Electronic supplementary materials *Mendeleev Commun.*, 2022, **32**, 588–590

Tripodal 1,2,3-triazole click ligand based on the triphenylphosphine oxide platform: atrane-type lanthanide complexes in solutions

Anna G. Matveeva, Olga V. Bykhovskaya, Margarita P. Pasechnik, Anna V. Vologzhanina, Rinat R. Aysin, Sergey V. Matveev, Ivan A. Godovikov, Igor Y. Kudryavtsev, Tatyana V. Baulina and Valery K. Brel

Table of content

Experimental

Compound **1** was prepared according to the literature procedure [S1].

Multinuclear ^{1}H, ^{13}C, and $^{31}P\{^{1}H\}$ NMR spectra were recorded on a Bruker Avance 400 spectrometer (operating at 400.23, 100.61, and 161.98 MHz, respectively), and a Bruker Avance 500 instrument (operating at 500.15, 125.75 and 202.46 MHz, respectively) at ambient temperature using $CDCl_3$ (c = 0.01 M) or CD_3CN (c = 0.01 M) solutions. Chemical shifts (ppm) refer to the residual protic solvent peaks (for ^{1}H and ^{13}C), and 85% H_3PO_4 (for ^{31}P) as external standards and coupling constants are expressed in hertz (Hz), the band width at half-height ($W_{1/2}$) is given in ppm (for $^{31}P\{^{1}H\}$ NMR spectra). IR spectra were obtained on a Bruker Tensor 37 FTIR spectrometer in the region 400–4000 cm^{-1} for solid samples, 950–4000 cm^{-1} for solutions in $CDCl_3$ and CD_3CN. The solid samples were KBr pellets and mulls in Nujol. The concentrations of solutions were 0.01 M in $CDCl_3$, and 0.03 M in CD_3CN, CaF_2 cuvettes were used, d = 0.23 mm and 0.06 mm for different solutions. Raman spectra of the crystalline and solid samples were obtained in the region 100–3500 cm^{-1} on a Jobin-Ivon LabRAM 300 spectrometer, equipped with a microscope and laser CCD detector. The He–Ne laser emission line at 632.8 nm was used for excitation at a power not higher than 2 mW. The content of C, H, and N was determined on a Carlo Erba 1106 instrument. Melting points were determined in open capillary tubes on a Stanford Research Systems MPA120 EZ-melt automated melting point apparatus and were not corrected.

Computation

Geometry optimization for complex **4** was performed in Gaussian software [S2] at the theory level PBE0/Def2-TZVP [S3,S4] in approximation of isolated molecule and SMD solvation model [S5] with parameters of acetonitrile solvent. The QTAIM analysis [S6] was performed using AIMAll program [S7]. The strength of intramolecular H-bonds was assessed using Espinosa–Lecomte correlation [S8]

Tris(2-propargyloxyphenyl)phosphine oxide (2)

^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.42 (s, 3H, CH); 4.52 (s, 6H, OCH_2); 7.09–7.16 (m, 6H, H^3, H^5); 7.54 (t, $^{3}J_{HH}$ = 7.6, 3H, H^4); 7.68 (dd, $^{3}J_{HH}$ = 7.6, $^{3}J_{PH}$ = 14.6, 3H, H^6).

^{13}C NMR (100 MHz, $CDCl_3$) δ: 55.93 (s, CH_2O); 75.32 (s, CH); 78.46 (s, $OCH_2\boldsymbol{C}$); 112.88 (d, $^{3}J_{PC}$ = 6.5, C^3); 121.45 (d, $^{3}J_{PC}$ = 12.5, C^5); 122.0 (d, $^{1}J_{PC}$ = 109.5, C^1); 133.01 (s, C^4); 134.79 (d, $^{2}J_{PC}$ = 8.6, C^6); 159.28 (s, C^2).

^{31}P{H} NMR (162 MHz, $CDCl_3$) δ: 24.62 (s).

Found (%): C 73.71; H 4.84; P 7.03. Calcd. for $C_{27}H_{21}O_4P$ (%): C 73.70; H 4.81; P 7.05.

Tris[2-(1-phenyl-1,2,3-triazol-4-ylmethoxy)phenyl]phosphine oxide (3).

^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.19 (s, 6H, OCH_2), 6.90 (t, $^{3}J_{HH}$ = 7.0, 3H, H^3), 7.08 (t, $^{3}J_{HH}$ = 7.6, 3H, H^5); 7.41–7.47 (m, 12H, H^4, H^6, $H^{2''}$); 7.48–7.56 (m, 9H, $H^{3''}$, $H^{4''}$); 7.70 (s, 3H, $H^{5'}$).

^{13}C NMR (100 MHz, $CDCl_3$) δ: 62.49 (s, CH_2O); 112.32 (d, $^{3}J_{PC}$ = 6.2, C^3); 120.03 (s, $C^{2''}$); 120.92 (d, $^{1}J_{PC}$ = 101.5, C^1); 121.05 (d, $^{3}J_{PC}$ = 12.5, C^5); 121.14 (s, $C^{5'}$); 128.74 (s, $C^{4''}$); 129.68 (s, $C^{3''}$); 133.66 (s, C^4); 134.60 (d, $^{2}J_{PC}$ = 8.7, C^6); 136.70 (s, $C^{1''}$); 144.39 (s, $C^{4'}$); 159.81 (s, C^2).

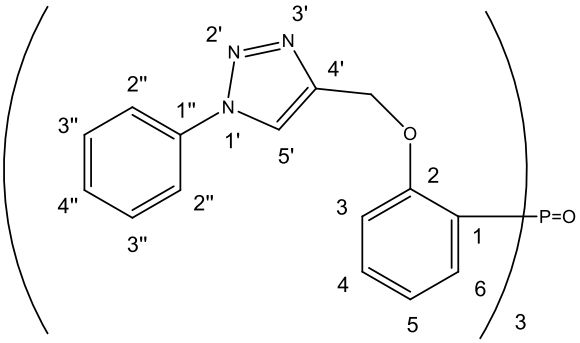
^{31}P{H} NMR (162 MHz, $CDCl_3$) δ: 26.03 (s), ($W_{½}$ = 0.2 ppm).

Found (%): C 67.65; H 4.59; N 15.59; P 3.81. Calcd. for $C_{45}H_{36}N_9O_4P$ (%): C 67.75; H 4.52; N 15.81; P 3.89.

^{1}H NMR (500 MHz, CD_3CN, c < 0.005 M), δ: 5.13 (s, 6H, OCH_2); 6.91 (t, 3H, H^3, $^{3}J_{HH}$ = 7.5); 7.16 (m, 3H, H^5); 7.41-7.51 (m, 6H, H^4, H^6); 7.48–7.51 (m, 3H, $H^{4''}$); 7.55–7.58 (m, 6H, $H^{2''}$); 7.63–7.64 (m, 6H, $H^{3''}$); 7.80 (s, 3H, $H^{5'}$).

^{13}C NMR (125 MHz, CD_3CN, c < 0.005 M) δ: 62.14 (s, CH_2O); 112.60 (d, C^3, $^{3}J_{PC}$ = 6.2); 120.14 (s, $C^{2''}$); 121.05 (d, C^5, $^{3}J_{PC}$ = 12.5); 121.14 (s, $C^{5'}$); 128.74 (s, $C^{4''}$); 129.68 (s, $C^{3''}$); 133.66 (s, C^4); 134.60 (d, C^6, $^{2}J_{PC}$ = 8.7); 136.70 (s, $C^{1''}$); 144.39 (s, $C^{4'}$); 159.81 (s, C^2). No signal of C-1 nucleus expected due to shift at ~117 ppm was observed because it is obscured by the solvent signal.

^{31}P {H} NMR (202 MHz, CD_3CN, c < 0.005 M), δ: 22.0 s ($W_{½}$ = 0.2 ppm).



Scheme S1. Atom numbering for **3–5.**

{Tris[2-(1-phenyl-1,2,3-triazol-4-ylmethoxy)phenyl]phosphine oxide}lanthanum trinitrate trihydrate, La(3)$(NO_3)_3\cdot 3H_2O$ (4).

^{1}H NMR (500 MHz, CD_3CN, 0.01 M), δ: 5.08 (s, 6H, OCH_2); 6.72 (t, 3H, H^3, $^{3}J_{HH}$ = 7.5); 7.09 (t, 3H, H^5, $^{3}J_{HH}$ = 5.0); 7.28–7.37 (m, 6H, H^4, H^6); 7.50–7.53 (m, 3H, $H^{4''}$); 7.56–7.59 (m, 6H, $H^{3''}$); 7.69–7.71 (m, 6H, $H^{2''}$); 7.84 (s, 1H, $H^{5'}$).

^{13}C NMR (125 MHz, CD_3CN, 0.01 M) δ: 61.92 (s, CH_2O); 112.82 (d, C^3, $^{3}J_{PC}$ = 6.2); 120.36 (s, $C^{2''}$); 121.00 (d, $^{3}J_{PC}$ = 11.3, C^5); 121.81 (s, $C^{5'}$); 128.95 (s, $C^{4''}$); 129.84 (s, $C^{3''}$); 133.98 (d, $^{2}J_{PC}$ = 8.8, C^6); 136.63 (s, C^4); 136.70 (s, $C^{1''}$); 143.24 (s, $C^{4'}$); 160.03 (d, C^2, $^{2}J_{PC}$ = 8.8). No signal of C-1 nucleus expected due to shift at ~117 ppm was observed because it is obscured by the solvent signal.

^{31}P {H} NMR (202 MHz, CD_3CN, 0.01 M), δ: 31.4 s ($W_{½}$ = 0.2 ppm).

Found (%): C 45.92; H 3.21; N 14.57. Calcd. for $C_{45}H_{36}N_9O_4P\cdot La(NO_3)_3\cdot 3H_2O$ (%): C 45.91; H 3.57; N 14.28.

^{1}H NMR (500 MHz, $CDCl_3$,0.01 M), δ: 5.04 (s, 6H, OCH_2); 6.6 (br s, 3H, H^3); 6.9 (br s, 3H, H^5); 7.2 (br s, 3H, H^{Ar}); 7.4 (br s, 3H, H^{Ar}); 7.38–7.41 (m, 3H, $H^{4''}$); 7.45–7.48 (m, 6H, $H^{2''}$); 7.62–7.64 (br d, 6H, $H^{3''}$); 7.7 (br s, 3H, $H^{5'}$).
^{13}C NMR (125 MHz, $CDCl_3$, 0.01 M) δ: 61.64 (s, CH_2O); 112.10 (s. C^3); 117.80 (d, C^1, $^1J_{PC}$ = 107.5); 120.10 (s, $C^{2''}$); 121.63 (d, C^5, $^3J_{PC}$ = 12.5); 121.47 (s, $C^{5'}$); 128.62 (s, $C^{4''}$); 129.66 (s, $C^{3''}$); 134.07 (s, C^4); 134.37 (d, $^2J_{PC}$ = 7.5, C^6); 136.64 (s, $C^{1''}$); 143.53 (s, $C^{4'}$); 159.96 (s, C^2). Minor signals are present in spectrum.
^{31}P {H} NMR (202 MHz, $CDCl_3$, 0.01 M), δ: 31 ($W_{½}$ = 1.3 ppm).

{Tris[2-(1-phenyl-1,2,3-triazol-4-ylmethoxy)phenyl]phosphine oxide}lutetium trinitrate trihydrate, $Lu(3)(NO_3)_3·3H_2O$ (5).
^{1}H NMR (500 MHz, CD_3CN, 0.01 M), δ: 5.1 (vbr s, ~6H, OCH_2); 6.8 (vbr s, ~3H, H^{Ar}); 7.1 (br s, 3H, H^{Ar}); 7.4 (vbr s, 6H, H^{Ar}, H^{Ar}); 7.52–7.68 (br m, ~15H, $H^{2''}$, $H^{3''}$, $H^{4''}$); 7.80 (s, ~3H, $H^{5'}$).
^{13}C NMR (125 MHz, CD_3CN, 0.01 M) δ: 61.32 s (CH_2O); 112.52 (d, $^3J_{PC}$ = 5.2, C^3); 120.36 (s, $C^{2''}$); 120.84 (d, $^3J_{PC}$ = 12.5, C^5); 122.03 (s, $C^{5'}$); 129.02 (s, $C^{4''}$); 129.84 (s, $C^{3''}$); 134.07 (d, $^2J_{PC}$ = 10.0, C^6); 134.56 (s, C^4); 136.59 (s, $C^{1''}$); 143.18 (s, $C^{4'}$); 159.96 (s, C^2). No signal of C-1 nucleus expected due to shift at ~117 ppm was observed because it is obscured by the solvent signal.
^{31}P {H} (202 MHz, CD_3CN, 0.01 M): δ_P 34.1 ($W_{½}$ = 0.2 ppm).
Found (%): C 44.10; H 3.27; N 13.49. Calcd. for $C_{45}H_{36}N_9O_4P·Lu(NO_3)_3·3H_2O$ (%): C 44.55; H 3.47; N 13.86.

X-ray diffraction analysis

Comment for Figure 1 (main text). Intermolecular hydrogen bonds are observed in crystal structure **3**·H_2O. Water molecules form O-H...O and O-H...N interactions with the phosphine oxide and triazole rings (r(O...O) = 2.738(3) Å, r(O...N) = 2.971(5) Å, OHO = 168.9(2)°, OHN = 156.7(2)°) to form H-bonded dimers additionally stabilized by C-H...O interactions (r(C...O) = 3.327(6) Å, CHO = 165.4(3)°).

Comment for Figure 2 (main text). The asymmetric molecular conformation is additionally supported by some hydrophobic interactions. π...π Interaction between two phenyl rings between two 'up' chains can be proposed with intercentroid distance as short as 3.946(3) Å, and two C-H...π interactions can be proposed with the distance between carbon atom of a heterocycle and a phenyl ring centroid equal to 3.674(3) – 3.807(3) Å.

Table S1. Selected geometrical parameters (Å, °) of compound **3**.

Parameter	Value	Parameter	Value
P=O (Å)	1.482(2)	N–N (Å)	1.341(4) – 1.359(3)
P–C (Å)	1.805(3) – 1.806(3)	C–N (Å)	1.341(3) – 1.442(4)
C^{Ar}–O (Å)	1.365(4) – 1.367(3)	O1-P1-C2-O2(°)	–59.5(2)
$C(H_2)$–O (Å)	1.418(4) – 1.432(3)	O1-P1-C17-O3(°)	–52.7(2)
N=N (Å)	1.308(4) – 1.315(4)	O1-P1-C32-O4 (°)	–178.2(2)

IR and Raman spectra for solid 2–5

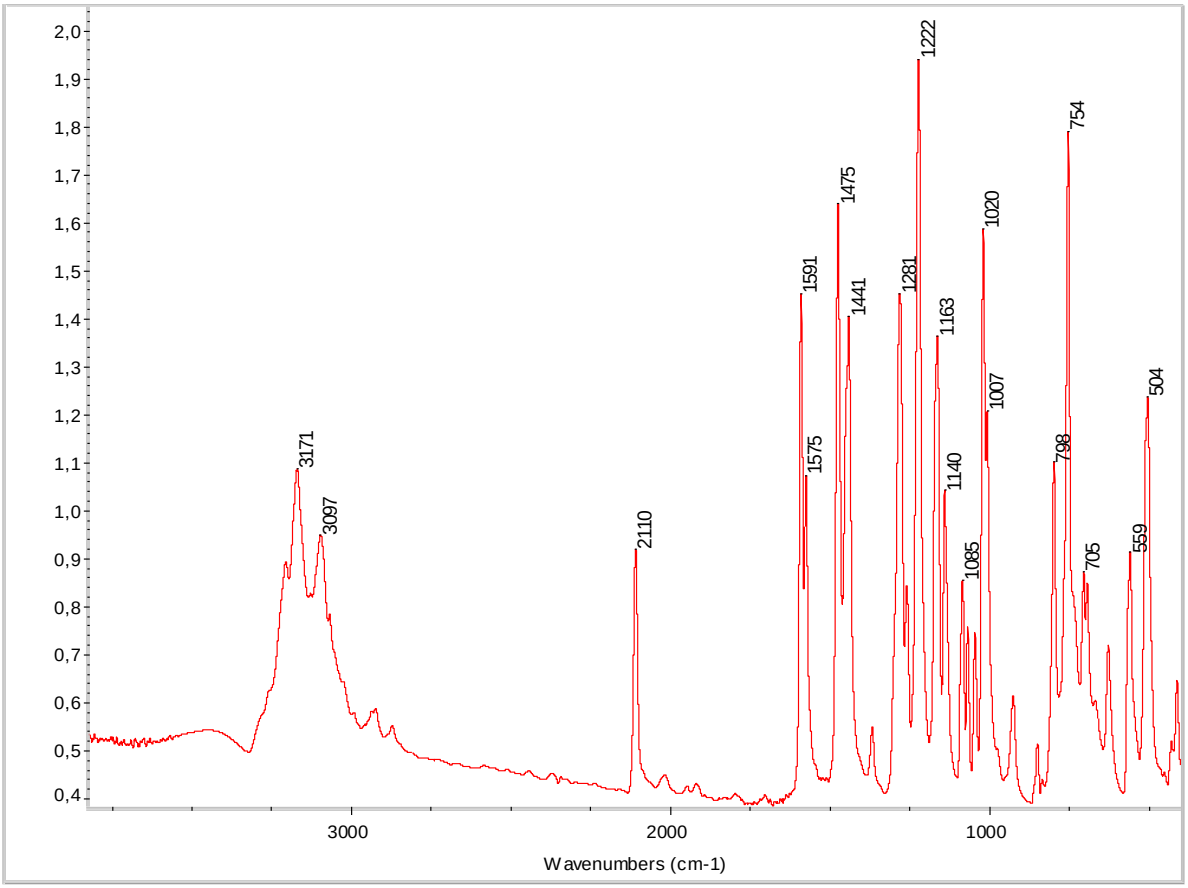


Fig. S1. IR spectrum of solid compound **2** (KBr disk).

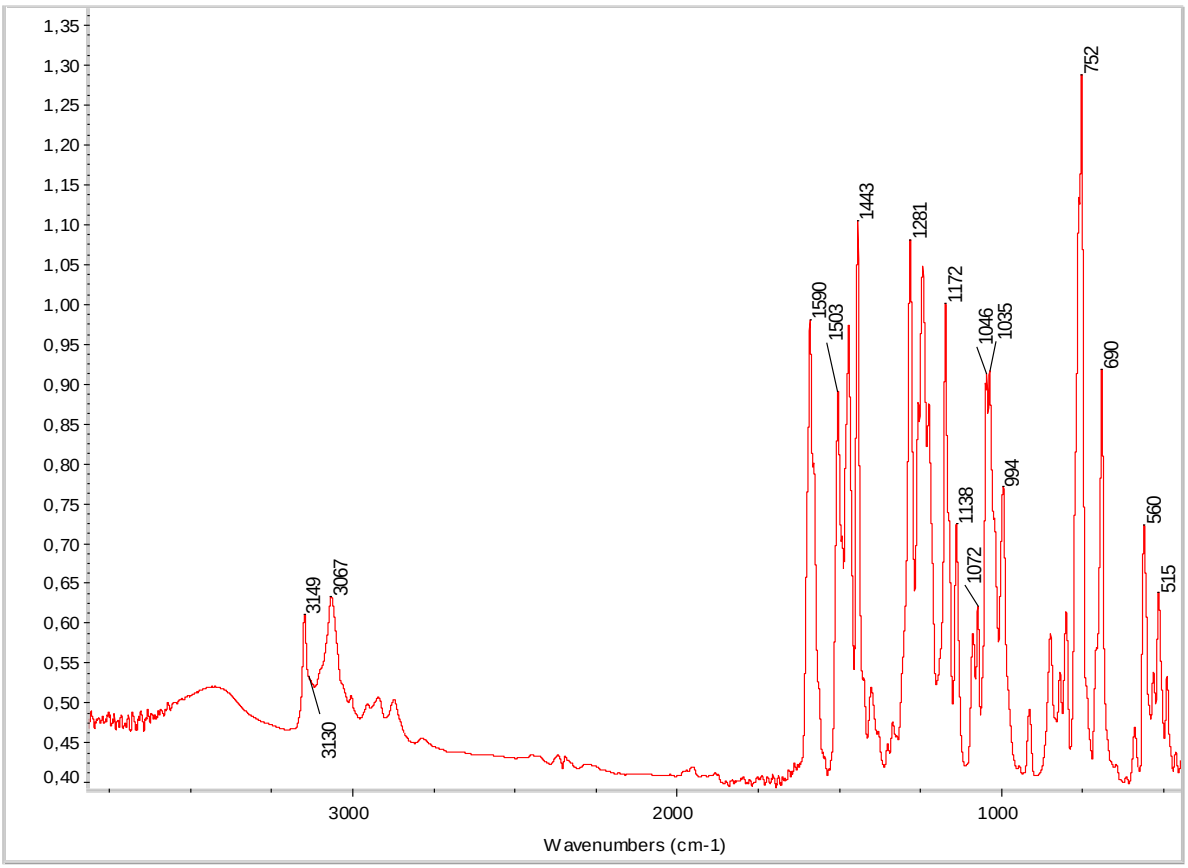


Fig. S2. IR spectrum of the solid ligand **3** (KBr disk).

