

Electronic Supplementary Information

**Experimental and Theoretical Studies on Extraction
behavior of Di-*n*-Alkyl Phosphine Oxides towards
Actinides**

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2.2.1. Di-n-hexyl phosphine oxide (DHePO): 7.8 g (326.09 mmol) of Mg, 53.8 g (326.09 mmol) of 1-bromohexane and 15 g (108.69 mmol) of diethyl phosphite. Product: 19.6g, Yield: 82%, M.P: 75-77°C, **IR** (cm⁻¹): (P=O) 1161.15. **¹H NMR** (δ, 400 MHz, CDCl₃): 0.89-0.92 (t, CH₃CH₂, 6 H), 1.81-1.88 (m, P-CH₂, 4 H), 1.32-1.79 (m, CH₃CH₂, 16 H), 6.8 (d, ¹J_{P-H}: 448.8 Hz, 1 H). **³¹P{¹H}-NMR** (δ, 400 MHz, CDCl₃): 36.14 (d, ¹J_{P-H}: 458.46 Hz) . **¹³C-NMR** (δ, 100 MHz, CDCl₃): 31.30, 30.43, 28.24 (d), 22.38, 21.74 (d), 13.98. **Mass (EI, M/Z):** 218.2

2.2.2. Di-n-heptyl phosphine oxide (DHpPO): 7.8 g (326.09 mmol) of Mg, 58.37 g (326.09 mmol) of 1-bromoheptane and 15 g (108.69 mmol) of diethyl phosphite. Product: 23.43 g, Yield: 88%, M.P: 83-85°C, **IR** (cm⁻¹): (P=O) 1157.29. **¹H-NMR** (δ, 400 MHz, CDCl₃): 0.82-0.86 (t, CH₃CH₂, 6 H), 1.78 (m, P-CH₂, 4 H), 1.24-1.68 (m, CH₃CH₂, 20 H), 6.86 (d, ¹J_{P-H}: 446 Hz, 1 H). **³¹P{¹H}-NMR** (δ, 162 MHz, CDCl₃): 35.69 (d, ¹J_{P-H}: 443.88 Hz). **¹³C-NMR** (δ, 100 MHz, CDCl₃): 31.52, 30.70, 30.57, 28.77, 22.55, 21.78, 14.07. **Mass (EI, M/Z):** 245.27

2.2.3. Di-n-octyl phosphine oxide (DOPO): M.P: 84-86 °C, **IR** (cm⁻¹): (P=O) 1159.22. **¹H-NMR** (δ, 400 MHz, CDCl₃): 0.86-0.89 (t, CH₃CH₂, 6 H), 1.85-1.9 (m, P-CH₂, 4 H), 1.26-1.62 (m, CH₃CH₂, 24 H), 6.91 (d, ¹J_{P-H}: 445 Hz, 1 H). **³¹P{¹H}-NMR** (δ, 162 MHz, CDCl₃): 35.03 (d, ¹J_{P-H}: 447.12 Hz). **¹³C-NMR** (δ, 100 MHz, CDCl₃): 31.77, 30.63 (d), 29.01 (d), 27.95(d), 21.61, 21.76(d), 14.07. **Mass (EI, M/Z):** 274.5

2.2.4. Di-n-decyl phosphine oxide (DDPO): 7.8 g (326.09 mmol) of Mg, 72 g (326.09 mmol) of 1-bromodecane and 15 g (108.69 mmol) of diethyl phosphite. Product: 28.22 g, Yield: 79%, M.P: 95-97°C **IR** (cm⁻¹): (P=O) 1155.36. **¹H-NMR** (δ, 400 MHz, CDCl₃): 0.85-0.88 (t, CH₃CH₂, 6H), 1.74-1.95 (m, P-CH₂, 4H), 1.24-1.63 (m, CH₃CH₂, 32H), 6.83 (d, ¹J_{P-H}: 444 Hz, 1 H). **³¹P{¹H}-NMR** (δ, 162 MHz, CDCl₃): 35.03 (d, ¹J_{P-H}: 445.5 Hz). **¹³C-NMR** (δ, 100 MHz,

CDCl₃):31.87, 30.77 (d), 29.52, 29.31 (d), 29.13, 28.25(d), 22.67, 21.76, 14.1. **Mass (EI, M/Z):**
329.4

2.3.2. [Th(NO₃)₄(DHpPO)₂] (2): [Th(NO₃)₄.5H₂O (0.2 g, 0.35 mmol) and DHpPO (0.172 g, 0.7 mmol)], Product: 0.33 g (low melting solid), Yield: 87.1%, **IR** (cm⁻¹): (P=O) 1078.21, **³¹P{¹H}-NMR** (δ, 162 MHz, CDCl₃): 49.2 (d, ¹J_{P-H}: 479.52 Hz). **¹H-NMR** (δ, 400 MHz, CDCl₃): 0.860.89 (t, CH₃CH₂, 6 H), 1.98 (m, P-CH₂, 4 H), 1.28-1.6 (m, CH₃CH₂, 20 H), 6.93 (d, ¹J_{P-H}: 484 Hz, 1 H).

2.3.3. [Th(NO₃)₄(DOPO)₂] (3): [Th(NO₃)₄.5H₂O (0.2 g, 0.35 mmol) and DOPO (0.193 g, 0.7 mmol)], Product: 0.32 g (low melting solid), Yield: 81.2%, **IR** (cm⁻¹): (P=O) 1085.92, **³¹P{¹H}-NMR**(δ, 162 MHz, CDCl₃): 49.73 (d, ¹J_{P-H}: 502 Hz), **¹H-NMR** (δ, 400 MHz, CDCl₃): 0.86-0.89 (t, CH₃CH₂, 6 H), 1.93 (m, P-CH₂, 4 H), 1.27-1.56 (m, CH₃CH₂, 24 H), 6.94 (d, ¹J_{P-H}: 484 Hz, 1 H).

2.3.4. [Th(NO₃)₄(DDPO)₂] (4): [Th(NO₃)₄.5H₂O (0.2 g, 0.35 mmol) and DDPO (0.231 g, 0.7 mmol)], Product: 0.37 g (low melting solid), Yield: 84.7%, **IR** (cm⁻¹): (P=O) 1083.99, **³¹P{¹H}-NMR** (δ, 162 MHz, CDCl₃): 49.05 (d, ¹J_{P-H}: 490.86 Hz). **¹H-NMR** (δ, 400 MHz, CDCl₃): δ = 0.85-0.89 (t, CH₃CH₂, 6 H), 1.97 (m, P-CH₂, 4 H), 1.25-1.57 (m, CH₃CH₂, 32 H), 6.94 (d, ¹J_{P-H}: 484 Hz, 1 H).

2.3.5. [LaCl₃(DHePO)₃] (5):[LaCl₃.7H₂O (0.2 g, 0.54 mmol) and DHePO (0.35 g, 1.62 mmol)], Product: 0.49 g, Yield: 88%, M.P: 65-67°C, **IR** (cm⁻¹): (P=O) 1145.72, **³¹P{¹H}-NMR** (δ, 162 MHz, CDCl₃): 36.93 (d, ¹J_{P-H}: 455.22 Hz). **¹H-NMR** (δ, 400 MHz, CDCl₃): δ = 0.86-0.89 (t, CH₃CH₂, 6 H), 1.9 (m, P-CH₂, 4 H), 1.27-1.63 (m, CH₃CH₂, 16 H), 6.9 (d, ¹J_{P-H}: 452 Hz, 1 H).

2.3.6. [LaCl₃(DHpPO)₃] (6): [LaCl₃·7H₂O (0.2 g, 0.54 mmol) and DHpPO (0.39 g, 1.62 mmol)], Product: 0.51 g, Yield: 84.6%, M.P: 70-72°C, **IR** (cm⁻¹): (P=O) 1138.00, **³¹P{¹H}-NMR** (δ, 162 MHz, CDCl₃, 25°C): 38.56 (d, ¹J_{P-H}: 461.7 Hz). **¹H-NMR** (δ, 400 MHz, CDCl₃): 0.85-0.88 (t, **CH₃CH₂**, 6 H), 1.96 (m, **P-CH₂**, 4 H), 1.26-1.59 (m, **CH₃CH₂**, 20 H), 6.95 (d, ¹J_{P-H}: 460 Hz, 1 H).

2.3.7. [LaCl₃(DOPO)₃] (7): [LaCl₃·7H₂O (0.2 g, 0.54 mmol) and DOPO (0.45 g, 1.62 mmol)], Product: 0.55 g, Yield: 85%, M.P: 70-72°C, **IR** (cm⁻¹): (P=O) 1139.93. **³¹P{¹H}-NMR** (δ, 162 MHz, CDCl₃): 37.6 (d, ¹J_{P-H}: 455 Hz). **¹H-NMR** (δ, 400 MHz, CDCl₃): δ = 0.84-0.87 (t, **CH₃CH₂**, 6 H), 2.07 (m, **P-CH₂**, 4 H), 1.21-1.64 (m, **CH₃CH₂**, 32 H), 7.01 (d, ¹J_{P-H}: 472 Hz, 1 H).

2.3.8. [LaCl₃(DDPO)₃] (8) : [LaCl₃·7H₂O (0.2 g, 0.54 mmol) and DDPO (0.54 g, 1.62 mmol)], Product: 0.63 g, Yield: 86%, M.P: 83-84°C, **IR**(cm⁻¹): (P=O) 1153.43, **³¹P{¹H}-NMR** (δ, 162 MHz, CDCl₃): 40.54 (d, ¹J_{P-H}: 469.8 Hz), **¹H-NMR** (δ, 400 MHz, CDCl₃): 0.85-0.88 (t, **CH₃CH₂**, 6 H), 1.91 (m, **P-CH₂**, 4 H), 1.39-1.61 (m, **CH₃CH₂**, 32 H), 6.9 (d, ¹J_{P-H}: 456 Hz, 1 H).

RK-G-HPO

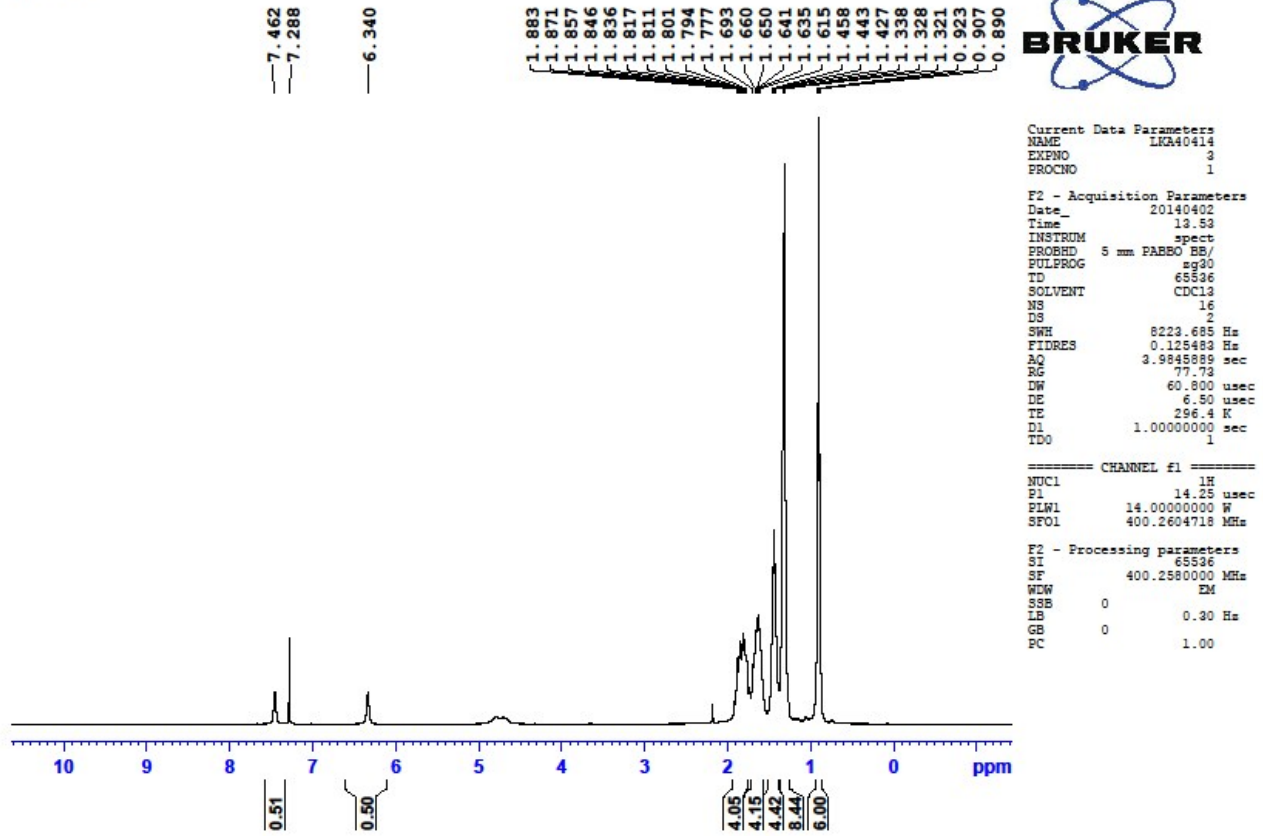


Fig. S1 ¹H-NMR of Di-*n*-hexyl phosphine oxide(DHePO)

RK-G-HPO

— 37.56
— 34.73



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PROCNO        1

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PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            32
DS            4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5111808 sec
RG            199.6
DW            7.800 usec
DE            6.50 usec
TE            296.4 K
D1            2.00000000 sec
TDO           1
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P1            14.50 usec
PLW1          15.00000000 W
SFO1          162.0193069 MHz
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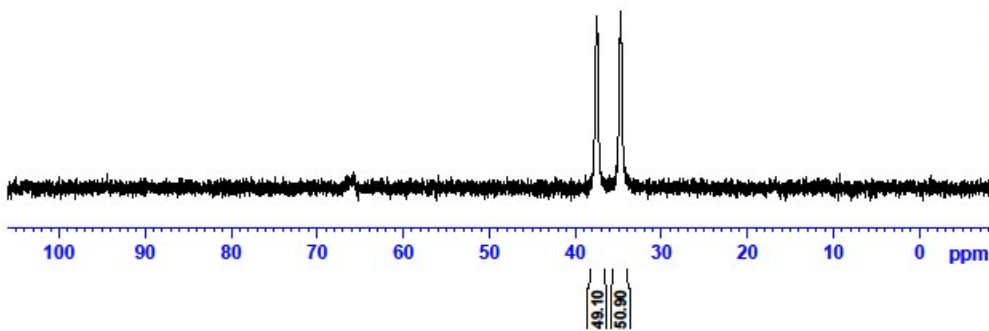


Fig. S2 ^{31}P -NMR of Di-*n*-hexyl phosphine oxide(DHePO)

Signature SIF VIT VELLORE
DJ-DHPO

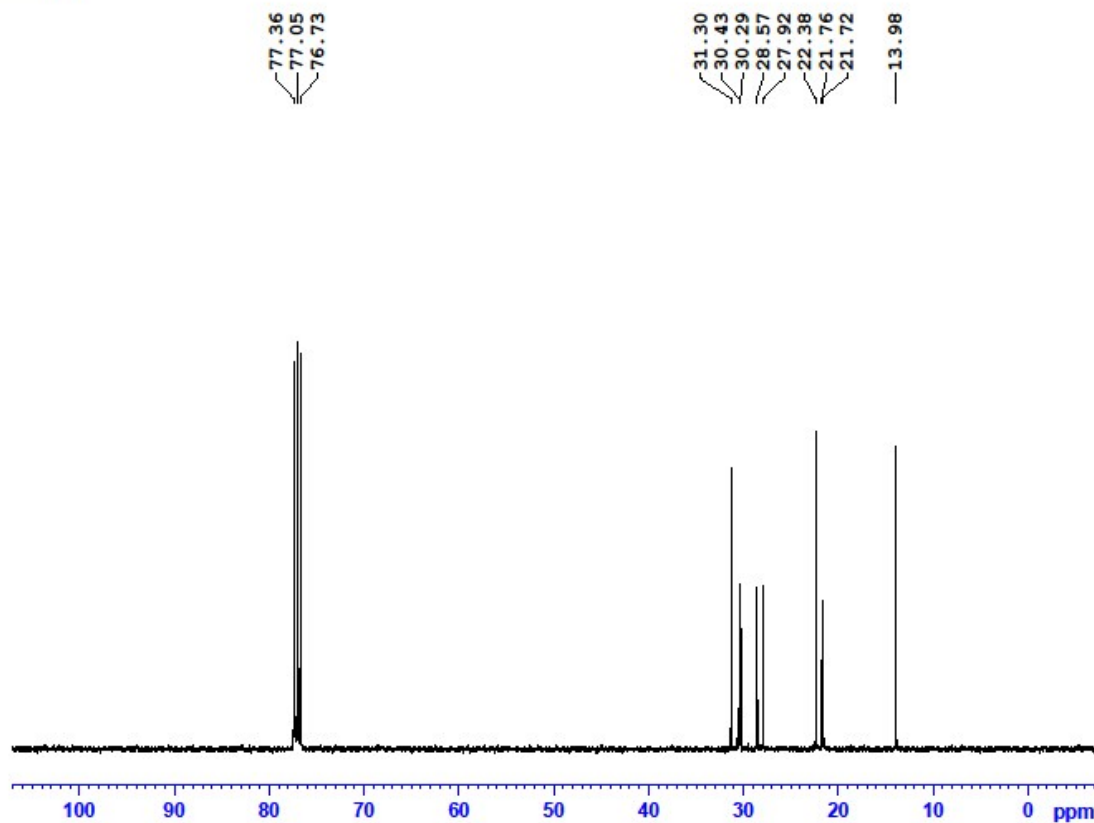


Fig. S3 ¹³C-NMR of Di-*n*-hexyl phosphine oxide(DHePO)

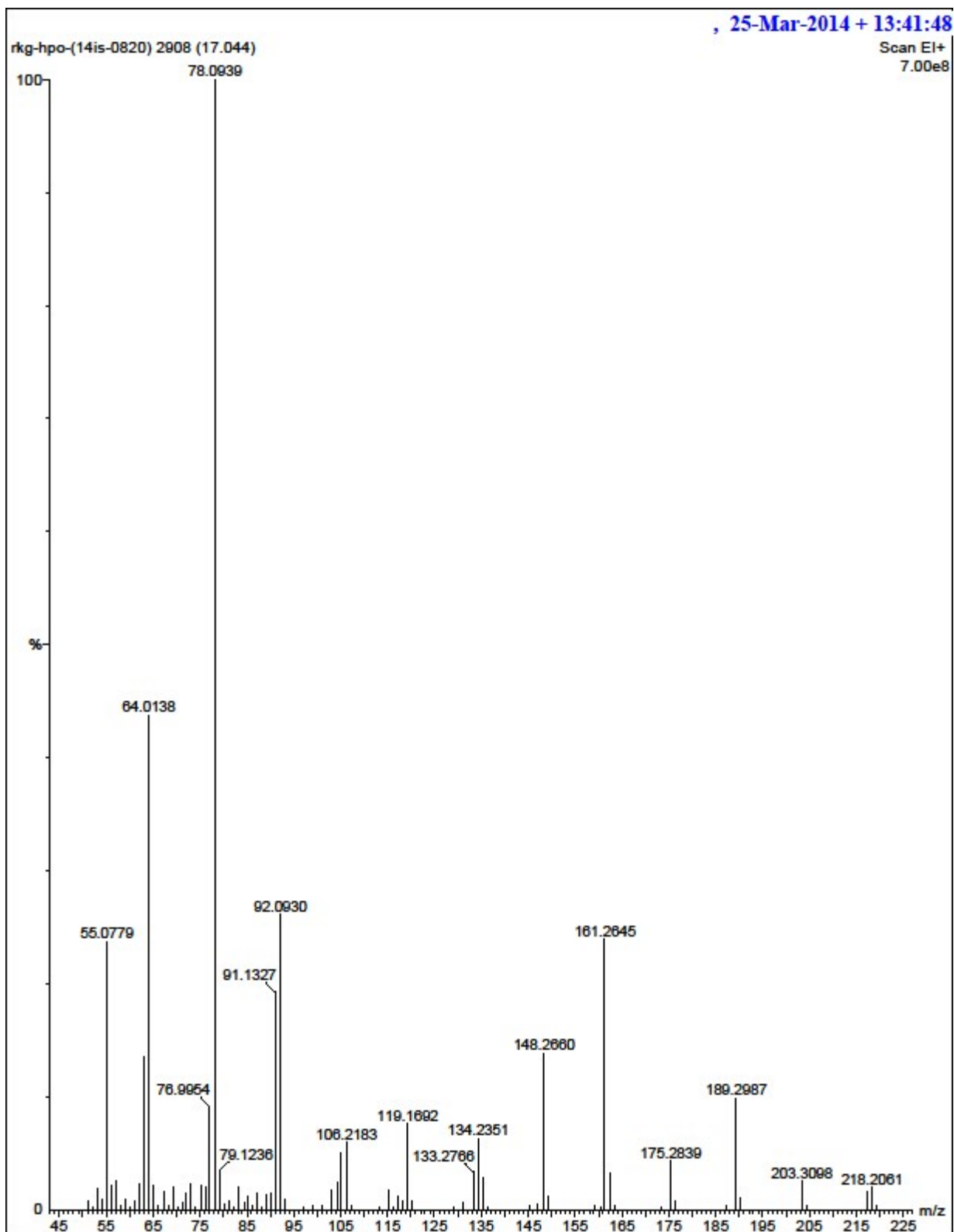


Fig. S4 EI mass spectra of Di-*n*-hexyl phosphine oxide(DHePO)

