Electronic Supplementary Information

Oxyphosphoranes as precursors to bridging phosphate-catecholate ligands

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General information

All manipulations were carried out on a Schlenk line or in an argon atmosphere glovebox. Solvents were dried using a MBraun solvent purification system, and stored over 3 Å sieves. Unless otherwise stated, commercial reagents were used without further purification. UV spectra were recorded on a Shimadzu UV2600 spectrometer. ^{1}H, ^{31}P and ^{13}C NMR spectra were recorded on a Bruker AV-500M (liguid-state) or a Bruker AV-800M (solid-state) spectrometer. Mass spectra were measured using ThermoScientific Q Exactive Plus mass spectrometer. IR spectra were recorded on a Nicolet 6700 spectrometer. Elemental analysis was recorded on an Elementar vario EL cube analyzer. Powder X-ray diffraction data were collected on a Rigaku SmartLab XE diffractometer (Cu X-ray source at room temperature). The single-crystal X-ray diffraction data were collected on a Bruker D8 QUEST diffractometer using Cu (60W, Diamond, $\mu K\alpha = 12.894\ mm^{-1}$) micro-focus X-ray sources at 100 K. The structure was solved and refined using Full-matrix least-squares based on F^2 with program SHELXS and SHELXL[S1] within OLEX2.[S2]

Table. S1 Crystal data and refinement details for compounds **2, 3, 4**, and **5**

	2	**3·thf**	**4**	**5**
CCDC	2041784	2023193	2041786	2023174
empirical formula	$C_{12}H_{13}Cl_6O_6PZr$	$C_{40}H_{58}Cl_{10}O_{16}P_2V_2$	$C_{2.82}H_{3.53}Cl_{1.18}O_{1.65}P_{0.24}V_{0.24}$	$C_{32}H_{42}C_{l8}Ni_2O_{14}P_2$
formula weight	588.11	1313.18	124.80	1113.61
temp, K	100.0	100.0	199.0	103.0
cryst syst	monoclinic	triclinic	triclinic	triclinic
space group	$P2_1/c$	P-1	P-1	P-1
a, Å	9.6112(5)	14.4834(9)	12.0697(6)	8.9110(5)
b, Å	11.6372(6)	14.9881(9)	12.2097(6)	11.1675(6)
c, Å	18.1370(10)	15.5710(10)	16.6508(8)	11.8597(7)
α, deg	90	107.350(2)	72.3790(10)	108.4832(15)
β, deg	99.301(2)	117.247(2)	73.2710(10)	97.6582(16)
γ, deg	90	98.551(2)	60.5460(10)	100.3215(15)
V, Å^3	2001.91(18)	2701.5(3)	2007.62(17)	1078.12(11)
Z	4	2	17	1
D_{calcd}, g/cm^3	1.951	1.614	1.755	1.715
μ, mm^{-1}	12.894	8.563	11.316	6.897
F(000)	1160	1344	1064	568
2θ range, deg	9.06 - 144.89	7.02 - 144.59	5.65 - 145.72	8.03 - 146.93
index range	$-11 \le h \le 11$, $-14 \le k \le 14$, $-22 \le l \le 22$	$-17 \le h \le 17$, $-18 \le k \le 18$, $-19 \le l \le 19$	$-14 \le h \le 14$, $-15 \le k \le 15$, $-20 \le l \le 20$	$-11 \le h \le 10$, $-13 \le k \le 13$, $-14 \le l \le 14$
reflns collected/unique	49347 / 3948 [R(int) = 0.0704]	82763 / 10538 [R(int) = 0.0543]	62077 / 7917 [R(int) = 0.0491]	32977 / 4260 [R(int) = 0.0585]
data/restraints/param	3948/0/236	10538/0/633	7917/0/475	4260/0/263
GOF on F^2	1.073	1.044	1.051	1.060
final R indices [I >2σ(I)]	R1 = 0.0291, wR2 = 0.0777	R1 = 0.0424, wR2 = 0.1157	R1 = 0.0331, wR2 = 0.0874	R1 = 0.0325, wR2 = 0.0853
R indices (all data)	R1 = 0.0306, wR2 = 0.0787	R1 = 0.0438, wR2 = 0.1174	R1 = 0.0334, wR2 = 0.0876	R1 = 0.0329, wR2 = 0.0856
largest diff peak/hole, e/Å^3	1.33 / -0.40	0.89 / -0.76	0.76 / -0.69	0.75/-0.43