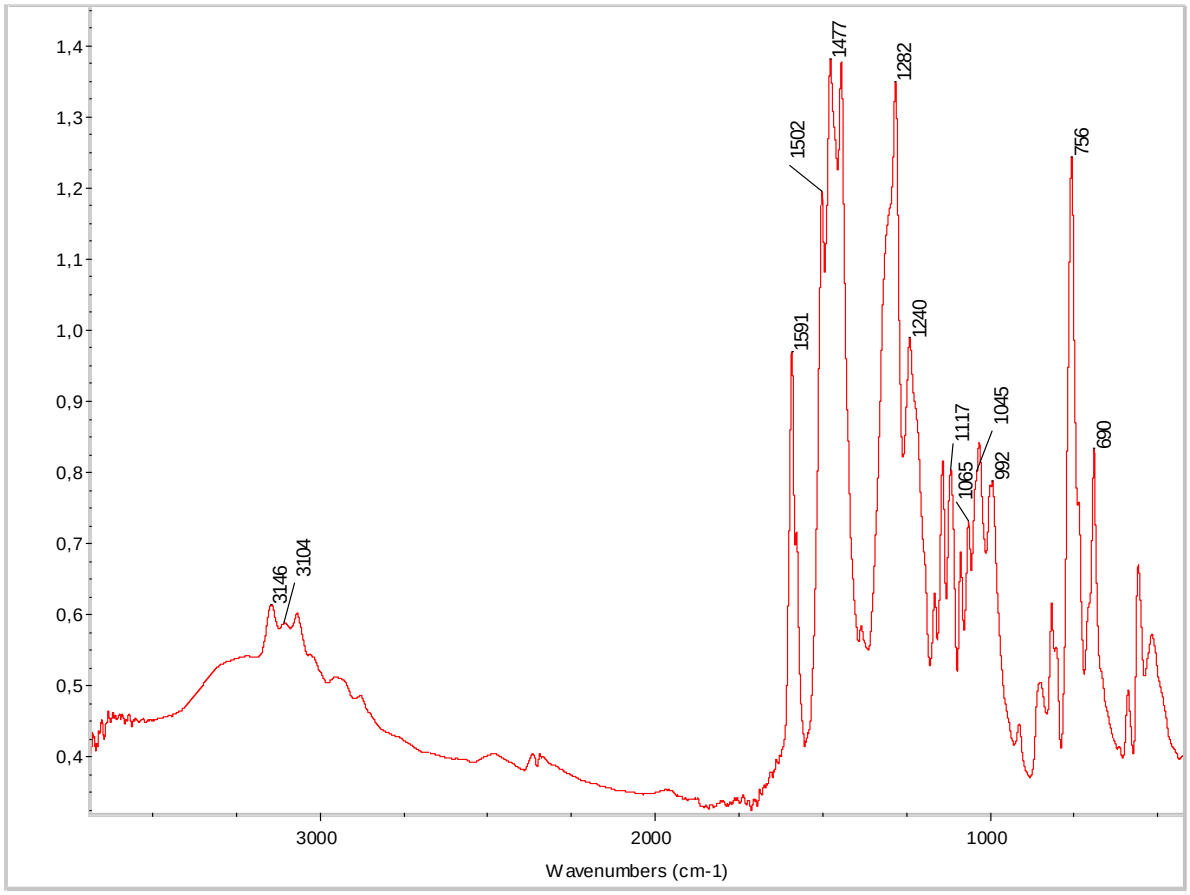


Fig. S3. IR spectrum of the solid complex **4** (KBr disk).

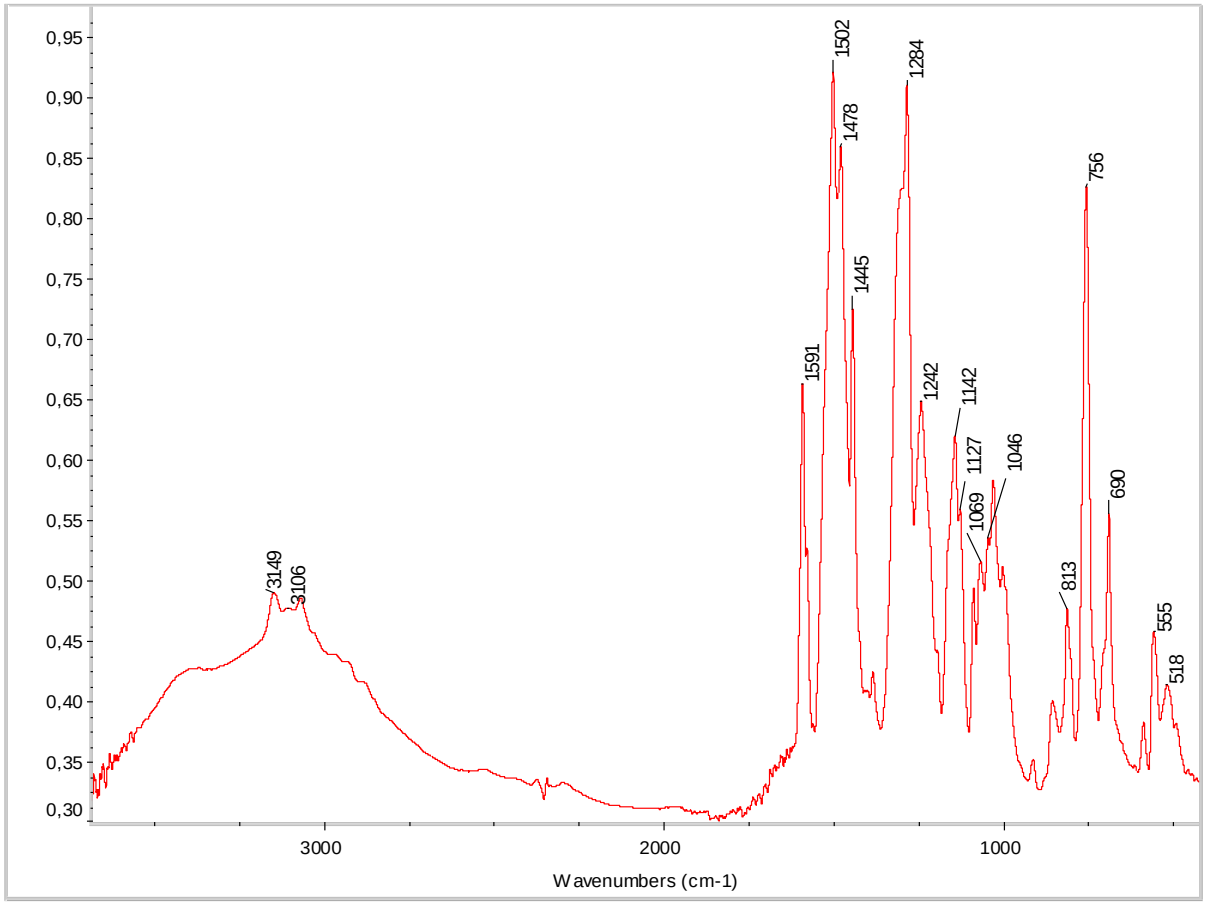


Fig. S4. IR spectrum of the solid complex **5** (KBr disk).

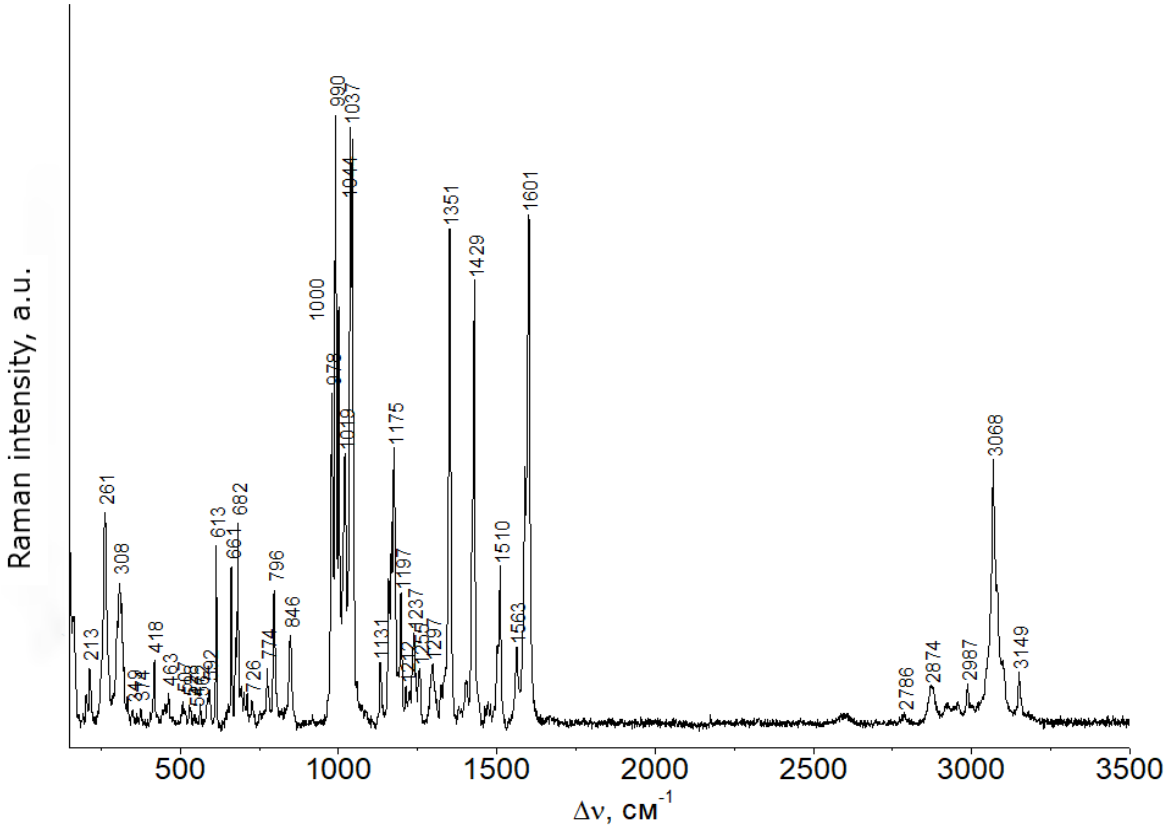


Fig. S5. Raman spectrum of the ligand **3**.

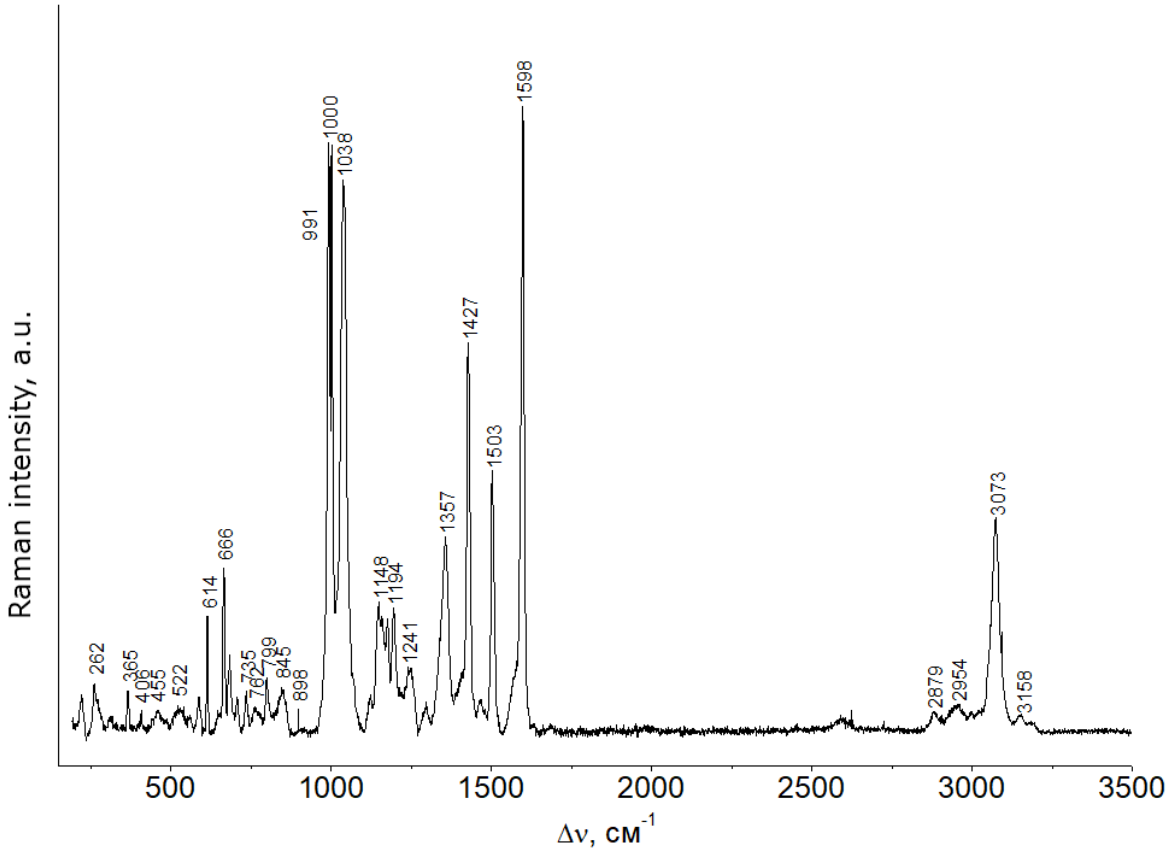


Fig. S6. Raman spectrum of the complex **4**.

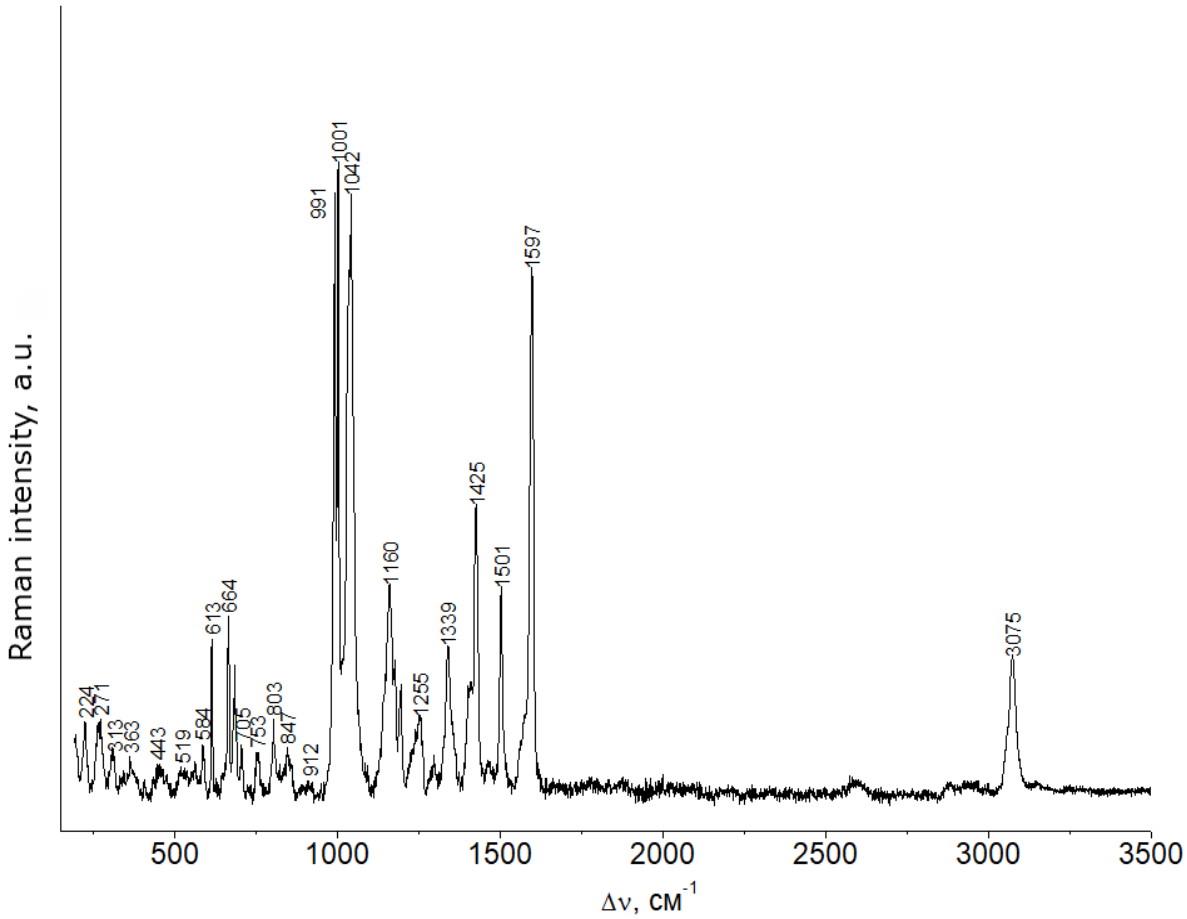


Fig. S7. Raman spectrum of the complex **5**.

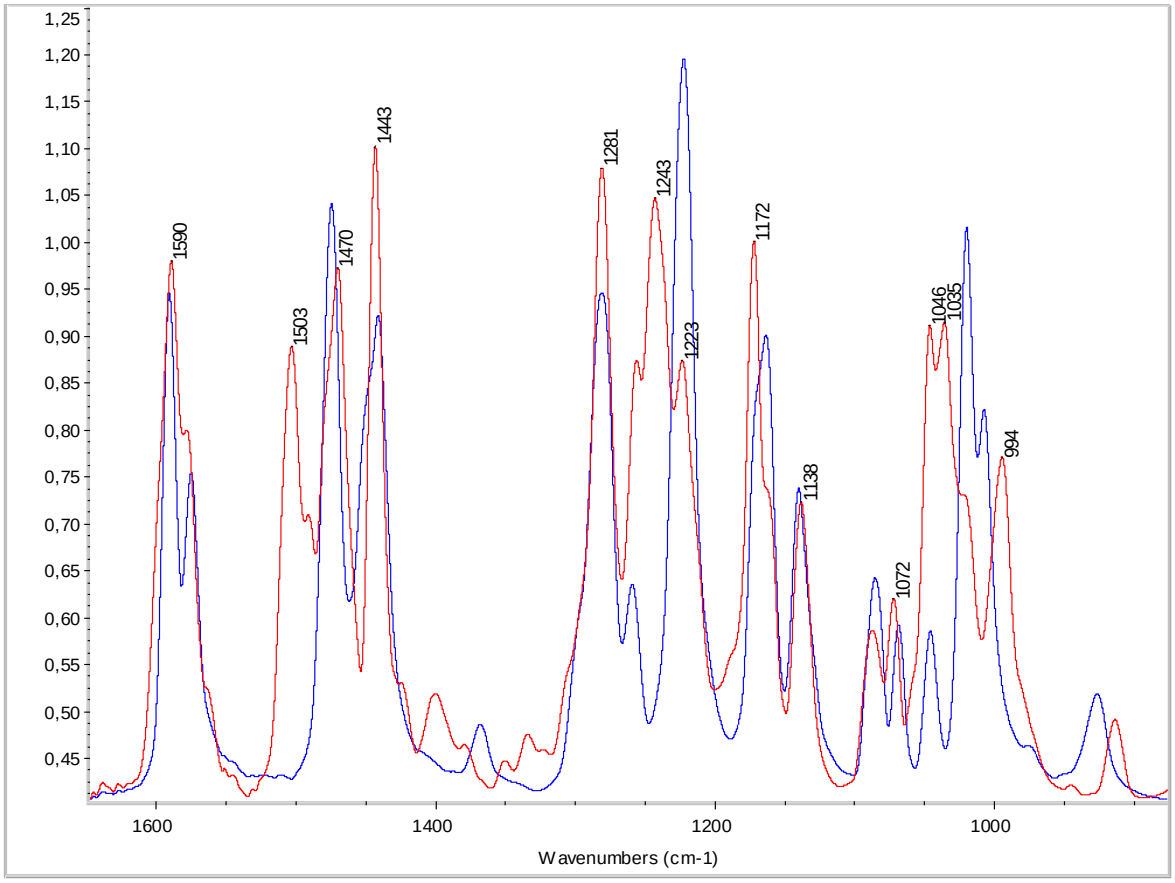


Fig. S8. IR spectra of solid compounds **2** (blue) and **3** (red) (KBr disk).

