536	-1.653676	4.268356
H	1.162192	1.357458	5.287041
H	-0.517884	1.966296	5.240621
H	0.588621	2.290535	3.877803
O	-0.271287	-0.369707	-2.691161
H	-0.004193	-1.271861	-2.932470
H	0.345248	0.227542	-3.143979

0

Ni	-0.010815	-0.065890	-0.062121
N	2.010398	-0.022297	-0.376252
N	0.824829	-1.254035	2.542281
H	1.505321	-1.759825	1.987257
N	0.001731	-0.375267	1.936042
C	-0.770306	0.122106	2.905529
H	-1.526209	0.860287	2.659461
C	-0.437312	-0.439288	4.142405
H	-0.883365	-0.234269	5.105886
C	0.591002	-1.318814	3.868483
H	1.164543	-1.973895	4.512056
N	-2.024853	0.028879	-0.380304
N	-1.010441	-2.866502	-0.043397
N	0.839286	2.624761	0.930354
H	1.365845	2.087222	1.608590
N	0.020343	1.981603	0.074649

N	-0.047008	-2.058897	-0.531755
C	-0.573552	2.942863	-0.635763
H	-1.277084	2.678545	-1.417242
C	-0.879748	-4.129791	-0.493603
H	-1.567573	-4.910805	-0.194904
C	0.223141	-4.151745	-1.323012
H	0.619562	-5.000642	-1.862774
C	-0.140413	4.208801	-0.228147
H	-0.442614	5.171440	-0.616971
H	-1.708692	-2.479923	0.580914
C	0.705021	-2.839730	-1.312222
H	1.552879	-2.417161	-1.838368
C	0.761714	3.963454	0.786461
H	1.338944	4.633759	1.410843
C	3.056121	0.183510	-0.865341
N	4.220652	0.415899	-1.383355
C	5.087183	-0.676821	-1.842805
C	4.702431	1.791397	-1.565411
H	6.047442	-0.621856	-1.318058
H	5.254543	-0.582234	-2.921652
H	4.617324	-1.640602	-1.630903
H	4.876046	1.978458	-2.631074
H	5.639692	1.923685	-1.013389
H	3.956632	2.497981	-1.191813
C	-3.094237	0.258525	-0.801552
N	-4.280634	0.521955	-1.251465
C	-4.966402	1.766894	-0.881523
C	-4.998442	-0.419776	-2.120206
H	-5.251519	0.079276	-3.062152
H	-5.917991	-0.747610	-1.622304
H	-4.368791	-1.287343	-2.331244
H	-5.877821	1.531264	-0.320469
H	-5.230852	2.317026	-1.791526
H	-4.309682	2.383960	-0.262474

trans-**I**

Ni	0.535269	-0.568848	-0.084977
N	-1.605865	-0.428355	-0.140552
N	1.692223	2.006873	0.959834
N	-0.823475	-3.251504	0.151413
H	-1.608973	-2.651797	0.387343
N	0.305993	-2.658363	-0.281032
N	0.723851	1.485939	0.185165
C	1.160776	-3.659527	-0.515132
H	2.154906	-3.436521	-0.886501
C	1.565925	3.341848	1.097802
H	2.264966	3.919498	1.689080
C	0.455171	3.716673	0.369342
H	0.060188	4.715743	0.246307
C	0.575007	-4.897834	-0.225838
H	1.014050	-5.881327	-0.324284

H	2.386504	1.381644	1.351412
C	-0.031154	2.523511	-0.178295
H	-0.880402	2.364183	-0.833748
C	-0.703181	-4.592059	0.201104
H	-1.521912	-5.224193	0.521169
N	2.653834	-0.751139	-0.044800
N	0.922793	-1.878339	2.640010
N	0.141660	-1.249905	-3.004887
H	-0.304201	-2.080007	-2.632618
N	0.647817	-0.347314	-2.145109
N	0.428677	-0.807297	1.990681
C	1.207400	0.591733	-2.907840
H	1.684978	1.445935	-2.440000
C	0.704258	-1.806788	3.969371
H	1.037434	-2.587673	4.641119
C	0.032488	-0.624649	4.202754
H	-0.300891	-0.239301	5.156510
C	1.060525	0.288004	-4.267324
H	1.402530	0.861561	-5.117914
H	1.373679	-2.612756	2.105965
C	-0.114023	-0.041763	2.938063
H	-0.578471	0.900194	2.662569
C	0.370165	-0.906254	-4.289106
H	0.030613	-1.525011	-5.109986
C	-2.631310	0.142659	-0.141229
N	-3.767428	0.772724	-0.135340
C	-4.404697	1.161221	1.127968
C	-4.527083	0.986224	-1.372626
H	-5.330395	0.590718	1.268349
H	-4.639138	2.231054	1.099258
H	-3.726897	0.962990	1.962382
H	-4.775593	2.049486	-1.462412
H	-5.452548	0.398997	-1.346513
H	-3.928402	0.682718	-2.234825
C	3.777994	-0.864148	-0.355428
N	5.021394	-0.988322	-0.716834
C	5.450754	-0.581228	-2.059159
C	6.053701	-1.444575	0.218716
H	6.783390	-0.643231	0.384474
H	6.565343	-2.317524	-0.202140
H	5.598497	-1.720537	1.172993
H	5.966188	-1.418593	-2.542978
H	6.134536	0.272897	-1.988047
H	4.579894	-0.301759	-2.658257

cis-**I**

Ni	-0.021036	-0.138633	-0.003059
N	-1.103043	1.349378	-1.131213
N	-1.337046	0.969065	2.471892
N	1.318837	0.811093	-2.529748
H	0.431735	1.302564	-2.610293

N	1.461037	-0.046839	-1.502550
N	-1.503598	0.068271	1.485892
C	2.722480	-0.478105	-1.579133
H	3.102074	-1.179010	-0.841938
C	-2.462287	1.147962	3.190179
H	-2.494010	1.827490	4.032699
C	-3.425197	0.323369	2.641926
H	-4.444848	0.191560	2.978436
C	3.388165	0.099823	-2.667526
H	4.403396	-0.076527	-2.996945
H	-0.437529	1.440246	2.529526
C	-2.776794	-0.323168	1.582152
H	-3.177032	-1.045936	0.877976
C	2.448559	0.924658	-3.254531
H	2.498959	1.562467	-4.128166
N	1.085466	1.401779	1.030505
N	-1.601990	-2.731872	-0.264934
N	1.496193	-2.739514	0.420068
H	1.192222	-2.947964	-0.524671
N	1.077808	-1.598923	1.009242
N	-1.119851	-1.656282	-0.924650
C	1.666534	-1.588493	2.206124
H	1.479533	-0.766620	2.888579
C	-2.396400	-3.489461	-1.051578
H	-2.862785	-4.393761	-0.681009
C	-2.432581	-2.882583	-2.289767
H	-2.962407	-3.221686	-3.169385
C	2.469320	-2.722058	2.385538
H	3.054337	-2.991850	3.254126
H	-1.362743	-2.861590	0.712008
C	-1.622253	-1.748120	-2.156715
H	-1.370153	-0.993954	-2.894073
C	2.335675	-3.437964	1.213993
H	2.760795	-4.381926	0.896556
C	-2.144097	1.827296	-0.858757
N	-3.294318	2.341748	-0.561738
C	-4.538476	1.712423	-1.016960
C	-3.400099	3.535850	0.281776
H	-5.085735	2.402930	-1.668443
H	-5.156184	1.466118	-0.144988
H	-4.308749	0.796461	-1.569044
H	-3.941455	3.279986	1.201130
H	-3.944175	4.319360	-0.257411
H	-2.400937	3.898702	0.536193
C	2.146990	1.820852	0.740370
N	3.322936	2.263605	0.428768
C	3.497237	3.424137	-0.449404
C	4.528815	1.591851	0.924951
H	5.150008	1.294693	0.071559
H	4.246624	0.701472	1.494614

H	5.095630	2.273669	1.568931
H	4.049366	3.116001	-1.345765
H	4.060145	4.202922	0.077250
H	2.520158	3.817834	-0.740755

II

Ni	0.001660	-0.015324	-0.332113
N	1.659927	-0.510744	0.827533
N	0.663172	1.991458	-2.512112
N	-1.291861	-1.106382	0.885172
N	1.212861	1.155464	-1.610445
C	1.558152	2.877484	-2.990855
H	1.282984	3.614392	-3.734917
C	2.761703	2.610113	-2.368747
H	3.703890	3.119140	-2.519598
H	-0.325561	1.894932	-2.718842
C	2.490961	1.534287	-1.514976
H	3.148289	1.013801	-0.827400
N	-0.330802	1.746543	0.731207
N	1.469258	-1.760628	-2.334443
N	-2.169210	-0.575738	-2.375713
H	-1.593512	-1.389637	-2.565614
N	-1.688775	0.365838	-1.541065
N	0.449032	-1.750588	-1.454954
C	-2.659239	1.279637	-1.447263
H	-2.514226	2.143557	-0.808283
C	1.816274	-3.012472	-2.691416
H	2.611941	-3.198653	-3.401786
C	0.979358	-3.872598	-2.008160
H	0.966301	-4.952714	-2.060712
C	-3.760763	0.925776	-2.235535
H	-4.684042	1.472049	-2.372371
H	1.873949	-0.872850	-2.613224
C	0.152263	-3.037181	-1.248161
H	-0.640064	-3.293579	-0.553865
C	-3.407734	-0.277108	-2.814514
H	-3.935756	-0.924475	-3.503325
C	2.403432	-1.060639	1.543087
N	3.241497	-1.674651	2.328848
C	3.779381	-2.988313	1.968798
C	3.755065	-1.039103	3.543533
H	3.591352	-3.694959	2.785400
H	4.860090	-2.915598	1.796534
H	3.291400	-3.352381	1.060631
H	4.835980	-0.877854	3.451920
H	3.559501	-1.688040	4.405031
H	3.258993	-0.078038	3.698817
C	-0.193806	2.724277	1.357580
N	-0.043478	3.821162	2.044076
C	0.797733	4.908817	1.539972
C	-0.791012	4.056892	3.280512