RK-G-HPO-TH-1H

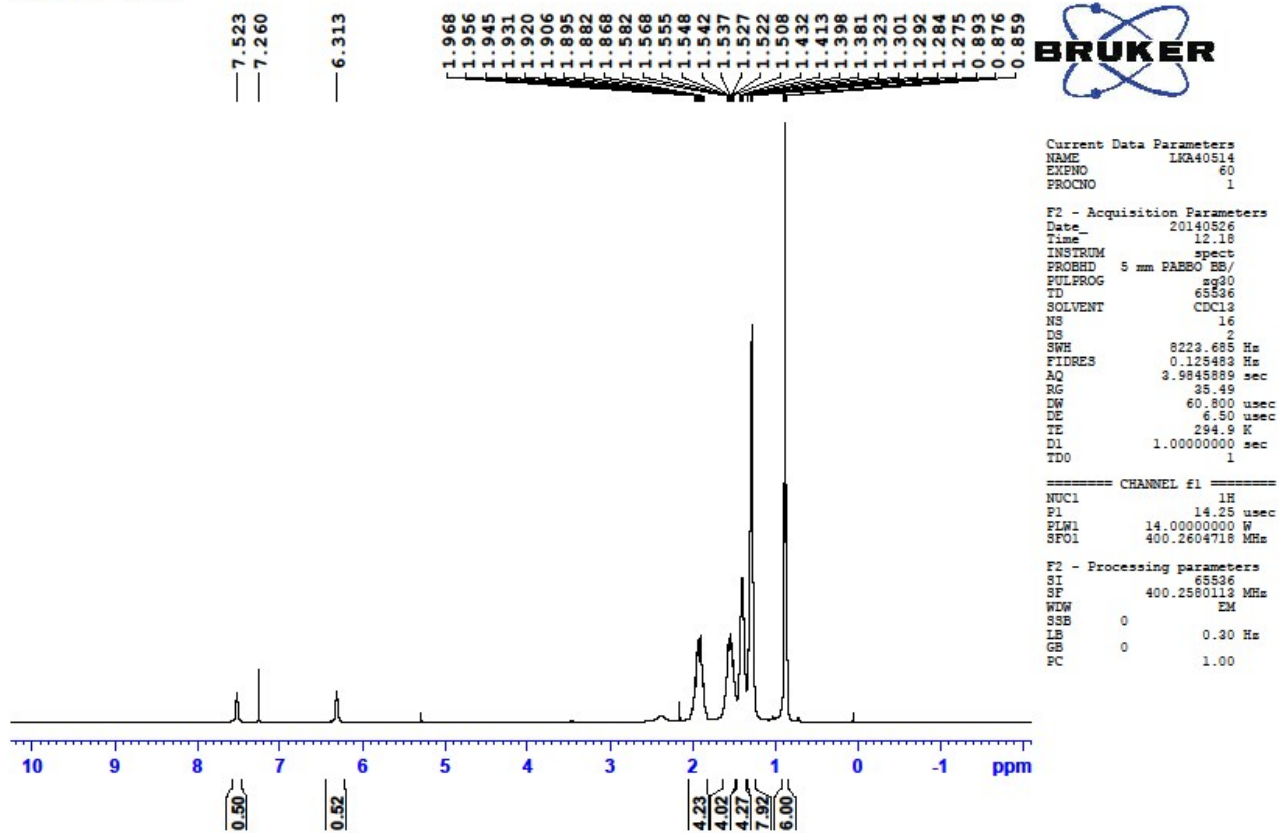


Fig. S5 $^1\text{H-NMR}$ of Thorium-DHePO complex

RK-G-HPO-TH-31P

—49.08
—46.09



Current Data Parameters
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EXPNO 61
PROCNO 1

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Time 12.20
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PULPROG zg30
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SOLVENT CDCl3
NS 32
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 199.6
DM 7.800 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
TD0 1

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F2 - Processing parameters
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PC 1.40

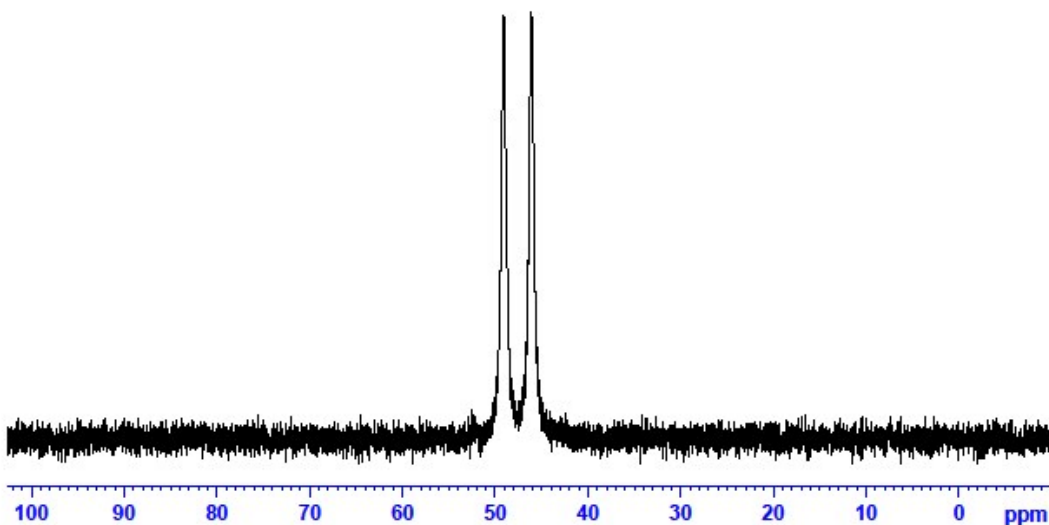
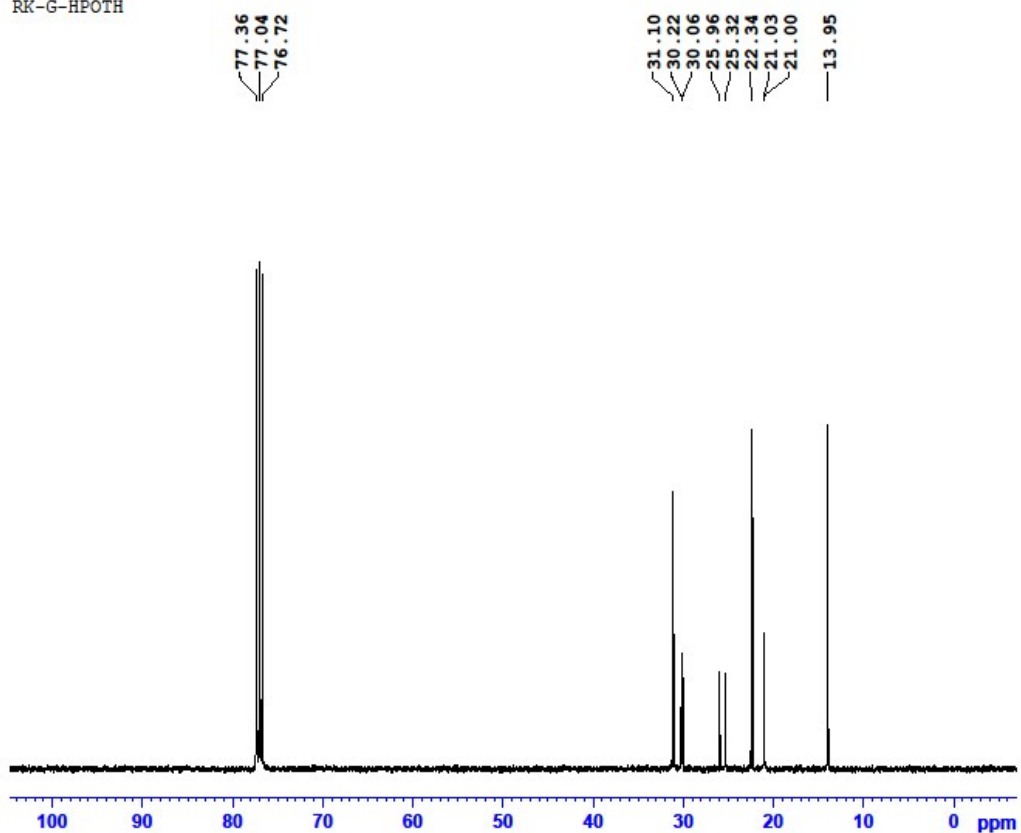


Fig. S6 ^{31}P -NMR of Thorium-DHePO complex

RK-G-HPOTH



Current Data Parameters
NAME LKA40215
EXPNO 185
PROCNO 1

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Time 13.37
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PULPROG zgpg30
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SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 175.97
DW 20.800 usec
DE 6.50 usec
TE 303.1 K
D1 2.0000000 sec
D11 0.0200000 sec
TDO 1

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P1 9.80 usec
PLW1 58.0000000 W
SFO1 100.6550182 MHz

==== CHANNEL f2 =====
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NUC2 1H
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.35097000 W
PLW13 0.28428999 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
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LB 1.00 Hz
GB 0
PC 1.40

Fig. S7 ¹³C-NMR of Thorium-DHePO complex

RK-G-LAHPO-1H

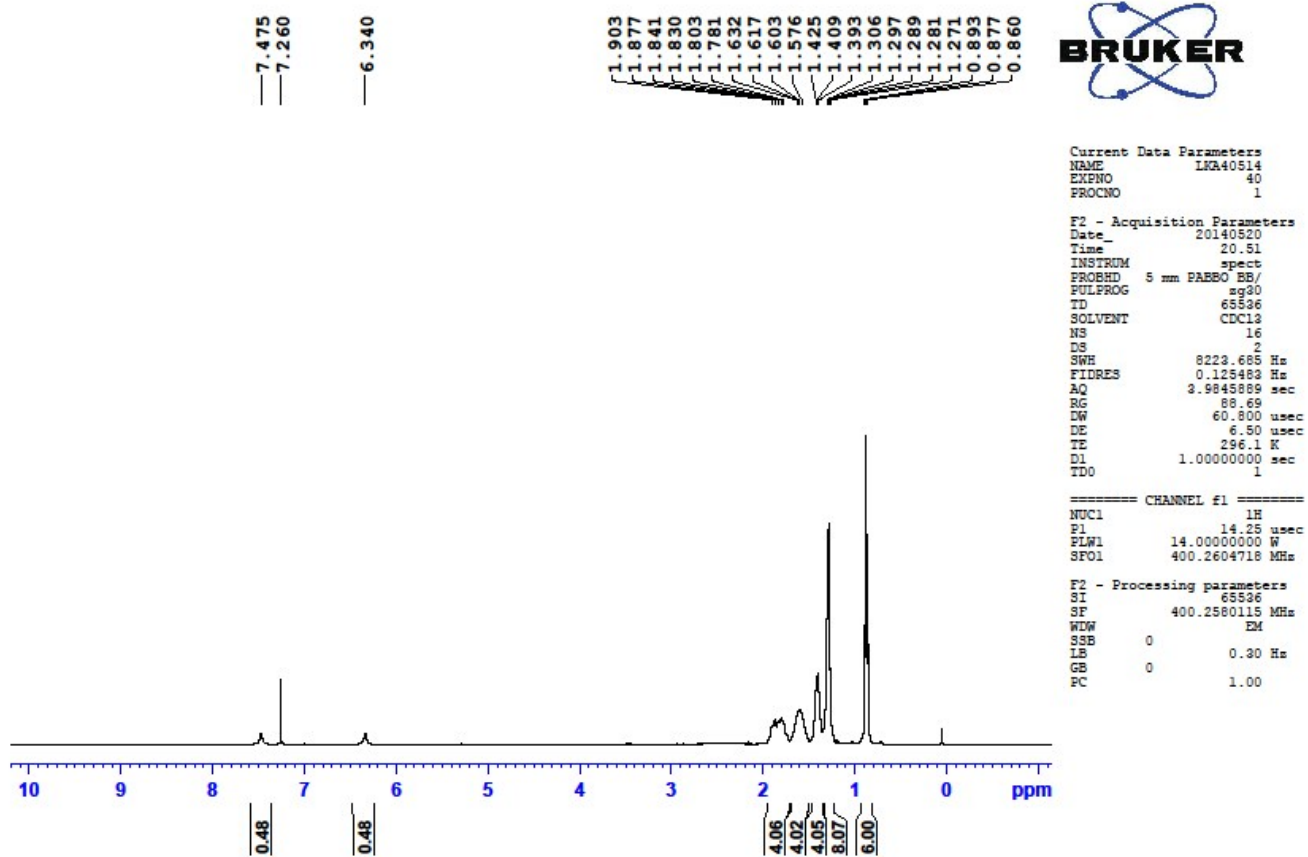
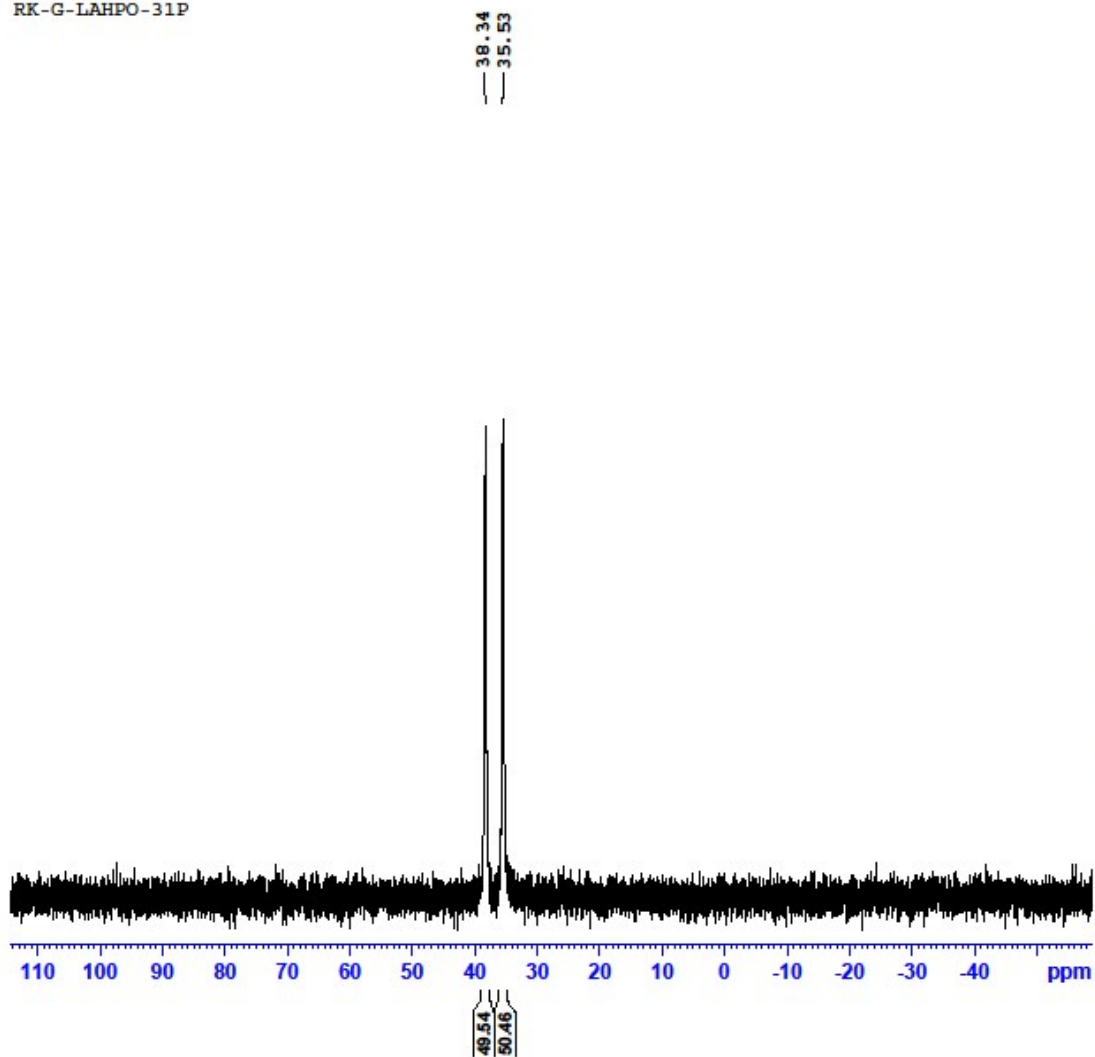


Fig. S8 ¹H-NMR of Lanthanum-DHePO complex

RK-G-LAHPO-31P



Current Data Parameters
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EXPNO 41
PROCNO 1

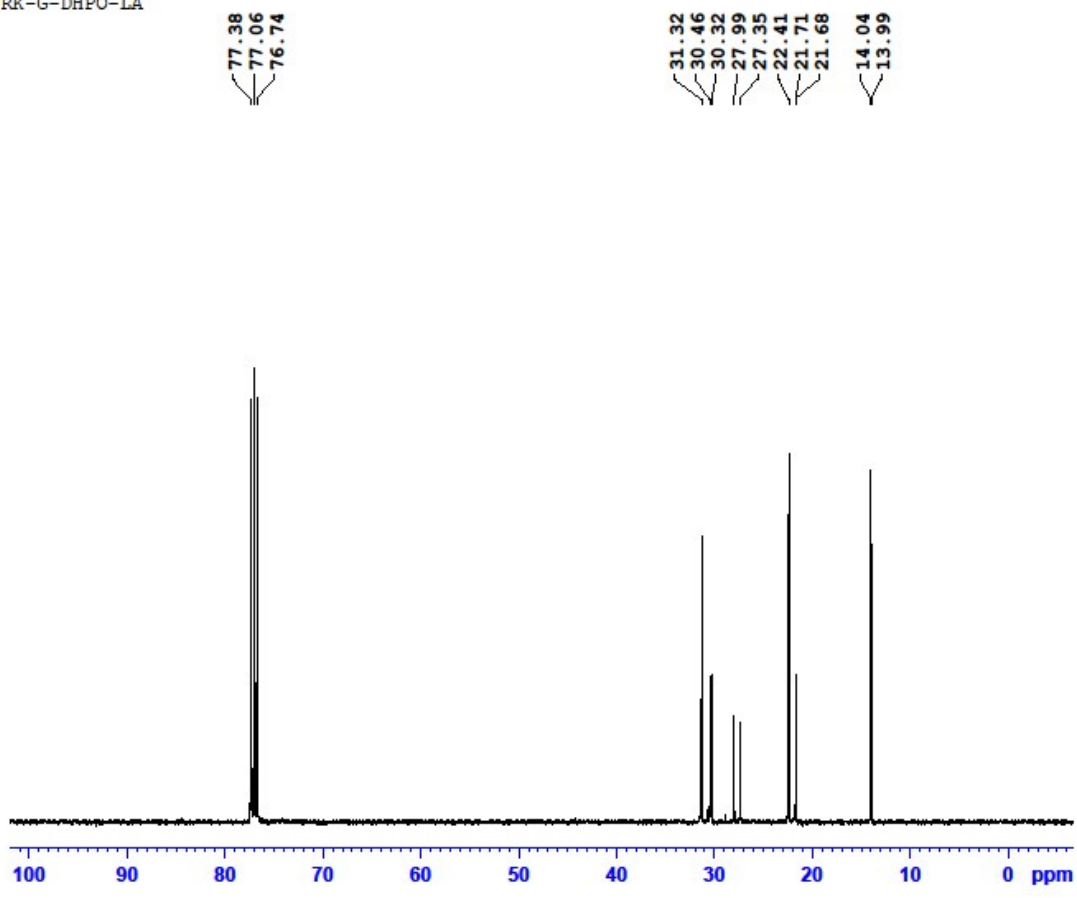
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SOLVENT CDCl3
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DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 199.6
DW 7.800 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 31P
P1 14.50 usec
PLW1 15.00000000 W
SFO1 162.0193069 MHz

F2 - Processing parameters
SI 32768
SF 162.0274080 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig. S9 ^{31}P -NMR of Lanthanum-DHePO complex

RK-G-DHPO-LA



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Current Data Parameters
NAME          LKA40215
EXPNO         186
PROCNO        1

F2 - Acquisition Parameters
Date_         20150302
Time          14.08
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PULPROG       zgpg30
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SOLVENT       CDCl3
NS            512
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            199.6
DW            20.800 usec
DE            6.50 usec
TE            303.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

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PLW1          58.00000000 W
SFO1          100.6550182 MHz

===== CHANNEL f2 =====
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NUC2           1H
PCPD2          90.00 usec
PLW2          14.00000000 W
PLW12         0.35097000 W
PLW13         0.28428999 W
SFO2          400.2596010 MHz

F2 - Processing parameters
SI            32768
SF            100.6449540 MHz
NUW           EM
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Fig. S10 ¹³C-NMR of Lanthanum-DHPO complex