Table S2. Selected IR and Raman spectra data (ν, cm^{-1}) of the solid ligand **3**, their complexes **4**, **5** and model compounds: 1-Ph-4-Pr-1,2,3-triazole (**L1**) and their complex *trans*-Pd(**L**)$_2$Cl$_2$ [S9]; {2-[Me$_2$NC(O)CH$_2$O]C$_6$H$_4$}$_3$P(O) (**L2**) and their complexes La(**L2**)(NO$_3$)$_3$, and Lu(**L2**)(NO$_3$)$_3$ [S10]

Compound	Triazole ring vibrations			ν(P=O)
	IR	Raman		IR
3	1046[a], 1059	1563	1510	1172
4	1046[a], 1065	1570	1503	1117
5	1046[a], 1069br	1570br, 1580	1502	1127
L [S9]	1048	1554	1507	–
Pd(**L1**)$_2$Cl$_2$ [S9]	1074	1564	1500	–
L2 [S10]	–	–	–	1172
La(L2)(NO$_3$)$_3$ [S10]	–	–	–	1122
Lu(L2)(NO$_3$)$_3$ [S10]	–	–	–	1131

[a] Bands of triazole rings distortion are overlapping with platform vibrations

IR and ^{1}H, ^{13}C and ^{31}P NMR spectra for 3–5 in solution

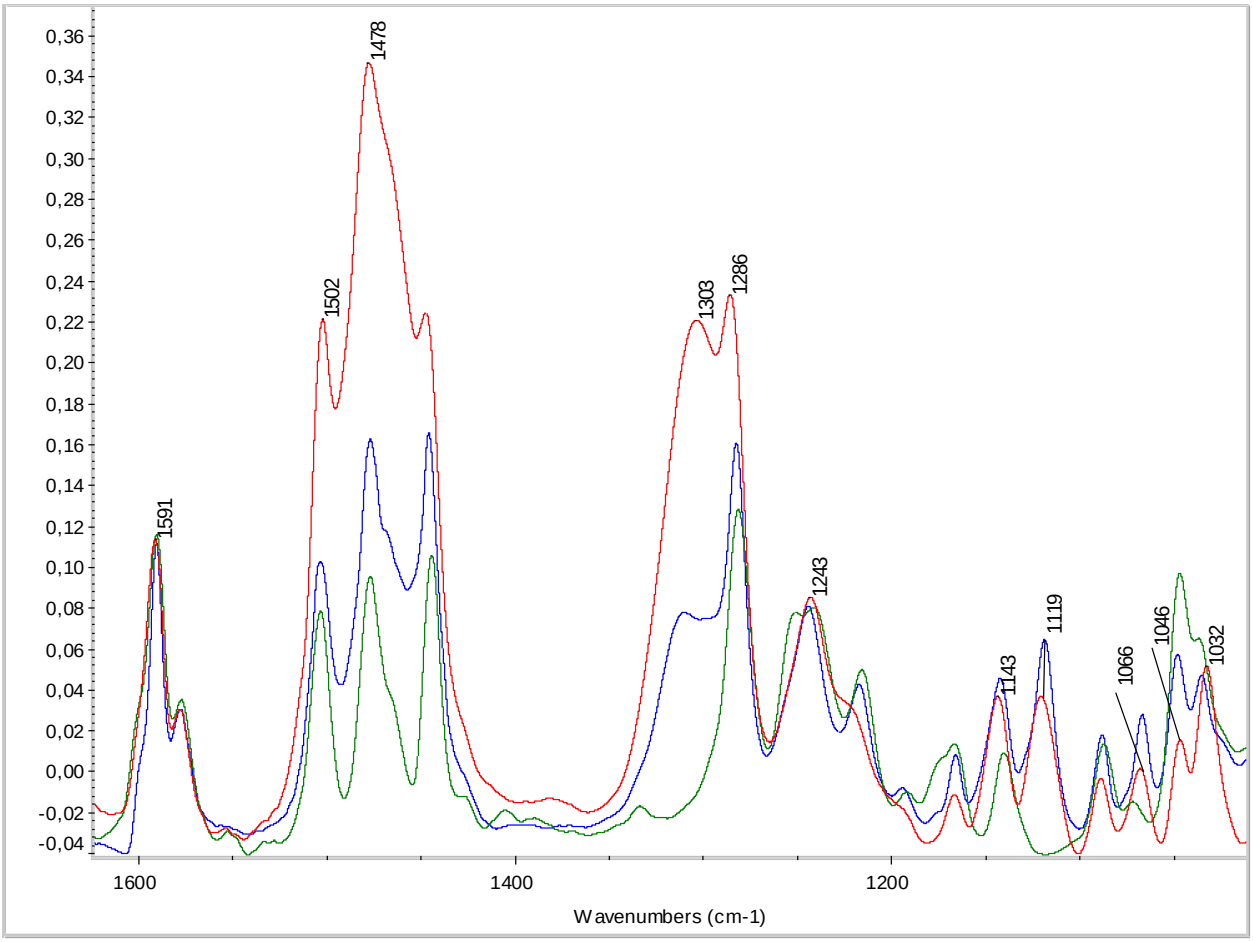


Fig. S9. Fragments of spectra of ligand **3** in $CDCl_3$ (green), complex **4** in $CDCl_3$ (blue), and complex **5** in CD_3CN (red).

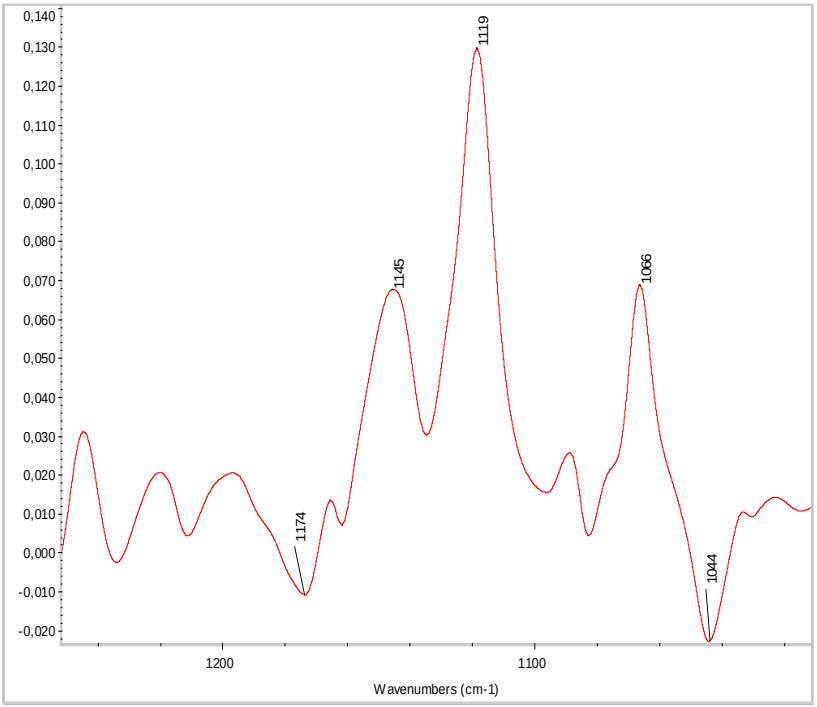


Fig. S10. The result of subtraction of spectrum of **3** from spectrum of **4** ($CDCl_3$). Negative absorption at 1174 and 1044 cm^{-1} belongs to ν(P=O) and ν(triazole) of the ligand, and new bands at 1119 and 1066 cm^{-1} belong to these vibrations for the complex.

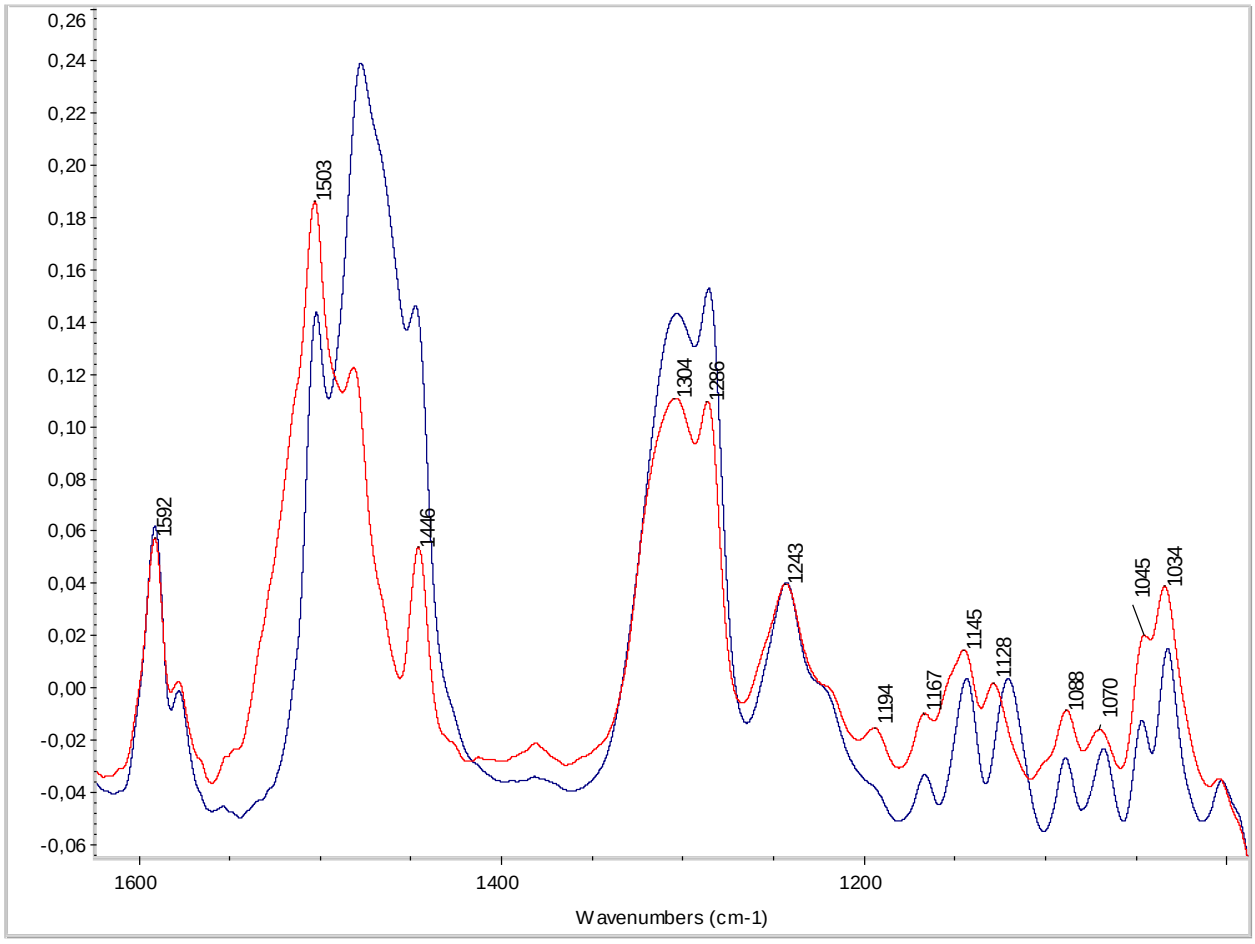


Fig. S11. Fragments of the spectra of the complexes **4** (blue) and **5** (red) in the CD_3CN solutions.

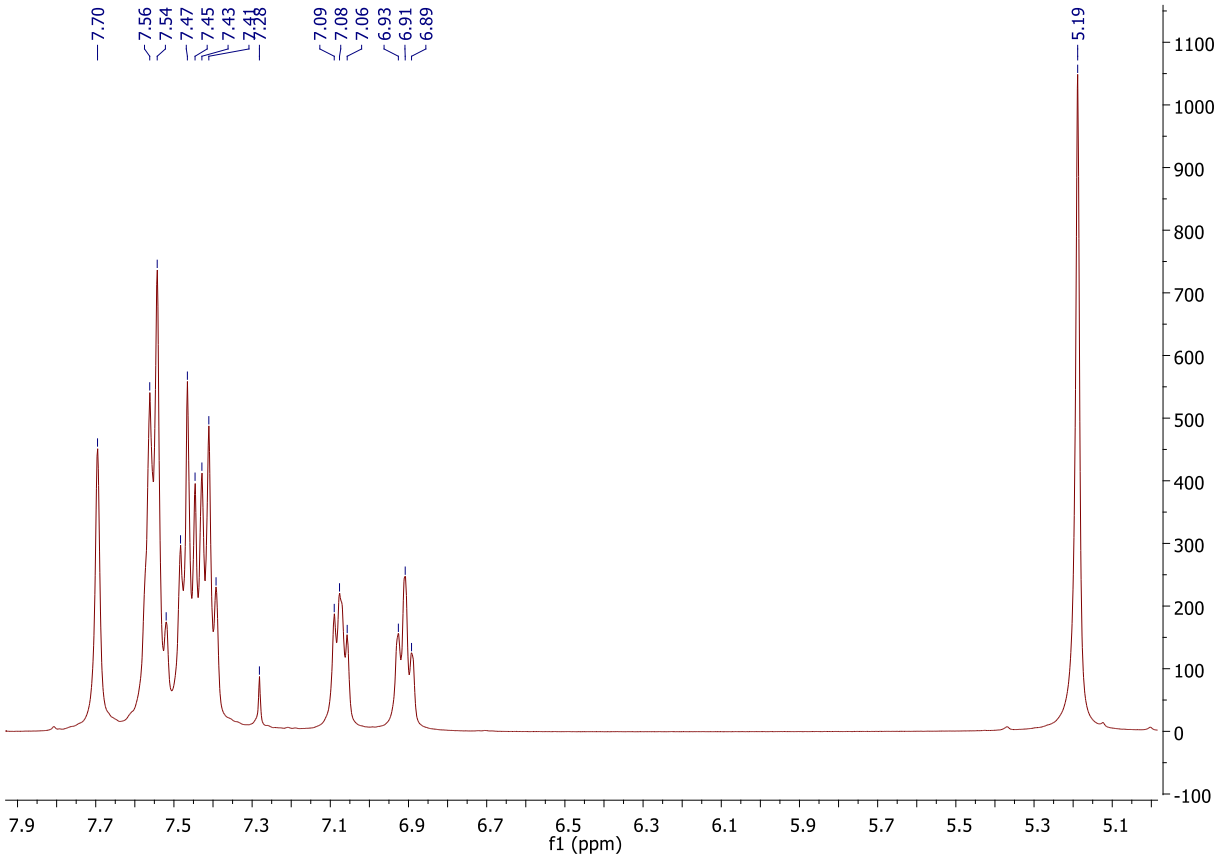


Fig S12. ^{1}H NMR spectrum for ligand **3** ($CDCl_3$, 400.13 MHz).

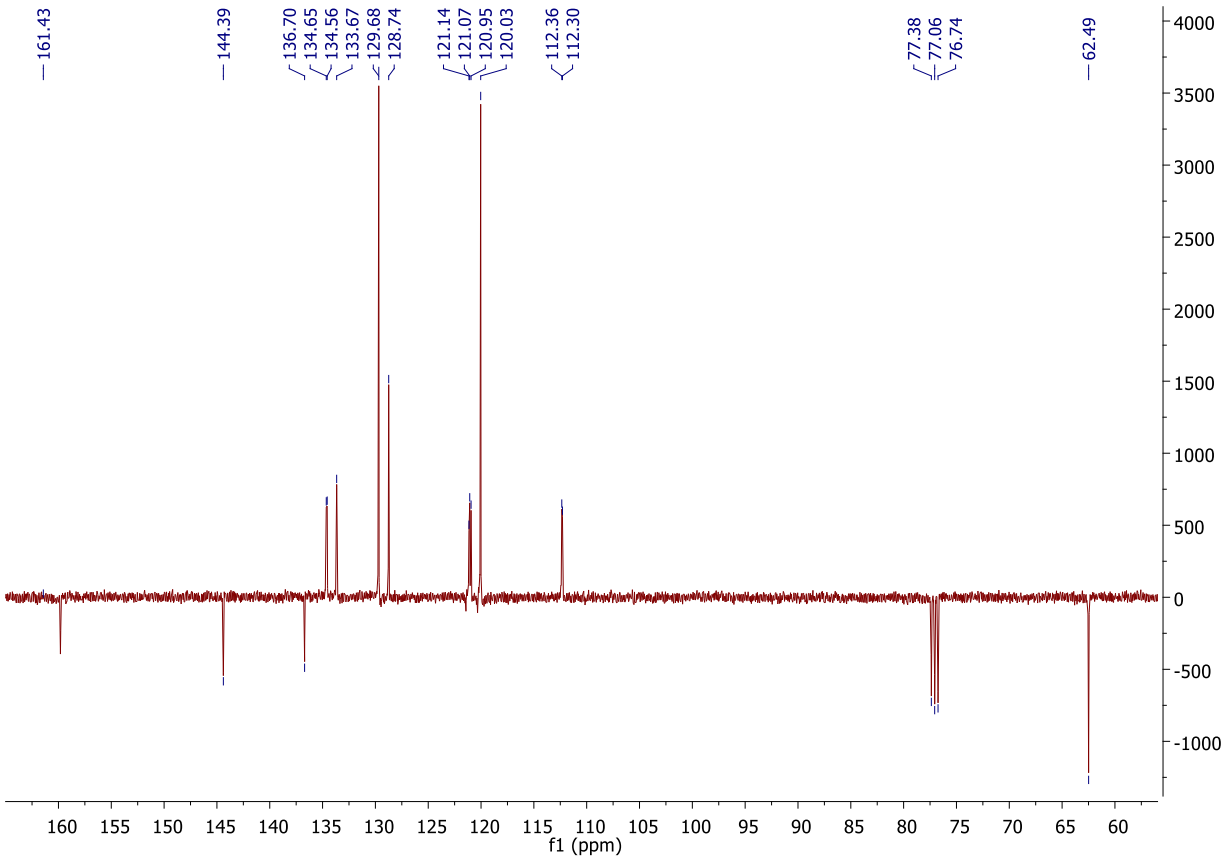


Fig S13. $^{13}C\{^{1}H\}$ NMR spectrum for ligand **3** ($CDCl_3$, 100.61 MHz)