H	-1.484875	4.895178	3.143798
H	-0.090762	4.297241	4.088769
H	-1.355780	3.161330	3.550410
H	1.540964	5.175930	2.300059
H	0.180030	5.786913	1.315476
H	1.314418	4.587150	0.631659
C	-2.171283	-1.427122	1.585795
N	-3.157318	-1.790792	2.355606
C	-4.544671	-1.656380	1.906235
C	-2.919776	-2.450346	3.640759
H	-4.574973	-1.124023	0.951736
H	-5.114897	-1.089666	2.651308
H	-4.996815	-2.648153	1.783998
H	-3.293278	-3.480993	3.606982
H	-3.444051	-1.903102	4.432631
H	-1.849667	-2.461282	3.861160

trans-**III**

N	-1.567672	-0.177537	-1.460018
N	-2.715804	-0.391971	-0.754883
N	-1.695492	0.352141	1.155389
H	-1.769374	0.985594	1.949226
N	0.105554	2.153451	-0.368463
N	-0.596823	2.698021	-1.379574
H	-1.178932	2.089107	-1.942959
N	-4.060170	0.477022	0.967933
C	-2.823160	0.194777	0.529311
C	-2.879159	-1.672043	-2.540976
H	-3.234464	-2.368669	-3.288380
C	-1.677367	-0.942713	-2.539437
H	-0.885500	-0.941684	-3.281360
C	-3.511035	-1.307599	-1.379450
H	-4.451500	-1.628332	-0.948428
C	0.801060	3.162488	0.155862
H	1.457124	2.988613	1.002237
C	-0.358107	4.020110	-1.507504
H	-0.840048	4.611369	-2.275661
C	0.543683	4.360741	-0.522458
H	0.956564	5.339767	-0.321913
C	-4.243434	0.805864	2.376837
H	-3.609940	0.167363	3.001043
H	-5.286817	0.614795	2.644862
H	-4.022105	1.863383	2.580524
C	-5.191968	0.824340	0.104072
H	-5.554568	1.820600	0.384175
H	-6.011305	0.107208	0.233659
H	-4.895158	0.854437	-0.945980
Ni	0.025462	0.083663	-0.021963
N	1.537335	0.250363	1.413048
N	2.768180	0.235704	0.835529
N	1.741271	-0.202180	-1.162799

H	1.823659	-0.606589	-2.091887
N	4.094900	-0.456904	-0.985504
C	2.861640	-0.184781	-0.515222
C	3.053582	1.150759	2.821340
H	3.489096	1.609750	3.698694
C	1.709488	0.789424	2.609275
H	0.861065	0.910405	3.274572
C	3.697478	0.800822	1.663169
H	4.729682	0.923601	1.363102
C	5.138296	-1.130537	-0.205865
H	4.786112	-1.382529	0.796700
H	6.038628	-0.508057	-0.137063
H	5.403806	-2.067233	-0.711321
C	4.281800	-0.521583	-2.429717
H	5.344486	-0.376030	-2.646040
H	3.725266	0.283262	-2.920884
H	3.978389	-1.495910	-2.841611
N	-0.121933	-2.002533	0.303815
N	-0.568427	-2.482212	1.478586
H	-0.909142	-1.823920	2.168295
C	0.233554	-3.078698	-0.397136
H	0.633884	-2.963316	-1.398422
C	-0.502805	-3.828677	1.536046
H	-0.823453	-4.375850	2.413398
C	0.013537	-4.254900	0.330586
H	0.202677	-5.274022	0.022572

cis-**IIIa**

Ni	0.000000	0.187630	0.000000
N	1.648560	0.008268	1.254167
H	1.760363	0.333516	2.210885
N	2.460086	-1.271859	-0.457956
N	3.810451	-0.953525	1.450591
N	-1.307526	1.564805	2.433559
H	-1.071453	0.724758	2.946325
N	-0.995821	1.654750	1.124425
N	1.200905	-1.297837	-0.965646
C	-1.517691	2.814073	0.723132
H	-1.396968	3.125173	-0.308682
C	3.368350	-1.712511	-1.379101
H	4.430830	-1.725295	-1.175419
C	2.666202	-2.076311	-2.498951
H	3.066786	-2.489971	-3.414844
C	-2.164787	3.471899	1.776546
H	-2.671313	4.426913	1.752556
C	2.635483	-0.716815	0.834739
C	1.321339	-1.798354	-2.185784
H	0.433717	-1.943962	-2.793490
C	-2.013259	2.634569	2.860332
H	-2.346678	2.719669	3.886810
C	4.176276	-0.111995	2.583551

H	3.696491	-0.444186	3.516415
H	5.260620	-0.169077	2.718530
H	3.917508	0.932201	2.380293
C	4.528086	-2.230971	1.386076
H	3.982312	-2.965100	0.789468
H	5.535551	-2.094224	0.974849
H	4.622071	-2.631156	2.403069
N	-1.648560	0.008274	-1.254167
H	-1.760362	0.333527	-2.210884
N	-2.460086	-1.271862	0.457950
N	-3.810451	-0.953517	-1.450596
N	1.307528	1.564817	-2.433551
H	1.071456	0.724773	-2.946322
N	0.995821	1.654755	-1.124417
N	-1.200905	-1.297842	0.965640
C	1.517690	2.814076	-0.723117
H	1.396967	3.125171	0.308698
C	-3.368351	-1.712519	1.379091
H	-4.430830	-1.725303	1.175409
C	-2.666203	-2.076327	2.498939
H	-3.066788	-2.489994	3.414829
C	2.164785	3.471909	-1.776527
H	2.671311	4.426923	-1.752532
C	-2.635482	-0.716810	-0.834742
C	-1.321340	-1.798363	2.185776
H	-0.433719	-1.943973	2.793483
C	2.013259	2.634585	-2.860318
H	2.346678	2.719691	-3.886796
C	-4.176275	-0.111980	-2.583552
H	-3.696489	-0.444166	-3.516417
H	-5.260619	-0.169061	-2.718531
H	-3.917506	0.932214	-2.380288
C	-4.528087	-2.230963	-1.386088
H	-3.982313	-2.965096	-0.789485
H	-5.535551	-2.094218	-0.974861
H	-4.622071	-2.631141	-2.403084

cis-**IIIb**

Ni	-0.051239	0.240043	0.053349
N	-1.695928	-0.096834	1.273168
H	-2.016364	0.555053	1.985974
N	-2.262710	-1.610829	-0.343260
N	-3.878339	-1.033814	1.272327
N	1.497076	2.737370	1.017537
H	1.479828	3.052451	0.055755
N	0.870135	1.592058	1.351380
N	-1.181668	-1.194977	-1.056293
C	1.052670	1.466048	2.666193
H	0.649268	0.599679	3.178927
C	-2.666815	-2.850761	-0.752729
H	-3.487175	-3.369020	-0.273047

C	-1.845224	-3.227344	-1.783134
H	-1.890358	-4.145943	-2.352618
C	1.791109	2.538300	3.181036
H	2.088942	2.710249	4.206165
C	-2.635484	-0.847566	0.792834
C	-0.934041	-2.163565	-1.924675
H	-0.102769	-2.063195	-2.615509
C	2.058795	3.336377	2.089139
H	2.596913	4.271285	1.997135
C	-4.186344	-0.534012	2.607113
H	-4.420228	0.540638	2.598298
H	-5.060570	-1.073115	2.984164
H	-3.350417	-0.727870	3.287029
C	-5.049287	-1.320102	0.439338
H	-4.785696	-1.349490	-0.619874
H	-5.512105	-2.270701	0.730930
H	-5.785093	-0.519092	0.580759
N	1.150737	-1.293169	0.794933
H	0.856324	-2.070240	1.380905
N	2.646287	-0.457313	-0.713796
N	3.242596	-2.383656	0.509154
N	-1.381276	1.714016	-2.251881
H	-1.213837	0.846539	-2.747665
N	-1.004424	1.810011	-0.961206
N	1.632517	0.268016	-1.259583
C	-1.451739	2.999829	-0.555749
H	-1.277499	3.318866	0.466729
C	3.860028	0.033128	-1.097996
H	4.786549	-0.388042	-0.729566
C	3.625083	1.080913	-1.951693
H	4.362254	1.687664	-2.460349
C	-2.118308	3.669722	-1.589587
H	-2.581422	4.646454	-1.559005
C	2.309257	-1.448121	0.245607
C	2.224045	1.185734	-2.013827
H	1.618211	1.892789	-2.572363
C	-2.057989	2.807630	-2.663913
H	-2.438268	2.891377	-3.674191
C	3.085807	-3.190246	1.713108
H	2.384271	-4.024066	1.561368
H	4.061923	-3.607504	1.978507
H	2.747514	-2.565386	2.545913
C	4.136750	-2.959591	-0.498831
H	3.960606	-2.522111	-1.483862
H	5.186496	-2.815773	-0.215717
H	3.942491	-4.037082	-0.569330

IV

Ni	0.044910	0.348914	0.148165
N	-1.740070	0.123910	1.294401
N	-2.441207	0.206367	-1.759608