RK-G-HEPPO

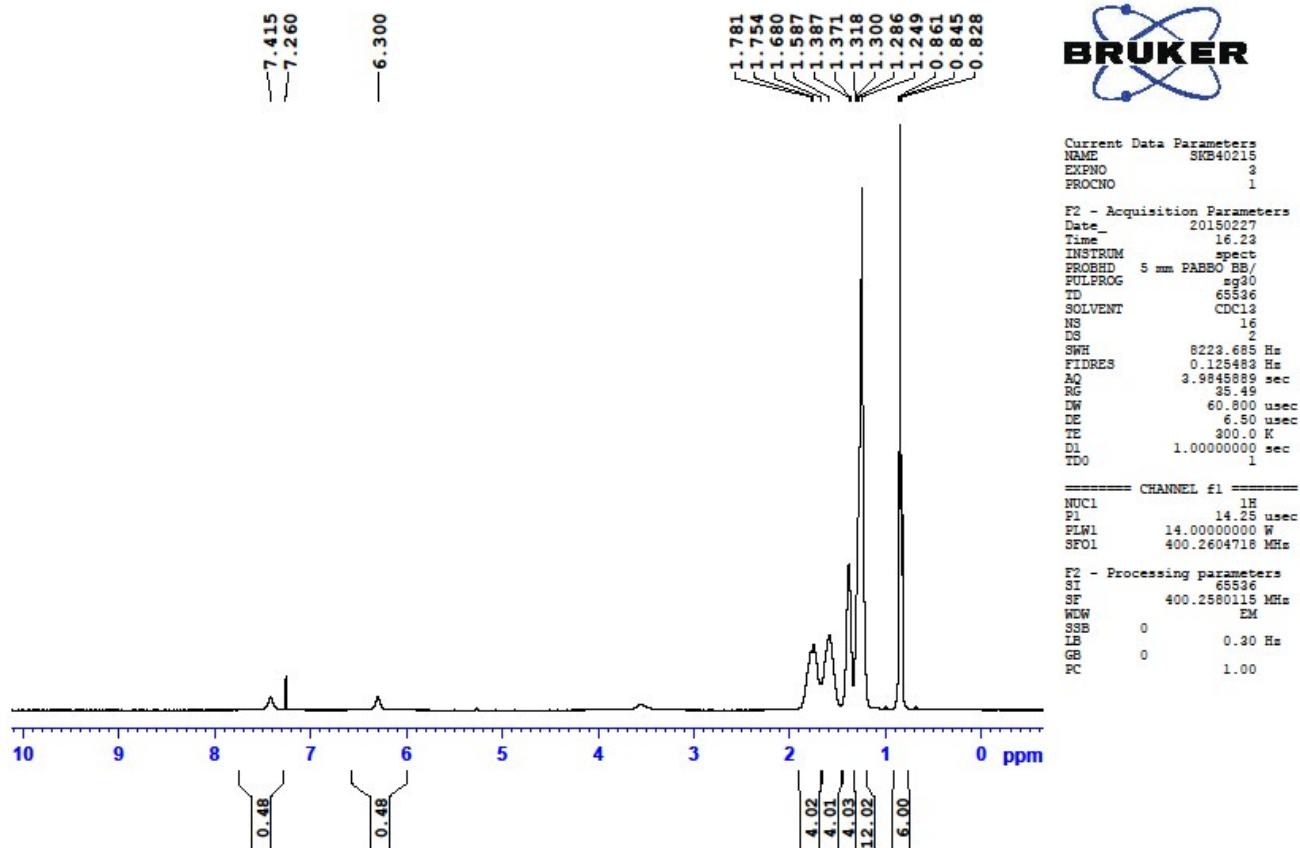


Fig. S11 ¹H-NMR of Di-*n*-heptyl phosphine oxide(DHpPO)