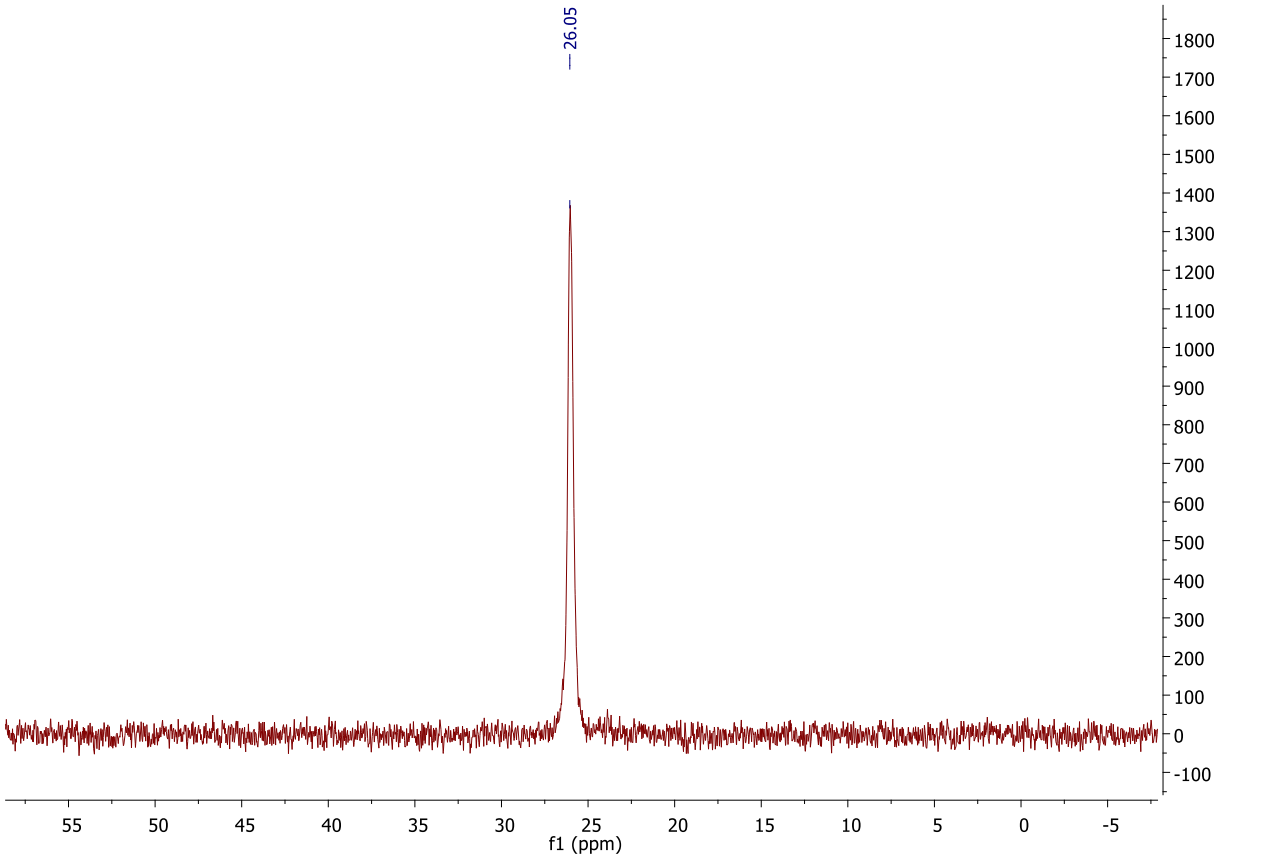


Fig S14. $^{31}P\{^{1}H\}$ NMR spectrum for ligand **3** ($CDCl_3$, 161.98 MHz).

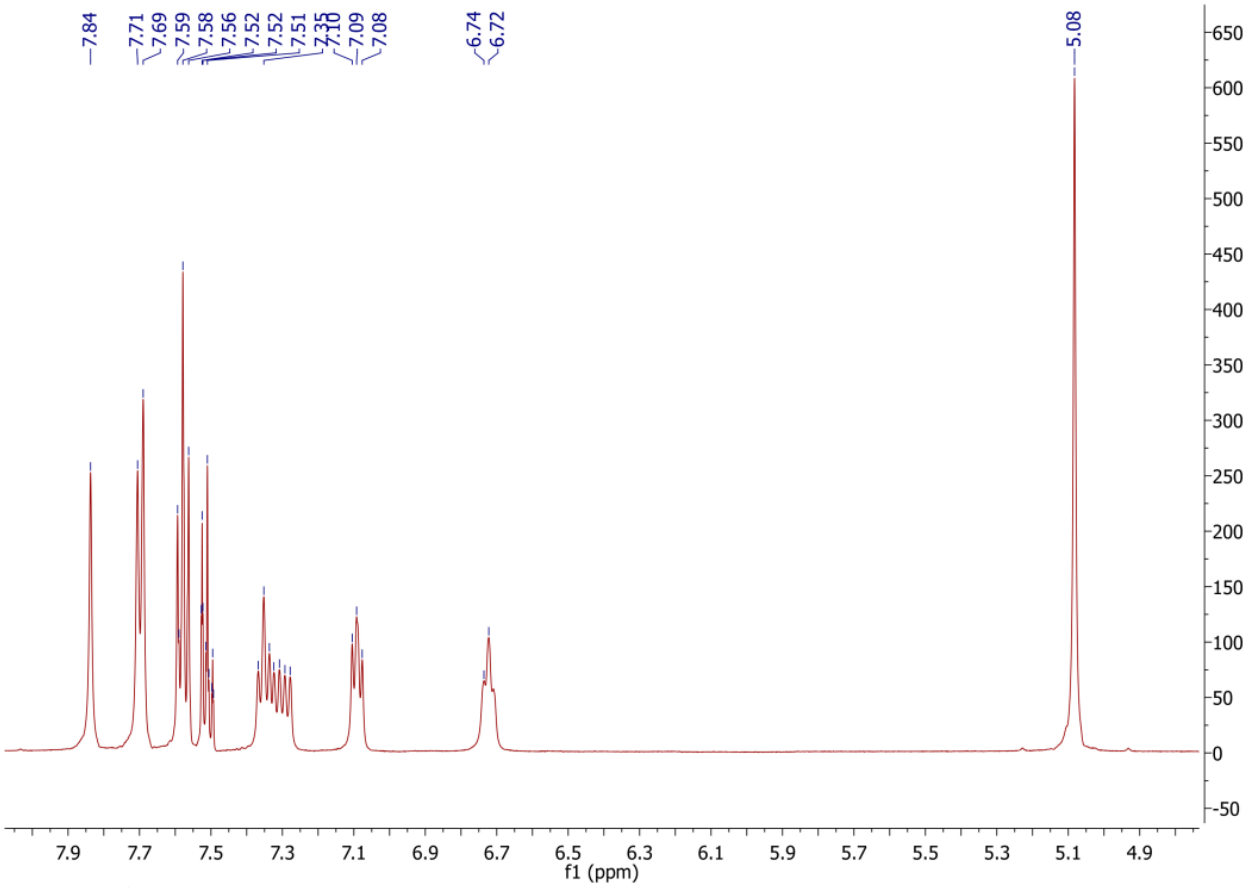


Fig S15. ^{1}H NMR spectrum for complex **4** (CD_3CN, 0.01 M, 500.13 MHz).

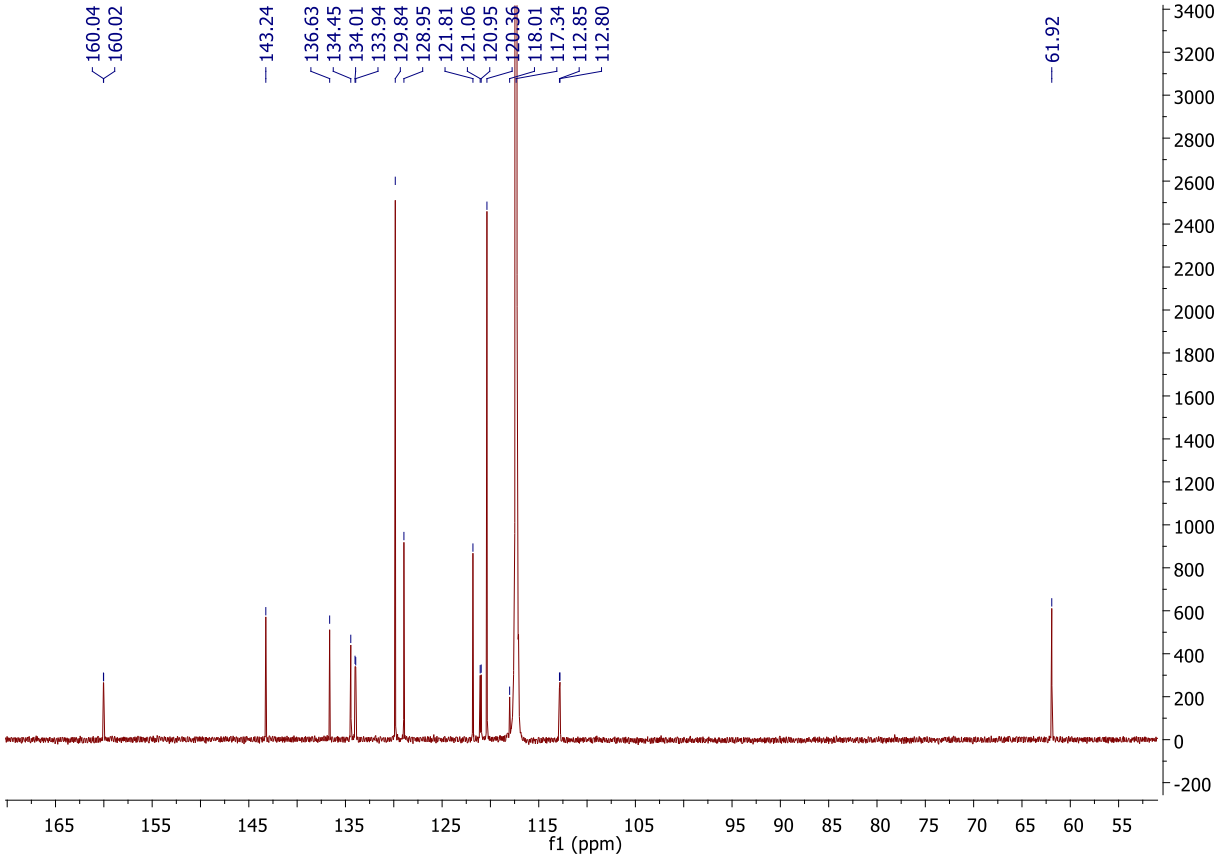


Fig S16. $^{13}C\{^{1}H\}$ NMR spectrum for complex **4** (CD_3CN, 0.01 M, 125.75 MHz)

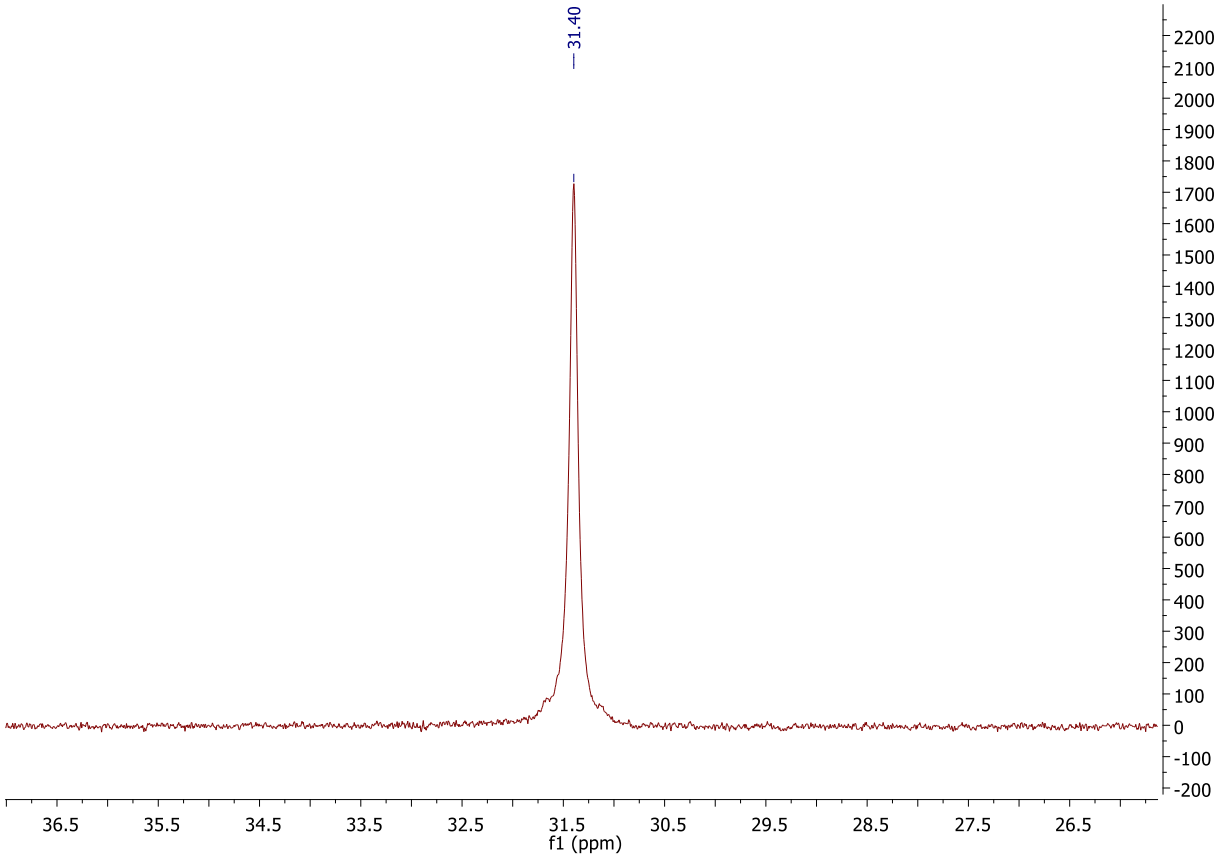


Fig S17. $^{31}P\{^{1}H\}$ NMR spectrum for complex **4** (CD_3CN, 0.01 M, 202.46 MHz).

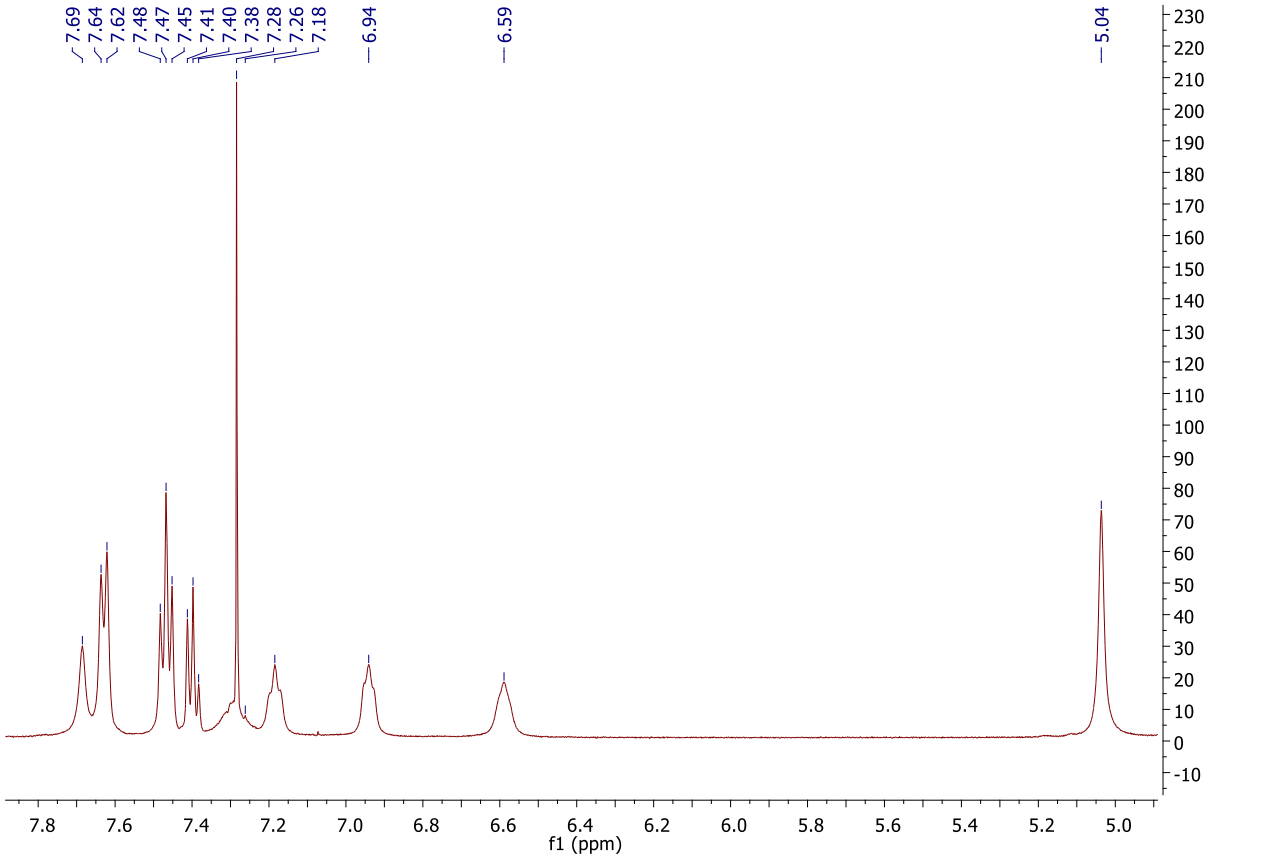


Fig S18. ^{1}H NMR spectrum for complex **4** ($CDCl_3$, 0.01 M, 500.13 MHz).