N	0.426574	0.508466	3.129827
H	-0.587837	0.578474	3.067639
N	1.087925	0.178745	2.004351
N	-1.055476	0.578926	-1.653696
C	2.382901	0.174006	2.349170
H	3.134805	-0.075170	1.607028
C	-2.834193	0.520244	-2.960322
H	-3.851222	0.334272	-3.290455
C	-1.766388	1.109815	-3.713745
H	-1.773596	1.473796	-4.736156
C	2.544824	0.506268	3.698877
H	3.464847	0.572165	4.263786
C	-0.667761	1.099879	-2.776173
H	0.347209	1.454779	-2.921697
C	1.259303	0.715393	4.165354
H	0.888742	0.982258	5.147158
N	1.871044	0.472413	-0.900402
N	0.950943	3.111925	1.097271
N	0.534619	-2.553364	0.813834
H	0.825443	-2.157296	1.701163
N	0.049049	-1.724810	-0.127098
N	-0.002295	2.417600	0.443878
C	-0.239771	-2.505058	-1.168374
H	-0.647355	-2.067536	-2.072972
C	0.636743	4.420764	1.203398
H	1.291557	5.121139	1.706125
C	-0.579700	4.594189	0.578544
H	-1.133072	5.516514	0.467977
C	0.056524	-3.846382	-0.890017
H	-0.079259	-4.705594	-1.532730
H	1.734607	2.613036	1.504085
C	-0.933497	3.316645	0.127352
H	-1.824742	2.999004	-0.404161
C	0.553634	-3.836382	0.397683
H	0.906271	-4.634869	1.038210
C	-2.812116	-0.304052	1.073424
N	-3.993811	-0.813897	0.903005
C	2.491670	-0.596727	-1.222313
N	3.702269	-0.988155	-1.535852
C	4.854429	-0.082115	-1.514438
C	3.931749	-2.343519	-2.035276
C	-4.102494	-2.238152	0.572416
C	-5.122917	0.046789	0.544053
H	-3.237096	-2.777129	0.969134
H	-4.149467	-2.369677	-0.517079
H	-5.012813	-2.637466	1.031010
H	-6.019301	-0.314592	1.058206
H	-5.286976	0.019620	-0.541451
H	-4.921676	1.073789	0.858928
H	4.270407	-2.312427	-3.077839

H	2.995677	-2.908054	-1.972146
H	4.696728	-2.838409	-1.425779
H	4.634650	0.787766	-0.886554
H	5.104572	0.253109	-2.528490
H	5.716593	-0.609748	-1.092285
H	2.376828	1.357521	-1.040905

trans-**I•••**N(CN)(Me)$_2$

Ni	0.858251	0.180098	0.061630
N	-0.587393	1.696079	0.001042
N	1.757571	0.096502	2.972169
N	-1.143229	-0.636378	-2.081716
H	-1.869648	-0.412188	-1.387110
N	0.163632	-0.512349	-1.782556
N	1.525041	0.883435	1.905174
C	0.821535	-0.919033	-2.871583
H	1.906398	-0.901714	-2.877933
C	2.174349	0.807614	4.041136
H	2.400759	0.329883	4.985836
C	2.224029	2.128541	3.648360
H	2.520645	2.978860	4.246807
C	-0.067082	-1.309982	-3.877745
H	0.166644	-1.680558	-4.866334
H	1.567741	-0.895147	2.899983
C	1.809258	2.120257	2.310228
H	1.704799	2.945833	1.615073
C	-1.319264	-1.115378	-3.326535
H	-2.311613	-1.281199	-3.726616
N	2.314074	-1.393649	0.081083
N	-0.585833	-2.405165	0.724500
N	1.907859	2.188757	-1.954885
H	0.949282	2.184258	-2.280396
N	2.241935	1.405932	-0.914554
N	-0.484347	-1.101866	1.041782
C	3.542877	1.620217	-0.718348
H	4.052110	1.111570	0.093451
C	-1.514278	-3.034941	1.471977
H	-1.712235	-4.092795	1.353848
C	-2.051846	-2.089658	2.322870
H	-2.811071	-2.242653	3.078071
C	4.046595	2.545207	-1.641552
H	5.057152	2.920820	-1.724696
H	0.031330	-2.778954	0.012324
C	-1.379318	-0.901689	2.007073
H	-1.492767	0.090387	2.431370
C	2.961440	2.889139	-2.421197
H	2.863995	3.570411	-3.256712
C	-1.631001	2.220978	0.053508
N	-2.756548	2.877430	0.124572
C	-3.441891	2.975402	1.413743
C	-3.569511	3.059153	-1.077870

H	-4.162776	2.154080	1.526803
H	-3.968184	3.934542	1.458606
H	-2.710873	2.939830	2.226347
H	-4.000282	4.065961	-1.065306
H	-4.372124	2.310333	-1.107754
H	-2.944469	2.950400	-1.968366
C	3.414201	-1.785684	-0.019130
N	4.639688	-2.204368	-0.156398
C	5.291761	-2.154549	-1.468293
C	5.329610	-2.920999	0.919399
H	6.314652	-2.468431	1.078090
H	5.455268	-3.976427	0.648966
H	4.751794	-2.850951	1.844112
H	5.364216	-3.161222	-1.897730
H	6.298399	-1.738891	-1.348732
H	4.719949	-1.509129	-2.141433
N	-3.523779	-0.216806	-0.423502
C	-4.597282	-0.668483	-0.275998
N	-5.799191	-1.153333	-0.095977
C	-6.940821	-0.644476	-0.854071
C	-6.025721	-2.302323	0.776744
H	-7.736992	-0.344727	-0.162218
H	-7.324805	-1.420974	-1.527505
H	-6.637878	0.223198	-1.446029
H	-6.395294	-3.153339	0.190778
H	-6.768327	-2.045901	1.541970
H	-5.089020	-2.583351	1.265352

trans-**I**•••$(H_2O)_3$

Ni	-0.474221	-0.243383	0.039924
N	1.411098	-0.997766	-0.414222
N	-2.309710	-2.391072	1.100616
N	1.563041	2.038112	-0.250765
H	2.322999	1.331675	-0.309943
N	0.250873	1.722672	-0.242502
N	-1.184436	-2.168125	0.397403
C	-0.393664	2.898892	-0.190649
H	-1.477537	2.914355	-0.181866
C	-2.530190	-3.707137	1.294287
H	-3.394427	-4.062985	1.840602
C	-1.494225	-4.381620	0.680495
H	-1.349517	-5.452009	0.629048
C	0.508441	3.965374	-0.157926
H	0.285368	5.023066	-0.121456
H	-2.851591	-1.586589	1.396597
C	-0.684859	-3.376508	0.135962
H	0.230795	-3.463944	-0.436962
C	1.756313	3.366346	-0.202528
H	2.764489	3.772196	-0.215927
N	-2.469676	0.485901	0.430562
N	0.135197	1.095991	2.719655

N	-0.525798	0.447617	-2.901200
H	0.115971	1.177993	-2.615210
N	-1.026978	-0.370448	-1.959312
N	-0.003351	-0.087307	2.093601
C	-1.856887	-1.188719	-2.604564
H	-2.384939	-1.960151	-2.054173
C	0.350968	0.946178	4.041450
H	0.480899	1.799834	4.694616
C	0.353669	-0.411050	4.297501
H	0.488587	-0.897149	5.254293
C	-1.892216	-0.889252	-3.973194
H	-2.464492	-1.382234	-4.747072
H	0.074492	1.948042	2.170344
C	0.123510	-1.010223	3.051756
H	0.043148	-2.062438	2.795822
C	-1.022013	0.170351	-4.124802
H	-0.724713	0.736601	-4.998218
C	2.428278	-1.461437	-0.759557
N	3.530477	-2.029058	-1.158169
C	4.577622	-2.340903	-0.178518
C	3.977225	-1.797027	-2.535171
H	5.336373	-1.548153	-0.192496
H	5.031091	-3.301309	-0.443552
H	4.142533	-2.397978	0.822029
H	4.553596	-2.668389	-2.861732
H	4.604039	-0.897157	-2.577417
H	3.111480	-1.680779	-3.192840
C	-3.494617	1.017930	0.225890
N	-4.627440	1.607935	-0.020838
C	-5.308661	1.398126	-1.303095
C	-5.333866	2.376608	1.008410
H	-6.272730	1.873840	1.269416
H	-5.555821	3.378043	0.622998
H	-4.711231	2.464845	1.902029
H	-5.547923	2.371296	-1.746214
H	-6.235655	0.833805	-1.146066
H	-4.655339	0.844802	-1.983367
O	4.032242	0.817822	-0.330559
H	4.044330	0.539060	0.605860
H	4.563046	1.639727	-0.378032
O	3.207336	-0.276501	2.058070
O	5.059947	3.440078	-0.433150
H	3.359508	-0.307788	3.011769
H	2.270173	-0.491272	1.934096
H	5.651040	3.788973	0.248819
H	5.441878	3.748954	-1.266826

V•••$N(H)(CN)(Me)_2^+$

Ni	0.258915	0.084372	0.160061
N	-1.687762	0.737388	-0.572797
N	0.740741	0.873233	3.012491