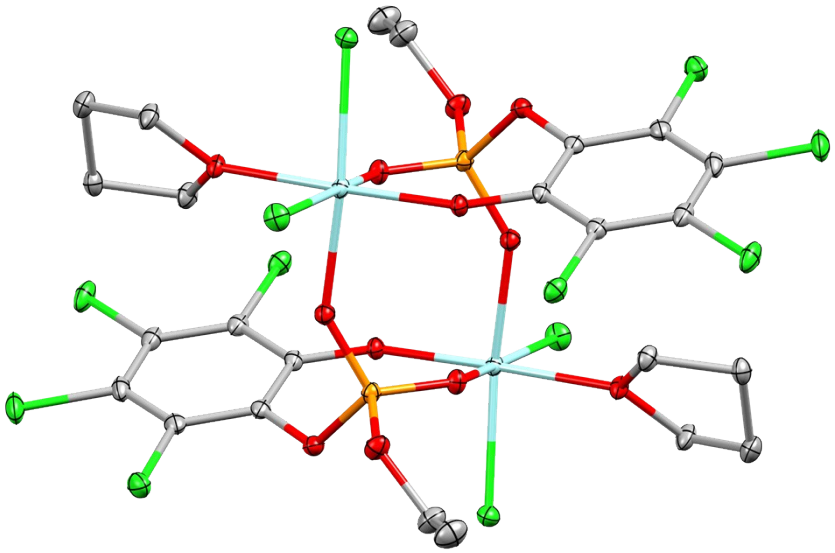

Fig. S1 Thermal ellipsoid plot for **2** with the anisotropic displacement parameters depicted at the 30% probability level. Hydrogen atoms are omitted for clarity.

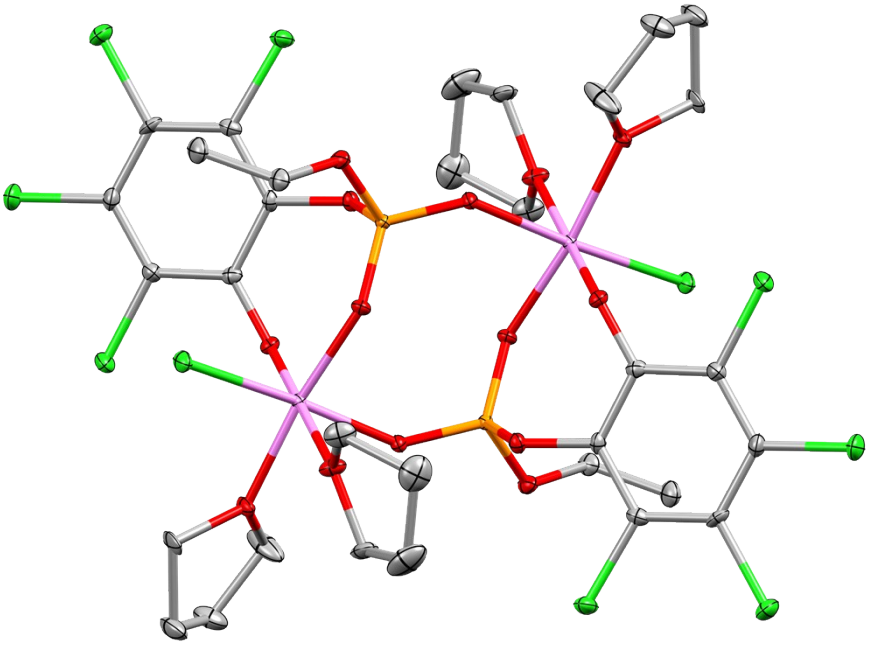

Fig. S2 Thermal ellipsoid plot for **3** with the anisotropic displacement parameters depicted at the 30% probability level. Hydrogen atoms are omitted for clarity.