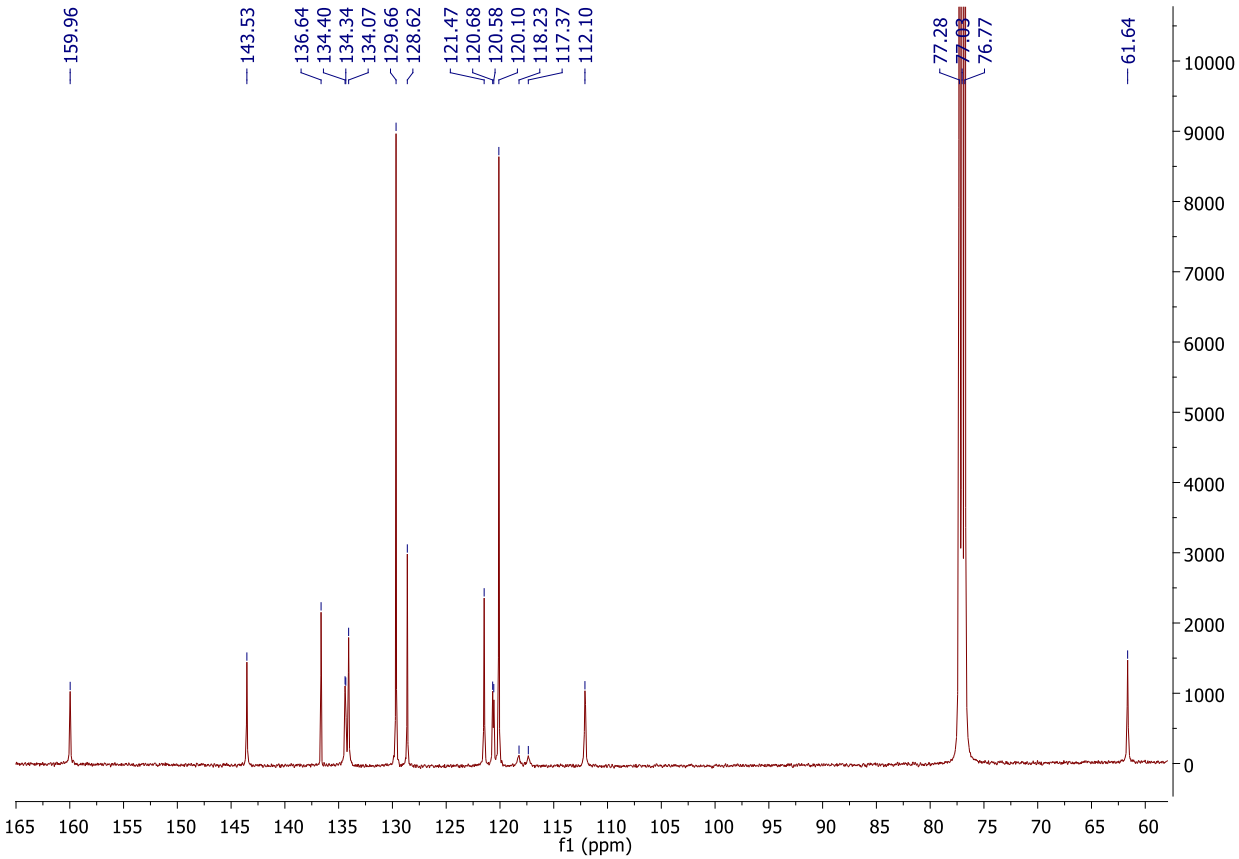


Fig S19. $^{13}C\{^{1}H\}$ NMR spectrum for complex **4** ($CDCl_3$, 0.01 M, 125.75 MHz)

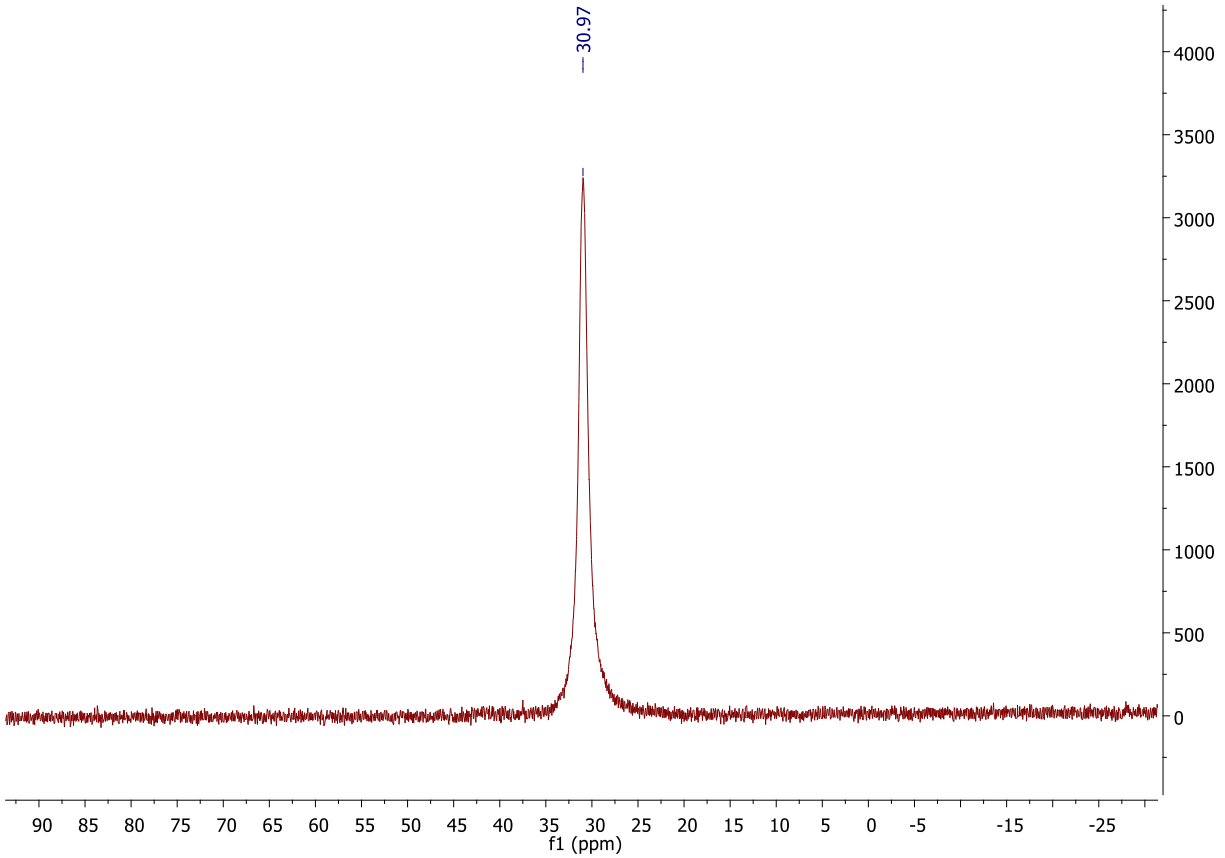


Fig S20. $^{31}P\{^{1}H\}$ NMR spectrum for complex **4** ($CDCl_3$, 0.01 M, 202.46 MHz).

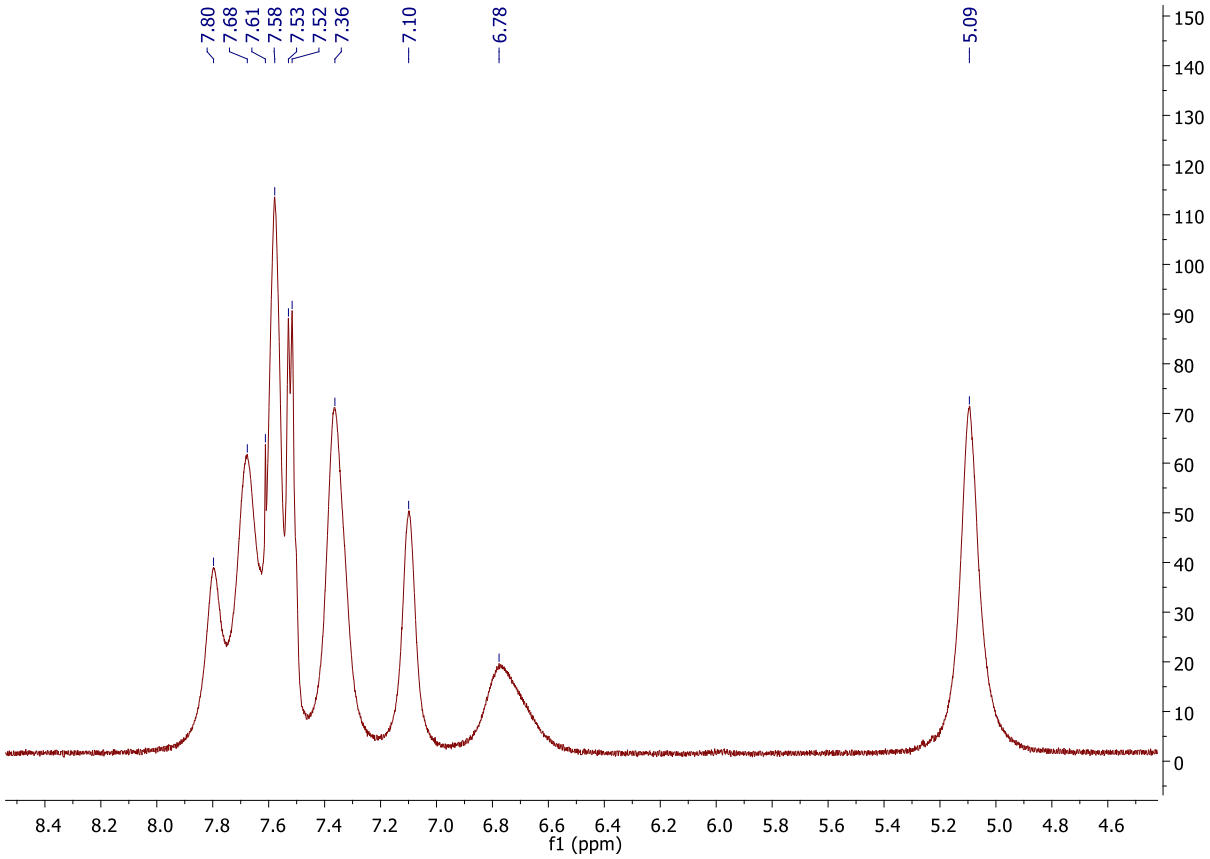


Fig S21. ^{1}H NMR spectrum for complex **5** (CD_3CN, 0.01 M, 500.13 MHz).

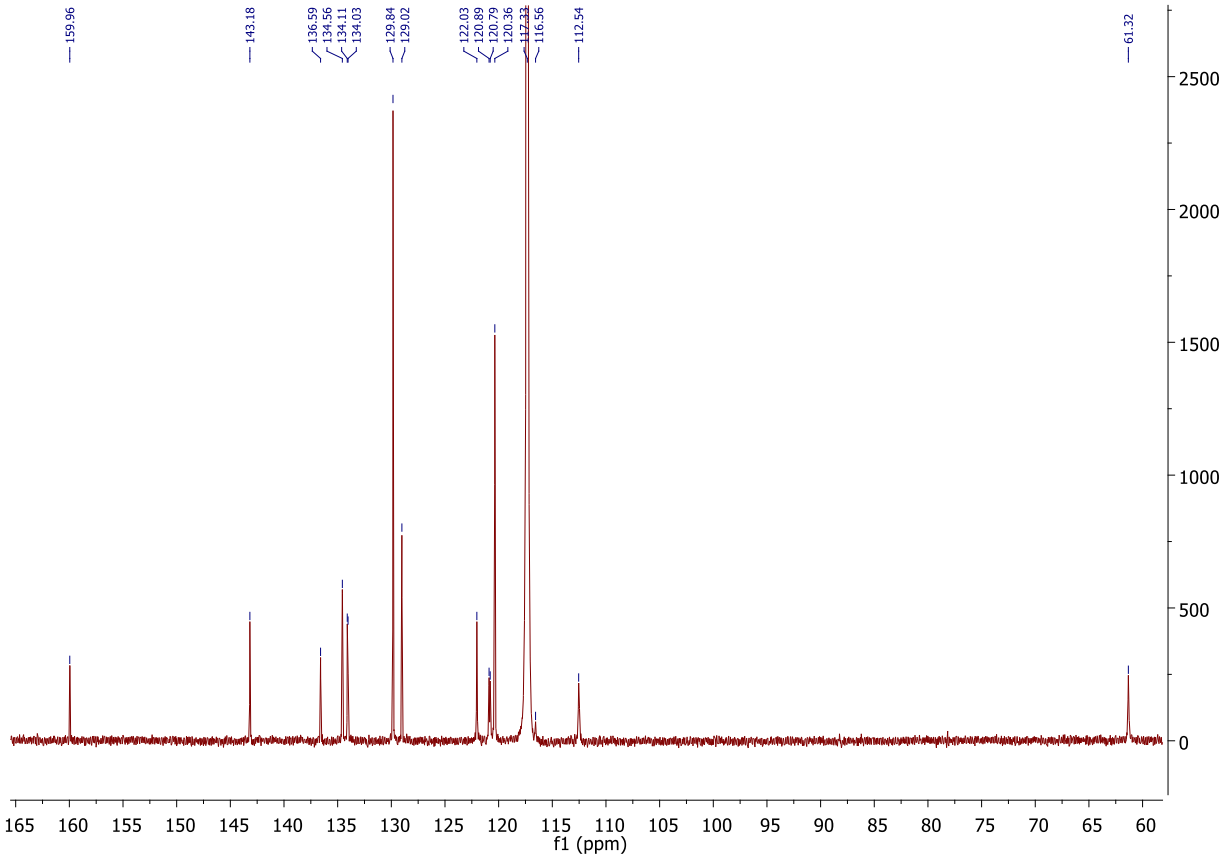


Fig S22. $^{13}C\{^{1}H\}$ NMR spectrum for complex **5** (CD_3CN, 0.01 M, 125.75 MHz)

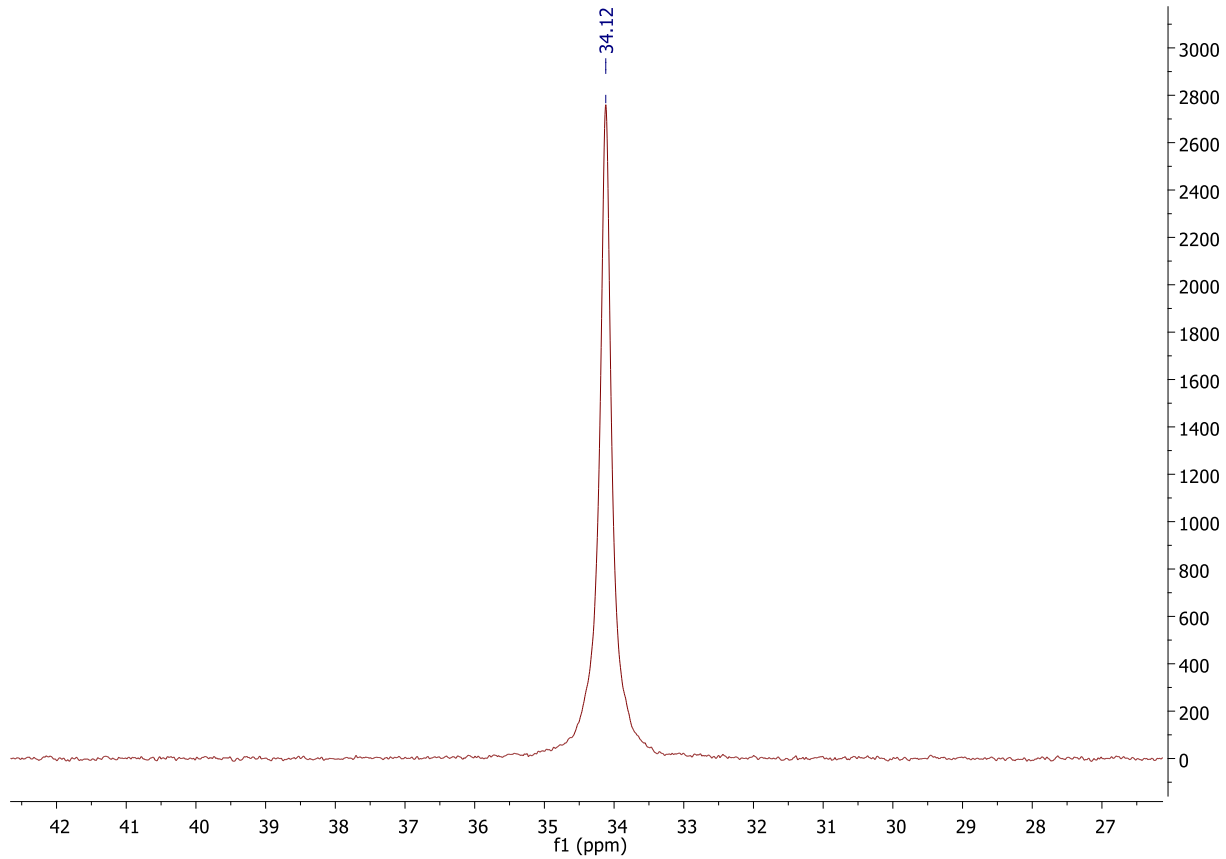


Fig S23. $^{31}P\{^{1}H\}$ NMR spectrum for complex **5** (CD_3CN, 0.01 M, 202.46 MHz).

DFT results for complex La(L)$(NO_3)_3$ at PBE0/def2-TZVP level

In DFT computations, we used model ligand [2-(1-Me-1,2,3-triazol-4-yl-CH_2O)C_6H_4]$_3$P(O) (**L)** where Ph substituent in triazole rings of ligand **3** is replaced by Me.

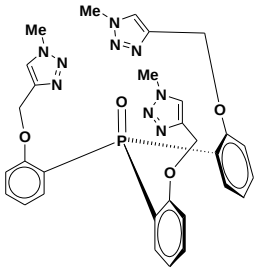


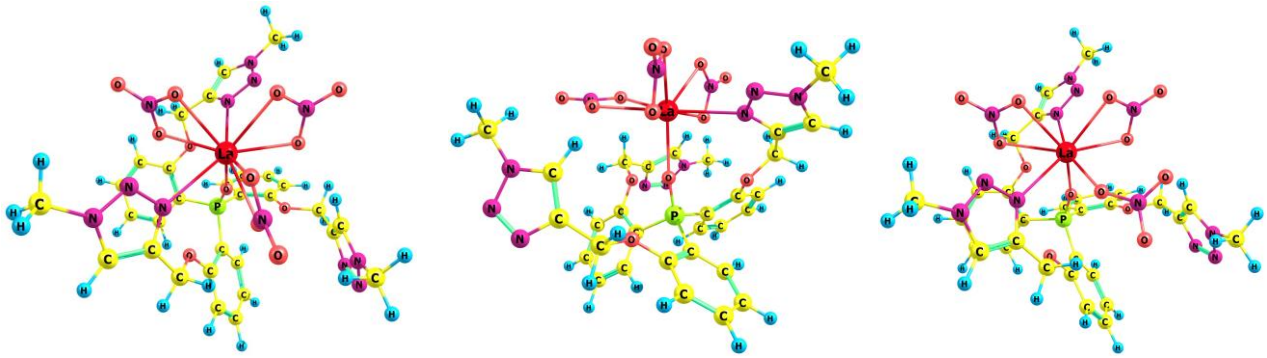
Fig. S24. Model ligand **L.**

Geometry optimization for complexes of ligand **L** with La$(NO_3)_3$ was performed in Gaussian software [S2] at the theory level PBE0/Def2-TZVP [S3,S4] in approximation of isolated molecule and SMD solvation model (acetonitrile).

Table S3. Relative energies of isomeric complexes La(**L**)$(NO_3)_3$ calculated at the PBE0/Def2-TZVP level (***isolated molecule***).

Type of complex	Ligand denticity	NO_3^- denticity	CN*	E_{tot}, a.u.	ΔE, kcal/mol	Comment
A	4	3 mono	7	-3166.836794	28.5	
B	4	1 bi + 2 mono	8	-3166.847290	21.9	
C	4	2 bi + 1 mono	9	-3166.858318	14.9	
D	4	3 bi	10	–	–	Unstable
E	**3**	**3 bi**	9	-3166.882203	**0.0**	**The most stable**
F	3	2bi + 1 mono	8	-3166.870617	7.2	
G	2	3 bi	8	-3166.876612	3.5	

* Coordination number.



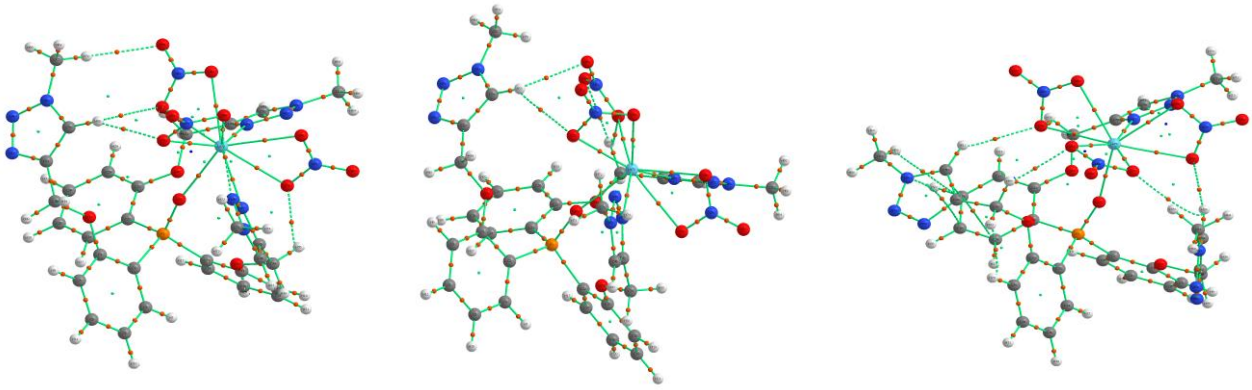
E **G** **F**

Fig. S25. Complexes of type E, G, F (***isolated molecule***). The most stable complex **E**.

Table S4. Interatomic distances (Å) in optimized complexes (types **A**-**C**, **E**–**G)** at the PBE0/Def2-TZVP level ***(isolated molecule***).