N	-0.472033	-1.614347	-2.140115
H	-1.950736	-1.698479	-1.249694
N	0.545026	-0.883987	-1.615209
N	-0.176141	0.921041	2.028964
C	1.670266	-1.159500	-2.312976
H	2.607800	-0.669329	-2.060933
C	0.217015	1.200236	4.209655
H	0.821350	1.215251	5.107708
C	-1.118045	1.482212	4.000604
H	-1.847614	1.783810	4.739596
C	1.393965	-2.079254	-3.315450
H	2.070472	-2.491909	-4.052362
H	1.673901	0.554471	2.767334
C	-1.310855	1.290734	2.627130
H	-2.224975	1.368313	2.049666
C	0.031073	-2.330032	-3.157543
H	-0.606284	-2.987915	-3.743092
N	2.303893	-0.215983	0.835629
N	0.372056	-2.899947	0.511901
N	1.063671	2.064184	-1.958310
H	0.851169	1.268649	-2.555348
N	0.965599	1.891662	-0.628949
N	-0.254493	-1.808363	0.995102
C	1.337482	3.050510	-0.088369
H	1.334169	3.164758	0.990432
C	0.232767	-3.964686	1.325998
H	0.677731	-4.922744	1.087313
C	-0.534012	-3.552886	2.399480
H	-0.844292	-4.144909	3.249878
C	1.685788	3.976905	-1.082913
H	2.029525	4.994255	-0.953247
H	0.873901	-2.814633	-0.368023
C	-0.800169	-2.199602	2.149630
H	-1.359660	-1.488576	2.749380
C	1.500122	3.302551	-2.273438
H	1.648981	3.605892	-3.302231
C	-2.209933	1.790832	-0.590216
N	-2.810135	2.942865	-0.622709
C	-3.938520	3.226965	0.269580
C	-2.285450	4.039056	-1.441601
H	-4.759565	3.653238	-0.317536
H	-3.637782	3.943716	1.043594
H	-4.283132	2.300436	0.738796
H	-1.926006	4.847519	-0.793456
H	-3.080030	4.419932	-2.093096
H	-1.455489	3.675591	-2.054941
C	3.442234	-0.284048	0.557878
N	4.698441	-0.315900	0.225626
C	5.306056	0.847821	-0.428331
C	5.572887	-1.432469	0.594871

H	6.336891	-1.087568	1.301540
H	6.061651	-1.822881	-0.304742
H	4.984859	-2.227448	1.059485
H	5.807862	0.523646	-1.347239
H	6.039868	1.314398	0.239704
H	4.527731	1.575983	-0.678620
N	-3.825412	-0.844327	1.046708
C	-3.369448	-1.355751	0.112318
N	-2.873530	-2.002662	-1.013192
C	-3.696807	-1.669904	-2.235180
C	-2.777365	-3.491949	-0.777557
H	-4.720276	-2.020107	-2.082558
H	-3.223831	-2.177137	-3.079799
H	-3.658578	-0.587922	-2.377708
H	-2.218797	-3.904194	-1.622140
H	-3.786596	-3.907370	-0.726443
H	-2.237625	-3.659570	0.159659

V•••$H_3O(H_2O)_2^+$

Ni	-0.427590	0.316579	-0.053464
N	1.463838	0.954846	0.613470
N	-1.822921	2.457054	-1.672977
N	1.019379	-2.286968	0.568947
H	2.466850	-1.728563	0.379999
N	-0.130903	-1.572708	0.729001
N	-0.768015	2.219124	-0.872508
C	-1.048369	-2.394090	1.270531
H	-2.050121	-2.030609	1.484246
C	-1.844960	3.731252	-2.112829
H	-2.630936	4.092671	-2.763720
C	-0.742976	4.361979	-1.571272
H	-0.447631	5.393555	-1.705289
C	-0.507873	-3.657097	1.486139
H	-0.988973	-4.526854	1.913532
H	-2.470588	1.690110	-1.832171
C	-0.109239	3.375933	-0.804265
H	0.783878	3.447963	-0.194685
C	0.795904	-3.534746	1.024733
H	1.590095	-4.274976	0.999630
N	-2.419460	-0.196597	-0.755566
N	0.663932	-1.552213	-2.225315
N	-0.993611	0.368015	2.914900
H	-0.395155	-0.451361	2.905054
N	-1.299320	0.940236	1.737780
N	0.359949	-0.268193	-1.959580
C	-2.143921	1.927632	2.031674
H	-2.527720	2.560735	1.238687
C	0.919621	-1.748500	-3.532173
H	1.174513	-2.727398	-3.918795
C	0.771802	-0.527836	-4.163878
H	0.886338	-0.315809	-5.218409

C	-2.390539	1.982785	3.410169
H	-3.025150	2.676108	3.944869
H	0.713852	-2.196534	-1.430676
C	0.414444	0.359680	-3.141100
H	0.193487	1.420913	-3.198536
C	-1.633153	0.960567	3.944116
H	-1.504503	0.618786	4.963160
C	2.516531	1.303823	0.983671
N	3.685308	1.704486	1.396778
C	4.494911	2.604178	0.573384
C	4.311839	1.106801	2.575366
H	5.342287	2.059307	0.138624
H	4.868359	3.423849	1.197142
H	3.885383	3.016362	-0.235062
H	4.657466	1.903085	3.243962
H	5.167551	0.489063	2.274572
H	3.586652	0.485131	3.106352
C	-3.369282	-0.854675	-0.549927
N	-4.428025	-1.558777	-0.281046
C	-5.216918	-1.259157	0.917902
C	-4.916843	-2.601655	-1.185886
H	-5.907048	-2.326246	-1.567480
H	-4.988972	-3.550531	-0.642312
H	-4.226577	-2.718750	-2.024545
H	-5.340749	-2.176079	1.505898
H	-6.204143	-0.875868	0.633642
H	-4.695770	-0.510316	1.523058
O	3.425293	-1.476024	0.247309
H	3.502561	-0.881990	-0.571588
H	3.980880	-2.315986	0.180251
O	3.362375	0.271446	-1.673558
O	4.617768	-3.806861	0.253862
H	3.667837	0.158697	-2.585770
H	2.409096	0.471184	-1.736598
H	5.048716	-4.269282	-0.478524
H	5.090344	-4.082444	1.052250

VI

N	-0.760135	1.917474	1.094129
N	-1.167744	3.063757	0.517444
N	-1.629112	0.241992	-1.455768
N	-1.182121	-1.026320	1.149361
N	-2.329302	-0.636605	1.738587
H	-2.534115	0.355328	1.789701
N	-3.838735	-0.870108	-1.408170
C	-2.684466	-0.277970	-1.427236
C	-1.144746	3.488168	2.669062
H	-1.232746	3.978280	3.629019
C	-0.743367	2.173531	2.407140
H	-0.445802	1.391751	3.099653
C	-1.402839	4.031198	1.426227

H	-1.733458	5.018645	1.129743
C	-1.140164	-2.348298	1.309457
H	-0.304446	-2.915033	0.912970
C	-2.999850	-1.676556	2.280070
H	-3.927093	-1.533368	2.821084
C	-2.261090	-2.810401	2.013835
H	-2.490433	-3.826169	2.306075
C	-3.927136	-2.332833	-1.466991
H	-2.931139	-2.758403	-1.617406
H	-4.579263	-2.626936	-2.296770
H	-4.337841	-2.712888	-0.523081
C	-5.076848	-0.125264	-1.161574
H	-5.473396	-0.382598	-0.170962
H	-5.814777	-0.391556	-1.926004
H	-4.884258	0.949009	-1.214319
Ni	-0.017460	0.308624	-0.007866
N	0.961386	-1.301453	-0.948807
N	2.093651	-1.660363	-0.287868
N	1.683588	0.057648	1.160615
H	2.063495	0.746503	1.805411
N	3.811158	-0.996867	1.186823
C	2.558040	-0.796682	0.736264
C	1.616214	-3.354931	-1.614554
H	1.642859	-4.300764	-2.138806
C	0.680711	-2.311732	-1.754791
H	-0.186193	-2.254311	-2.404550
C	2.493943	-2.913902	-0.658670
H	3.352193	-3.395521	-0.208939
C	4.939024	-1.381779	0.332757
H	4.636156	-1.464753	-0.713221
H	5.379452	-2.328613	0.668026
H	5.707676	-0.601891	0.396316
C	4.190908	-0.388539	2.456346
H	5.056292	-0.928894	2.851689
H	3.375462	-0.482114	3.180802
H	4.469758	0.669241	2.338669
N	0.930323	1.671084	-1.290111
N	0.729049	1.634435	-2.620566
H	-0.004427	1.030755	-2.977020
C	1.891150	2.577774	-1.104740
H	2.232552	2.800307	-0.099157
C	1.533041	2.495827	-3.275341
H	1.494511	2.599839	-4.352267
C	2.306637	3.128180	-2.322732
H	3.060551	3.885343	-2.488954
H	-1.191725	3.119890	-0.494312

VII

Ni	0.000950	0.002035	-0.227989
N	0.771780	2.674194	0.585401
N	-1.403661	-1.128890	-1.257005

N	1.048589	1.402406	0.976577
N	1.692648	-0.641168	-1.243190
N	1.928192	-2.009244	0.570299
N	0.686941	-1.617669	0.961083
N	-0.275107	1.790372	-1.241818
N	-2.704816	-0.667665	0.562690
N	-3.667047	-1.848803	-1.238215
N	-1.744390	0.207413	0.961002
N	3.444371	-2.245236	-1.221080
N	0.237379	4.109253	-1.209123
C	2.363560	-1.613897	-0.719060
C	0.975244	3.554330	1.610745
H	0.766145	4.610876	1.506579
C	1.459786	1.496093	2.230612
H	1.752211	0.599356	2.768563
C	1.435726	2.831210	2.680378
H	1.714810	3.211263	3.653969
C	1.345585	5.051312	-1.026870
H	0.997306	5.977852	-0.554595
H	1.761443	5.300225	-2.011170
H	2.146780	4.612572	-0.428301
C	-2.580599	-1.230629	-0.731906
C	-3.576058	-0.931434	1.581869
H	-4.386815	-1.639490	1.471250
C	3.706242	-3.677356	-1.050433
H	4.680606	-3.842744	-0.574908
H	3.718983	-4.153159	-2.038958
H	2.923079	-4.157463	-0.459863
C	1.726362	-2.681664	2.658727
H	1.913311	-3.122022	3.628962
C	0.559006	-2.031737	2.211239
H	-0.365610	-1.841958	2.747880
C	-2.039487	0.516088	2.213294
H	-1.412244	1.216910	2.755913
C	-3.187094	-0.171886	2.654654
H	-3.662611	-0.120305	3.624935
C	0.225965	2.856531	-0.709668
C	4.129514	-1.636913	-2.354262
H	3.627179	-1.858904	-3.307882
H	5.145178	-2.041480	-2.400443
H	4.204025	-0.553550	-2.214984
C	-5.039213	-1.364292	-1.062140
H	-5.064787	-0.448155	-0.468294
H	-5.666558	-2.129010	-0.588280
H	-5.460583	-1.134794	-2.048776
C	-3.481970	-2.737410	-2.378281
H	-3.425068	-2.184146	-3.327838
H	-4.338784	-3.416170	-2.428663
H	-2.579647	-3.342797	-2.244363
C	-0.620166	4.400026	-2.350961