RK-G-HEPPO

36.96
34.22



```
Current Data Parameters
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EXPNO         4
PROCNO        1

F2 - Acquisition Parameters
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Time          16.25
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PULPROG       zg30
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SOLVENT       CDCl3
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DS            4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5111808 sec
RG            199.6
DW            7.800 usec
DE            6.50 usec
TE            300.0 K
DL            2.00000000 sec
TDO           1

===== CHANNEL f1 =====
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P1            14.50 usec
PLW1          15.00000000 W
SFO1          162.0193069 MHz

F2 - Processing parameters
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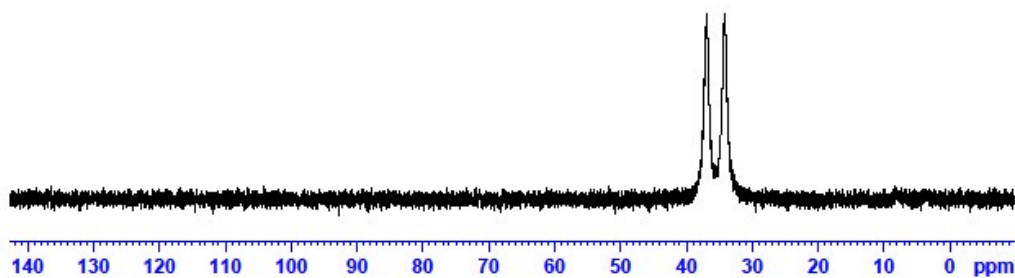


Fig. S12 ^{31}P -NMR of Di-*n*-heptyl phosphine oxide (DHpPO) complex

RK-G-HEPPO

77.39
77.07
76.75

31.52
30.70
30.57
28.77
22.55
21.78
14.00

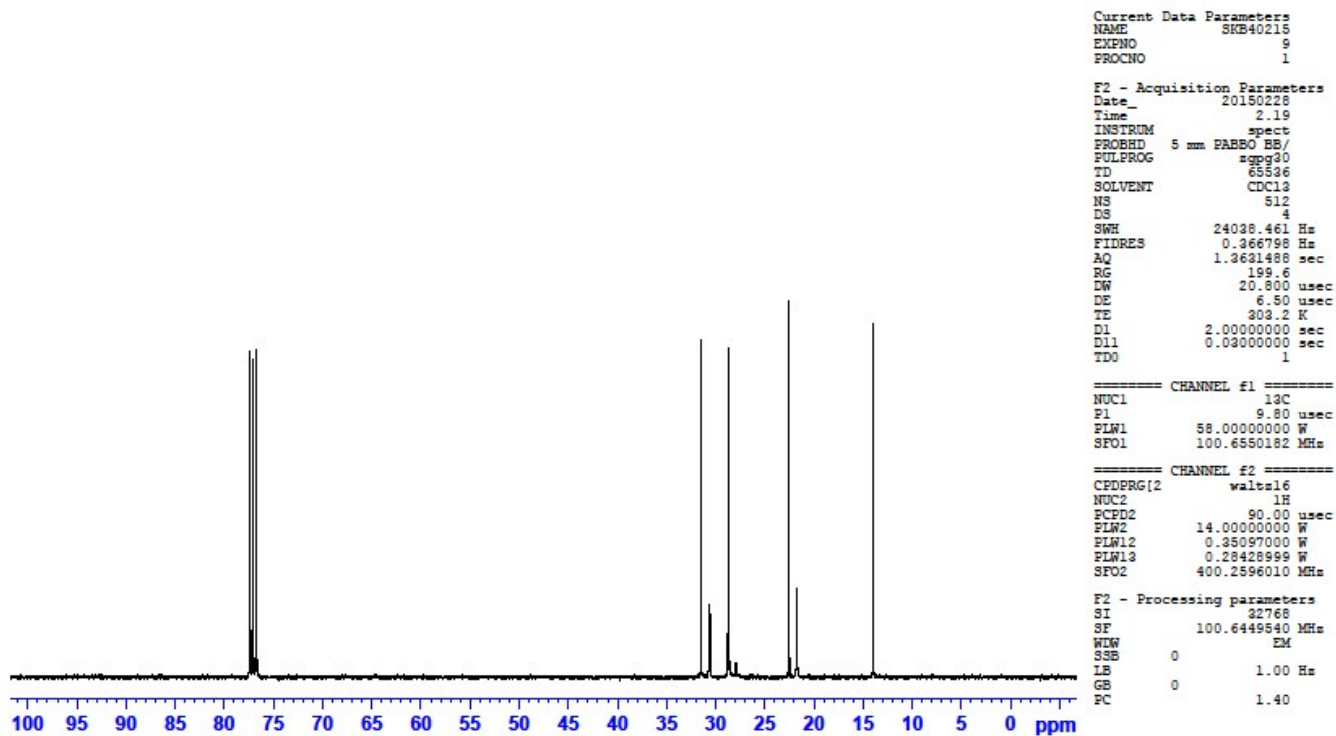


Fig. S13 ^{13}C -NMR of Di-*n*-heptyl phosphine oxide(DHpPO)

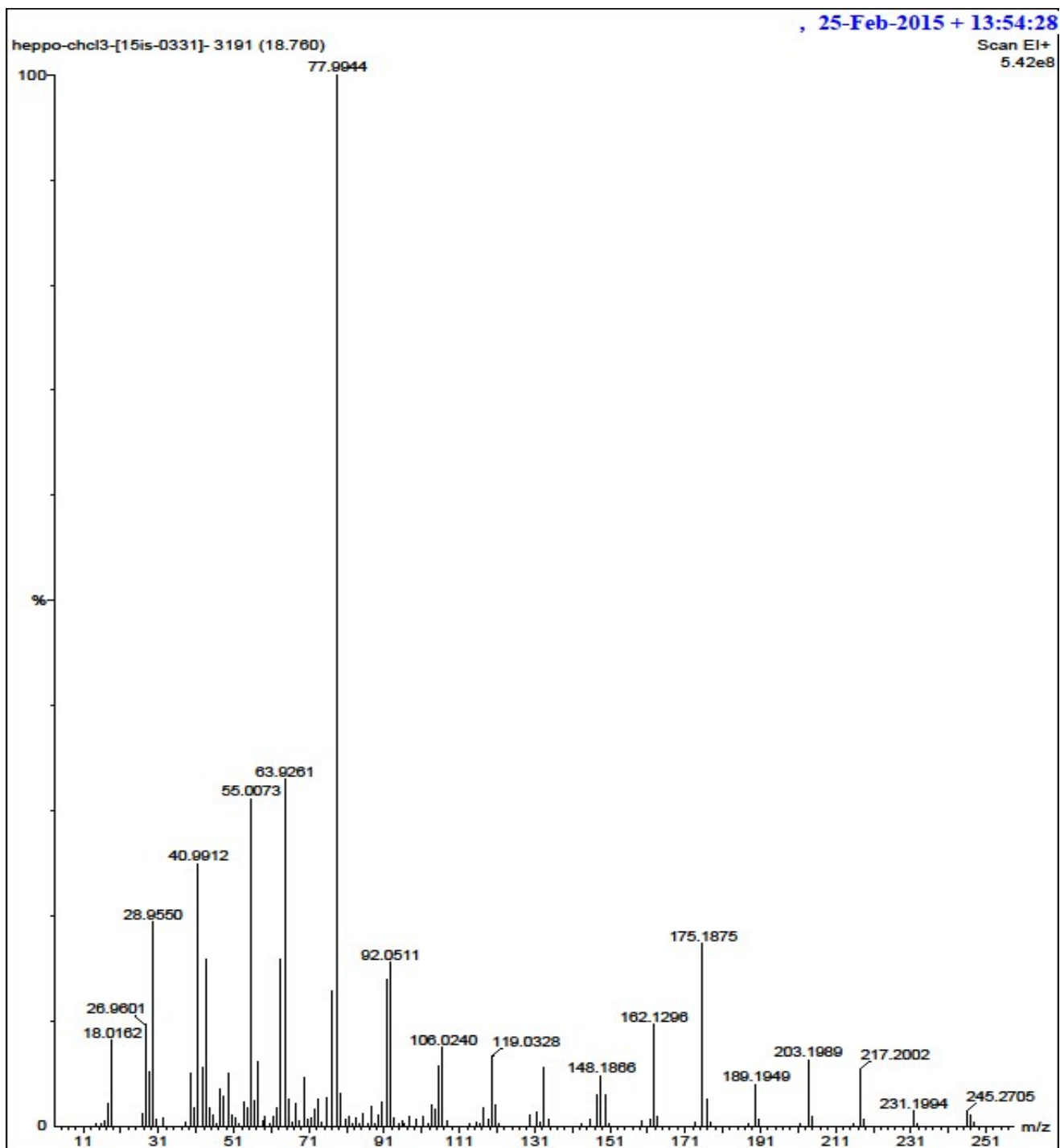


Fig.S14 EI mass spectra of Di-*n*-heptyl phosphine oxide(DHpPO)

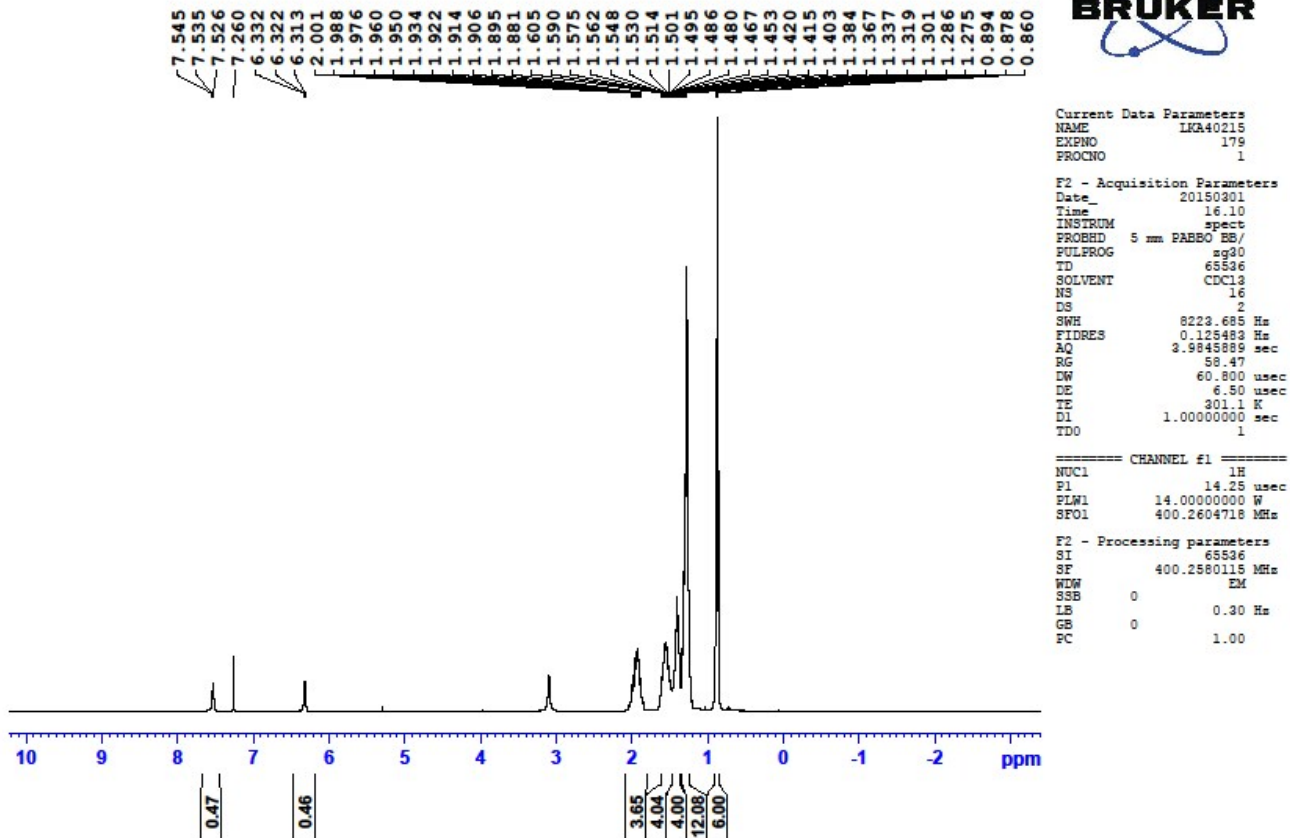


Fig. S15 ¹H-NMR of Thorium-DHpPO complex

HEPPOTH

— 50.68
— 47.72

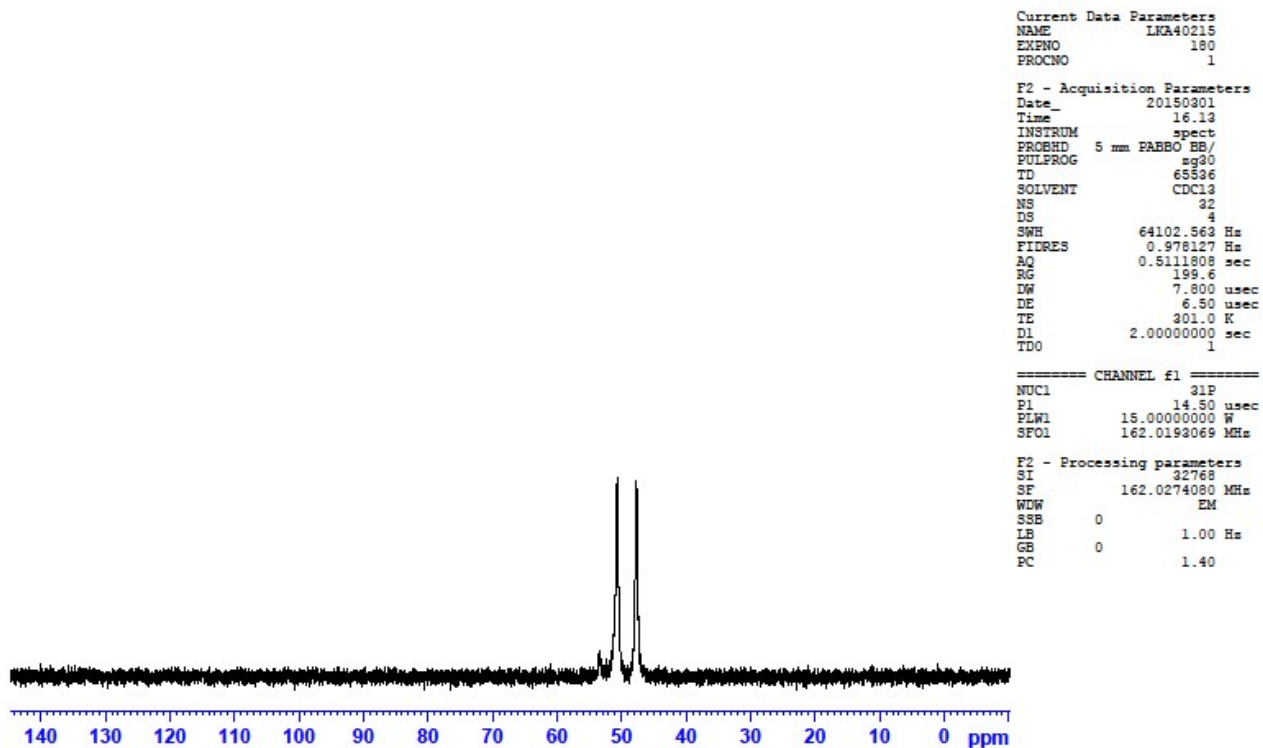
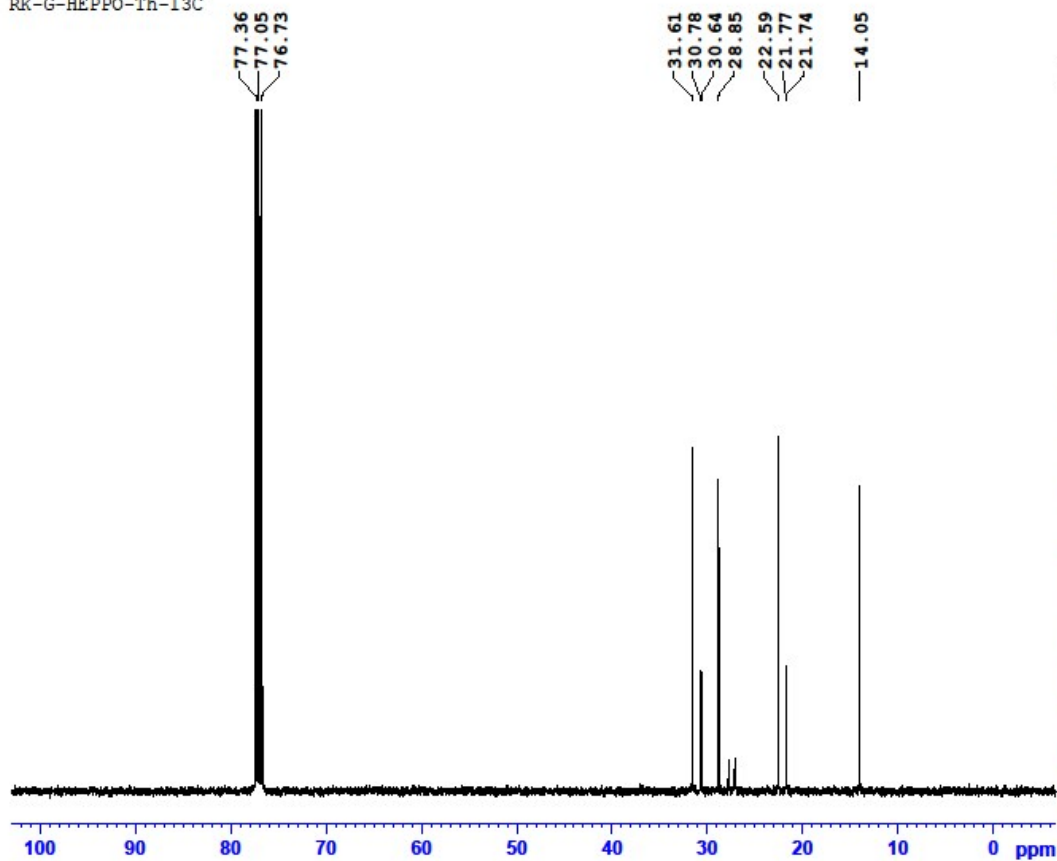


Fig. S16 ^{31}P -NMR of Thorium-DHpPO complex

RK-G-HEPPO-Th-13C



Current Data Parameters
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EXPNO 184
PROCNO 1

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NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.266798 Hz
AQ 1.3621488 sec
RG 175.97
DW 20.800 usec
DE 6.50 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO1 100.6550182 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.35097000 W
PLW13 0.28428999 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig. S17 ¹³C-NMR of Thorium-DHpPO complex

RK-G-HEPPO-La

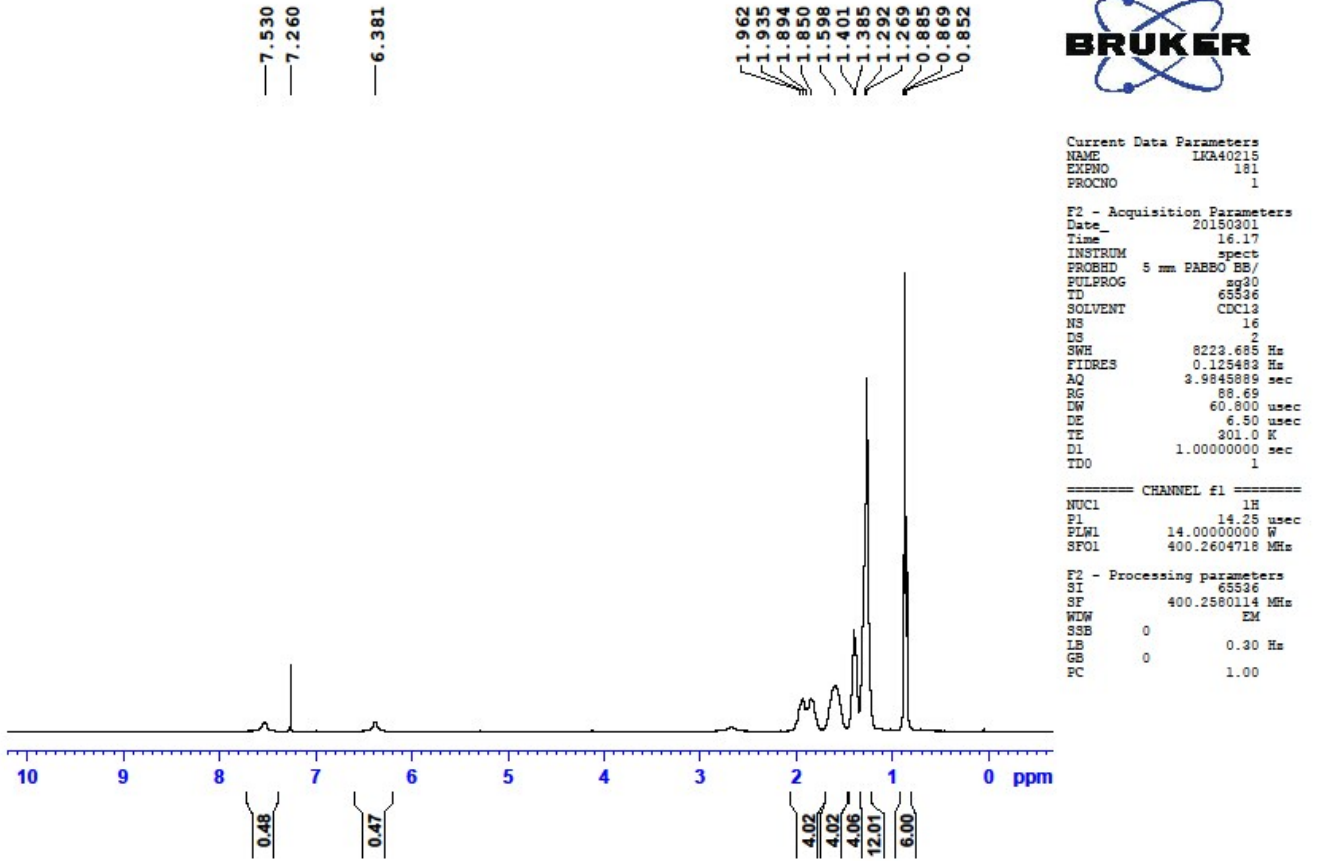
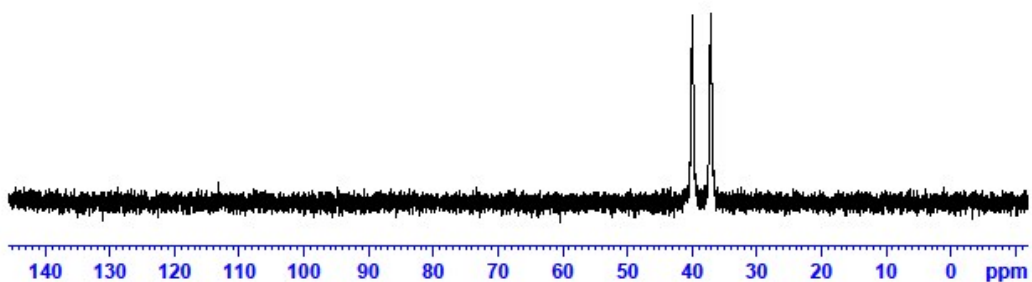


Fig. S18 ¹H-NMR of Lanthanum-DHpPO complex

RK-G-HEPPO-La

— 39.99
— 37.14



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Current Data Parameters
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PROCNO        1