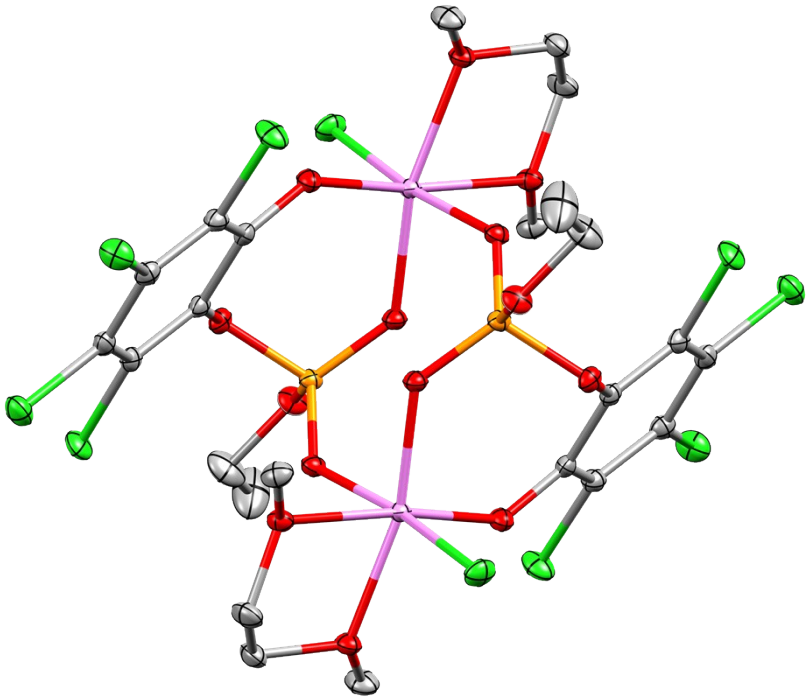

Fig. S3 Thermal ellipsoid plot for **4** with the anisotropic displacement parameters depicted at the 30% probability level. Hydrogen atoms are omitted for clarity.

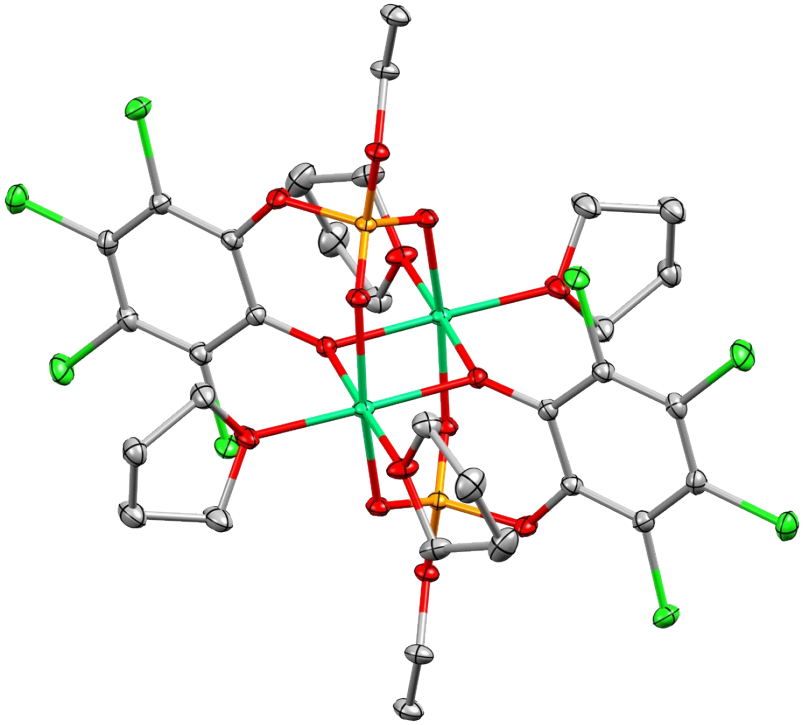

Fig. S4 Thermal ellipsoid plot for **5** with the anisotropic displacement parameters depicted at the 30% probability level. Hydrogen atoms are omitted for clarity.