H	-0.776912	5.481989	-2.397446
H	-1.597138	3.922935	-2.222469
H	-0.166880	4.077086	-3.300320
C	2.585962	-2.634327	1.592031
H	3.605884	-2.980375	1.487510
H	1.945145	-0.439162	-2.206578
H	-1.355784	-1.440457	-2.223062
H	-0.566011	1.910021	-2.208087

VIII

N	2.837258	0.654480	0.789456
N	2.965703	-0.581825	0.238319
N	1.234069	-0.449696	-1.314019
H	1.039696	-0.561691	-2.309587
N	0.073833	2.250159	-0.908027
N	1.305995	2.716049	-0.625889
H	1.957821	2.095125	-0.123911
N	3.223202	-1.604173	-1.839290
C	2.435037	-0.861825	-1.036013
C	3.974022	-0.724518	2.188536
H	4.521955	-1.075358	3.052983
C	3.449630	0.567752	1.957255
H	3.505960	1.440129	2.599024
C	3.652030	-1.435205	1.065803
H	3.845377	-2.462046	0.778557
C	-0.545079	3.239471	-1.564435
H	-1.557316	3.105258	-1.928860
C	1.471321	3.968672	-1.082546
H	2.402694	4.501604	-0.938711
C	0.293402	4.346138	-1.700336
H	0.076783	5.288737	-2.183573
Ni	-0.467840	0.357901	-0.434048
N	-1.389257	-1.528939	-0.477274
N	-2.705532	-1.446026	-0.152316
N	-2.463505	0.817141	-0.288446
H	-2.892530	1.726639	-0.435027
N	-4.649074	-0.102377	-0.205373
C	-3.309037	-0.164842	-0.236077
C	-2.113846	-3.521491	0.296244
H	-2.127612	-4.561488	0.593709
C	-1.036132	-2.781001	-0.220447
H	-0.018205	-3.100957	-0.421613
C	-3.159466	-2.634390	0.342156
H	-4.173994	-2.756617	0.698051
N	-0.088538	0.411171	1.549432
N	0.319545	-0.605199	2.330718
H	0.487465	-1.515900	1.923353
C	-0.216577	1.458926	2.362646
H	-0.543583	2.411621	1.960430
C	0.457964	-0.221212	3.617595
H	0.776292	-0.917295	4.383283

C	0.118027	1.113759	3.677455
H	0.104499	1.747587	4.553476
C	-5.538618	-1.105257	-0.801255
C	-5.275225	1.190996	0.053303
C	4.688926	-1.539191	-1.829451
C	2.653029	-2.211249	-3.034465
H	-6.174069	-1.569549	-0.037518
H	-4.973328	-1.873233	-1.333619
H	-6.185140	-0.603511	-1.530814
H	-4.730673	1.726945	0.837303
H	-6.293016	1.013636	0.412887
H	-5.331883	1.806070	-0.856411
H	5.033132	-1.185800	-2.809110
H	5.114656	-2.532593	-1.645966
H	5.048338	-0.844239	-1.068706
H	2.598246	-1.499855	-3.871647
H	1.653247	-2.607473	-2.822846
H	3.292364	-3.045533	-3.338638

IX

Ni	-0.024285	-0.294388	0.094760
N	-1.491959	-1.017605	-1.157381
H	-1.475197	-1.935617	-1.594115
N	-2.728363	0.712470	-0.327578
N	-3.770689	-0.806850	-1.795426
N	1.485979	-1.484512	-0.681520
N	-1.823854	0.846338	0.682112
C	-3.429769	1.866705	-0.514631
H	-4.170193	1.958974	-1.299535
C	-2.994216	2.764939	0.426953
H	-3.350309	3.774749	0.580897
C	-2.656059	-0.457091	-1.126802
C	-1.993780	2.080861	1.139596
H	-1.387154	2.433615	1.968122
C	-3.656188	-1.802332	-2.853891
H	-3.642005	-2.826518	-2.453093
H	-4.521577	-1.704081	-3.516154
H	-2.753096	-1.622641	-3.446302
C	-5.130253	-0.605229	-1.288730
H	-5.122417	-0.101851	-0.319892
H	-5.724478	-0.019484	-2.000307
H	-5.609518	-1.583494	-1.158537
N	0.521603	1.328040	-1.113436
H	0.493078	1.325167	-2.129703
N	1.591394	2.012710	0.782640
N	2.050288	3.143821	-1.235017
N	-1.357404	-1.475140	2.518797
H	-2.018063	-0.725043	2.348916
N	-0.364245	-1.659004	1.627923
N	1.211401	0.839465	1.352867
C	0.349384	-2.679261	2.103700

H	1.219025	-3.024727	1.557556
C	1.961246	2.918092	1.737689
H	2.258932	3.926830	1.482263
C	1.849037	2.293802	2.953036
H	2.076705	2.711074	3.924814
C	-0.190184	-3.154957	3.305408
H	0.165574	-3.973089	3.916436
C	1.383728	2.151383	-0.612702
C	1.373532	1.000511	2.655905
H	1.143246	0.181150	3.329865
C	-1.289115	-2.354731	3.539132
H	-2.017181	-2.351347	4.340349
C	3.411735	3.560112	-0.889714
H	4.057892	3.411445	-1.763733
H	3.438796	4.622164	-0.617019
H	3.814702	2.960551	-0.070759
C	1.616737	3.529330	-2.571452
H	0.523321	3.543628	-2.625292
H	1.979200	4.541783	-2.773912
H	2.019242	2.857743	-3.344427
C	2.363703	-2.139148	-1.090729
N	3.352803	-2.860596	-1.536136
C	3.392310	-3.322482	-2.925619
C	4.374216	-3.377440	-0.621318
H	2.598776	-2.840529	-3.501806
H	3.259000	-4.410476	-2.963645
H	4.362044	-3.062050	-3.364543
H	5.367282	-3.120660	-1.006989
H	4.288959	-4.467985	-0.540454
H	4.250310	-2.928783	0.367825

TS1

N	-2.680894	0.502023	-1.327165
N	-2.978335	-0.388644	-0.343230
N	-1.369782	0.288368	1.184222
H	-1.253277	0.677223	2.119136
N	-0.013643	2.383787	-0.471089
N	-1.229024	2.933654	-0.668528
H	-2.000266	2.286510	-0.865477
N	-3.516813	-0.361568	1.926031
C	-2.588106	-0.121814	0.981275
C	-3.808430	-1.276331	-2.174648
H	-4.298673	-1.930230	-2.883364
C	-3.190900	-0.030981	-2.425198
H	-3.111816	0.501875	-3.366427
C	-3.659436	-1.472954	-0.829046
H	-3.964333	-2.283205	-0.177279
C	0.842640	3.414324	-0.420691
H	1.896100	3.228793	-0.248102
C	-1.152221	4.270101	-0.770737
H	-2.031156	4.872140	-0.964421

C	0.173954	4.624709	-0.598138
H	0.592616	5.621556	-0.603601
Ni	0.317692	0.415161	-0.011419
N	1.553801	-0.391453	1.478630
N	2.869856	-0.362720	1.130079
N	2.215852	0.564568	-0.846202
H	2.398245	0.712189	-1.835812
N	4.435102	-0.250940	-0.635030
C	3.183252	-0.012456	-0.208947
C	2.840669	-0.628470	3.319269
H	3.135386	-0.754256	4.352340
C	1.539206	-0.562104	2.793698
H	0.593262	-0.628125	3.320094
C	3.664438	-0.477060	2.234492
H	4.743136	-0.421293	2.168899
N	-0.006965	-1.377182	-0.930932
N	-0.135842	-2.540160	-0.264427
H	-0.038045	-2.543228	0.743101
C	-0.111611	-1.692752	-2.221025
H	-0.051859	-0.911258	-2.971391
C	-0.310493	-3.581575	-1.105951
H	-0.420723	-4.593814	-0.738013
C	-0.306129	-3.069842	-2.386105
H	-0.425034	-3.617546	-3.310850
C	4.879867	0.397286	-1.864666
C	5.249699	-1.394943	-0.215563
C	-4.962305	-0.253847	1.701226
C	-3.118849	-0.391014	3.325786
H	-5.455232	-1.208800	1.917619
H	-5.180223	0.041824	0.673705
H	-5.368156	0.511021	2.374248
H	-2.162223	-0.914090	3.436494
H	-3.874438	-0.943975	3.891895
H	-3.041557	0.619116	3.754027
H	4.526340	1.432805	-1.898090
H	4.539757	-0.144825	-2.758944
H	5.973684	0.415598	-1.867633
H	5.526747	-1.970273	-1.107047
H	4.692113	-2.058998	0.448308
H	6.169600	-1.061021	0.279616

TS2

N	2.471566	0.408588	1.170081
N	3.044372	-0.472948	0.308909
N	1.071510	-1.542060	-0.267666
H	0.622453	-2.452057	-0.353940
N	0.908719	1.331672	-1.293416
N	0.885420	2.656120	-1.054935
H	0.400883	2.989975	-0.228704
N	3.112703	-2.727502	-0.290096
C	2.358299	-1.635313	-0.086827