Type of complex	Ligand denticity	NO_3^- denticity	La...O(P=O)	La...N^3	La...O (NO_3)
A	4	3 mono	2.416	2.728 2.824 2.830	2.380 2.404 2.379
B	4	1 bi + 2 mono	2.452	2.729 2.869 2.917	2.394 2.408 2.587, 2.550
C	4	2 bi + 1 mono	2.450	2.755 2.970 2.985	2.416 2.568, 2.600 2.570, 2.591
E	3	3 bi	2.425	2.822 2.869	2.565, 2.561 2.569, 2.596 2.591, 2.606
F	3	2 bi + 1 mono	2.410	2.827 2.846	2.433 2.532, 2.433 2.565, 2.620
G	2	3 bi	2.375	2.781	2.584, 2.565 2.558, 2.565 2.535, 2.559

In complexes of type **E**, **F,** and **G (*isolated molecule)*,** the C–H bond of uncoordinated at La triazole ring forms hydrogen bonds with nitrates of type C–H...O_N (Fig. S26).



E **F** **G**

Fig. S26. Complexes of type **E**, F, and **G** (***isolated molecule)***.

The strength of these bonds (Table S5) was assessed using Espinosa–Lecomte correlation [S8].

Table S5. Assessment of strength of C–H...O_N hydrogen bonds in complexes **E**, **F,** and **G**

Type of complex	ρ(**r**), a.u.	V(**r**), a.u.	E_{cont}, kcal/mol
E*	0.008099	-0.004315	1.3
	0.004584	-0.002528	0.8
F*	0.005177	-0.002631	0.8
	0.007730	-0.004341	1.4
G	0.011059	-0.006819	2.1

* Bifurcate hydrogen bond.

On the use of SMD nonspecific solvation model with acetonitrile solvent parameters, complexes **A**, **C**, **D,** and **F** do not correspond to the minimum on potential curve and transfer to the most stable complex **E**. Complex **G** (ΔE = 7.8 kcal/mol) becomes the second in stability, complex **B** (ΔE = 14.3 kcal/mol) becomes the third (Table S6).

Table S6. Relative energies of optimized complexes **A**–**G** calculated at the PBE0/Def2-TZVP level, SMD solvation model (acetonitrile)

Type of complex	Ligand denticity	NO_3^- denticity	CN	E_{tot}, a.u.	ΔE, kcal/mol	Comment
A	4	3 mono	7	–	–	Unstable
B	4	1bi + 2 mono	8	–3166.940658	14.3	
C	4	2 bi + 1 mono	9	–	–	Unstable
D	4	3 bi	10	–	–	Unstable
E	3	3 bi	9	–3166.963391	**0.0**	**The most stable**
F	3	2bi + 1 mono	8	–	–	Unstable
G	2	3 bi	8	–3166.951009	7.8	

Table S7. Interatomic distances (Å) in optimized complexes **B, E,** and **G** at the PBE0/Def2-TZVP level, SMD solvation model (acetonitrile)

Type of complex	Ligand denticity	NO_3^- denticity	La...O (P=O)	La...N^3	La...O (NO_3)
B	4	1bi + 2 mono	2.399	2.810 2.804 2.858	2.660, 2.579 2.459 2.433
E	3	3 bi	2.471	2.830 2.789	2.684, 2.614 2.601, 2.634 2.611, 2.594
G	2	3 bi	2.350	2.723	2.619, 2.675 2.626, 2.606 2.719, 2.722

Geometry optimization (Fig. S27 and Table S8) of cationic complex of La^{3+} with two nitrates and tetradentate ligand (type **H**) was performed in Gaussian software at theory level PBE0/Def2-TZVP using SMD solvation model with acetonitrile solvent parameters.

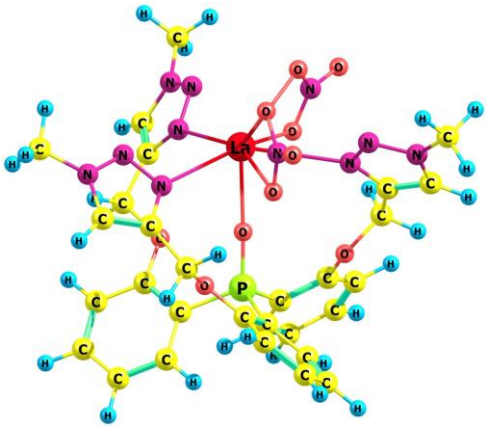


Fig. S27. Optimized structure of cationic complex **H** [SMD solvation model (MeCN)].

Table S8. Interatomic distances (Å) in optimized complexes **E** and **H** at the PBE0/Def2-TZVP level, SMD solvation model (acetonitrile)

Type of complex	Ligand denticity	NO_3^- denticity	La...O(P=O)	La...N^3	La...O (NO_3)
E	3	3 bi	2.471	2.830 2.789	2.684, 2.614 2.601, 2.634 2.611, 2.594
H (cationic complex)	4	2 bi	2.376	2.972 2.945 2.937	2.624, 2.625 2.668, 2.600

To compare stability of complex **H** with the most stable neutral complex **E** (in reaction **E** = **H** + NO_3^-), we calculated ΔH^o_{298} and ΔG^o_{298} values on the same theory level (Table S9). According to the obtained data, the dissociation of complex **E** to cationic **H** and free NO_3^- is profitable due to entropy factor, the value of ΔG^o_{298} is –4.9 kcal/mol.

Table S9. Calculated energetic parameters at the PBE0/Def2TZVP level, SMD solvation model (MeCN).

Type of complex	E_{tot} + ZPVE, a.u.	H^o_{298}, a.u.	G^o_{298}, a.u.
H	–2886.049280	–2885.998718	–2886.137113
NO_3^-	–280.267777	–280.263709	–280.293227
E	–3166.330079	–3166.276684	–3166.422510
Δ, kcal/mol	8.2	8.9	–4.9

References

S1. I.Yu. Kudryavtsev, T.V. Baulina, V.N. Khrustalev, P.V. Petrovskii, M.P. Pasechnik, E.E. Nifant'ev, Dokl. Chem., 2013, **448**, 55.

S2. M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheese- man, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Car- icato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery Jr., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, O. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, D.J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford CT, 2013 .

S3. F. Weigend, Phys. Chem. Chem. Phys. 8 (2006) 1057–1065.

S4. C. Adamo, V. Barone, J. Chem. Phys. 110 (1999) 6158–6169.

S5. A.V. Marenich, C.J. Cramer, and D.G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378.

S6. R.F.W. Bader, Atoms in Molecules. A Quantum Theory, Clarendron Press, Oxford, 1990.

S7. T.A. Keith, AIMAll (Ver. 19.10.12), TK Gristmill Software, Overland Park, KS, USA, 2019 aim.tkgristmill.com.

S8. (a) E. Espinosa, E. Molins, C. Lecomte, Chem. Phys. Lett. 285 (1998) 170; (b) E. Espinosa, I. Alkorta, I. Rozas, J. Elguero, E. Molins, Chem. Phys. Lett. 336 (2001) 457.].

S9. A.G. Matveeva, A.V. Vologzhanina, M.P. Pasechnik, R.R. Aysin, S.V. Matveev , Y.V. Zubavichus, O.I. Artyushin, E.V. Sharova, I.A. Godovikov and V.K. Brel, *Polyhedron*, 2022, **215**, 115680.

S10. A.G. Matveeva, I.Yu. Kudryavtsev, M.P. Pasechnik, A.V. Vologzhanina, T.V. Baulina, A.V. Vavina, G.Ya. Sukat, S.V. Matveev, I.A. Godovikov, A.N. Turanov, K. Karandashev, and V.K. Brel, *Polyhedron*, 2018, **142**, 71.

xyz-Optimized Cartesian coordinates for model complex La(L)$(NO_3)_3$

$La(NO_3)_3$-L, type A, Etot = -3166.83679446

P	1.835121000000	1.554584000000	0.144715000000
C	3.010832000000	1.029390000000	-1.112857000000
C	2.493026000000	0.722139000000	-2.382709000000
C	4.355918000000	0.802994000000	-0.853224000000
C	3.306744000000	0.145211000000	-3.348874000000
C	5.180239000000	0.260309000000	-1.826998000000
H	4.754200000000	1.036342000000	0.127702000000
C	4.644728000000	-0.079221000000	-3.060546000000
H	2.900301000000	-0.134336000000	-4.312139000000
H	6.227924000000	0.084101000000	-1.616778000000
H	5.276956000000	-0.528135000000	-3.818438000000
C	2.678051000000	1.707971000000	1.728939000000
C	3.008659000000	0.528499000000	2.414227000000
C	2.843269000000	2.932384000000	2.367651000000
C	3.433555000000	0.584523000000	3.735667000000
C	3.305072000000	2.993355000000	3.672588000000
H	2.582985000000	3.844432000000	1.842956000000
C	3.579513000000	1.816854000000	4.353448000000
H	3.652746000000	-0.325980000000	4.278372000000
H	3.426287000000	3.951601000000	4.162362000000
H	3.915449000000	1.854003000000	5.383642000000
C	1.311769000000	3.220562000000	-0.330248000000
C	0.088545000000	3.746754000000	0.111892000000
C	2.083987000000	3.970535000000	-1.212259000000
C	-0.359319000000	4.970982000000	-0.375957000000
C	1.656604000000	5.205470000000	-1.672119000000
H	3.026603000000	3.565318000000	-1.562498000000
C	0.426208000000	5.692308000000	-1.260724000000
H	-1.311489000000	5.370024000000	-0.050438000000
H	2.271416000000	5.772215000000	-2.360319000000
H	0.070369000000	6.649242000000	-1.625917000000
O	0.697557000000	0.581595000000	0.252838000000
O	2.925759000000	-0.606609000000	1.697639000000
C	2.577331000000	-1.827744000000	2.344729000000
H	1.680482000000	-1.677924000000	2.958074000000
H	3.397061000000	-2.179780000000	2.979742000000
O	1.206499000000	1.055125000000	-2.566751000000
C	0.448385000000	0.483181000000	-3.622116000000
H	0.608775000000	-0.601137000000	-3.655502000000
H	0.734288000000	0.922814000000	-4.584635000000
O	-0.583752000000	3.031810000000	1.031679000000
C	-1.997306000000	3.140127000000	1.082325000000
H	-2.306473000000	4.087799000000	1.536860000000
H	-2.400846000000	3.090141000000	0.064313000000
C	2.325177000000	-2.820527000000	1.272470000000
C	2.962981000000	-4.002268000000	1.004201000000
H	3.782991000000	-4.509610000000	1.483964000000
N	1.376502000000	-3.672683000000	-0.474589000000
C	-2.504146000000	2.008942000000	1.894733000000
C	-3.364273000000	1.997904000000	2.960338000000
H	-3.883124000000	2.781617000000	3.485598000000

N	-2.741378000000	-0.049422000000	2.502516000000
C	-0.974660000000	0.796487000000	-3.326336000000
C	-1.985039000000	1.193122000000	-4.161766000000
H	-2.021197000000	1.383342000000	-5.220993000000
N	-2.757719000000	1.018619000000	-2.116485000000
N	1.357804000000	-2.665090000000	0.332906000000
N	2.332259000000	-4.491759000000	-0.081453000000
N	-2.154042000000	0.724785000000	1.652054000000
N	-3.475875000000	0.696541000000	3.292836000000
N	-3.066052000000	1.303909000000	-3.363307000000
N	-1.503469000000	0.696002000000	-2.081107000000
C	-4.280746000000	0.066906000000	4.313934000000
H	-4.204399000000	0.631901000000	5.242213000000
H	-5.320184000000	0.015905000000	3.987909000000
H	-3.889362000000	-0.939133000000	4.456873000000
C	-4.430563000000	1.639397000000	-3.701453000000
H	-5.079531000000	1.104470000000	-3.008568000000
H	-4.591931000000	2.715728000000	-3.623062000000
H	-4.634247000000	1.310620000000	-4.719010000000
C	2.560498000000	-5.715955000000	-0.812044000000
H	1.850274000000	-5.729833000000	-1.636702000000
H	3.578741000000	-5.738879000000	-1.201330000000
H	2.391719000000	-6.577721000000	-0.165622000000
La	-0.995181000000	-1.125482000000	0.016148000000
O	-0.935946000000	-2.387431000000	2.061708000000
O	-3.330036000000	-1.375235000000	-0.371667000000
O	-0.545067000000	-2.150681000000	-2.083322000000
N	-0.155365000000	-3.095328000000	-2.872792000000
O	-0.668242000000	-4.187639000000	-2.776223000000
O	0.716910000000	-2.818223000000	-3.689308000000
N	-4.460971000000	-0.791129000000	-0.579527000000
O	-4.925212000000	-0.087670000000	0.303270000000
O	-5.010327000000	-0.973089000000	-1.652954000000
N	-1.132662000000	-2.293687000000	3.332274000000
O	-0.346644000000	-1.608787000000	3.981176000000
O	-2.067962000000	-2.888699000000	3.823842000000

$La(NO_3)_3$-L, type B, E_{tot} = -3166.84728998

P	1.809052000000	1.536172000000	0.356656000000
C	3.034058000000	1.338648000000	-0.953857000000
C	2.558403000000	1.317637000000	-2.274730000000
C	4.374713000000	1.071733000000	-0.711983000000
C	3.405600000000	0.975373000000	-3.320041000000
C	5.232760000000	0.761361000000	-1.756644000000
H	4.743000000000	1.084816000000	0.307434000000
C	4.738416000000	0.699292000000	-3.050550000000
H	3.032635000000	0.935793000000	-4.335906000000
H	6.276548000000	0.550983000000	-1.558520000000
H	5.399301000000	0.438575000000	-3.869704000000
C	2.616733000000	1.384424000000	1.959665000000
C	2.983221000000	0.100153000000	2.390763000000
C	2.716078000000	2.450866000000	2.847345000000
C	3.372215000000	-0.111502000000	3.707543000000
C	3.145405000000	2.250179000000	4.149171000000

H	2.429430000000	3.443446000000	2.519721000000
C	3.451270000000	0.966174000000	4.575324000000
H	3.610723000000	-1.108874000000	4.053489000000
H	3.215052000000	3.086415000000	4.833799000000
H	3.758342000000	0.795743000000	5.601093000000
C	1.231443000000	3.248132000000	0.240485000000
C	-0.000398000000	3.627313000000	0.795632000000
C	1.968352000000	4.195233000000	-0.462941000000
C	-0.492156000000	4.912769000000	0.587842000000
C	1.497678000000	5.486131000000	-0.642075000000
H	2.919239000000	3.907326000000	-0.896786000000
C	0.259352000000	5.832685000000	-0.126282000000
H	-1.450647000000	5.201907000000	0.999286000000
H	2.085930000000	6.207959000000	-1.195032000000
H	-0.129801000000	6.834092000000	-0.272983000000
O	0.718213000000	0.519456000000	0.208535000000
O	2.968354000000	-0.854726000000	1.445693000000
C	2.691240000000	-2.205792000000	1.805008000000
H	1.791725000000	-2.243600000000	2.429954000000
H	3.533513000000	-2.641140000000	2.353497000000
O	1.275409000000	1.689287000000	-2.429579000000
C	0.496892000000	1.190692000000	-3.508947000000
H	0.670359000000	0.117141000000	-3.631676000000
H	0.745816000000	1.707836000000	-4.441976000000
O	-0.632392000000	2.706993000000	1.543672000000
C	-2.040403000000	2.785622000000	1.686505000000
H	-2.326621000000	3.607281000000	2.352474000000
H	-2.495545000000	2.954465000000	0.703328000000
C	2.500199000000	-2.945178000000	0.534146000000
C	3.210806000000	-4.001208000000	0.030069000000
H	4.043926000000	-4.565395000000	0.414257000000
N	1.644909000000	-3.420143000000	-1.393606000000
C	-2.502712000000	1.496199000000	2.252387000000
C	-3.364580000000	1.235550000000	3.284411000000
H	-3.911356000000	1.874553000000	3.956672000000
N	-2.672200000000	-0.649210000000	2.414908000000
C	-0.921405000000	1.449454000000	-3.150120000000
C	-1.911498000000	2.086520000000	-3.849473000000
H	-1.937212000000	2.539119000000	-4.826266000000
N	-2.689230000000	1.436880000000	-1.904179000000
N	1.545463000000	-2.627797000000	-0.378522000000
N	2.636278000000	-4.260188000000	-1.160758000000
N	-2.108162000000	0.304439000000	1.751671000000
N	-3.433971000000	-0.109185000000	3.336396000000
N	-2.985923000000	2.041416000000	-3.036987000000
N	-1.453873000000	1.060258000000	-1.964301000000
C	-4.220458000000	-0.963841000000	4.195092000000
H	-4.181160000000	-0.592154000000	5.218316000000
H	-5.252654000000	-0.992913000000	3.844176000000
H	-3.783895000000	-1.960119000000	4.143737000000
C	-4.334692000000	2.509169000000	-3.261147000000
H	-5.000492000000	1.866951000000	-2.685076000000
H	-4.438449000000	3.548714000000	-2.945843000000
H	-4.570387000000	2.421591000000	-4.320449000000

C	2.947538000000	-5.283244000000	-2.128952000000
H	2.228939000000	-5.184048000000	-2.939801000000
H	3.959816000000	-5.149813000000	-2.512686000000
H	2.852136000000	-6.270750000000	-1.676642000000
La	-0.986399000000	-1.185237000000	-0.241350000000
O	-0.614459000000	-2.659176000000	1.625835000000
O	-3.339363000000	-1.183594000000	-0.681812000000
O	-0.459745000000	-1.641078000000	-2.694512000000
N	-0.827802000000	-2.861565000000	-2.731771000000
O	-1.288721000000	-3.326222000000	-1.662055000000
O	-0.728306000000	-3.512069000000	-3.737059000000
N	-4.447177000000	-0.530777000000	-0.717730000000
O	-4.868914000000	-0.032903000000	0.315673000000
O	-5.026594000000	-0.441816000000	-1.788211000000
N	-0.852726000000	-2.882199000000	2.872701000000
O	-0.082194000000	-2.392256000000	3.693246000000
O	-1.806630000000	-3.568985000000	3.174148000000

$La(NO_3)_3$-L, type C, E_{tot} = -3166.85831800

P	1.540413000000	1.802384000000	0.336157000000
C	2.496938000000	1.788059000000	1.865508000000
C	3.113829000000	0.590267000000	2.263807000000
C	2.509989000000	2.874434000000	2.733455000000
C	3.681649000000	0.486076000000	3.528625000000
C	3.104801000000	2.783701000000	3.982079000000
H	2.027450000000	3.797056000000	2.432671000000
C	3.673910000000	1.583424000000	4.376113000000
H	4.130228000000	-0.443740000000	3.852739000000
H	3.103633000000	3.637079000000	4.648779000000
H	4.121841000000	1.492992000000	5.359408000000
C	0.683950000000	3.398302000000	0.290058000000
C	-0.599557000000	3.556306000000	0.835662000000
C	1.268175000000	4.475667000000	-0.369180000000
C	-1.285829000000	4.755152000000	0.656735000000
C	0.602587000000	5.681839000000	-0.514306000000
H	2.256773000000	4.356372000000	-0.798277000000
C	-0.682129000000	5.808084000000	-0.011521000000
H	-2.284937000000	4.874564000000	1.054888000000
H	1.076020000000	6.506288000000	-1.032971000000
H	-1.225466000000	6.738508000000	-0.133666000000
C	2.678122000000	1.828236000000	-1.062830000000
C	2.109573000000	1.767854000000	-2.345937000000
C	4.058872000000	1.779494000000	-0.929135000000
C	2.918887000000	1.608868000000	-3.463049000000
C	4.872882000000	1.649498000000	-2.044697000000
H	4.498373000000	1.825761000000	0.060786000000
C	4.295485000000	1.550281000000	-3.301309000000
H	2.480984000000	1.536374000000	-4.450463000000
H	5.949226000000	1.608867000000	-1.931303000000
H	4.924001000000	1.429620000000	-4.176625000000
O	0.626780000000	0.622122000000	0.256378000000
O	-1.093447000000	2.526201000000	1.544349000000
C	-2.498562000000	2.392465000000	1.658887000000
H	-2.949866000000	2.459691000000	0.661699000000