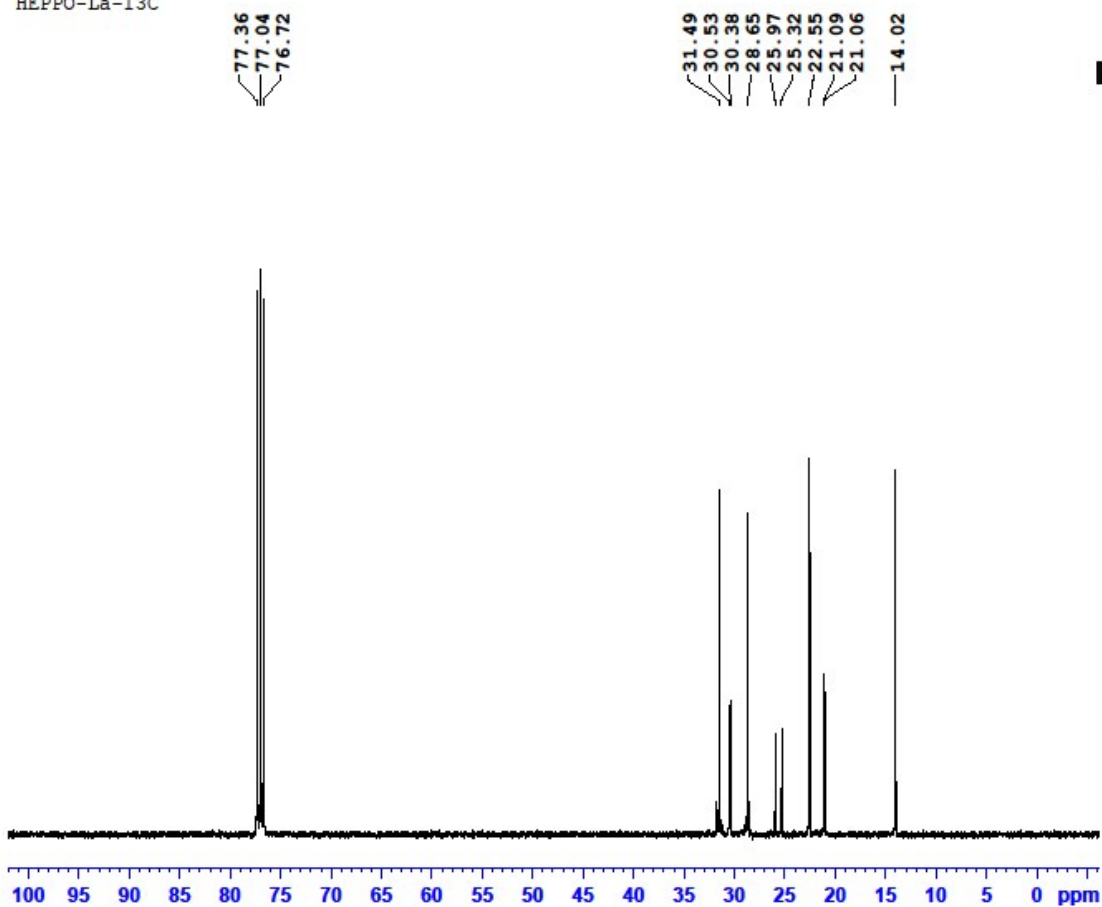
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SOLVENT       CDCl3
NS            32
DS            4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5111808 sec
RG            199.6
DW            7.800 usec
DE            6.50 usec
TE            301.0 K
D1            2.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          31P
P1            14.50 usec
PLW1          15.00000000 W
SFO1          162.0193069 MHz

F2 - Processing parameters
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WDW           EM
SSB           0
LB            1.00 Hz
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Fig. S19 ^{31}P -NMR of Lanthanum-DHpPO complex

HEPPO-La-13C



Current Data Parameters
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EXNO 183
PROCNO 1

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INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3621488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL #1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6250182 MHz

===== CHANNEL #2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.35097000 W
PLW13 0.28428999 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSE 0
LB 1.00 Hz
GB 0
PC 1.40

Fig. S20 ¹³C-NMR of Lanthanum-DHppO complex

Signature SIF VIT VELLORE
DJ-DOPO

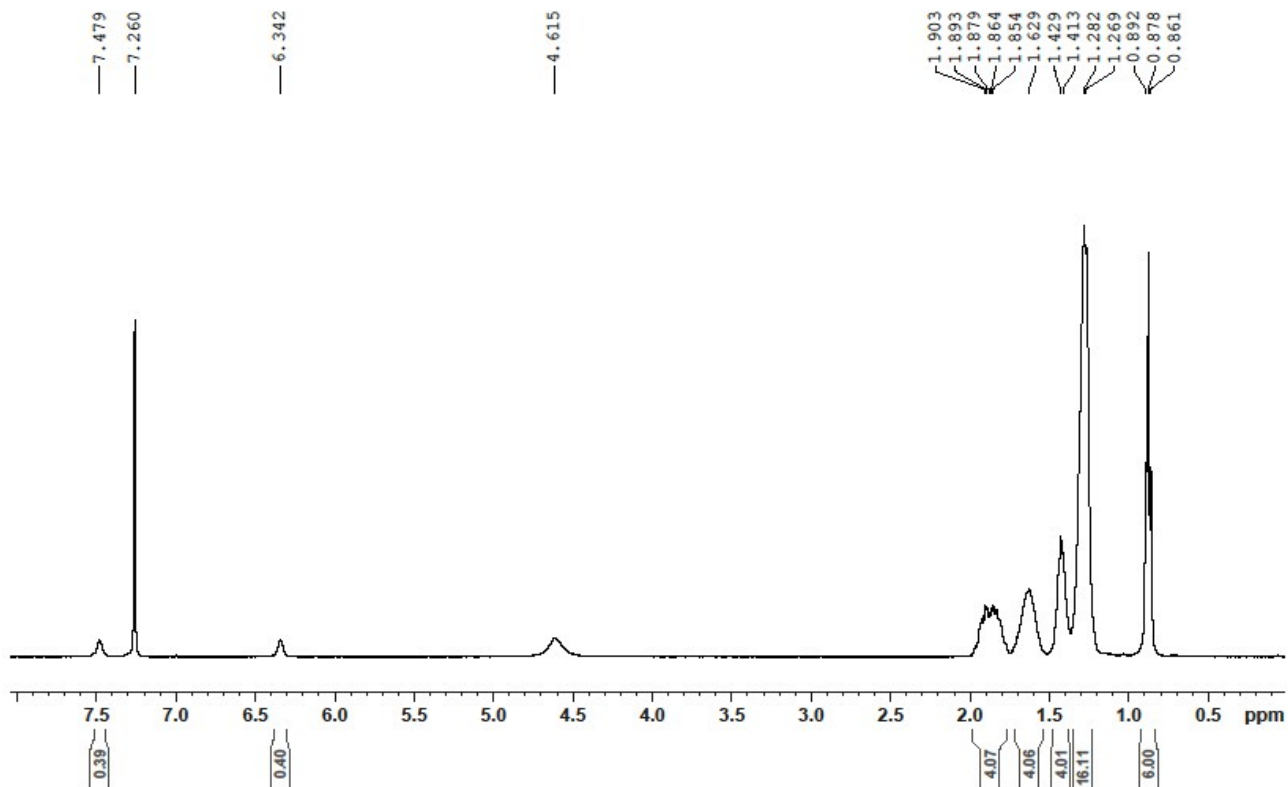


Fig. S21 ¹H-NMR of Di-*n*-octyl phosphine oxide(DOPO)

RK-G-DOPO

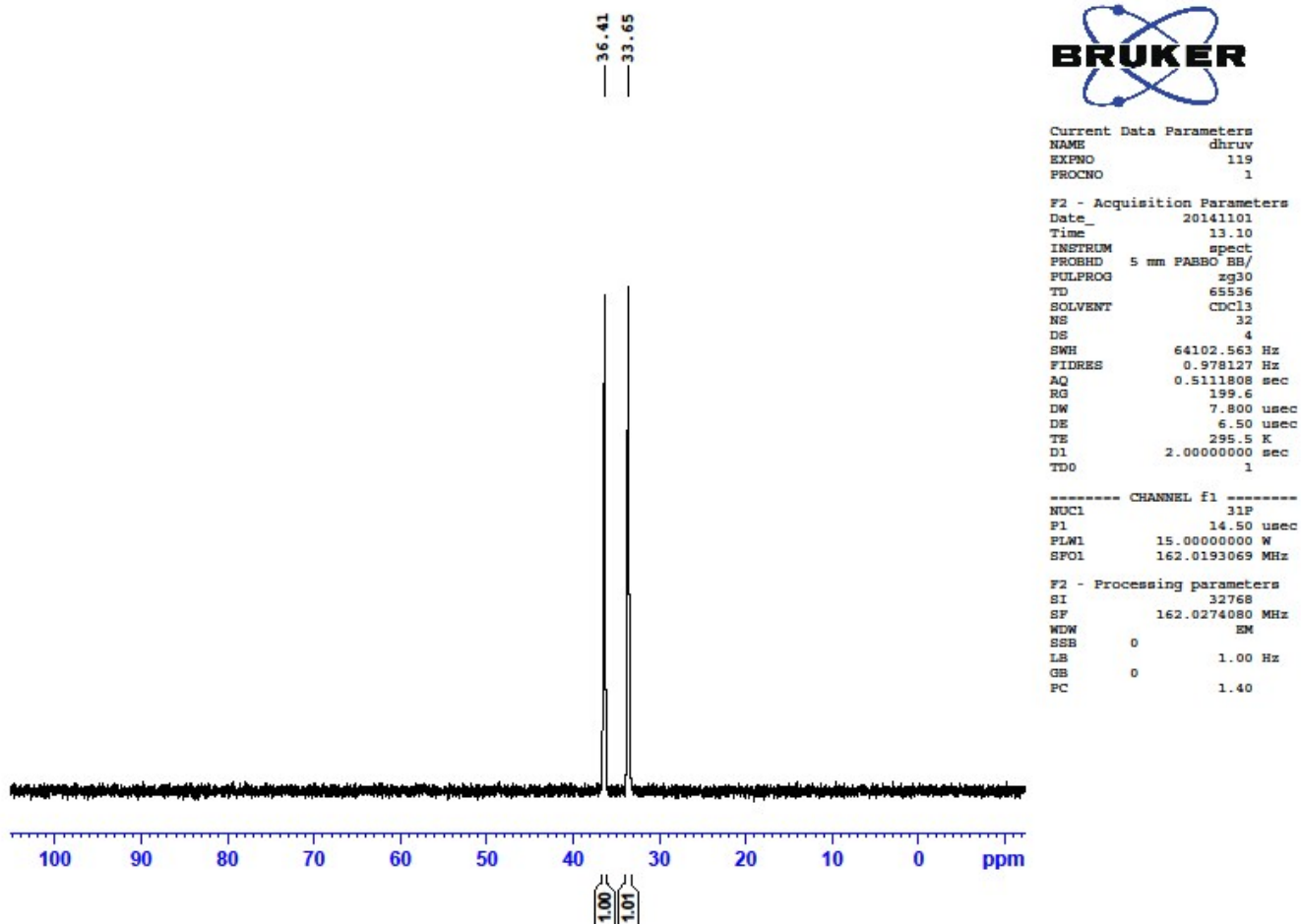


Fig. S22 ^{31}P NMR of Di-*n*-octyl phosphine oxide(DOPO)

Signature SIF VIT VELLORE
DU-OCT-PO

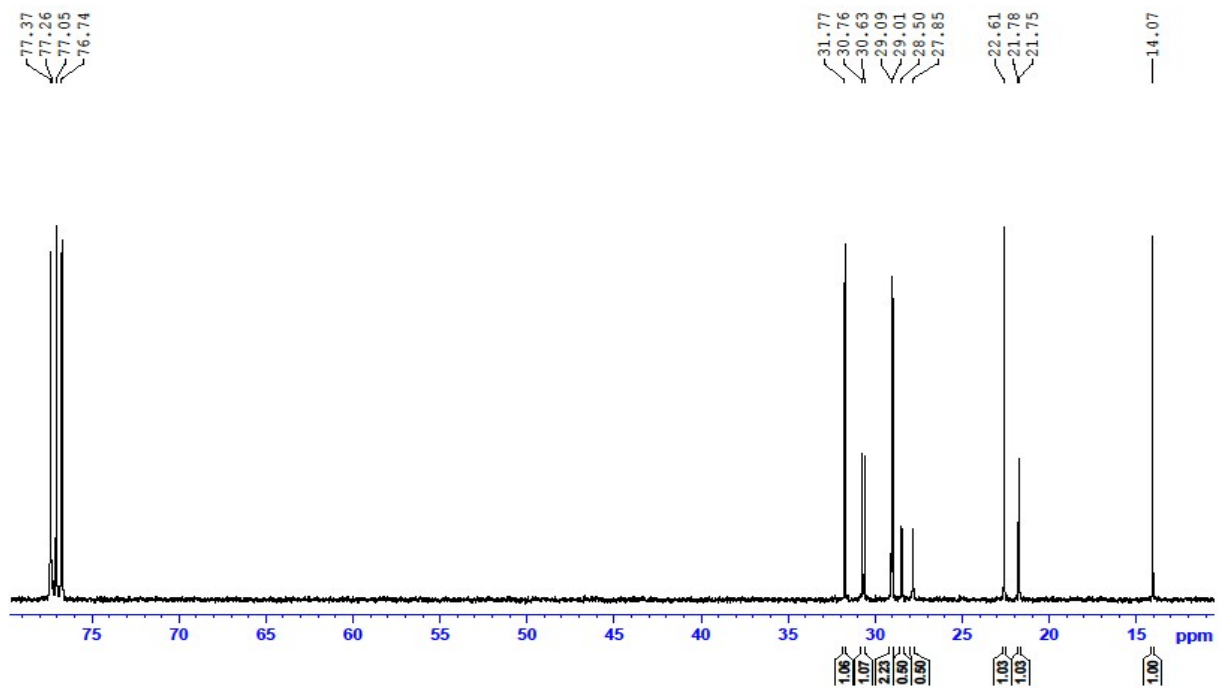


Fig. S23 ^{13}C NMR of Di-*n*-octyl phosphine oxide(DOPO)

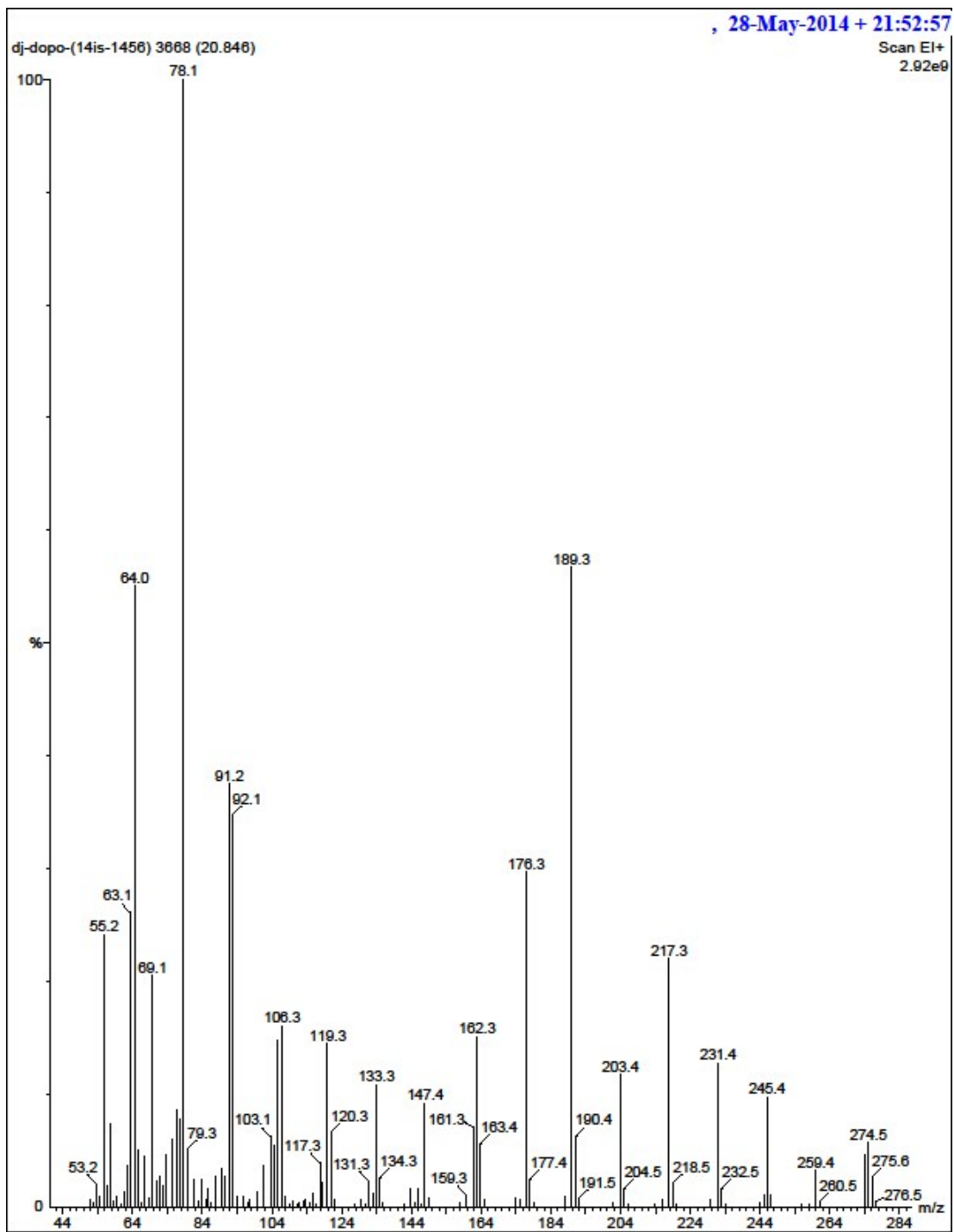


Fig.S24 EI mass spectra of Di-*n*-octyl phosphine oxide(DOPO)

RK-G-IH-OPO

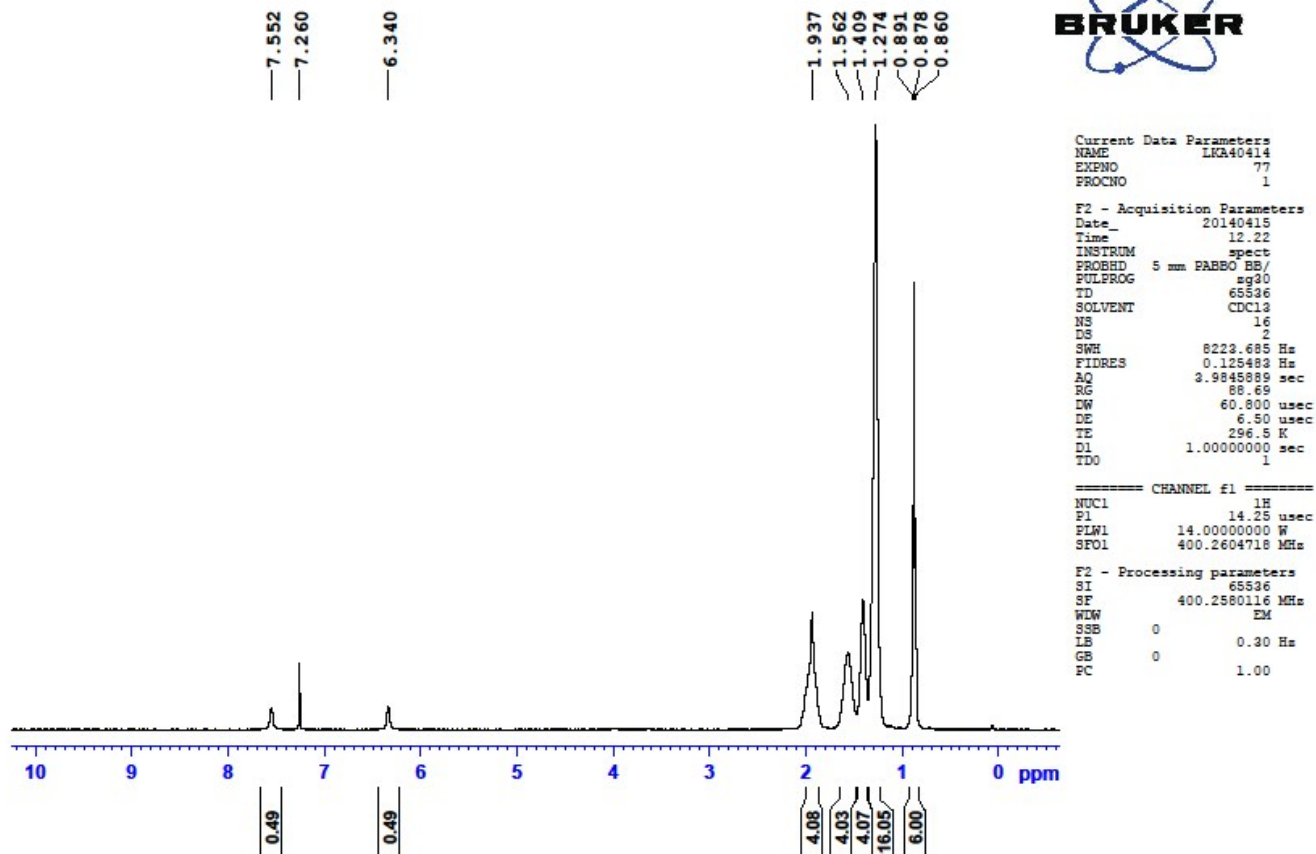


Fig. S25 ¹H-NMR of Thorium-DOPO complex

Signature SIF VIT VELLORE
DJ-DOPO-IH

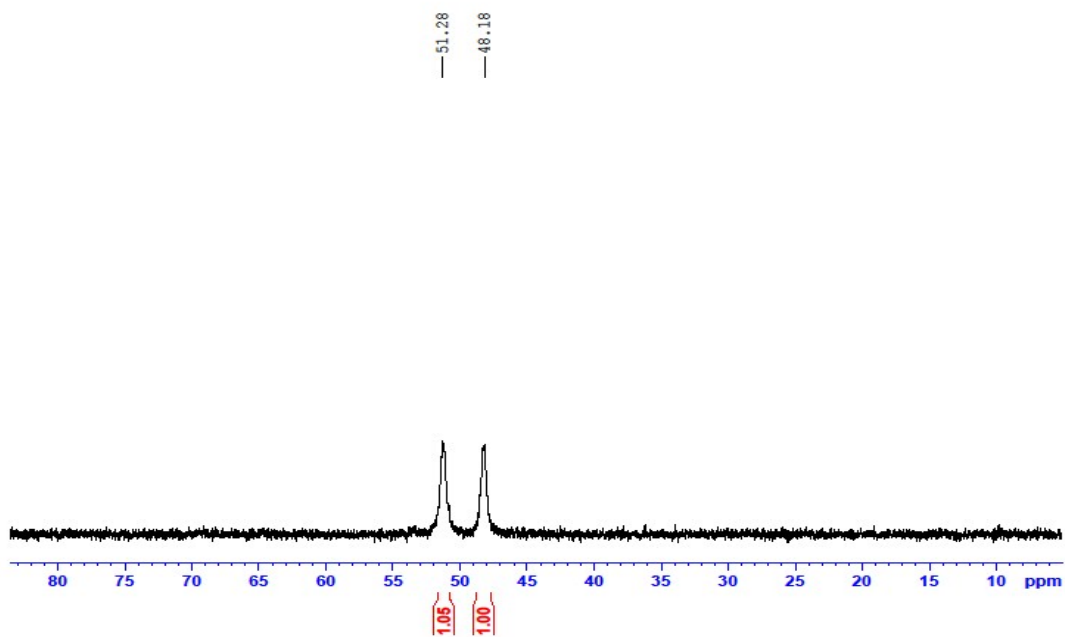


Fig. S26 ^{31}P NMR of Thorium-DOPO Complex

Signature SIF VIT VELLORE
DJ-DOPO-IN

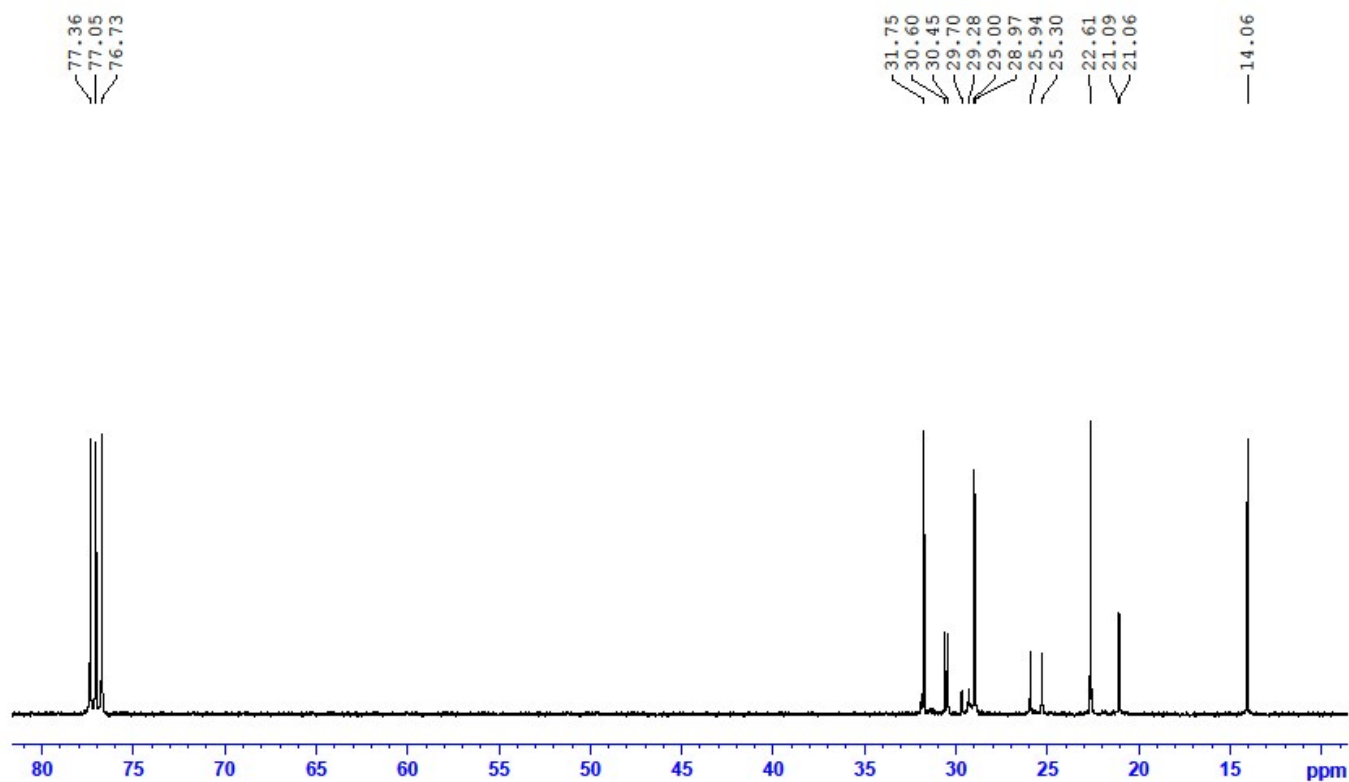


Fig. S27 ^{13}C -NMR of Thorium-DOPO complex

RK-G-DOPO-LA

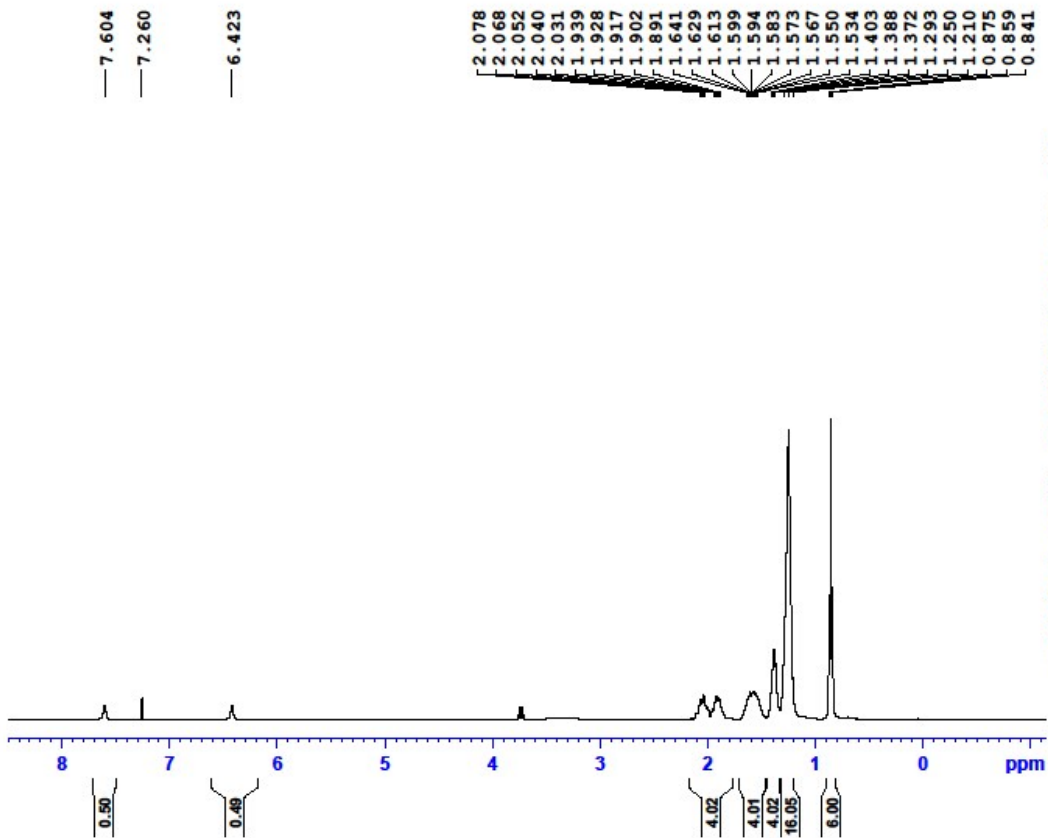


Fig. S28 ¹H-NMR of Lanthanum-DOPO complex

Signature SIF VIT VELLORE
DJ-LA-C

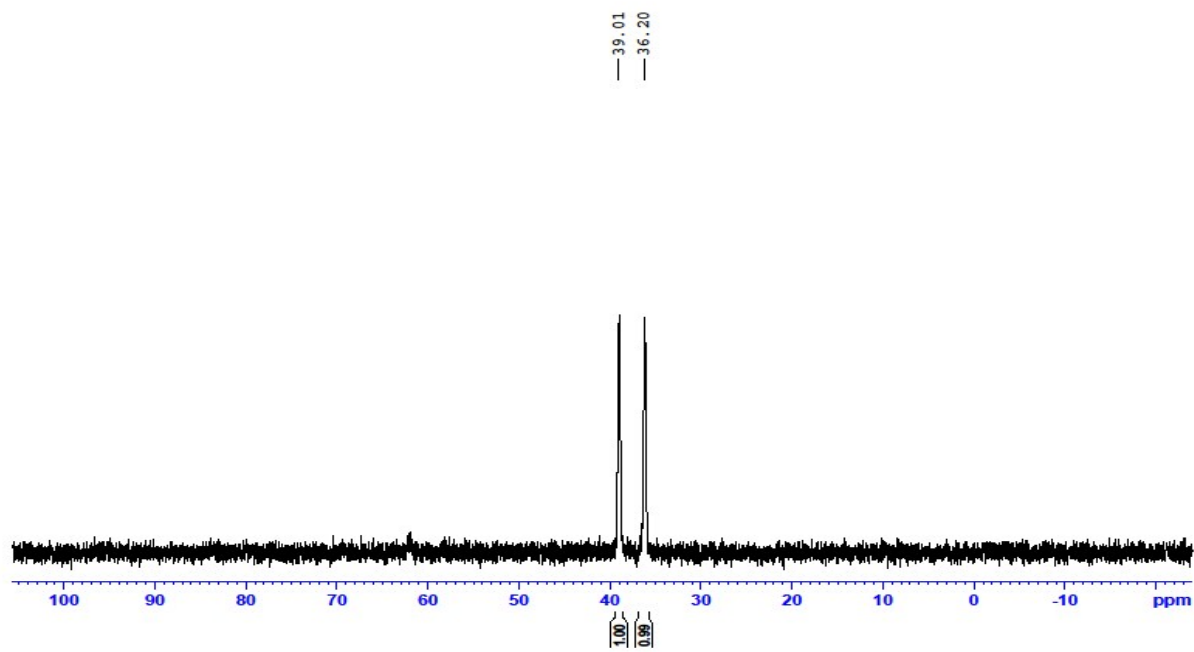
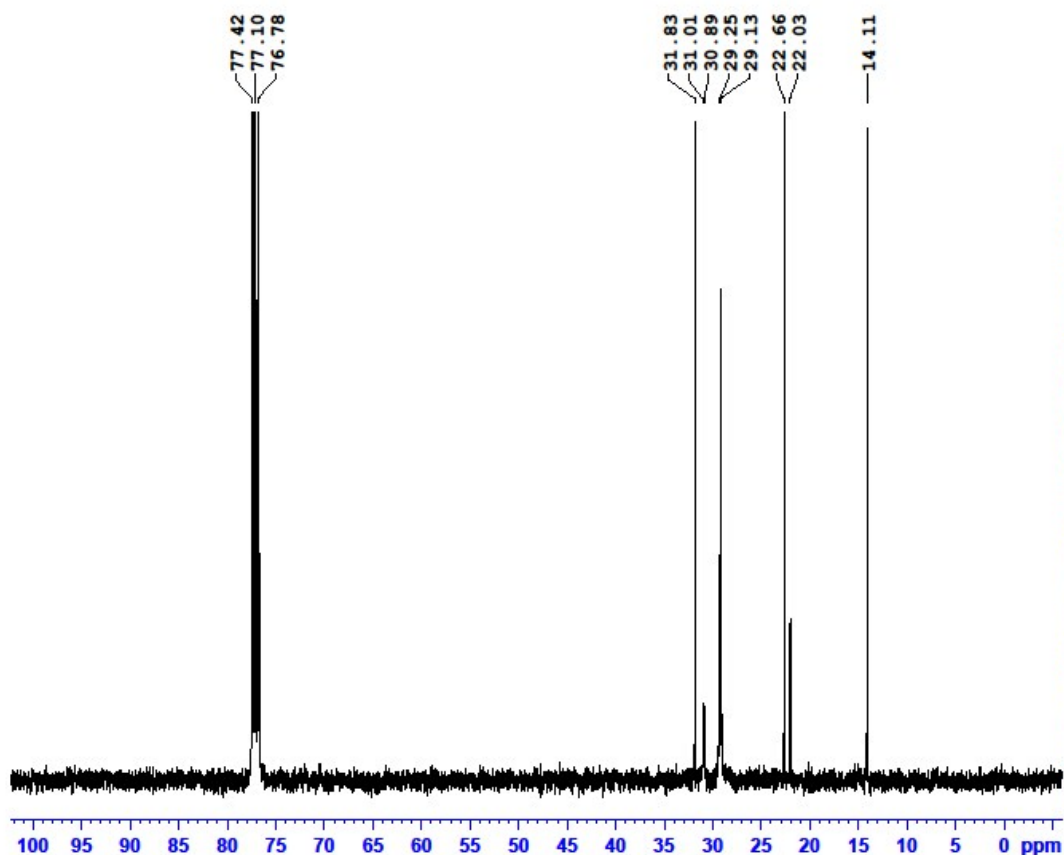


Fig. S29 ^{31}P NMR of Lanthanum-DOPO Complex

RK-G-DOPO-LA