C	4.418177	1.246810	0.352046
H	5.248988	1.917926	0.180786
C	3.307504	1.434092	1.202571
H	3.094085	2.279836	1.849452
C	4.215743	0.016936	-0.209221
H	4.786632	-0.545336	-0.938289
C	1.631204	1.183221	-2.404910
H	1.786877	0.191891	-2.816672
C	1.584900	3.343704	-1.980155
H	1.674937	4.421635	-1.935263
C	2.082323	2.421255	-2.877619
H	2.684288	2.619047	-3.753834
Ni	-0.214097	0.046365	-0.167302
N	-1.656977	-1.243101	0.763029
N	-2.896529	-0.991777	0.259773
N	-1.883660	0.336635	-1.289675
H	-1.862290	0.705424	-2.236945
N	-4.110255	-0.387863	-1.670841
C	-2.960887	-0.321931	-0.982782
C	-3.228428	-1.717660	2.313979
H	-3.688619	-2.036730	3.239461
C	-1.857385	-1.688097	1.993687
H	-1.007545	-1.968539	2.607364
C	-3.862557	-1.251156	1.192642
H	-4.911695	-1.077529	0.990167
N	-0.635487	1.408348	1.313062
N	0.038023	1.261749	2.474655
H	0.940769	0.780745	2.429510
C	-1.753810	2.071534	1.631174
H	-2.476924	2.306222	0.857656
C	-0.619917	1.826403	3.502944
H	-0.212417	1.821332	4.506255
C	-1.788197	2.365389	2.996496
H	-2.549352	2.907017	3.541221
C	-5.023761	-1.533973	-1.644641
C	-4.308249	0.531232	-2.786831
C	2.544025	-3.865378	-1.001794
C	4.367072	-3.006375	0.415232
H	-5.148073	-1.903469	-2.669432
H	-6.007786	-1.239828	-1.260230
H	-4.619384	-2.349102	-1.041084
H	-3.819878	0.170413	-3.703351
H	-3.932042	1.527068	-2.531142
H	-5.382056	0.615228	-2.978070
H	4.594316	-2.222150	1.139237
H	5.195723	-3.098755	-0.296768
H	4.262820	-3.955777	0.954137
H	3.363344	-4.453176	-1.426532
H	1.909120	-3.521259	-1.824852
H	1.965357	-4.517446	-0.331777

cis-**I•••**$(H_2O)_3$

Ni	0.685387	-0.071048	-0.041321
N	-1.025659	0.777224	0.787956
N	3.108098	0.364057	1.741590
N	-1.776879	-1.034013	-1.567812
H	-2.373754	-0.583943	-0.851227
N	-0.434427	-0.922421	-1.590645
N	1.829725	0.724662	1.522399
C	-0.038285	-1.633821	-2.656532
H	1.016542	-1.708929	-2.898410
C	3.607608	0.927231	2.860218
H	4.626040	0.745413	3.179246
C	2.600962	1.697924	3.404561
H	2.647533	2.293928	4.305659
C	-1.132601	-2.204690	-3.312354
H	-1.124491	-2.821479	-4.200683
H	3.559092	-0.252468	1.074672
C	1.517199	1.538215	2.531671
H	0.523623	1.967209	2.582831
C	-2.231873	-1.790820	-2.580651
H	-3.297603	-1.969106	-2.693920
N	1.040579	1.711094	-1.164747
N	0.052040	-3.014555	0.487276
N	3.045104	-0.239427	-1.916287
H	2.695896	0.685616	-2.154382
N	2.445047	-0.881669	-0.897331
N	0.451457	-1.863847	1.063889
C	3.077923	-2.056746	-0.800776
H	2.777802	-2.771441	-0.040362
C	0.141563	-4.059935	1.332448
H	-0.137984	-5.060537	1.027146
C	0.623851	-3.569704	2.531053
H	0.823737	-4.129188	3.434907
C	4.087309	-2.162875	-1.764512
H	4.766423	-2.988448	-1.928177
H	-0.243398	-2.994817	-0.484930
C	0.804656	-2.198389	2.309807
H	1.169387	-1.433211	2.988003
C	4.032739	-0.972946	-2.464602
H	4.621007	-0.602230	-3.294496
C	-1.992177	1.287324	1.205377
N	-3.027308	1.912761	1.691932
C	-3.781750	1.310050	2.797839
C	-3.790278	2.786519	0.795235
H	-4.644866	0.764684	2.395353
H	-4.118758	2.108841	3.466079
H	-3.144894	0.611378	3.344723
H	-4.267385	3.565466	1.398440
H	-4.549986	2.199811	0.263918
H	-3.115384	3.258881	0.075573

C	0.805484	2.846152	-1.345664
N	0.559276	4.106598	-1.547535
C	1.261164	5.137587	-0.775746
C	-0.255463	4.546314	-2.684266
H	0.375176	5.057525	-3.421599
H	-1.025136	5.239783	-2.327243
H	-0.735402	3.684171	-3.153788
H	0.528836	5.852876	-0.385426
H	1.975972	5.666202	-1.417842
H	1.793919	4.676732	0.060025
O	-3.939057	-0.369255	0.029791
H	-3.725925	-0.983258	0.759087
H	-4.615438	-0.815019	-0.521083
O	-2.538779	-1.621921	2.064566
O	-5.480730	-1.731979	-1.894074
H	-2.549612	-2.384990	2.657540
H	-1.602916	-1.418411	1.913170
H	-5.993410	-2.530290	-1.704896
H	-6.054516	-1.203769	-2.466604

cis-**I**(deprotonated)•••$H_3O(H_2O)_2^+$

Ni	0.650268	-0.080235	0.069397
N	-1.066231	0.618154	1.063883
N	2.710647	-1.093846	2.072968
N	-1.496420	-0.159262	-2.080567
H	-2.708195	-0.281905	-1.130263
N	-0.216199	0.185101	-1.764435
N	1.578820	-0.375893	1.941923
C	0.391569	0.589215	-2.889363
H	1.436424	0.885701	-2.873485
C	3.074980	-1.234857	3.363942
H	3.967055	-1.780431	3.644285
C	2.131864	-0.570996	4.120638
H	2.111171	-0.467447	5.196815
C	-0.489195	0.531437	-3.966421
H	-0.297391	0.787376	-4.999991
H	3.153439	-1.453682	1.234160
C	1.225877	-0.053410	3.185849
H	0.338606	0.546840	3.349313
C	-1.662056	0.052487	-3.402361
H	-2.619739	-0.154687	-3.871078
N	1.449259	1.906452	-0.044877
N	-0.647136	-2.670347	-0.905879
N	3.477757	0.068551	-1.016624
H	3.389009	1.011128	-0.646863
N	2.434472	-0.765692	-0.842697
N	-0.041550	-2.110786	0.159514
C	2.772799	-1.889795	-1.478863
H	2.088105	-2.731624	-1.488303
C	-0.770928	-4.003738	-0.769238
H	-1.230525	-4.611681	-1.538692

C	-0.212671	-4.342896	0.449990
H	-0.126647	-5.331541	0.880533
C	4.039384	-1.773614	-2.065125
H	4.576106	-2.515307	-2.640557
H	-0.972209	-2.036611	-1.645667
C	0.232126	-3.128300	0.986417
H	0.736191	-2.937307	1.928873
C	4.457373	-0.496058	-1.750882
H	5.367925	0.039168	-1.988564
C	-2.038363	1.017096	1.576258
N	-3.113852	1.460118	2.164768
C	-3.531960	0.905920	3.453658
C	-4.066018	2.306094	1.446001
H	-4.393464	0.239893	3.318319
H	-3.806192	1.726535	4.125668
H	-2.709928	0.338417	3.897929
H	-4.295442	3.190083	2.051528
H	-4.992297	1.749181	1.254635
H	-3.633881	2.622275	0.493140
C	1.280521	3.058800	-0.179992
N	1.099554	4.334803	-0.357851
C	1.434156	5.306729	0.685398
C	0.737323	4.849485	-1.681653
H	1.581489	5.397823	-2.117321
H	-0.118285	5.526572	-1.580679
H	0.461596	4.019441	-2.338082
H	0.578516	5.972027	0.846775
H	2.301381	5.903454	0.377537
H	1.666273	4.786752	1.617946
O	-3.549268	-0.402742	-0.602999
H	-3.379872	-1.061727	0.147219
H	-4.285537	-0.699202	-1.225996
O	-2.811733	-1.843789	1.437606
O	-5.284817	-1.025551	-2.463216
H	-2.995887	-2.780564	1.600691
H	-1.840332	-1.768760	1.387904
H	-5.706249	-1.877263	-2.643854
H	-5.906730	-0.352754	-2.774517

IX•••$NCNMe_2$

Ni	0.772854	0.030617	0.207778
N	-0.620071	1.134286	-0.839468
H	-1.592104	0.834244	-0.941537
N	0.867440	2.833607	-0.476944
N	-1.279873	3.371173	-1.283684
N	-0.249703	-1.762228	-0.021200
N	1.604028	1.985784	0.286301
C	1.610973	3.914485	-0.860124
H	1.205943	4.681149	-1.507882
C	2.851834	3.772416	-0.296994
H	3.689243	4.451831	-0.380552