H	-2.923155000000	3.181403000000	2.290057000000
O	3.138314000000	-0.390466000000	1.346899000000
C	3.300358000000	-1.735444000000	1.772514000000
H	2.574786000000	-1.952185000000	2.562222000000
H	4.315473000000	-1.902846000000	2.149625000000
O	0.775857000000	1.914272000000	-2.387463000000
C	0.024515000000	1.415182000000	-3.482324000000
H	0.110662000000	2.081790000000	-4.348018000000
H	0.383705000000	0.416258000000	-3.745411000000
C	-2.788186000000	1.071323000000	2.266802000000
C	-3.702175000000	0.736295000000	3.229665000000
H	-4.410665000000	1.315636000000	3.796838000000
N	-2.639168000000	-1.061882000000	2.567810000000
C	-1.390614000000	1.356786000000	-3.030232000000
C	-2.529182000000	1.785569000000	-3.660358000000
H	-2.701170000000	2.248564000000	-4.617355000000
N	-3.047722000000	0.934101000000	-1.707437000000
C	3.070992000000	-2.606592000000	0.594144000000
C	3.921033000000	-3.517189000000	0.024508000000
H	4.924243000000	-3.824981000000	0.267164000000
N	2.030210000000	-3.476001000000	-1.087517000000
N	-2.166024000000	-0.067972000000	1.890639000000
N	-3.569168000000	-0.596075000000	3.370876000000
N	-1.764422000000	0.829770000000	-1.835530000000
N	-3.525656000000	1.489964000000	-2.802848000000
N	3.226041000000	-4.029597000000	-1.008407000000
N	1.919541000000	-2.619624000000	-0.127143000000
C	-4.952781000000	1.662737000000	-2.949101000000
H	-5.261608000000	2.642509000000	-2.580693000000
H	-5.216736000000	1.567211000000	-4.001066000000
H	-5.435993000000	0.869863000000	-2.378217000000
C	3.605441000000	-5.045972000000	-1.959421000000
H	2.806164000000	-5.108449000000	-2.694845000000
H	4.538273000000	-4.770758000000	-2.452105000000
H	3.721208000000	-6.009011000000	-1.460610000000
C	-4.355750000000	-1.509893000000	4.161958000000
H	-3.789668000000	-2.433457000000	4.258551000000
H	-4.540050000000	-1.082543000000	5.147030000000
H	-5.300176000000	-1.714216000000	3.655889000000
La	-0.765594000000	-1.362045000000	-0.098382000000
O	-3.116153000000	-1.749441000000	-0.499446000000
O	0.280415000000	-1.378770000000	-2.443229000000
O	0.254118000000	-1.879070000000	2.226466000000
N	-0.082210000000	-3.099166000000	2.266434000000
O	-0.758181000000	-3.522699000000	1.293306000000
O	0.243419000000	-3.812091000000	3.184341000000
N	-0.101914000000	-2.541902000000	-2.799299000000
O	0.200936000000	-2.992877000000	-3.874593000000
O	-0.797946000000	-3.167516000000	-1.969596000000
N	-4.334353000000	-1.353893000000	-0.516922000000
O	-4.844984000000	-0.961469000000	0.525163000000
O	-4.937915000000	-1.385985000000	-1.578657000000

$La(NO_3)_3$-L, type E, E_{tot} = -3166.882203

P	-1.046353000000	0.856050000000	1.686021000000
C	-2.078021000000	2.304518000000	1.385446000000
C	-3.041982000000	2.269412000000	0.358860000000
C	-1.909526000000	3.475360000000	2.115085000000
C	-3.777818000000	3.416149000000	0.065634000000
C	-2.656187000000	4.609435000000	1.837236000000
H	-1.177290000000	3.498333000000	2.913427000000
C	-3.578823000000	4.572075000000	0.804662000000
H	-4.508615000000	3.408001000000	-0.731236000000
H	-2.512667000000	5.512447000000	2.417483000000
H	-4.163476000000	5.454170000000	0.567562000000
C	0.146176000000	1.317903000000	2.959643000000
C	1.207782000000	2.168853000000	2.611121000000
C	0.101214000000	0.786719000000	4.242656000000
C	2.214335000000	2.444616000000	3.527673000000
C	1.093626000000	1.074187000000	5.167225000000
H	-0.717114000000	0.129266000000	4.513271000000
C	2.148938000000	1.893237000000	4.798572000000
H	3.044128000000	3.083993000000	3.255883000000
H	1.048184000000	0.651651000000	6.163339000000
H	2.937676000000	2.113379000000	5.509227000000
C	-2.122507000000	-0.410793000000	2.384145000000
C	-1.678906000000	-1.740809000000	2.466752000000
C	-3.435806000000	-0.118089000000	2.736566000000
C	-2.565466000000	-2.746119000000	2.836391000000
C	-4.311898000000	-1.113128000000	3.136252000000
H	-3.782622000000	0.906369000000	2.671901000000
C	-3.873658000000	-2.425762000000	3.165499000000
H	-2.246207000000	-3.778960000000	2.866704000000
H	-5.335222000000	-0.867713000000	3.390176000000
H	-4.556345000000	-3.220115000000	3.444796000000
O	-0.351912000000	0.377931000000	0.442387000000
O	1.141621000000	2.698441000000	1.377520000000
C	2.293490000000	3.270199000000	0.784363000000
H	3.153839000000	2.617451000000	0.955348000000
H	2.496339000000	4.260707000000	1.207533000000
O	-3.199895000000	1.095071000000	-0.257754000000
C	-4.154916000000	0.979138000000	-1.315924000000
H	-3.828457000000	1.605267000000	-2.152506000000
H	-5.137509000000	1.313530000000	-0.970009000000
O	-0.374174000000	-1.955276000000	2.202704000000
C	0.055021000000	-3.280055000000	1.951778000000
H	-0.095782000000	-3.913931000000	2.832642000000
H	-0.515369000000	-3.691489000000	1.111958000000
C	2.009167000000	3.395369000000	-0.668192000000
C	2.023674000000	4.509954000000	-1.463089000000
H	2.245192000000	5.544110000000	-1.259622000000
N	1.446689000000	2.762770000000	-2.659884000000
C	1.503987000000	-3.244940000000	1.632831000000
C	2.526728000000	-3.959979000000	2.198068000000
H	2.553161000000	-4.683151000000	2.995710000000
N	3.322245000000	-2.675257000000	0.606688000000
C	-4.254037000000	-0.443291000000	-1.703208000000
C	-3.381565000000	-1.226157000000	-2.416417000000

H	-2.429482000000	-1.011560000000	-2.876246000000
N	-5.121123000000	-2.413945000000	-1.760879000000
N	1.650100000000	2.345454000000	-1.453038000000
N	1.673605000000	4.061588000000	-2.684481000000
N	2.046230000000	-2.471066000000	0.660551000000
N	3.625948000000	-3.573483000000	1.522840000000
N	-3.960403000000	-2.435431000000	-2.420587000000
N	-5.301976000000	-1.212783000000	-1.322624000000
C	4.994417000000	-4.005832000000	1.678121000000
H	5.318036000000	-3.861024000000	2.708862000000
H	5.093026000000	-5.056470000000	1.403082000000
H	5.601441000000	-3.394433000000	1.014417000000
C	-3.472717000000	-3.666122000000	-2.994228000000
H	-4.245820000000	-4.417152000000	-2.846932000000
H	-3.287711000000	-3.536673000000	-4.061187000000
H	-2.551629000000	-3.978316000000	-2.500034000000
C	1.534015000000	4.788352000000	-3.923914000000
H	1.199961000000	4.076571000000	-4.675694000000
H	0.795363000000	5.582715000000	-3.813928000000
H	2.492652000000	5.213864000000	-4.222175000000
La	1.242092000000	-0.480591000000	-1.170746000000
O	3.069696000000	0.376435000000	0.462044000000
O	-0.447220000000	-2.462347000000	-1.079312000000
O	-0.456708000000	0.191756000000	-2.965290000000
N	0.364743000000	0.276403000000	-3.936557000000
O	1.555794000000	-0.029357000000	-3.675734000000
O	0.010505000000	0.631530000000	-5.028141000000
N	0.221917000000	-3.261843000000	-1.800062000000
O	1.279315000000	-2.810023000000	-2.305311000000
O	-0.143939000000	-4.399944000000	-1.980810000000
N	4.058385000000	0.168254000000	-0.305905000000
O	3.791404000000	-0.309652000000	-1.438882000000
O	5.184440000000	0.424320000000	0.037629000000

$La(NO_3)_3$-L, type F, E_{tot} = -3166.870617

P	-0.559635000000	0.910281000000	1.845274000000
C	-1.338624000000	2.531645000000	1.769899000000
C	-2.393040000000	2.757687000000	0.862187000000
C	-0.856421000000	3.591974000000	2.529420000000
C	-2.885491000000	4.052334000000	0.697548000000
C	-1.373987000000	4.869411000000	2.391922000000
H	-0.054612000000	3.412482000000	3.235894000000
C	-2.376345000000	5.090366000000	1.461540000000
H	-3.668647000000	4.253448000000	-0.019604000000
H	-0.988769000000	5.682613000000	2.994363000000
H	-2.779433000000	6.087940000000	1.325293000000
C	0.872947000000	1.074769000000	2.928921000000
C	2.008196000000	1.749405000000	2.447711000000
C	0.918353000000	0.487093000000	4.186606000000
C	3.165431000000	1.802700000000	3.213804000000
C	2.067088000000	0.550648000000	4.960688000000
H	0.043186000000	-0.036235000000	4.555160000000
C	3.184818000000	1.201607000000	4.464025000000
H	4.047360000000	2.308131000000	2.842469000000

H	2.090838000000	0.086650000000	5.938899000000
H	4.092049000000	1.248146000000	5.055904000000
C	-1.725632000000	-0.227940000000	2.604474000000
C	-1.515218000000	-1.614876000000	2.507197000000
C	-2.914134000000	0.238028000000	3.157341000000
C	-2.516096000000	-2.493754000000	2.905776000000
C	-3.895537000000	-0.637196000000	3.589628000000
H	-3.081178000000	1.306806000000	3.221843000000
C	-3.695293000000	-1.999159000000	3.441715000000
H	-2.390805000000	-3.561114000000	2.787360000000
H	-4.822039000000	-0.257101000000	4.000447000000
H	-4.470347000000	-2.696315000000	3.738940000000
O	-0.137539000000	0.423233000000	0.485828000000
O	1.866473000000	2.339493000000	1.246959000000
C	3.005314000000	2.769123000000	0.523353000000
H	3.777500000000	1.995612000000	0.562658000000
H	3.399669000000	3.702632000000	0.940754000000
O	-2.868475000000	1.682488000000	0.229233000000
C	-3.911513000000	1.845857000000	-0.738913000000
H	-3.485669000000	2.320385000000	-1.627978000000
H	-4.702080000000	2.476887000000	-0.324502000000
O	-0.313496000000	-2.008715000000	2.041306000000
C	-0.131547000000	-3.369979000000	1.683738000000
H	-0.315262000000	-4.022828000000	2.544039000000
H	-0.820087000000	-3.631906000000	0.871549000000
C	2.573192000000	2.990919000000	-0.881641000000
C	2.689412000000	4.109632000000	-1.662273000000
H	3.098320000000	5.087856000000	-1.473073000000
N	1.709783000000	2.515094000000	-2.810987000000
C	1.277481000000	-3.542993000000	1.250111000000
C	2.186929000000	-4.488361000000	1.644414000000
H	2.131834000000	-5.297858000000	2.352664000000
N	3.103559000000	-3.172068000000	0.145788000000
C	-4.509268000000	0.531689000000	-1.052828000000
C	-4.104791000000	-0.459994000000	-1.912341000000
H	-3.249854000000	-0.563287000000	-2.561751000000
N	-5.986312000000	-1.030402000000	-0.912288000000
N	1.964181000000	2.038749000000	-1.635773000000
N	2.145952000000	3.759112000000	-2.844652000000
N	1.891244000000	-2.759446000000	0.329252000000
N	3.294012000000	-4.218434000000	0.925474000000
N	-5.050469000000	-1.404093000000	-1.786637000000
N	-5.664616000000	0.136983000000	-0.464510000000
C	4.566479000000	-4.899192000000	0.916462000000
H	4.985434000000	-4.925827000000	1.922569000000
H	4.449879000000	-5.915479000000	0.538502000000
H	5.226805000000	-4.337402000000	0.259768000000
C	-5.151220000000	-2.681355000000	-2.453732000000
H	-6.069674000000	-3.148255000000	-2.104594000000
H	-5.197097000000	-2.536754000000	-3.533458000000
H	-4.288861000000	-3.300966000000	-2.208901000000
C	2.002018000000	4.536896000000	-4.052440000000
H	1.463787000000	3.920035000000	-4.768541000000
H	1.434127000000	5.444972000000	-3.849160000000

H	2.982084000000	4.795773000000	-4.454258000000
La	1.080263000000	-0.612634000000	-1.287953000000
O	3.355361000000	-0.155873000000	-0.092982000000
O	-0.373368000000	-2.553158000000	-1.383465000000
O	-0.775634000000	0.504612000000	-2.640665000000
N	-0.276446000000	0.262543000000	-3.781806000000
O	0.815129000000	-0.378855000000	-3.781679000000
O	-0.801952000000	0.628710000000	-4.795435000000
N	-1.485747000000	-2.981472000000	-1.864206000000
O	-1.831431000000	-2.615201000000	-2.973393000000
O	-2.142266000000	-3.748548000000	-1.169740000000
N	4.087234000000	-0.552616000000	-1.047862000000
O	3.483584000000	-0.956518000000	-2.080489000000
O	5.287793000000	-0.535748000000	-0.972659000000

$La(NO_3)_3$-L, type G, E_{tot} = -3166.876612

P	-0.637162000000	0.899656000000	1.477588000000
C	0.257831000000	1.068643000000	3.031897000000
C	1.528272000000	1.677480000000	3.037220000000
C	-0.254478000000	0.559358000000	4.219697000000
C	2.259675000000	1.732607000000	4.221852000000
C	0.467708000000	0.627475000000	5.400552000000
H	-1.236254000000	0.100792000000	4.217247000000
C	1.724891000000	1.208762000000	5.388840000000
H	3.239883000000	2.188665000000	4.238863000000
H	0.052463000000	0.228020000000	6.317385000000
H	2.304995000000	1.264555000000	6.303334000000
C	-2.140576000000	-0.040443000000	1.850655000000
C	-2.094007000000	-1.434714000000	2.010352000000
C	-3.372457000000	0.599462000000	1.945845000000
C	-3.262384000000	-2.153253000000	2.233690000000
C	-4.538944000000	-0.111086000000	2.182645000000
H	-3.421288000000	1.673907000000	1.818922000000
C	-4.475846000000	-1.486569000000	2.320886000000
H	-3.233867000000	-3.228684000000	2.347577000000
H	-5.486285000000	0.409825000000	2.241955000000
H	-5.379119000000	-2.057808000000	2.505464000000
C	-1.210319000000	2.525801000000	0.984217000000
C	-1.871867000000	2.684010000000	-0.248433000000
C	-1.094794000000	3.613184000000	1.845227000000
C	-2.445507000000	3.912135000000	-0.561458000000
C	-1.633319000000	4.843512000000	1.513731000000
H	-0.582362000000	3.486976000000	2.791420000000
C	-2.316248000000	4.977026000000	0.315134000000
H	-3.006151000000	4.044834000000	-1.475460000000
H	-1.528724000000	5.684759000000	2.186997000000
H	-2.761999000000	5.928861000000	0.049364000000
O	0.210065000000	0.212936000000	0.434679000000
O	-0.870683000000	-2.003304000000	1.965974000000
C	-0.780571000000	-3.404711000000	1.813105000000
H	-1.409520000000	-3.721187000000	0.973301000000
H	-1.116347000000	-3.923818000000	2.718030000000
O	1.939694000000	2.190399000000	1.873313000000
C	3.243368000000	2.774170000000	1.788485000000

H	3.987424000000	2.003843000000	2.015666000000
H	3.332492000000	3.592083000000	2.509582000000
O	-1.881998000000	1.602015000000	-1.047390000000
C	-2.731539000000	1.521972000000	-2.199044000000
H	-2.857339000000	2.498288000000	-2.666059000000
H	-2.182995000000	0.885568000000	-2.892042000000
C	0.643363000000	-3.733899000000	1.553237000000
C	1.473076000000	-4.616037000000	2.191746000000
H	1.326122000000	-5.276472000000	3.029673000000
N	2.565285000000	-3.634559000000	0.559215000000
C	-4.047887000000	0.927679000000	-1.867450000000
C	-4.387744000000	-0.397754000000	-1.752722000000
H	-3.815849000000	-1.306313000000	-1.860644000000
N	-6.133990000000	0.879553000000	-1.320505000000
C	3.425725000000	3.323384000000	0.428989000000
C	3.665699000000	2.680935000000	-0.759826000000
H	3.795704000000	1.640552000000	-1.010226000000
N	3.492098000000	4.854972000000	-1.083697000000
N	1.361429000000	-3.158062000000	0.557792000000
N	2.645172000000	-4.517162000000	1.533549000000
N	-5.148927000000	1.668967000000	-1.592079000000
N	-5.686002000000	-0.375429000000	-1.414049000000
N	3.692189000000	3.670230000000	-1.665024000000
N	3.327213000000	4.651207000000	0.180314000000
C	-6.578446000000	-1.481915000000	-1.183560000000
H	-6.700791000000	-2.071494000000	-2.093180000000
H	-6.191069000000	-2.120503000000	-0.388824000000
H	-7.539309000000	-1.066267000000	-0.887672000000
C	3.884704000000	3.582189000000	-3.092481000000
H	3.764090000000	4.585528000000	-3.494663000000
H	4.887429000000	3.216097000000	-3.317977000000
H	3.142641000000	2.911972000000	-3.526142000000
C	3.885675000000	-5.220933000000	1.764582000000
H	4.613660000000	-4.828778000000	1.058117000000
H	4.230600000000	-5.046890000000	2.783789000000
H	3.748795000000	-6.289460000000	1.596984000000
La	0.984225000000	-1.161748000000	-1.340621000000
O	-1.375654000000	-2.212983000000	-1.202071000000
O	1.774986000000	0.802790000000	-2.776081000000
O	3.381051000000	-0.740608000000	-0.550510000000
N	3.936379000000	-1.580692000000	-1.326990000000
O	3.166298000000	-2.179699000000	-2.132344000000
O	5.115570000000	-1.791325000000	-1.292004000000
N	0.781874000000	0.833575000000	-3.562617000000
O	-0.086845000000	-0.074613000000	-3.385989000000
O	0.667921000000	1.668725000000	-4.414287000000
N	-1.151598000000	-3.179491000000	-1.999642000000
O	0.012650000000	-3.246064000000	-2.476766000000
O	-2.006374000000	-3.981423000000	-2.267611000000

$La(NO_3)_3$-L, type B, SMD (MeCN) E_{tot} = -3166.940658

P	2.304520000000	0.827149000000	0.457819000000
C	3.418311000000	0.315379000000	-0.857392000000
C	2.965726000000	0.506949000000	-2.173001000000