```
Current Data Parameters
NAME LRA40215
EXPNO 187
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150303
Time 15.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.266798 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 302.8 K
DL 2.00000000 sec
D11 0.03000000 sec
TDO 1

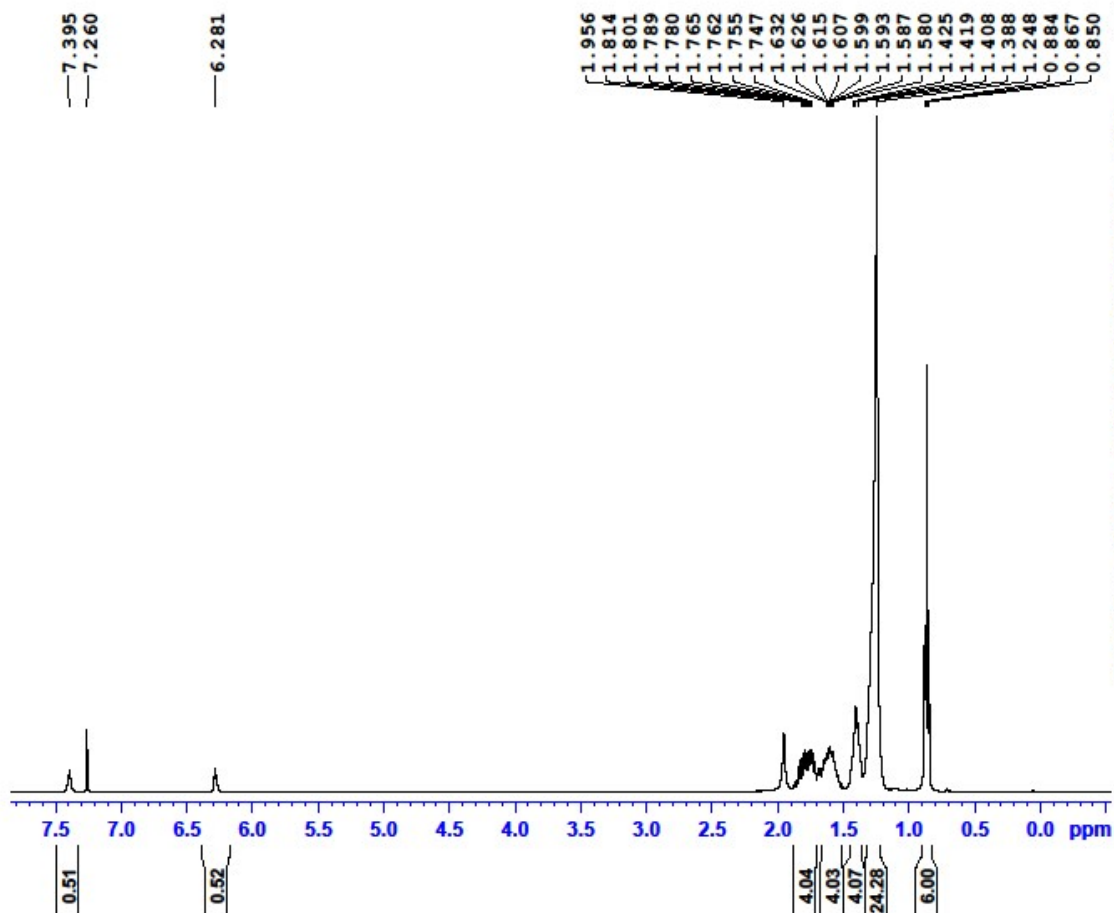
===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6550182 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.35097000 W
PLW13 0.28428999 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

Fig. S30 ^{13}C -NMR of Lanthanum-DOPO complex

DDPO



Current Data Parameters
NAME Desktop
EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150528
Time 17.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125482 Hz
AQ 3.9845889 sec
RG 71.13
DW 60.800 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLN1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig. S31 ¹H-NMR of Di-*n*-decyl phosphine oxide(DDPO)

DDPO

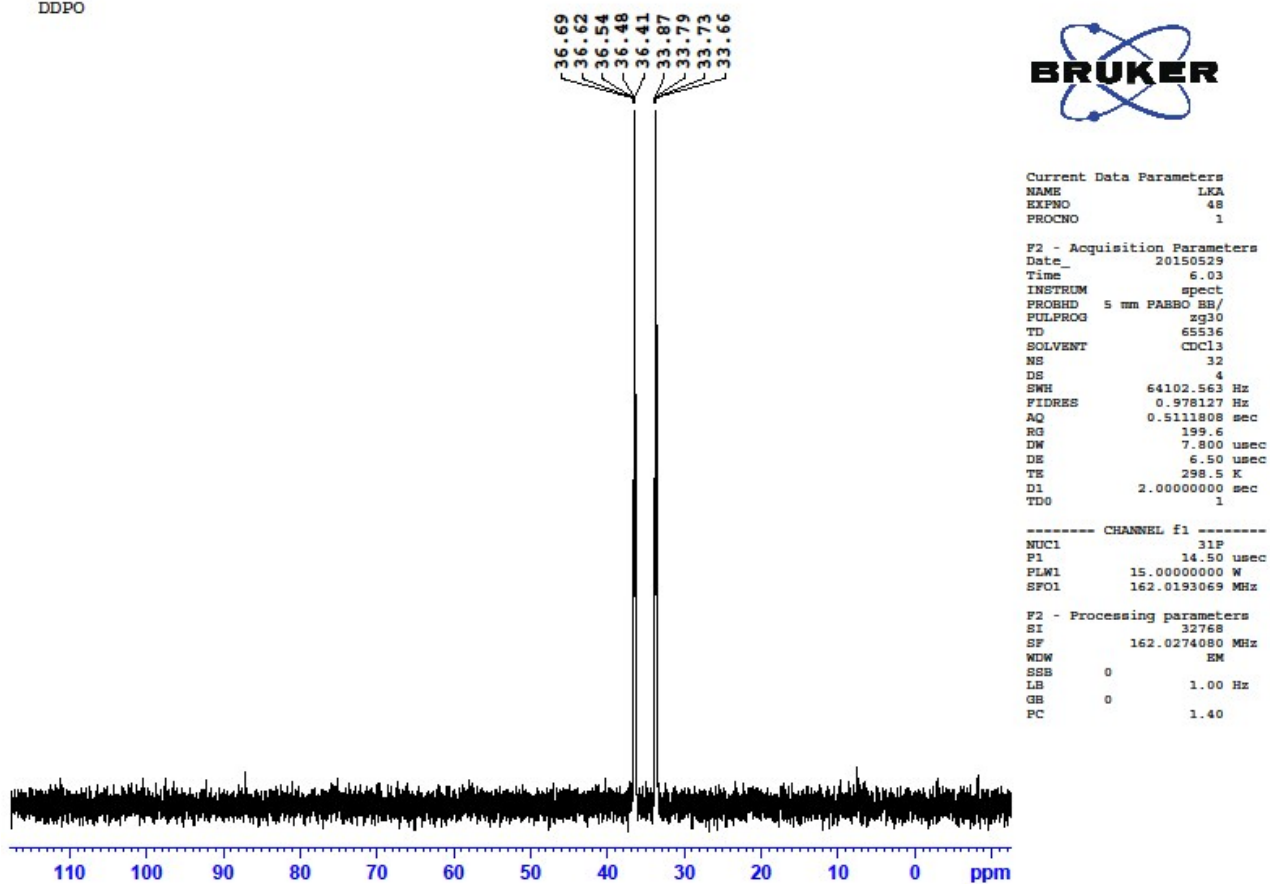
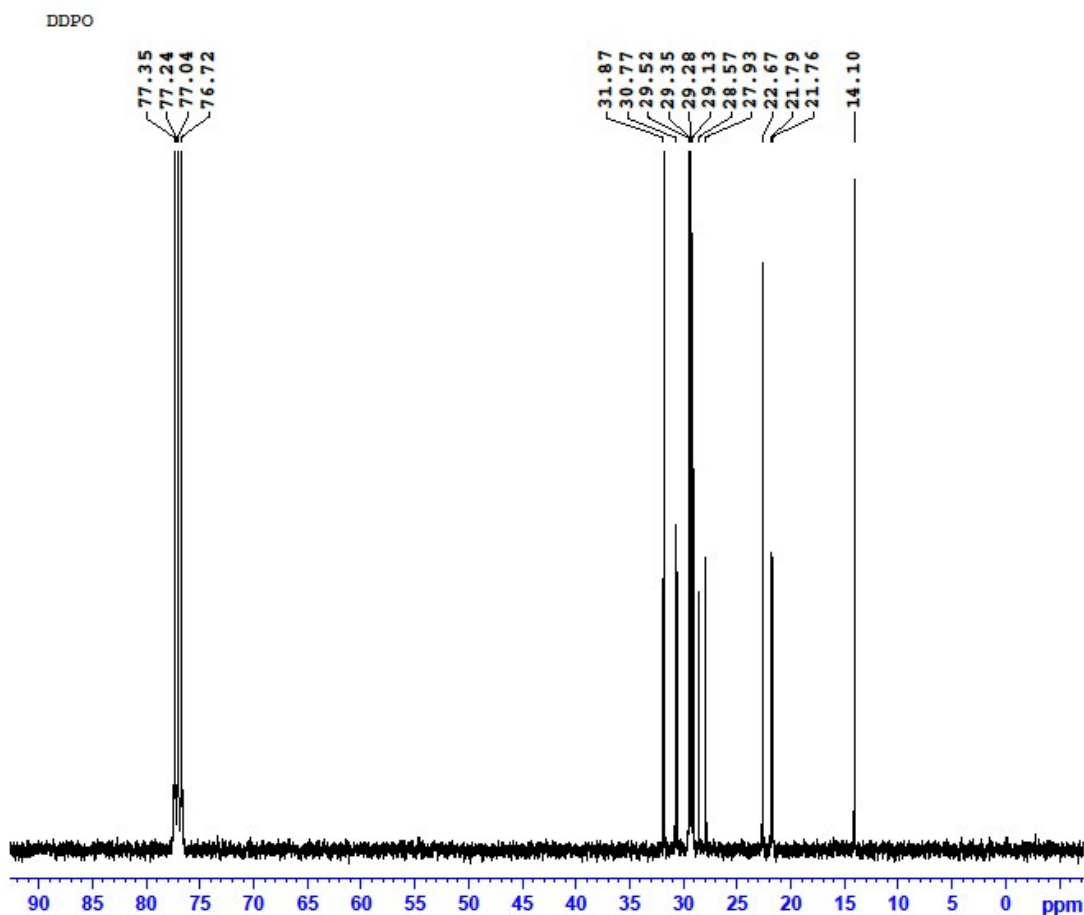


Fig. S32 ^{31}P -NMR of Di-*n*-decyl phosphine oxide(DDPO)



Current Data Parameters
NAME LKA
EXPNO 47
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150529
Time 6.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6250182 MHz

----- CHANNEL f2 -----
CFDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.35097000 W
PLW13 0.28428999 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SBB 0
LB 1.00 Hz
GB 0
PC 1.40

Fig. S33 ^{13}C -NMR of Di-*n*-decyl phosphine oxide(DDPO)

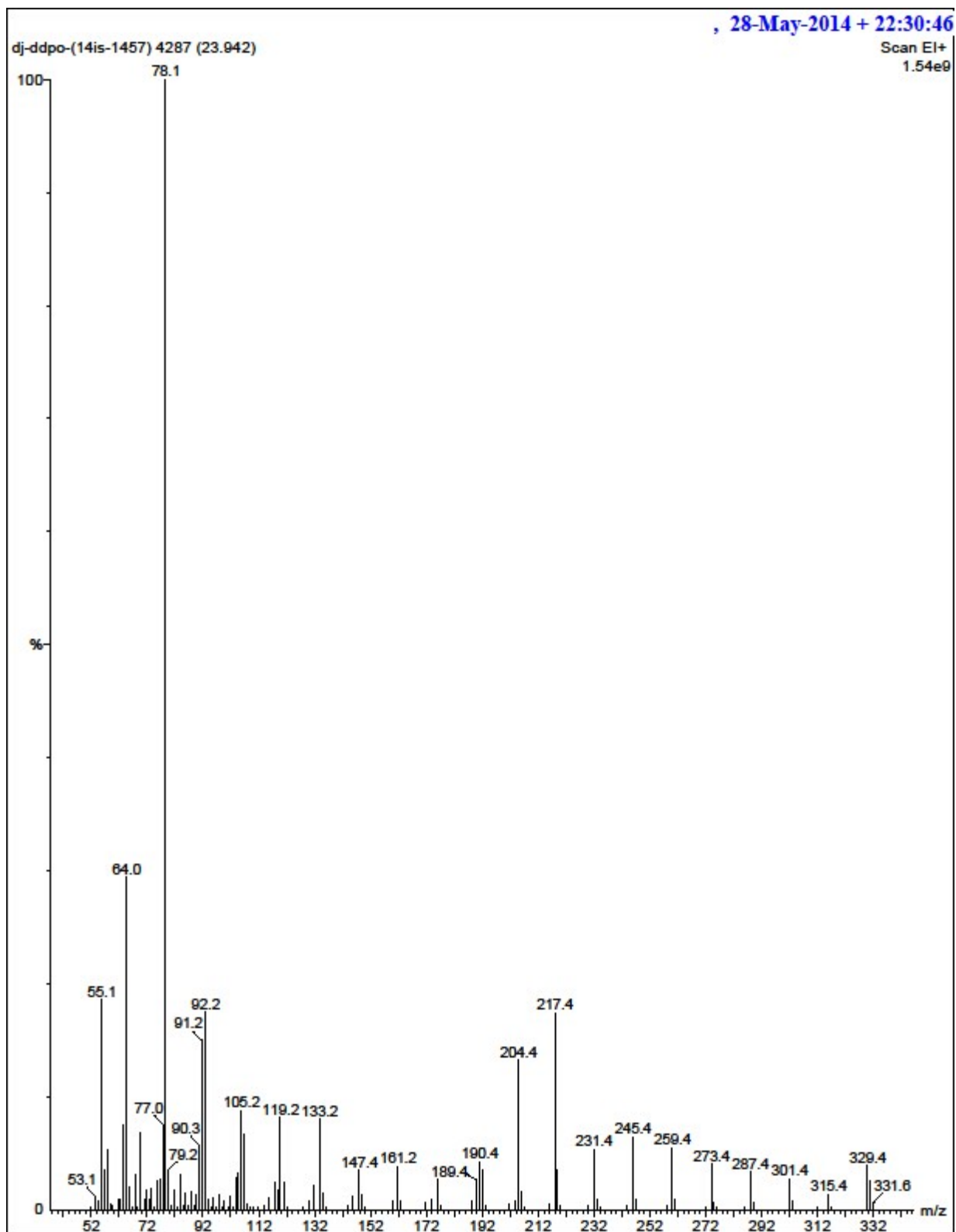


Fig. S34 EI mass spectra of Di-*n*-decyl phosphine oxide(DDPO)