C	-0.426824	2.408764	-0.869469
C	2.793231	2.550148	0.402069
H	3.567678	2.057683	0.982070
C	-2.485244	2.951011	-1.981828
H	-3.263178	2.607968	-1.282904
H	-2.872665	3.804056	-2.547656
H	-2.251658	2.147188	-2.687625
C	-1.354974	4.704939	-0.685658
H	-0.601004	4.833820	0.093497
H	-1.227825	5.481758	-1.449613
H	-2.341446	4.832962	-0.221805
N	2.014607	-0.404454	-1.421377
H	1.692580	-0.493214	-2.381313
N	3.457083	-1.081191	0.208937
N	3.988393	-1.581580	-2.033194
N	-1.544901	0.068020	2.154241
H	-2.076465	-0.304462	1.362853
N	-0.250162	0.390610	1.988324
N	2.470074	-0.851779	1.115319
C	0.119399	0.982653	3.124099
H	1.132884	1.355573	3.230776
C	4.670405	-1.192519	0.826673
H	5.584024	-1.335220	0.264347
C	4.451713	-1.068253	2.173988
H	5.188998	-1.119886	2.963802
C	-0.945051	1.039130	4.031717
H	-0.946755	1.451295	5.031341
C	3.111267	-1.031267	-1.165059
C	3.064043	-0.856708	2.297570
H	2.471875	-0.712881	3.194740
C	-1.998809	0.448896	3.364811
H	-3.024402	0.272761	3.662688
C	4.718855	-2.823476	-1.771134
H	4.404357	-3.581858	-2.499539
H	5.799687	-2.669572	-1.877116
H	4.501675	-3.208815	-0.772667
C	3.847862	-1.249915	-3.443938
H	3.627334	-0.184032	-3.561677
H	4.798994	-1.457012	-3.944135
H	3.063740	-1.848240	-3.932471
C	-0.976323	-2.675948	0.000212
N	-1.786852	-3.698001	0.014884
C	-2.913133	-3.768722	-0.911612
C	-1.561918	-4.834021	0.909025
H	-2.941474	-2.860743	-1.520584
H	-3.850535	-3.853199	-0.346287
H	-2.806209	-4.644318	-1.563847
H	-1.367441	-5.739259	0.321100
H	-2.450079	-4.992562	1.532106
H	-0.704126	-4.633681	1.555483

N	-3.375258	-0.327843	-0.228379
C	-4.521651	-0.397467	-0.476038
N	-5.795250	-0.453107	-0.771602
C	-6.299790	-1.432167	-1.732947
C	-6.781378	0.268810	0.033462
H	-5.477856	-1.810747	-2.346656
H	-7.029403	-0.944406	-2.389096
H	-6.788341	-2.268416	-1.215699
H	-7.358735	-0.431166	0.650791
H	-7.464863	0.807406	-0.632691
H	-6.276161	0.988915	0.681894

IX•••$(H_2O)_3$

Ni	0.471758	0.113627	-0.057338
N	0.863924	1.669934	-1.368811
H	0.187831	2.070728	-2.013332
N	2.668237	2.010624	-0.012025
N	2.191368	3.618960	-1.664732
N	-1.108756	-0.681272	-1.142965
N	2.153873	1.084582	0.837294
C	3.994938	2.221231	0.239972
H	4.587035	2.898924	-0.361353
C	4.333457	1.431380	1.307284
H	5.301333	1.357942	1.784551
C	1.838702	2.461968	-1.066252
C	3.149842	0.740903	1.635925
H	2.979898	0.008427	2.419067
C	1.580714	3.942029	-2.946201
H	0.576091	4.375001	-2.826100
H	2.212361	4.676905	-3.454776
H	1.526413	3.047838	-3.575685
C	2.748438	4.768570	-0.948462
H	2.877315	4.549772	0.113472
H	3.711301	5.066731	-1.380822
H	2.052547	5.612580	-1.035554
N	1.806297	-1.258794	-0.943829
H	2.032417	-1.288693	-1.934554
N	1.464782	-2.411076	0.995635
N	2.609963	-3.490035	-0.760140
N	-2.163720	0.909164	1.213374
H	-2.661914	0.436608	0.446766
N	-0.841540	1.158190	1.168117
N	0.550378	-1.464883	1.333443
C	-0.576725	1.865362	2.271902
H	0.441597	2.175363	2.477942
C	1.851349	-3.126165	2.094459
H	2.606603	-3.899079	2.034030
C	1.135578	-2.647125	3.161103
H	1.179548	-2.993177	4.185064
C	-1.736940	2.075703	3.023428
H	-1.833993	2.612242	3.957381

C	1.971326	-2.380681	-0.328595
C	0.342665	-1.608286	2.631542
H	-0.362841	-0.954848	3.135641
C	-2.737593	1.448319	2.303551
H	-3.803642	1.326728	2.477351
C	2.186183	-4.851943	-0.430330
H	1.894361	-5.367709	-1.354165
H	3.005690	-5.413563	0.034635
H	1.322570	-4.847489	0.238144
C	3.428515	-3.383806	-1.959568
H	4.000074	-2.450125	-1.945811
H	4.138921	-4.216254	-1.968336
H	2.824221	-3.436345	-2.877920
C	-1.965121	-1.213868	-1.731927
N	-2.877321	-1.848453	-2.420818
C	-3.548179	-1.144648	-3.515163
C	-3.659453	-2.891533	-1.750281
H	-2.860594	-0.431138	-3.976973
H	-4.435826	-0.617966	-3.140609
H	-3.849110	-1.880255	-4.268133
H	-3.957248	-3.634095	-2.497698
H	-4.546075	-2.447926	-1.280364
H	-3.046052	-3.381154	-0.989182
O	-4.316412	-0.071353	-0.322827
H	-4.834569	0.699910	-0.613618
H	-4.791380	-0.313759	0.500568
O	-5.750207	0.297681	1.974860
O	-6.498271	1.878090	-0.214102
H	-7.306843	1.697416	-0.714620
H	-6.464069	2.842648	-0.142754
H	-6.346390	-0.142183	2.594734
H	-6.296284	0.920049	1.458931

IX(deprotonated)•••N(H)(CN)$(Me)_2^+$

Ni	0.283731	0.075215	0.126506
N	-0.227863	1.604035	-1.180706
H	-1.106982	1.681224	-1.687450
N	1.573929	2.655999	-0.252473
N	0.205694	3.868254	-1.743907
N	-1.084272	-1.280571	-0.726090
N	1.628187	1.657727	0.665748
C	2.752337	3.348140	-0.292184
H	2.913549	4.158207	-0.991574
C	3.574400	2.799614	0.656790
H	4.578560	3.111718	0.910248
C	0.435417	2.707580	-1.091794
C	2.824417	1.747482	1.220408
H	3.102913	1.051319	2.005818
C	-0.757483	3.851398	-2.835979
H	-1.796441	3.859392	-2.471262
H	-0.600092	4.742858	-3.450478

H	-0.600509	2.970615	-3.467411
C	0.446434	5.189594	-1.160377
H	0.873663	5.108965	-0.158705
H	1.116138	5.780563	-1.796955
H	-0.509672	5.721717	-1.075863
N	1.817553	-0.664673	-1.144445
H	1.825750	-0.599586	-2.158890
N	2.425586	-1.824369	0.721694
N	3.510888	-2.327031	-1.309838
N	-1.920254	-0.437451	2.070167
H	-3.089339	-0.199653	1.002885
N	-0.976880	0.481998	1.709795
N	1.302713	-1.340464	1.316707
C	-0.625540	1.174367	2.811384
H	0.145223	1.936421	2.757586
C	3.303339	-2.300586	1.656090
H	4.274895	-2.689157	1.379694
C	2.708394	-2.151270	2.881305
H	3.114353	-2.435674	3.842814
C	-1.350194	0.730150	3.912784
H	-1.297931	1.084422	4.934280
C	2.571288	-1.596820	-0.667527
C	1.463908	-1.542984	2.613232
H	0.686315	-1.230269	3.303786
C	-2.152962	-0.279111	3.387219
H	-2.883722	-0.905027	3.893905
C	3.784419	-3.735091	-1.019291
H	3.551797	-4.334799	-1.908774
H	4.842227	-3.884639	-0.770163
H	3.162677	-4.097976	-0.198050
C	3.932543	-1.887496	-2.631437
H	4.042933	-0.798329	-2.650503
H	4.909305	-2.330861	-2.848820
H	3.229079	-2.202912	-3.417284
C	-1.784209	-2.058118	-1.241826
N	-2.646650	-2.886774	-1.789136
C	-2.974401	-2.722646	-3.211508
C	-2.786969	-4.235568	-1.225778
H	-2.916382	-1.664702	-3.483318
H	-3.997823	-3.075928	-3.374101
H	-2.290698	-3.304636	-3.842999
H	-2.108521	-4.941697	-1.721811
H	-3.819128	-4.569870	-1.375465
H	-2.568491	-4.212804	-0.154266
N	-3.299200	0.954159	-1.795013
C	-3.576555	0.570712	-0.736883
N	-3.906836	0.135149	0.534266
C	-4.871379	-1.023196	0.514715
C	-4.390868	1.288182	1.388193
H	-4.469444	-1.792707	-0.151198

H	-5.848712	-0.675299	0.171709
H	-4.922901	-1.395416	1.542075
H	-4.598047	0.878651	2.379634
H	-5.287757	1.715999	0.934552
H	-3.577435	2.015937	1.451602