C	4.620350000000	-0.344502000000	-0.636343000000
C	3.686452000000	-0.002932000000	-3.244069000000
C	5.357982000000	-0.833010000000	-1.705170000000
H	4.975814000000	-0.489600000000	0.377824000000
C	4.879383000000	-0.670169000000	-2.998058000000
H	3.331856000000	0.129345000000	-4.259157000000
H	6.293547000000	-1.349388000000	-1.526987000000
H	5.443835000000	-1.062240000000	-3.836960000000
C	2.967637000000	0.348800000000	2.060531000000
C	2.864993000000	-0.995806000000	2.439669000000
C	3.415999000000	1.284473000000	2.988928000000
C	3.140879000000	-1.380328000000	3.745844000000
C	3.729928000000	0.898745000000	4.282389000000
H	3.496956000000	2.326957000000	2.702980000000
C	3.572868000000	-0.428755000000	4.657322000000
H	3.036471000000	-2.415873000000	4.045063000000
H	4.075719000000	1.633998000000	4.999008000000
H	3.795576000000	-0.734182000000	5.673788000000
C	2.264269000000	2.628355000000	0.432403000000
C	1.184840000000	3.313341000000	1.008065000000
C	3.261595000000	3.355219000000	-0.210431000000
C	1.085846000000	4.695620000000	0.873962000000
C	3.186216000000	4.735174000000	-0.312501000000
H	4.099635000000	2.829780000000	-0.654276000000
C	2.088303000000	5.395032000000	0.218765000000
H	0.241986000000	5.229627000000	1.290624000000
H	3.969216000000	5.286966000000	-0.818470000000
H	2.006047000000	6.472692000000	0.128336000000
O	0.945683000000	0.210006000000	0.241753000000
O	2.536994000000	-1.853449000000	1.455781000000
C	1.674262000000	-2.952644000000	1.747266000000
H	0.792449000000	-2.598593000000	2.291939000000
H	2.188851000000	-3.704980000000	2.351038000000
O	1.837077000000	1.230466000000	-2.282645000000
C	1.018688000000	1.144753000000	-3.443465000000
H	0.817615000000	0.094479000000	-3.679699000000
H	1.507826000000	1.611802000000	-4.303325000000
O	0.298381000000	2.560566000000	1.685152000000
C	-1.006836000000	3.075915000000	1.890387000000
H	-0.996424000000	3.927666000000	2.577075000000
H	-1.416271000000	3.411908000000	0.930370000000
C	1.304231000000	-3.542780000000	0.440386000000
C	1.682368000000	-4.744356000000	-0.097052000000
H	2.282001000000	-5.554420000000	0.284272000000
N	0.451514000000	-3.651480000000	-1.546835000000
C	-1.849520000000	2.003257000000	2.470392000000
C	-2.681250000000	2.085118000000	3.555660000000
H	-2.890295000000	2.878434000000	4.254013000000
N	-2.843405000000	0.090251000000	2.660864000000
C	-0.238939000000	1.871307000000	-3.127103000000
C	-0.787483000000	2.972873000000	-3.728432000000
H	-0.481888000000	3.568492000000	-4.572625000000
N	-2.050838000000	2.365097000000	-2.039258000000
N	0.541120000000	-2.908191000000	-0.487225000000

N	1.130779000000	-4.761059000000	-1.321342000000
N	-1.983646000000	0.755255000000	1.953058000000
N	-3.272543000000	0.880803000000	3.622692000000
N	-1.903269000000	3.230301000000	-3.023309000000
N	-1.057326000000	1.531000000000	-2.099195000000
C	-4.278442000000	0.423165000000	4.553388000000
H	-4.013556000000	0.748018000000	5.558476000000
H	-5.252095000000	0.830411000000	4.278060000000
H	-4.308139000000	-0.663228000000	4.509929000000
C	-2.849922000000	4.309736000000	-3.197403000000
H	-3.811261000000	3.989313000000	-2.801748000000
H	-2.505620000000	5.197495000000	-2.665230000000
H	-2.942487000000	4.530871000000	-4.259047000000
C	1.208718000000	-5.793883000000	-2.328825000000
H	0.618264000000	-5.468978000000	-3.182533000000
H	2.246198000000	-5.940907000000	-2.629754000000
H	0.804300000000	-6.725490000000	-1.933360000000
La	-1.211803000000	-0.655451000000	-0.350803000000
O	-1.788454000000	-2.352159000000	1.295417000000
O	-3.579510000000	-0.153556000000	-0.787843000000
O	-1.106872000000	-1.293892000000	-2.847685000000
N	-1.864083000000	-2.312374000000	-2.829557000000
O	-2.317201000000	-2.651488000000	-1.717758000000
O	-2.126607000000	-2.907327000000	-3.851244000000
N	-4.501455000000	0.726786000000	-0.883234000000
O	-4.707167000000	1.479275000000	0.060446000000
O	-5.164958000000	0.758749000000	-1.912810000000
N	-2.263251000000	-2.767819000000	2.403912000000
O	-1.550692000000	-2.705519000000	3.401109000000
O	-3.390550000000	-3.238074000000	2.421352000000

$La(NO_3)_3$-L. type E. SMD (MeCN) E_{tot} = -3166.963391

P	-1.314146000000	0.359123000000	1.726392000000
C	-2.572272000000	1.649995000000	1.787940000000
C	-3.579094000000	1.713024000000	0.803997000000
C	-2.525858000000	2.637186000000	2.767965000000
C	-4.481905000000	2.773785000000	0.805842000000
C	-3.435511000000	3.683125000000	2.780174000000
H	-1.761118000000	2.588577000000	3.534642000000
C	-4.402897000000	3.747639000000	1.790404000000
H	-5.248263000000	2.844733000000	0.046043000000
H	-3.382079000000	4.442345000000	3.551189000000
H	-5.114367000000	4.566357000000	1.777753000000
C	-0.143956000000	0.720894000000	3.053999000000
C	0.846580000000	1.701464000000	2.869072000000
C	-0.196886000000	0.040957000000	4.266482000000
C	1.760278000000	1.976973000000	3.881509000000
C	0.709320000000	0.313286000000	5.279554000000
H	-0.960230000000	-0.713453000000	4.420027000000
C	1.683484000000	1.279035000000	5.078297000000
H	2.521754000000	2.734087000000	3.747672000000
H	0.653499000000	-0.225670000000	6.217716000000
H	2.397646000000	1.501829000000	5.863568000000
C	-2.105035000000	-1.205788000000	2.146465000000

C	-1.383983000000	-2.410920000000	2.053342000000
C	-3.451821000000	-1.252194000000	2.494022000000
C	-2.037342000000	-3.624235000000	2.249831000000
C	-4.096548000000	-2.458063000000	2.718407000000
H	-4.008657000000	-0.327062000000	2.582571000000
C	-3.384805000000	-3.638586000000	2.579666000000
H	-1.505079000000	-4.560716000000	2.158930000000
H	-5.146904000000	-2.473160000000	2.983322000000
H	-3.876640000000	-4.592935000000	2.733923000000
O	-0.663403000000	0.312122000000	0.365973000000
O	0.818037000000	2.336233000000	1.683278000000
C	1.814004000000	3.296584000000	1.363823000000
H	2.810792000000	2.866630000000	1.500003000000
H	1.717352000000	4.182922000000	1.997591000000
O	-3.610160000000	0.707890000000	-0.084974000000
C	-4.579092000000	0.750549000000	-1.134877000000
H	-4.422152000000	1.651688000000	-1.734920000000
H	-5.589551000000	0.774232000000	-0.715872000000
O	-0.064022000000	-2.310473000000	1.794936000000
C	0.653470000000	-3.499155000000	1.490643000000
H	0.602580000000	-4.202653000000	2.326339000000
H	0.208626000000	-3.972688000000	0.609173000000
C	1.584883000000	3.662308000000	-0.054243000000
C	1.470360000000	4.901215000000	-0.624739000000
H	1.521401000000	5.898188000000	-0.218864000000
N	1.215971000000	3.359658000000	-2.167829000000
C	2.081355000000	-3.173810000000	1.242540000000
C	3.179163000000	-3.784611000000	1.794224000000
H	3.284137000000	-4.562811000000	2.532336000000
N	3.836941000000	-2.277849000000	0.343770000000
C	-4.432169000000	-0.470101000000	-1.959874000000
C	-3.454114000000	-0.819921000000	-2.859976000000
H	-2.556203000000	-0.322517000000	-3.194126000000
N	-4.962106000000	-2.415073000000	-2.730152000000
N	1.425503000000	2.743279000000	-1.041204000000
N	1.250892000000	4.654287000000	-1.926743000000
N	2.536911000000	-2.250491000000	0.357542000000
N	4.230167000000	-3.199805000000	1.199270000000
N	-3.828999000000	-2.025613000000	-3.306362000000
N	-5.331307000000	-1.480452000000	-1.910047000000
C	5.636828000000	-3.476284000000	1.386100000000
H	5.880260000000	-3.420891000000	2.446543000000
H	5.872751000000	-4.469748000000	1.004135000000
H	6.199694000000	-2.725100000000	0.836573000000
C	-3.149181000000	-2.885188000000	-4.247561000000
H	-3.850363000000	-3.651879000000	-4.570066000000
H	-2.823523000000	-2.299999000000	-5.106691000000
H	-2.285334000000	-3.351821000000	-3.771947000000
C	1.064818000000	5.605719000000	-2.998891000000
H	0.832947000000	5.046797000000	-3.902500000000
H	0.240605000000	6.275172000000	-2.754498000000
H	1.978669000000	6.182472000000	-3.143415000000
La	1.379184000000	-0.085469000000	-0.966581000000
O	3.553196000000	0.838699000000	0.308097000000

O	-0.118531000000	-2.226654000000	-1.299283000000
O	-0.321126000000	0.526117000000	-2.827477000000
N	0.515158000000	0.796330000000	-3.740091000000
O	1.725867000000	0.694882000000	-3.433987000000
O	0.154211000000	1.136549000000	-4.844242000000
N	0.558915000000	-2.740431000000	-2.223120000000
O	1.550121000000	-2.079540000000	-2.628119000000
O	0.269006000000	-3.812519000000	-2.710878000000
N	4.363909000000	0.617128000000	-0.628683000000
O	3.882567000000	0.139564000000	-1.685739000000
O	5.548028000000	0.837865000000	-0.508486000000

$La(NO_3)_3$-L, type G, SMD (MeCN) E_{tot} = -3166.951009

P	-0.704553000000	0.281393000000	1.553851000000
C	0.286820000000	0.595236000000	3.025618000000
C	1.236784000000	1.633812000000	3.033523000000
C	0.178125000000	-0.230953000000	4.140814000000
C	2.068817000000	1.800116000000	4.137559000000
C	0.998487000000	-0.058725000000	5.244638000000
H	-0.559777000000	-1.024682000000	4.145926000000
C	1.945310000000	0.953536000000	5.229918000000
H	2.814292000000	2.583819000000	4.153330000000
H	0.900217000000	-0.713276000000	6.102319000000
H	2.602586000000	1.096952000000	6.080708000000
C	-1.699435000000	-1.185692000000	1.881362000000
C	-1.124684000000	-2.466302000000	1.797014000000
C	-3.047139000000	-1.074296000000	2.212329000000
C	-1.906670000000	-3.598392000000	2.002040000000
C	-3.824457000000	-2.199697000000	2.436514000000
H	-3.497343000000	-0.091808000000	2.291425000000
C	-3.249374000000	-3.455907000000	2.320167000000
H	-1.474287000000	-4.587528000000	1.926541000000
H	-4.871954000000	-2.093640000000	2.692265000000
H	-3.847544000000	-4.345638000000	2.484201000000
C	-1.865607000000	1.641220000000	1.362630000000
C	-2.700018000000	1.723980000000	0.232953000000
C	-1.985489000000	2.597050000000	2.369060000000
C	-3.623224000000	2.761487000000	0.137114000000
C	-2.899988000000	3.631890000000	2.269976000000
H	-1.356636000000	2.526720000000	3.248390000000
C	-3.713002000000	3.705376000000	1.149009000000
H	-4.287529000000	2.836016000000	-0.712619000000
H	-2.977498000000	4.367532000000	3.061464000000
H	-4.440158000000	4.504645000000	1.054736000000
O	0.206249000000	0.091465000000	0.356960000000
O	0.193748000000	-2.507067000000	1.537622000000
C	0.811942000000	-3.761470000000	1.294821000000
H	0.295869000000	-4.273998000000	0.476345000000
H	0.772575000000	-4.400907000000	2.180888000000
O	1.262715000000	2.423879000000	1.945697000000
C	2.180382000000	3.519993000000	1.918904000000
H	3.205767000000	3.142447000000	1.948189000000
H	2.012189000000	4.161900000000	2.788690000000
O	-2.540175000000	0.758474000000	-0.692109000000

C	-3.411005000000	0.689479000000	-1.827858000000
H	-3.557748000000	1.677353000000	-2.268002000000
H	-2.858427000000	0.080155000000	-2.541468000000
C	2.225511000000	-3.485343000000	0.944673000000
C	3.364883000000	-4.062272000000	1.439637000000
H	3.530250000000	-4.826930000000	2.180855000000
N	3.907901000000	-2.553592000000	-0.057827000000
C	-4.724598000000	0.066076000000	-1.521091000000
C	-5.036931000000	-1.252397000000	-1.284290000000
H	-4.442390000000	-2.151222000000	-1.254496000000
N	-6.856196000000	-0.024992000000	-1.172224000000
C	1.945274000000	4.296639000000	0.681353000000
C	2.529275000000	4.192908000000	-0.557698000000
H	3.295427000000	3.546207000000	-0.953276000000
N	1.034944000000	5.804187000000	-0.568434000000
N	2.607508000000	-2.564410000000	0.025444000000
N	4.366560000000	-3.455428000000	0.784089000000
N	-5.873631000000	0.778563000000	-1.441511000000
N	-6.358168000000	-1.253721000000	-1.071228000000
N	1.933091000000	5.141497000000	-1.291409000000
N	1.036953000000	5.299990000000	0.625606000000
C	-7.218924000000	-2.379239000000	-0.788708000000
H	-7.209855000000	-3.073470000000	-1.629272000000
H	-6.877380000000	-2.888474000000	0.112386000000
H	-8.226510000000	-1.998308000000	-0.637345000000
C	2.166068000000	5.488839000000	-2.673760000000
H	1.473573000000	6.285206000000	-2.937266000000
H	3.192073000000	5.833843000000	-2.803524000000
H	1.987679000000	4.621719000000	-3.309528000000
C	5.787324000000	-3.693741000000	0.909337000000
H	6.303498000000	-2.975988000000	0.276091000000
H	6.088614000000	-3.559135000000	1.947582000000
H	6.017576000000	-4.708761000000	0.585921000000
La	1.334528000000	-0.703777000000	-1.555367000000
O	-0.393011000000	-2.636693000000	-1.558670000000
O	0.882332000000	1.631611000000	-2.621357000000
O	3.350994000000	0.636027000000	-0.639897000000
N	4.219302000000	0.208759000000	-1.452438000000
O	3.808349000000	-0.573219000000	-2.354451000000
O	5.378247000000	0.528844000000	-1.369708000000
N	-0.101595000000	1.285293000000	-3.333860000000
O	-0.437156000000	0.064594000000	-3.275481000000
O	-0.694010000000	2.070602000000	-4.028548000000
N	0.169084000000	-3.372320000000	-2.417041000000
O	1.251186000000	-2.942425000000	-2.902028000000
O	-0.303713000000	-4.430142000000	-2.754632000000

$La(NO_3)_2$-L, cation type H, SMD (MeCN) E_{tot} =-2886.66834390

P	1.113099000000	-1.221441000000	1.358934000000
C	0.706524000000	-0.959926000000	3.091456000000
C	-0.641065000000	-0.802021000000	3.454638000000
C	1.695612000000	-0.786072000000	4.055459000000
C	-0.973194000000	-0.432218000000	4.753819000000
C	1.365127000000	-0.445186000000	5.357790000000

H	2.736783000000	-0.904538000000	3.777983000000
C	0.032066000000	-0.259165000000	5.694205000000
H	-2.008088000000	-0.292356000000	5.038975000000
H	2.143737000000	-0.311515000000	6.099182000000
H	-0.237716000000	0.021088000000	6.706700000000
C	2.900010000000	-1.028085000000	1.204701000000
C	3.489779000000	0.240702000000	1.064062000000
C	3.720969000000	-2.153629000000	1.208656000000
C	4.866908000000	0.351046000000	0.889333000000
C	5.093573000000	-2.043920000000	1.055302000000
H	3.274660000000	-3.134534000000	1.325236000000
C	5.656836000000	-0.788361000000	0.886782000000
H	5.329370000000	1.322407000000	0.771215000000
H	5.714372000000	-2.931792000000	1.059346000000
H	6.728685000000	-0.684775000000	0.756959000000
C	0.747955000000	-2.926453000000	0.921506000000
C	0.903898000000	-3.319265000000	-0.420313000000
C	0.269437000000	-3.845366000000	1.848493000000
C	0.556759000000	-4.606873000000	-0.813657000000
C	-0.065140000000	-5.134540000000	1.461197000000
H	0.154938000000	-3.547954000000	2.884648000000
C	0.074952000000	-5.502384000000	0.131409000000
H	0.669339000000	-4.916985000000	-1.844623000000
H	-0.438469000000	-5.842581000000	2.191313000000
H	-0.190605000000	-6.505757000000	-0.183691000000
O	0.339942000000	-0.261323000000	0.490133000000
O	2.669193000000	1.306862000000	1.125648000000
C	3.157171000000	2.550050000000	0.636889000000
H	3.586668000000	2.403685000000	-0.360680000000
H	3.935491000000	2.952889000000	1.291294000000
O	-1.545891000000	-1.062665000000	2.493730000000
C	-2.838844000000	-0.475109000000	2.598935000000
H	-2.732510000000	0.594902000000	2.801684000000
H	-3.409403000000	-0.935557000000	3.409981000000
O	1.416939000000	-2.390007000000	-1.243937000000
C	1.358777000000	-2.591359000000	-2.648623000000
H	2.073810000000	-3.359140000000	-2.957827000000
H	0.352082000000	-2.911156000000	-2.932194000000
C	2.030094000000	3.511919000000	0.577259000000
C	1.978806000000	4.797053000000	1.056113000000
H	2.679915000000	5.394897000000	1.615111000000
N	0.106340000000	4.327855000000	0.015300000000
C	1.698836000000	-1.302112000000	-3.303376000000
C	2.602297000000	-1.054634000000	-4.306115000000
H	3.284461000000	-1.690482000000	-4.846295000000
N	1.598863000000	0.814947000000	-3.744903000000
C	-3.559506000000	-0.702742000000	1.323930000000
C	-4.750242000000	-1.358935000000	1.142671000000
H	-5.410554000000	-1.866565000000	1.826800000000
N	-4.031420000000	-0.598031000000	-0.783184000000
N	0.857006000000	3.269692000000	-0.053598000000
N	0.773059000000	5.252925000000	0.679635000000
N	1.110266000000	-0.123953000000	-2.991084000000
N	2.491216000000	0.261991000000	-4.546102000000

N	-4.996122000000	-1.260729000000	-0.171872000000
N	-3.152932000000	-0.253835000000	0.108195000000
C	3.237384000000	1.068387000000	-5.485648000000
H	4.185686000000	1.376049000000	-5.043098000000
H	3.424022000000	0.484690000000	-6.385082000000
H	2.643294000000	1.946218000000	-5.731096000000
C	-6.130411000000	-1.759733000000	-0.915186000000
H	-5.931928000000	-1.599717000000	-1.972583000000
H	-6.255950000000	-2.824123000000	-0.719391000000
H	-7.032467000000	-1.221916000000	-0.622492000000
C	0.201620000000	6.563666000000	0.891932000000
H	-0.868066000000	6.498111000000	0.705211000000
H	0.378789000000	6.872420000000	1.920917000000
H	0.653069000000	7.283610000000	0.208398000000
La	-0.822526000000	1.056162000000	-1.108604000000
O	-1.424450000000	-1.342290000000	-1.989230000000
O	-1.771671000000	2.187085000000	1.031386000000
N	-2.772732000000	2.760414000000	0.527715000000
O	-2.946781000000	2.621318000000	-0.711496000000
O	-3.538841000000	3.408742000000	1.207739000000
N	-2.151832000000	-0.989214000000	-2.949629000000
O	-2.686833000000	-1.795971000000	-3.676995000000
O	-2.310333000000	0.251751000000	-3.114540000000