Signature SIF VIT VELLORE
DJ-TH-DD

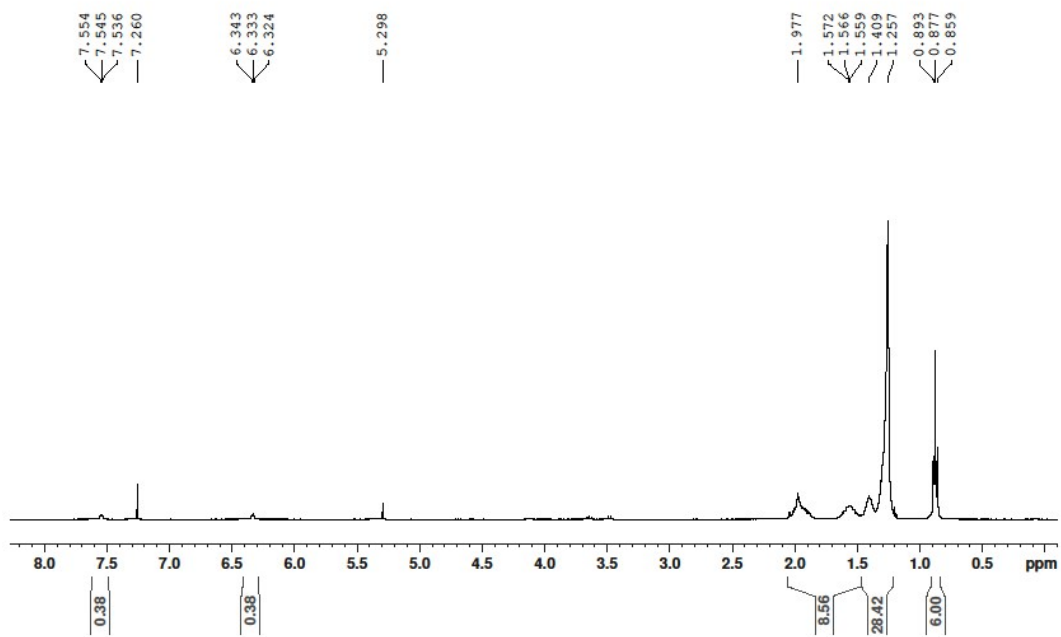


Fig. S35 ^1H NMR of Thorium-DDPO complex

Signature SIF VIT VELLORE
DJ-TH-DD

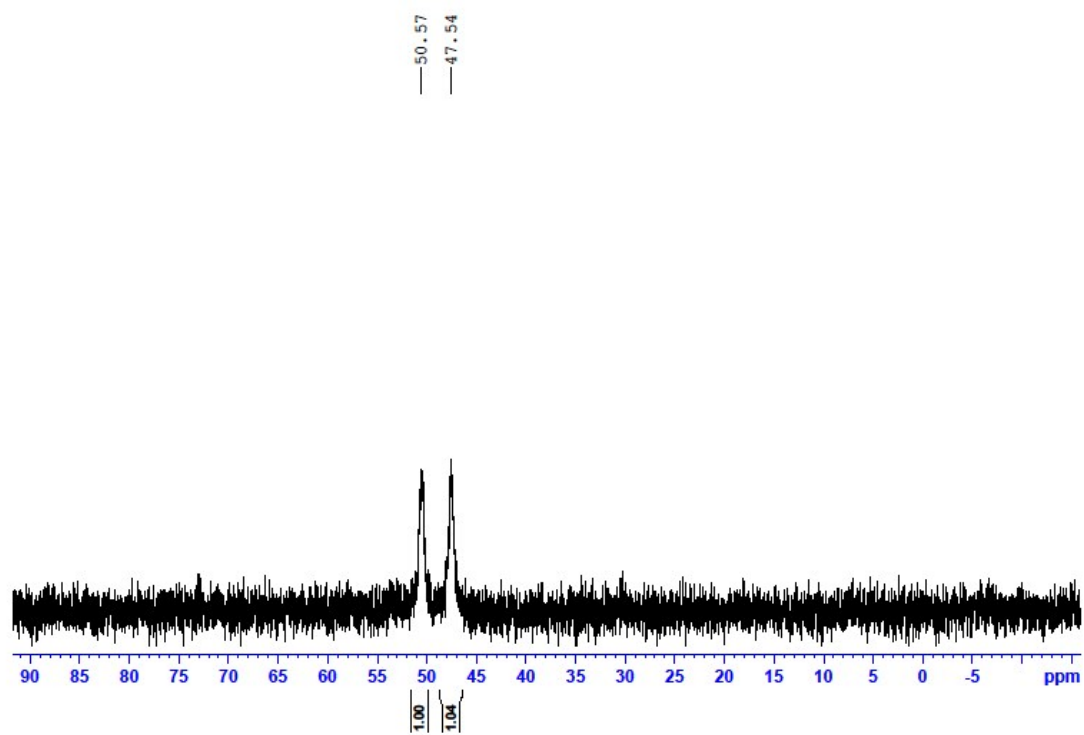


Fig. S36 ^{31}P NMR of Thorium-DDPO complex

Signature SIF VIT VELLORE
DJ-IH-DD

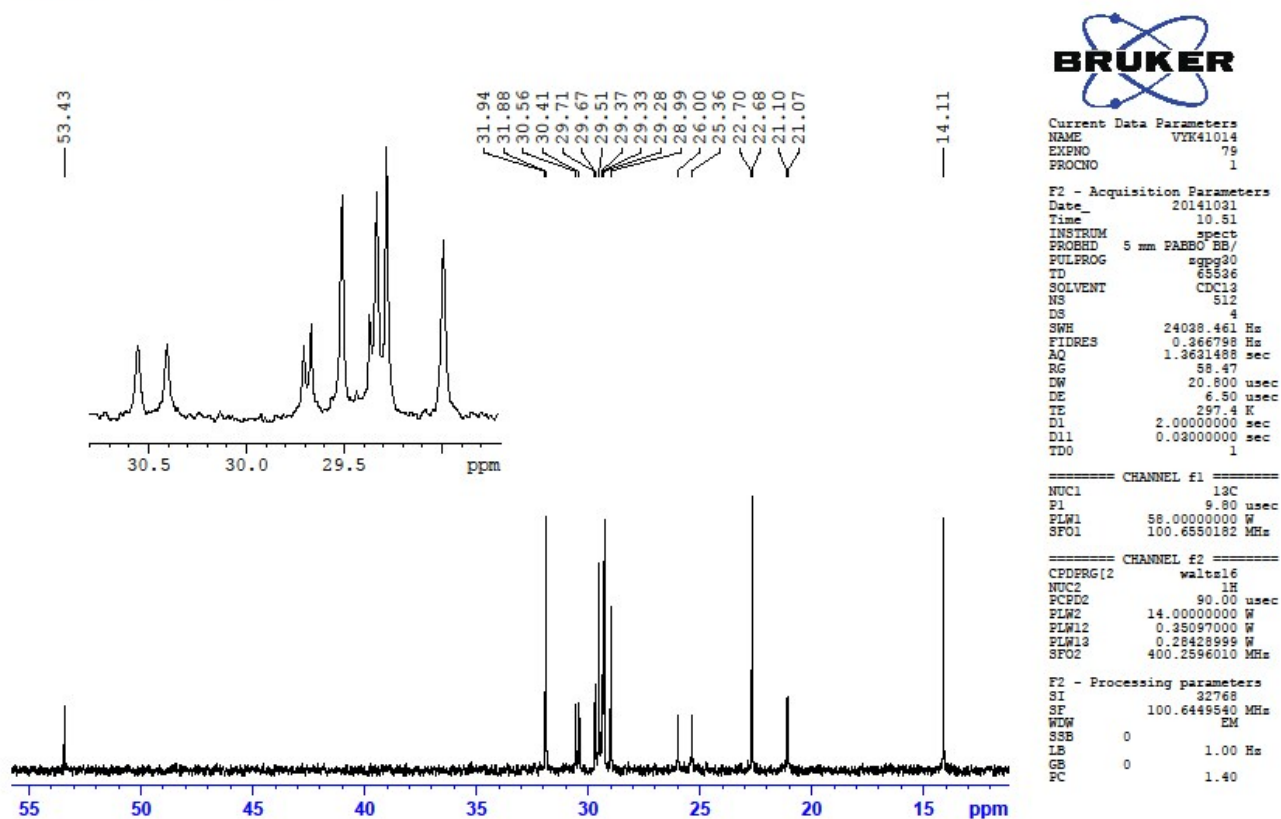


Fig. S37 ^{13}C -NMR of Thorium-DDPO complex

Signature SIF VIT VELLORE
DJ-LA-DD

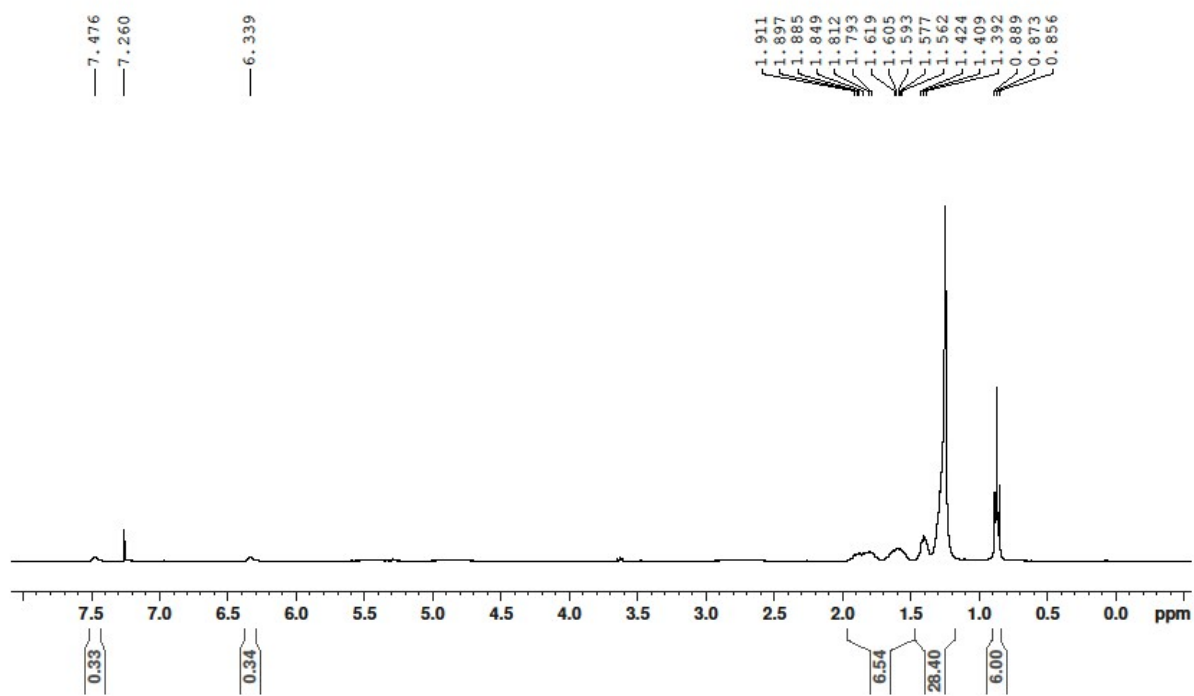
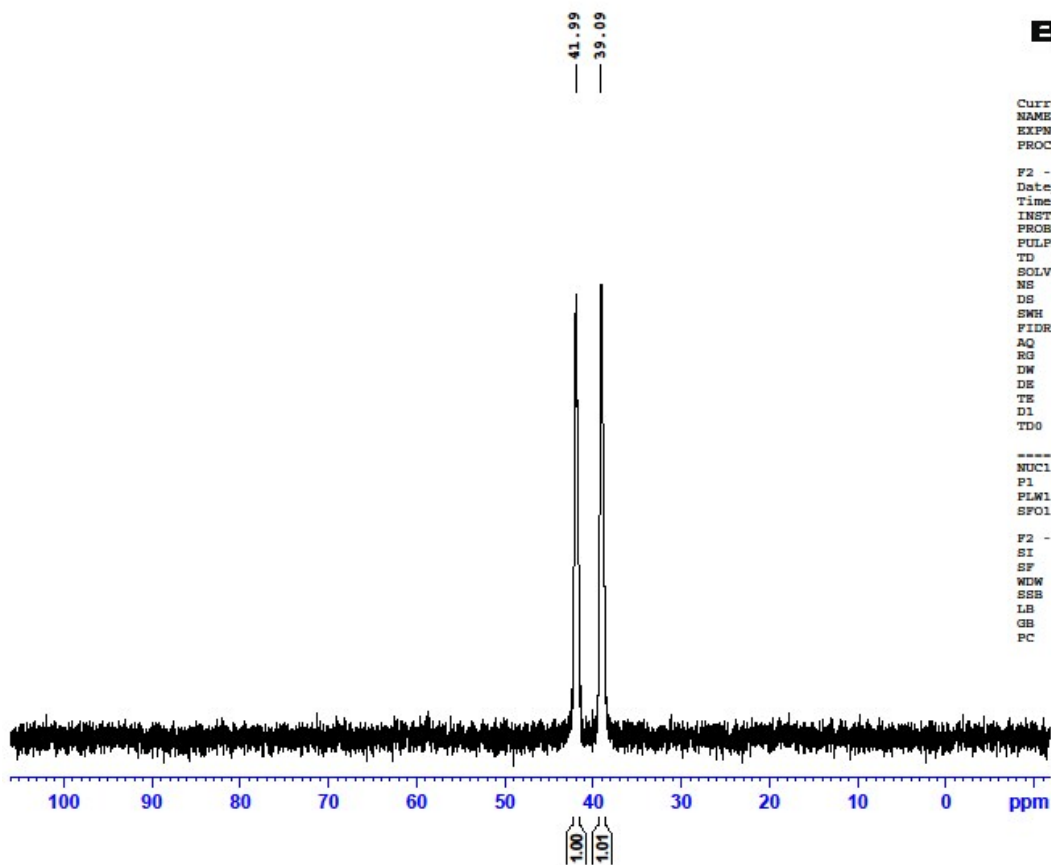