IX(deprotonated)•••$H_3O(H_2O)_2^+$

Ni	0.310088	0.094906	-0.092065
N	1.090157	1.444668	-1.466042
H	0.542152	1.918754	-2.178842
N	2.841032	1.551424	-0.004377
N	2.777860	3.087392	-1.787579
N	-1.270758	-0.508694	-1.335489
N	2.110046	0.810357	0.868073
C	4.164238	1.554837	0.342491
H	4.907884	2.062681	-0.257908
C	4.279285	0.821387	1.493013
H	5.181922	0.627610	2.056632
C	2.177978	2.061744	-1.143777
C	2.969297	0.379547	1.773700
H	2.617626	-0.231132	2.599227
C	2.321874	3.413464	-3.130446
H	1.408233	4.027404	-3.118837
H	3.109429	3.981735	-3.635145
H	2.144720	2.496938	-3.702611
C	3.475191	4.177044	-1.101187
H	3.490615	4.018984	-0.020716
H	4.503301	4.275049	-1.470462
H	2.945322	5.118157	-1.296615
N	1.459395	-1.566153	-0.760135
H	1.761196	-1.736386	-1.715824
N	0.840260	-2.438462	1.254873
N	1.964860	-3.839396	-0.269782
N	-2.109818	1.095228	1.324374
H	-3.202421	0.341790	0.537431
N	-0.857632	1.417641	0.932867
N	0.034199	-1.356069	1.412890
C	-0.457568	2.487054	1.640958
H	0.536837	2.898798	1.501553
C	1.086836	-3.040023	2.457953
H	1.741126	-3.898248	2.541628
C	0.389664	-2.340726	3.408917
H	0.344917	-2.549017	4.469539
C	-1.465396	2.894988	2.509304
H	-1.447036	3.714636	3.215814
C	1.438090	-2.619779	-0.016994
C	-0.244454	-1.295824	2.704038
H	-0.884343	-0.498140	3.069490
C	-2.487348	1.979210	2.272430
H	-3.462036	1.884032	2.747514
C	1.353543	-5.093778	0.170000

H	1.058712	-5.677327	-0.711851
H	2.064360	-5.689804	0.755599
H	0.457046	-4.909384	0.765682
C	2.878331	-3.970388	-1.394751
H	3.556972	-3.111971	-1.432624
H	3.480634	-4.872578	-1.249029
H	2.344964	-4.063893	-2.353182
C	-2.081819	-0.955617	-2.046699
N	-3.018472	-1.415252	-2.837377
C	-2.869666	-1.320227	-4.290388
C	-4.015439	-2.357494	-2.327807
H	-2.140161	-0.545726	-4.540330
H	-3.836730	-1.050627	-4.728977
H	-2.541010	-2.279627	-4.710749
H	-3.761150	-3.385363	-2.617868
H	-4.993115	-2.099645	-2.750050
H	-4.068366	-2.285515	-1.238892
O	-4.067796	0.174877	0.064934
H	-4.243683	1.077039	-0.334295
H	-4.778031	0.157852	0.794531
O	-5.725376	0.855644	1.902881
O	-4.577420	2.745563	0.075154
H	-4.802116	3.487634	-0.504611
H	-3.808294	3.031388	0.603169
H	-6.529082	0.518824	2.323198
H	-5.921827	1.747720	1.571867

cis-**IIIb$_N$**

Ni	0.472549	-0.066528	-0.488649
N	0.794513	1.538553	-1.802406
H	0.352152	1.729724	-2.699138
N	2.270591	2.219390	-0.218590
C	2.019050	3.663531	-2.193527
N	-0.891154	-1.062578	-1.742518
N	1.954429	1.097516	0.482241
C	3.156497	2.998041	0.480789
H	3.529403	3.934751	0.085773
C	3.414059	2.353299	1.658620
H	4.071322	2.679600	2.453239
C	1.638407	2.431731	-1.450361
C	2.636867	1.173514	1.607634
H	2.544142	0.386145	2.349118
N	2.037216	-1.289038	-1.300955
H	2.556774	-1.202343	-2.172367
N	1.734157	-2.442787	0.627914
C	3.518424	-3.236110	-0.867118
N	-2.094172	0.055447	0.991525
H	-3.113895	-0.450703	-0.123631
N	-1.012270	0.788395	0.621810
N	0.685764	-1.616253	0.894098
C	-0.938979	1.868278	1.417372

H	-0.123967	2.579942	1.318691
C	1.927593	-3.327064	1.656148
H	2.712552	-4.072474	1.627430
C	0.981614	-3.052579	2.605381
H	0.838688	-3.558607	3.550596
C	-2.001038	1.872667	2.320794
H	-2.206423	2.588987	3.106336
C	2.425280	-2.268115	-0.578006
C	0.231951	-1.975446	2.079555
H	-0.620715	-1.450950	2.499462
C	-2.692497	0.701386	2.010880
H	-3.598707	0.296758	2.454682
C	-1.602878	-1.642293	-2.445213
C	-2.503816	-2.365505	-3.317376
O	-3.891522	-0.384676	-0.748870
H	-3.975028	0.624390	-0.836924
H	-4.715308	-0.610579	-0.194701
O	-5.869733	-0.496354	0.911376
O	-4.219271	2.120948	-0.248070
H	-4.328683	2.947052	-0.738973
H	-3.610414	2.307187	0.492828
H	-6.545911	-1.168600	1.079024
H	-6.322546	0.359091	0.943613
H	-3.535893	-2.055871	-3.120177
H	-2.417076	-3.443204	-3.141761
H	-2.265749	-2.161080	-4.366760
H	3.973735	-3.020279	-1.837319
H	3.137501	-4.264773	-0.884833
H	4.303197	-3.181678	-0.102075
H	1.485266	3.715946	-3.146132
H	3.096229	3.679949	-2.401187
H	1.775471	4.562535	-1.613413

VII_N

Ni	0.658268	-1.465783	-0.622648
N	2.345584	-0.346780	-2.703298
N	-1.260023	-2.124814	-0.114459
N	2.364808	-0.477958	-1.347431
N	1.592328	-3.332946	-0.509224
N	2.057757	-2.680648	1.612393
N	1.373516	-1.531308	1.352973
N	0.374391	-1.468603	-2.695298
N	-1.691977	0.094753	0.061046
C	-3.543025	-1.441566	0.582834
N	-0.403700	0.321199	-0.319951
C	2.917834	-4.877782	0.912837
C	1.276260	-0.728282	-4.887121
C	2.163789	-3.636334	0.594293
C	3.460952	0.315371	-3.144108
H	3.628215	0.514601	-4.195379
C	3.483551	0.100318	-0.949178

H	3.730884	0.128043	0.107064
C	4.212527	0.617946	-2.042344
H	5.159987	1.139345	-2.019035
C	-2.131376	-1.231015	0.165426
C	-2.354125	1.276524	0.265123
H	-3.392679	1.303521	0.570909
C	2.131930	-1.514188	3.479684
H	2.327249	-1.185694	4.491626
C	1.417230	-0.830451	2.471621
H	0.936243	0.141138	2.519355
C	-0.266850	1.634571	-0.350985
H	0.686276	2.071955	-0.629966
C	-1.466939	2.285540	0.010106
H	-1.650300	3.349822	0.071522
C	1.263586	-0.888261	-3.408763
C	2.525053	-2.688874	2.900085
H	3.092520	-3.522095	3.295806
H	1.696101	-4.046169	-1.228778
H	-1.610998	-3.076257	-0.020596
H	-0.400452	-1.843318	-3.239786
H	2.940403	-5.545192	0.047298
H	2.452459	-5.415435	1.748615
H	3.952532	-4.646868	1.195816
H	0.385242	-1.181932	-5.329170
H	2.159730	-1.209053	-5.325914
H	1.296551	0.332470	-5.167101
H	-3.771265	-2.509321	0.636774
H	-4.236142	-0.978331	-0.130762
H	-3.730903	-0.999860	1.569540

IX$_N$(protonated)•••$H_3O(H_2O)_2^+$

Ni	0.472549	-0.066528	-0.488649
N	0.794513	1.538553	-1.802406
H	0.352152	1.729724	-2.699138
N	2.270591	2.219390	-0.218590
C	2.019050	3.663531	-2.193527
N	-0.891154	-1.062578	-1.742518
N	1.954429	1.097516	0.482241
C	3.156497	2.998041	0.480789
H	3.529403	3.934751	0.085773
C	3.414059	2.353299	1.658620
H	4.071322	2.679600	2.453239
C	1.638407	2.431731	-1.450361
C	2.636867	1.173514	1.607634
H	2.544142	0.386145	2.349118
N	2.037216	-1.289038	-1.300955
H	2.556774	-1.202343	-2.172367
N	1.734157	-2.442787	0.627914
C	3.518424	-3.236110	-0.867118
N	-2.094172	0.055447	0.991525
H	-3.113895	-0.450703	-0.123631

N	-1.012270	0.788395	0.621810
N	0.685764	-1.616253	0.894098
C	-0.938979	1.868278	1.417372
H	-0.123967	2.579942	1.318691
C	1.927593	-3.327064	1.656148
H	2.712552	-4.072474	1.627430
C	0.981614	-3.052579	2.605381
H	0.838688	-3.558607	3.550596
C	-2.001038	1.872667	2.320794
H	-2.206423	2.588987	3.106336
C	2.425280	-2.268115	-0.578006
C	0.231951	-1.975446	2.079555
H	-0.620715	-1.450950	2.499462
C	-2.692497	0.701386	2.010880
H	-3.598707	0.296758	2.454682
C	-1.602878	-1.642293	-2.445213
C	-2.503816	-2.365505	-3.317376
O	-3.891522	-0.384676	-0.748870
H	-3.975028	0.624390	-0.836924
H	-4.715308	-0.610579	-0.194701
O	-5.869733	-0.496354	0.911376
O	-4.219271	2.120948	-0.248070
H	-4.328683	2.947052	-0.738973
H	-3.610414	2.307187	0.492828
H	-6.545911	-1.168600	1.079024
H	-6.322546	0.359091	0.943613
H	-3.535893	-2.055871	-3.120177
H	-2.417076	-3.443204	-3.141761
H	-2.265749	-2.161080	-4.366760
H	3.973735	-3.020279	-1.837319
H	3.137501	-4.264773	-0.884833
H	4.303197	-3.181678	-0.102075
H	1.485266	3.715946	-3.146132
H	3.096229	3.679949	-2.401187
H	1.775471	4.562535	-1.613413