Fig. S38 ^1H NMR of Lanthanum-DDPO complex

DDPO-LA



```
Current Data Parameters
NAME          LKA
EXPNO         50
PROCNO        1

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Time          6.38
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PROBHD        5 mm PABBO BB/
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            32
DS            4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5111808 sec
RG            199.6
DW            7.800 usec
DE            6.50 usec
TE            298.5 K
D1            2.00000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          31P
P1            14.50 usec
PLM1          15.00000000 W
SFO1          162.0193069 MHz

F2 - Processing parameters
SI            32768
SF            162.0274080 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
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Fig. S39 ^{31}P NMR of Lanthanum-DDPO complex

Signature SIF VIT VELLORE
DJ-LA-DD

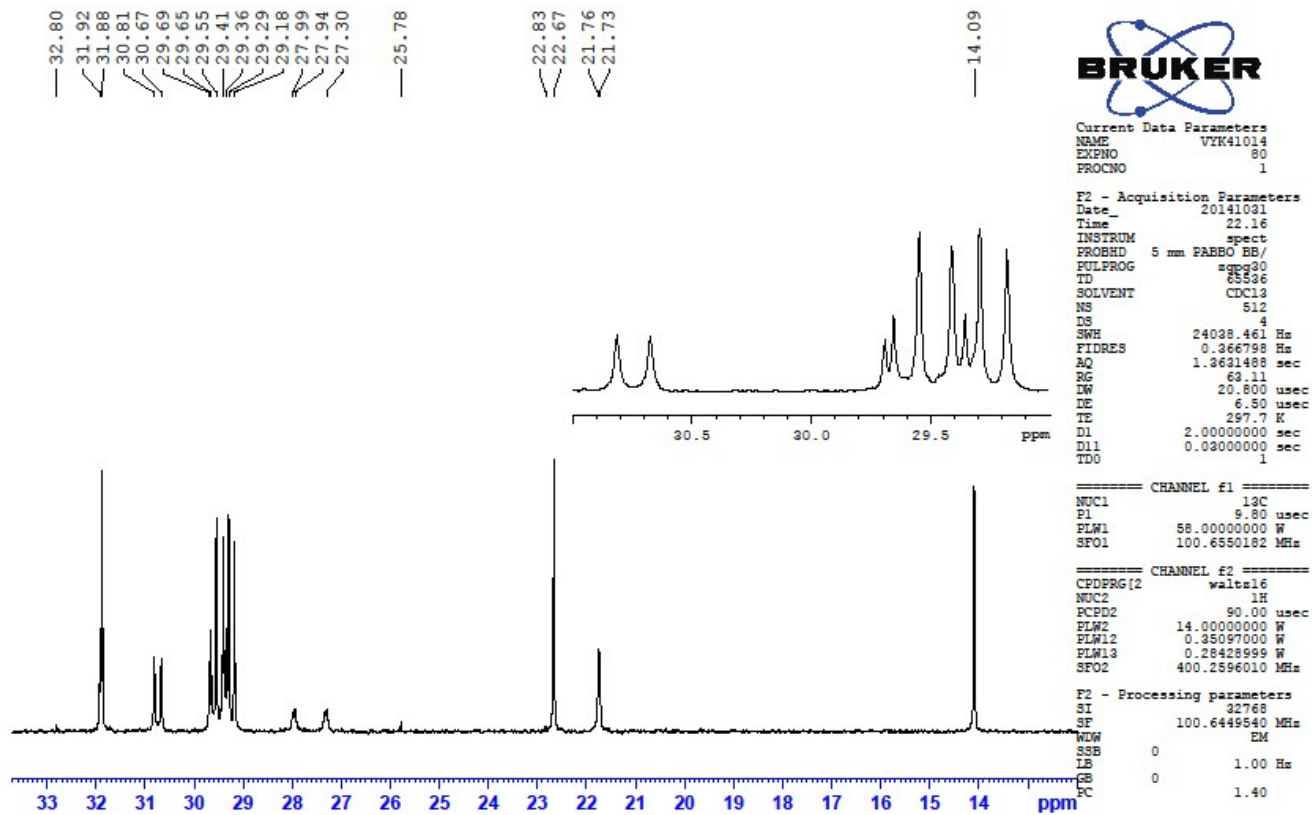
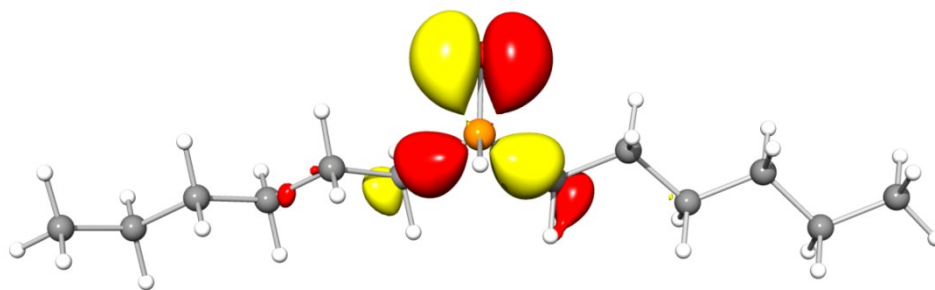
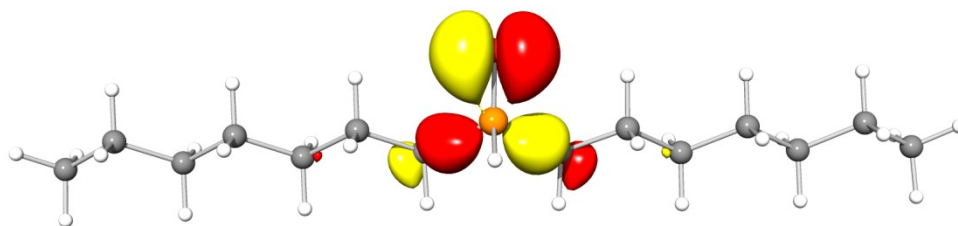


Fig. S40 ^{13}C -NMR of Lanthanum-DDPO complex

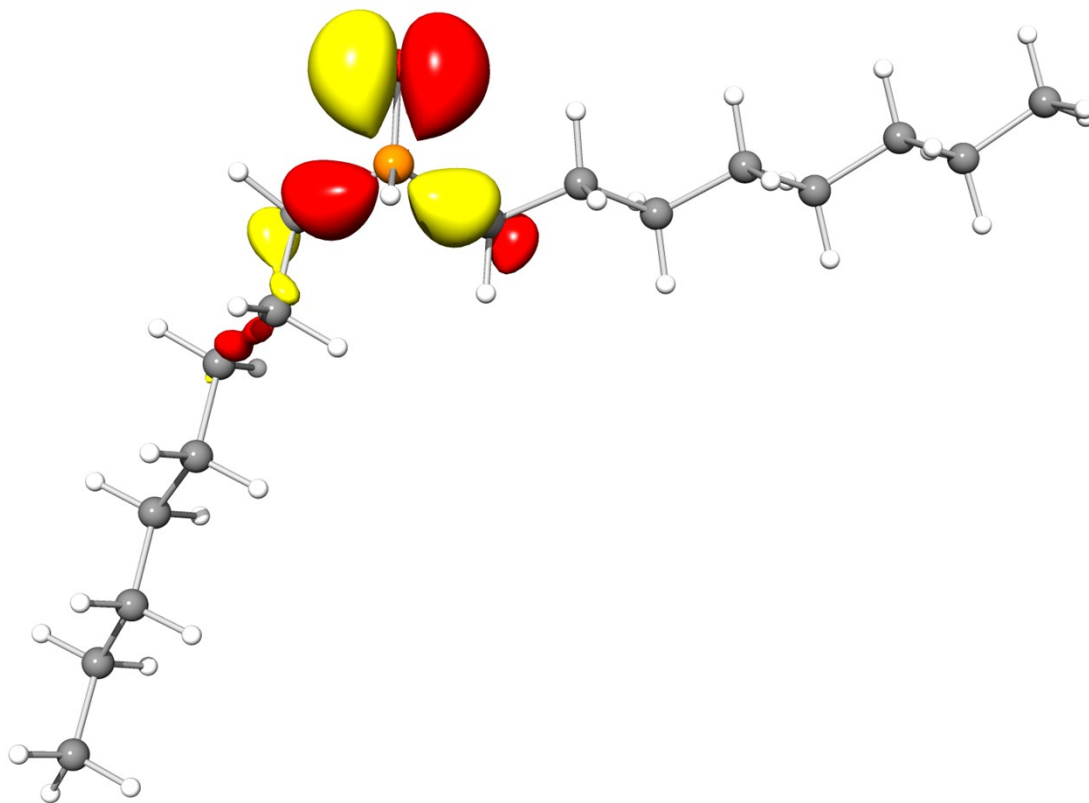


(a)

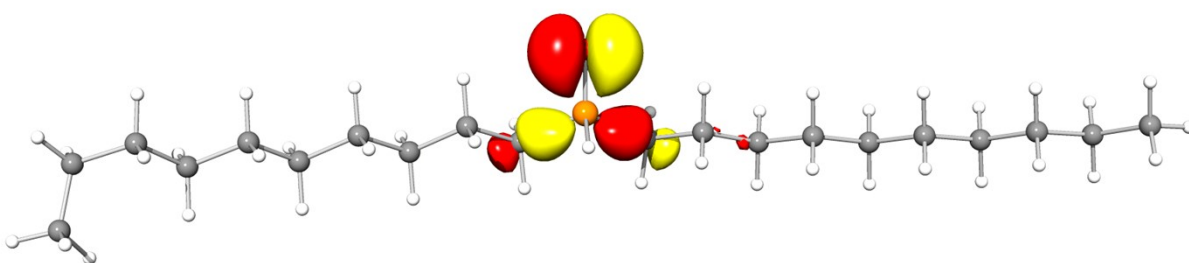


(b)

Fig.S41 Shape of highest occupied molecular orbital (HOMO) of di-hexyl (a) and di-heptyl(b) phosphine oxides at B3LYP/def2-TZVP level.



(a)



(b)

Fig.S42 Shape of highest occupied molecular orbital (HOMO) of di-octyl(a) and di-decyl(b) phosphine oxides at B3LYP/def2-TZVP level

COORDINATES OF OPTIMIZED GEOMETRIES

1. DHePO

C	0.85466779164257	2.03663831112894	-1.95530667196291
C	0.61169481680235	2.71646536585383	-0.60488793597144
C	-0.41042938982595	3.84972871938785	-0.68342987513490
C	-0.73836990438247	4.46127501274380	0.67769967622789
C	-1.74508374315715	5.60801410957609	0.61270709525244
C	-2.09449956015756	6.17912992705041	1.98696397270765
P	2.13584633795667	0.74352713600435	-1.91224209857824
O	3.53371421591322	1.22341500995243	-1.78266314512603
C	1.77784386299888	-0.31913603697694	-3.34449173119676
C	2.79369091644896	-1.44473790645466	-3.56163994553624
C	2.24323814877480	-2.53365288960958	-4.48266564967193
C	3.27239444104940	-3.58364156567576	-4.89510065548761
C	2.65783865685373	-4.73259094054047	-5.69271419623450
C	3.68537033434038	-5.74149111614215	-6.19977902404708
H	1.18463818038350	2.76448928178087	-2.70313719190847
H	-0.07191169142891	1.58655890011907	-2.32758841556171
H	0.77621697035231	-0.73275198024522	-3.17973462021271
H	1.71743737802659	0.31483766256410	-4.23412273185959
H	3.70937342084787	-1.01873393715721	-3.97762862075080
H	3.07839913692290	-1.89167581827657	-2.60330890332290
H	1.82614425220170	-2.07013990006808	-5.38438521060873
H	1.40199822329978	-3.02694694139022	-3.98205055365459
H	4.05679388088825	-3.10400456681866	-5.49098205912953
H	3.76916510309261	-3.98596913839208	-4.00441885646778
H	2.10128901953987	-4.32093745214329	-6.54162918371536
H	1.92061298562217	-5.24654544669285	-5.06614247165730
H	1.69931138584973	-0.07549169955184	-0.83632315166982
H	0.26093696076174	1.96855975055921	0.11399013589328
H	1.55757942546134	3.10364144355896	-0.21537833313511
H	-0.03107395608136	4.62794404159277	-1.35482527303662
H	-1.33213432466023	3.47086894565985	-1.14109868378729
H	-1.13129434836398	3.67883737467933	1.33723617753352
H	0.18491855422352	4.82161557032763	1.14583041325179
H	-1.34363602845813	6.40227598701178	-0.02535852086808
H	-2.65782252700871	5.25248450761550	0.12183864913176
H	3.20527207163533	-6.54663042768649	-6.76030800951190
H	4.41246071512595	-5.26105652462508	-6.85911647533792
H	4.23860769385354	-6.19409882660223	-5.37240511818511

H	-2.81724373840407	6.99374569742864	1.91219451075523
H	-2.53051478230961	5.41114758924565	2.63070247510181
H	-1.20639930603153	6.57185645990837	2.48811596617361

2. DHpPO

C	0.47187010053135	1.51329087976897	-1.43679085814918
P	1.99031728983123	0.55783906738324	-1.74705162430064
C	1.44771754499175	-0.77822975654778	-2.85463609550084
C	2.59361297816286	-1.66827707066401	-3.33760616964658
C	2.11771499686769	-2.74905596451174	-4.30588402392338
C	3.25311148853057	-3.59507546377203	-4.87612919179399
C	2.76886686475017	-4.66056664381667	-5.85595294046528
C	3.89459326088012	-5.48698676584245	-6.47455453175641
C	0.66202996416965	2.75221020507689	-0.56141626220843
C	-0.64991632770118	3.51032585475572	-0.34868066134308
C	-0.50465702825505	4.77877371580907	0.48705573888060
C	-1.82574858037945	5.52127378926655	0.68842418819716
C	-1.69460784973629	6.80029029397797	1.51157023960361
O	3.16972541774003	1.32798225690863	-2.21383486226888
H	0.07842977822160	1.80694458135574	-2.41557884135912
H	-0.25934322781666	0.82942741119277	-0.99066161206373
H	0.68228296280899	-1.36448597588081	-2.33473163752347
H	0.95963355115890	-0.29945984557329	-3.70966729050795
H	3.34698570572017	-1.04158022857636	-3.82007575964943
H	3.08783048813287	-2.13652240925165	-2.47957402103683
H	1.57445632902375	-2.27567468714043	-5.13177101083030
H	1.39526919278704	-3.39890731333184	-3.79843856543020
H	3.97120306411541	-2.93923802540149	-5.38089655097919
H	3.80035185591601	-4.07398951580509	-4.05623692157482
H	2.19831891012727	-4.17810876462709	-6.65834035432705
H	2.06690948012501	-5.32965241375980	-5.34433487328788
H	2.19841705006078	-0.11533157725686	-0.51370864538840
H	1.07821329243223	2.45917403001059	0.40843105372249
H	1.40181761834356	3.40587960630779	-1.02969992157874
H	-1.07425830226216	3.77336173610251	-1.32473996255514
H	-1.37711076685070	2.84444549683027	0.13028642191232
H	-0.07974030764127	4.52056184682449	1.46396818701333
H	0.21753551262257	5.44710327186881	0.00546714882017
H	-2.25568292093313	5.76927698415934	-0.28939090417501
H	-2.54476317618808	4.85267228103293	1.17626681030614
C	3.37999946392603	-6.53207814670122	-7.46221390881322
H	4.59553295171980	-4.81543346686104	-6.98158931393343

H	4.46350871323975	-5.97955316640549	-5.67877084458125
C	-3.02562593086179	7.52157265354724	1.71821018012025
H	-1.25632935250927	6.55431737860997	2.48478873442275
H	-0.98580460149064	7.47350718073293	1.01849730044349
H	4.19515807315558	-7.10251347028648	-7.91246680396815
H	2.71036089817842	-7.23892570668051	-6.96514790094639
H	2.81806180570363	-6.05818360551515	-8.27140689613996
H	-2.90170435633112	8.42778445217605	2.31404033423087
H	-3.47025020908872	7.81149767666812	0.76266705549655
H	-3.74304320922925	6.88004612714275	2.23619189633665

3. DOPO

C	2.56285461637794	3.30170160750105	-2.58206741039652
C	1.88033286621900	3.34966905427483	-1.20906956885377
C	0.62143855599068	4.21587597459707	-1.17982898121201
C	-0.01763586618914	4.27749764613380	0.20557119002695
C	-1.37980630793064	4.96640003876968	0.24518680787646
C	-1.97328523558771	5.01187754486110	1.65076199747059
C	-3.38352142750700	5.59399088545675	1.73103488139443
P	3.65603423400590	1.86470654849071	-2.82491441840128
O	4.66118559209093	1.99277954194296	-3.90956146483622
C	2.54286610101147	0.43731318408071	-3.01671942678124
C	3.30183932349401	-0.85919503696990	-3.31524712295233
C	2.39948588348882	-1.96983493829606	-3.85079846606276
C	3.17301668065579	-3.20646687356081	-4.30202579015922
C	2.29246792354995	-4.27280760240175	-4.95028547609154
C	3.08318149577950	-5.44444400682925	-5.52650189142326
C	2.21281702210388	-6.47489342682842	-6.24231771636691
H	3.17081988467543	4.19216282902069	-2.75705811918126
H	1.82214398774073	3.26785916725251	-3.38691242878953
H	1.90532714315327	0.34015299432878	-2.13372950589446
H	1.89028826180882	0.68482385135588	-3.86036909107000
H	4.07723026821454	-0.64162669329379	-4.05325782938145
H	3.82151033123424	-1.20074521557973	-2.41417573414115
H	1.82955450040240	-1.57981468989368	-4.70173646560831
H	1.65929667570029	-2.25011448986343	-3.09319804422150
H	3.94147790145465	-2.89825908253092	-5.01901532038463
H	3.71043404873960	-3.63864936016359	-3.45022332129431
H	1.70606345685039	-3.81114291530762	-5.75332006739943
H	1.56485989749439	-4.64476574212457	-4.22028739255975
H	3.82906816107302	-5.05856973934925	-6.23065888462277

H	3.64882357587693	-5.93643149923066	-4.72650076145236
H	4.20905647077398	1.67495258740531	-1.53117278998630
H	1.60233271284481	2.34068422555050	-0.88564387014037
H	2.59565632201559	3.71518580905101	-0.46673634956771
H	0.86314107731442	5.22699667289957	-1.52534643321003
H	-0.10161535784451	3.81105883839715	-1.89670223390766
H	-0.13016364790438	3.25738644831492	0.59151883041313
H	0.66605086948445	4.78519846539869	0.89496019950770
H	-1.29187234382476	5.98494146100518	-0.14950220272817
H	-2.06907030285194	4.43930575846973	-0.42415250978076
H	-1.98564292147788	3.99741278043906	2.06658041619268
H	-1.30885892538686	5.59256308453068	2.30075369681443
C	-3.90598041224949	5.65076737221874	3.16396407600292
H	-3.39509274015973	6.59870749274078	1.29522616420081
H	-4.05906137065787	4.99113836887931	1.11555646098022
H	-4.91633738891396	6.06195406221670	3.21206464754321
H	-3.92681856829843	4.65413679970726	3.61164375282989
H	-3.26487720295867	6.27721610554652	3.78888915969661
C	3.02356088979060	-7.59518197120309	-6.88717382816472
H	1.49561146814508	-6.90099761262979	-5.53239924245860
H	1.61689158856645	-5.96713895137629	-7.00845116574880
H	2.37992210728603	-8.30592932478025	-7.41018283035639
H	3.73440337816667	-7.19162877548232	-7.61248916555549
H	3.59578133326819	-8.14892936434248	-6.13787821250703

4. DDPO

C	-0.49573668592531	1.77127604802039	-2.05476378068504
P	-0.31704160046769	2.76792453830038	-0.54193685069698
C	-1.77847661525858	3.82526854277557	-0.30564530096600
C	-1.43446718960145	4.97207867433226	0.65420111445306
C	-2.63734383373871	5.78804662303932	1.12383099597027
C	-2.22271166355812	6.92786144068487	2.05232671154832
C	-3.38694437028298	7.73724752716035	2.61882076897040
C	-2.92685628972024	8.85512600404861	3.55217575406762
C	-4.06621589387689	9.66433401966529	4.16748651102595
C	-3.57607006728231	10.75844033595389	5.11314768220569
C	-4.69692381931281	11.56845742793875	5.76174360504463
C	0.82375950846474	1.03732605381166	-2.32740514300051
C	0.86533182951920	0.24118909072689	-3.63152130718856
C	2.23325985681346	-0.41375761283807	-3.82544442522001
C	2.41425999665139	-1.18111699474010	-5.13417837632221

C	3.80539523480216	-1.80593478335137	-5.23724727042000
C	4.06356748428343	-2.59115590245508	-6.52251106376091
C	5.44858180403976	-3.24038447345460	-6.53552675720529
C	5.75131174532991	-4.10454174877288	-7.76293698907243
C	5.92458610162835	-3.32001931654242	-9.06401006813364
O	0.06047119526324	2.00247434021518	0.67282359200009
H	-1.32050714071460	1.06566061424628	-1.92290848801439
H	-0.75969172036867	2.44126150194802	-2.88029966104601
H	-2.14074114338194	4.20540490928589	-1.26588718982731
H	-2.55885932554406	3.18679915080579	0.11956738976545
H	-0.92349328595724	4.55837446044842	1.52793133528718
H	-0.71702190586474	5.63915441832230	0.16484738617884
H	-3.33957358513229	5.12894603401788	1.64582583649920
H	-3.17619895890231	6.19335367310760	0.25978057722154
H	-1.63939043818337	6.51415260022161	2.88248035700865
H	-1.54554007768167	7.59995602219931	1.51256119469980
H	-4.06373306216713	7.06809261209963	3.16232443082448
H	-3.97309183733538	8.16515397936569	1.79748678302144
H	-2.32141227047020	8.42182652427987	4.35649688638261
H	-2.26064368260980	9.53030047291675	3.00260197448729
H	0.65669646109787	3.71135936605299	-0.96735947020550
H	1.63754294251944	1.77093224069623	-2.34458429637220
H	1.03984712515926	0.37646492942257	-1.48449893578994
H	0.08170875404400	-0.52449286197947	-3.63236193674565
H	0.64528566699584	0.90539844005761	-4.47533408045951
H	3.00455316604170	0.36238799762994	-3.75812237383444
H	2.42742742459143	-1.09121132859543	-2.98611786139726
H	1.65391277273984	-1.96640592759872	-5.21620092087991
H	2.24362747213180	-0.50648791910177	-5.98124198819434
H	4.55831804795106	-1.01524371011296	-5.13769941325287
H	3.96291347953928	-2.47031759000590	-4.37961031434277
H	3.30141761885463	-3.37172651577461	-6.63422280208627
H	3.94314202777521	-1.92513024626383	-7.38307029403976
H	-4.66808231424340	10.11481258762523	3.36987360617269
H	-4.73676561561780	8.99000679592428	4.71267827466806
H	6.21283257147429	-2.45929972661591	-6.44464535993919
H	5.54881341024312	-3.86024901932552	-5.63819226421422
H	6.66500160750355	-4.67511756479080	-7.57230888955153
H	4.95359153608602	-4.84502465194072	-7.88608511981984
H	6.20620253369342	-3.98166201258736	-9.88579413944365
H	5.00721523481435	-2.80329496222865	-9.35370991406927
H	6.70855528410323	-2.56475927343780	-8.96429340204741
H	-2.96257528975744	10.30404180862601	5.89997756573621
H	-2.91141424142113	11.43702974709129	4.56544637727339
C	-4.17144813118066	12.63966317230298	6.71546696075114
H	-5.30582887426464	12.03673648386557	4.98100718718802

H	-5.36367589950210	10.88955169592798	6.30420560821783
H	-4.98263633530955	13.20072858917549	7.18454527288259
H	-3.57255908392016	12.19020849090500	7.51191094706189
H	-3.53357954099962	13.35248547777236	6.18603071953047

5. DHePO-TS (*unimolecular*)

O	1.48411215469885	0.00271607722195	-0.60184991130590
H	2.11054395176783	0.00303850620448	0.65842237092383
C	-0.48795941972522	1.44229576751278	0.75494957031903
P	0.63797668582871	0.00067220565329	0.74919056872601
C	-0.48973726517723	-1.43941043424593	0.75067444216379
C	0.25015160124194	-2.77170115376546	0.62100581693722
C	-0.66401955793903	-3.93085444388931	0.22844510029543
C	0.09258842440554	-5.23573207800366	-0.01668852730590
C	-0.79034067912565	-6.35954717136762	-0.55708491687613
C	-0.01707056757252	-7.63641311036384	-0.88338613796660
C	0.25394114092899	2.77300935287323	0.61975117804486
C	-0.65861048420677	3.93309952771058	0.22628444468369
C	0.10100632337711	5.23473185366334	-0.02659202048135
C	-0.78027625765337	6.35949974610022	-0.56760497488650
C	-0.00422919474710	7.63317759094949	-0.89955422709170
H	-1.13630401628197	1.28653697333328	-0.11780637683744
H	-1.12398247423559	1.41304039360624	1.64417868675925
H	-1.13076979554791	-1.40782375785682	1.63622061225058
H	-1.13266132361318	-1.28312819662516	-0.12601247708457
H	1.02696989983474	-2.66283172761128	-0.13972914915826
H	0.76417581670468	-2.99904878175944	1.55982048023098
H	-1.20588928113014	-3.65835696047300	-0.68380665811857
H	-1.42689207986240	-4.08391324497641	0.99973157478946
H	0.90307228084054	-5.04614959910891	-0.72869871770795
H	0.57682738845003	-5.56195155463520	0.91104773037798
H	-1.30487550456728	-6.00540956274064	-1.45661515592547
H	-1.57680451886485	-6.58354367155494	0.17118572870264
H	0.77107084670424	3.00176296867493	1.55652109280326
H	1.02845118698504	2.66056707782961	-0.14279574951145
H	-1.20415999529940	3.65860610465634	-0.68318720814508
H	-1.41849730194779	4.09125561241089	0.99947232594709
H	0.59029645961057	5.56267192272832	0.89786782448598
H	0.90774387518277	5.03982510116465	-0.74142456995611
H	-1.29785535438149	6.00435282856738	-1.46499975381368
H	-1.56432982700025	6.58758455884662	0.16198366733571

H	-0.67672003434949	-8.41073322591931	-1.27985461411101
H	0.75776453517999	-7.44731214054526	-1.62999071617518
H	0.47700421747859	-8.03741874142753	0.00572642821017
H	-0.66238387128210	8.40768092557704	-1.29815567673927
H	0.49204333272901	8.03628857483619	-0.01262210857462
H	0.76910768256156	7.43917288674887	-1.64645599621422

6. DHePO-TS (*unimolecular*)

P	0.51924387757703	-1.67596379126344	-0.01435055842234
H	1.08813035646634	-0.27076857671437	-0.01680467059507
P	-0.55854513211341	1.47610000814530	-0.02591508147175
H	-1.19870569408578	-0.37908216967471	-0.02068634513289
O	-1.04586672785371	-1.45828383218971	-0.01574932072161
C	-0.95580733697580	2.56337748277823	1.40804349719915
C	-0.64836144805534	1.84439828990671	2.72366367463231
C	-1.21808561852277	2.51907863135977	3.96898629499817
C	-0.79838538877058	1.83960893689420	5.27073913175569
C	-1.42166094139271	2.46076173095916	6.51854967313237
C	-0.93049679504848	1.84432390740430	7.82527964893827
C	-0.95420927082170	2.56131111416687	-1.46176538917100
C	-0.64431178480924	1.84240675923448	-2.77690582350272
C	-1.21644576810217	2.51511651917851	-4.02221486205320
C	-0.79735557139957	1.83606756790277	-5.32439578274558
C	-1.42310456626159	2.45684149923924	-6.57119875548744
C	-0.93408596671592	1.84086090308851	-7.87892589392934
O	0.98768788294434	1.22823118541312	-0.02432206473436
C	0.98284239690961	-2.62713163494640	1.45650957419642
C	0.63058783413842	-1.86089516547620	2.73788599877369
C	1.24707898061998	-2.46901594931410	3.99455581014394
C	0.79951523046560	-1.78318712259599	5.28313722484507
C	1.43857270091402	-2.37792900670084	6.53599647238742
C	0.93969442620855	-1.75722046694624	7.83744611558478
C	0.98543579916023	-2.63040552573903	-1.48236192513042
C	0.63079191667847	-1.86845261347274	-2.76559646707236
C	1.24647571797786	-2.47860149897044	-4.02163588560190
C	0.79741677953577	-1.79442974075768	-5.31059676820129
C	1.43548517390637	-2.38984557742781	-6.56362214886212
C	0.93571828894527	-1.76935450722248	-7.86484725744970
H	-2.01911623428408	2.82191297709500	1.34799146152945
H	-0.38270982974202	3.49347197650554	1.33227782078776
H	-1.04327671475414	0.82343272975007	2.67250660612012

H 0.43695732526833	1.74868342325975	2.81742546072933
H -0.90446377908543	3.56875125201514	3.99215486781926
H -2.31230364240618	2.52148486910764	3.90267735751412
H -1.06749050007193	0.77830158798797	5.22803193602900
H 0.29399656852397	1.87818747281071	5.35535857092063
H -1.20951509376423	3.53549806345516	6.52433800197973
H -2.51060457288667	2.35576575493155	6.46014017799198
H -1.40271358151869	2.31871231258546	8.68819088429674
H -1.15630721738371	0.77606985726351	7.86892653301092
H 0.15117792919165	1.96093480187623	7.93313848534347
H -0.38249995168767	3.49223436986067	-1.38565011349105
H -2.01791991807993	2.81860364930733	-1.40328215452554
H 0.44129089727104	1.75011185965867	-2.87068928678007
H -1.03612830115308	0.82026000838798	-2.72539896496085
H -2.31059409407341	2.51554086977616	-3.95462652093465
H -0.90474352751672	3.56535166572386	-4.04626028817986
H 0.29486884358416	1.87602081637314	-5.41043655499981
H -1.06519853288481	0.77444634561178	-5.28153633767170
H -2.51189116313897	2.35130760956172	-6.51084087250948
H -1.21153657979909	3.53169174845965	-6.57727843832959
H -1.40826343132701	2.31510213114180	-8.74084293611465
H 0.14730676634225	1.95818513102240	-7.98885357029829
H -1.15939009606709	0.77247375231595	-7.92230573019301
H 2.06192836052675	-2.80473716755228	1.39198659652295
H 0.48819306325406	-3.60248527164665	1.42813997732046
H 0.96271308766408	-0.82335515593732	2.64303658266804
H -0.45717772230192	-1.82973822907375	2.83415917744382
H 0.99134431326976	-3.53365157640656	4.04545799079849
H 2.33891565979678	-2.40969996889333	3.91912142245127
H 1.03664554751499	-0.71586747870632	5.22867041705474
H -0.29102240016978	-1.85419272179320	5.36453497591831
H 1.24625500991068	-3.45649400478937	6.55364724982038
H 2.52518722742994	-2.25280676905566	6.47321908262525
H 1.41771214174876	-2.22159784994843	8.70243104518955
H 1.15349321522220	-0.68668681553169	7.87408094878800
H -0.14038060660196	-1.88537940125199	7.94599649276203
H 2.06503431556082	-2.80470643478017	-1.41750417116622
H 0.49347260987316	-3.60704325492429	-1.45126622374974
H -0.45714636793148	-1.83936574657893	-2.86071816506281
H 0.96143633595883	-0.83014807062860	-2.67386117446425
H 2.33836957659623	-2.41895103871495	-3.94731731282864
H 0.99078614227302	-3.54333185674989	-4.07077109501697
H -0.29316071693654	-1.86616188007793	-5.39091349481056
H 1.03401860644222	-0.72691386143585	-5.25733927078918
H 2.52217314773002	-2.26496274312944	-6.50167559567975
H 1.24285897062724	-3.46836238104014	-6.58081157890007

H	1.41307755934278	-2.23388685938011	-8.73011224339057
H	-0.14444124996631	-1.89750873599454	-7.97260681567214
H	1.14958358099004	-0.69883112778247	-7.90180166551859

7. Th(NO₃)₂.2DHePO (PBE0/def2-TZVP-ECP)

O	0.60502006267874	6.30446306838516	3.06994990814530
N	1.28767626435406	6.41583404891114	2.09721596964084
O	1.50960383878621	5.46026786037298	1.30120801427105
Th	2.88998686909698	6.75308031357211	-0.38939547960937
O	1.85810479966994	7.51460871660512	1.79103082350265
O	5.13624535954291	6.27304023318934	-1.41847517373390
N	5.02206513523436	7.02951012411388	-2.43502023716196
O	5.86606456506744	7.08727260769776	-3.28187861191116
O	3.95019121169587	7.69518220667998	-2.48890158411031
O	0.36431279497960	7.03767718573121	-0.63328874222942
N	0.39711985081015	8.20850426534990	-1.10360772083245
O	-0.58597277756546	8.84046635036938	-1.35140937686326
O	1.56899440713792	8.67381925812878	-1.29004067655875
O	3.79961371905059	4.40422687766464	0.10254595995150
N	4.45796471724061	4.72092723632285	1.13540971495594
O	5.11286908174644	3.93473962912403	1.75209519086168
O	4.37142244755601	5.94263999416183	1.47030575331140
O	2.16956813173238	5.30973211371393	-2.09131103810646
O	4.09508599822192	8.61753915275998	0.37707651727690
P	4.37412207709048	9.56317766924671	1.52815300915155
P	2.16549871804121	3.87504598331691	-2.58546492411048
H	1.30944353680932	3.77456947773671	-3.70032789105257
C	3.78404430581818	3.38278369513707	-3.15889714156162
C	1.51704309538137	2.75672122419027	-1.34941211524308
H	5.36097683236891	10.48755164036681	1.12630628856504
C	2.94262935610476	10.53763961264514	1.99269349388965
C	5.03488601538488	8.73143060774801	2.96593756308574
H	5.06125221837760	9.46256964672488	3.78136506836325
H	4.29609109111209	7.96760820459307	3.23015768958571
C	6.39556920492070	8.07984537307851	2.73075875079255
H	3.26831193223742	11.26086008833903	2.74722735286384
C	2.28596318184124	11.19604608365149	0.78237317448917
H	2.25047622799496	9.84102906220229	2.47816819115332
C	6.72623033784652	7.08777777514602	3.83370733068083

H	6.38497948960971	7.55280659899407	1.77255123405896
H	7.17088568461915	8.85074364272050	2.67101068702454
C	8.09125613810274	6.44304102937725	3.67497154127493
H	6.67179300872349	7.59203816040558	4.80624860761438
H	5.95764070052594	6.30764087478353	3.84121564767773
C	8.39570552391586	5.44433739709428	4.77835028471378
H	8.14194374234446	5.93811628622637	2.70347672575741
H	8.86664946382005	7.21935376514293	3.66276191866670
C	9.77434377675392	4.81960876111483	4.65772603192672
H	8.30571543608214	5.94735124860642	5.74867751282453
H	7.63163370314663	4.66017409715616	4.77113936000080
H	9.97472914208469	4.13166153000658	5.48113048664514
H	9.87604422866336	4.25412622210247	3.72748317177217
H	10.55127194422854	5.58841750001568	4.66724877361225
C	0.87335987147853	11.67693676025233	1.06102128078772
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C	4.20771353483420	4.14469936773184	-4.41336820561337
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