Experimental Section

Synthesis of 2 A solution of **1** (0.41 g, 1 mmol) and $ZrCl_4$ (0.23 g, 1 mmol) in 5 mL THF was stirred for 1 hour at room temperature. The reaction solution was filtrated, and colorless crystals of **2** (60 % yield) were obtained after 3 days at room temperature. ^{1}H NMR (500 MHz, thf-d_8, ppm): δ 4.58-4.47 (m, 8H, thf-OCH_2), 3.38 (q, J = 6.9 Hz, 4H, POCH_2), 1.39 (t, J = 7.0 Hz, 8H, thf-OCH$_2$CH_2), 1.11 (t, J = 6.9 Hz, 6H, CH_3). ^{13}C NMR (125 MHz, thf-d_8, ppm): δ 150.52 (*Ar*), 138.20 (d, $J_{C\text{-}P}$ = 9.1 Hz, *Ar*), 131.03, 125.30 (*Ar*), 125.18 (d, $J_{C\text{-}P}$ = 6.0 Hz, *Ar*), 123.77 (*Ar*), 70.08 (thf-O*C*H$_2$), 66.27 (PO*C*H$_2$), 26.22 (thf-OCH$_2$*C*H$_2$), 15.94 (d, J = 6.3 Hz, *C*H$_3$). ^{31}P NMR (202 MHz, thf-d_8, ppm): δ -10.12. IR (KBr, cm^{-1}): $\tilde{\nu}$ 2984.8, 1550.5, 1444.2, 1388.7, 1172.2, 1078.6, 1000.3, 872.1, 798.1, 670.0, 590.0. ESI-MS: *m/z* = 1173.5 $[M]^+$, 1174.5 $[M + H]^+$. Anal. calcd for $C_{24}H_{26}Cl_{12}O_{12}P_2Zr_2$: C, 24.51; H, 2.23. Found: C, 24.31; H, 2.28.

Synthesis of 3 and 4 A mixture of **1** (0.41 g, 1 mmol) and VCl_3 (0.16 g, 1 mmol) in 10 mL solvent (**3**: THF; **4**: DME) was sealed and heated to 80 °C without stir. Crystals (**3**: green; **4**: yellow) were obtained after continuous heating for 48 hours. The crystals were filtrated, washed with toluene for 3 times, and dried under vacuum to afford pure product (**3**: 72 % yield; **4**: 32 % yield). **3**: Solid ^{1}H NMR (800 MHz, ppm) δ 4.04 (br), 2.14 (br), 1.97 (br). Solid ^{13}C NMR (200 MHz, , ppm) δ 216.79, 162.10, 155.75, 137.01, 133.33, 110.92 (*Ar*), 76.09 (O*C*H$_2$), 69.24 (O*C*H$_2$), 31.58 (CH$_2$*C*H$_2$, CH$_2$*C*H$_3$), 27.18 (CH$_2$*C*H$_2$, CH$_2$*C*H$_3$). IR (KBr, cm^{-1}): $\tilde{\nu}$ 2980.8, 1424.8, 1384.6, 1239.7, 1088.9, 1056.0, 984.7, 859.6, 584.8. Anal. calcd for $C_{32}H_{42}Cl_{10}O_{14}P_2V_2$: C, 32.88; H, 3.62. Found: C, 32.74; H, 3.58. **4**: Solid ^{1}H NMR (800 MHz, ppm) δ 3.71 (br), 2.39 (br), 1.46 (br). Solid ^{13}C NMR (200 MHz, ppm) δ 262.24, 225.70, 212.97, 159.36, 146.36, 117.75 (*Ar*), 76.09 (O*C*H$_2$), 69.24 (O*C*H$_2$), 31.58 (CH$_2$*C*H$_2$, CH$_2$*C*H$_3$), 27.18 (CH$_2$*C*H$_2$, CH$_2$*C*H$_3$). IR (KBr, cm^{-1}): $\tilde{\nu}$ 2988.7, 2941.3, 1548.3, 1429.0, 1385.6, 1192.3, 1087.5, 1045.8, 982.5, 864.0, 762.9, 592.0. Anal. calcd for $C_{22}H_{25}Cl_{10}O_{13}P_2V_2$: C, 27.17; H, 2.85. Found: C, 27.23; H, 2.80.

Synthesis of 5 A mixture of **1** (0.21 g, 0.5 mmol) and $NiCl_2$ (0.16 g, 0.5 mmol) in 5 mL THF was sealed and heated to 70 °C without stir. Green crystals were obtained after continuous heating for 48 hours. The crystals were filtrated, washed with THF for 3 times, and dried under vacuum to afford pure **5** in 54 % yield. IR (KBr, cm^{-1}): $\tilde{\nu}$ 2978.4, 1540.9, 1433.3, 1385.6, 1215.0, 1062.9, 982.2, 962.7, 850.6, 772.6, 538.8. Anal. calcd for $C_{32}H_{42}Cl_8Ni_2O_{14}P_2$: C, 34.51; H, 3.80. Found: C, 34.52; H, 3.88.

Spectra

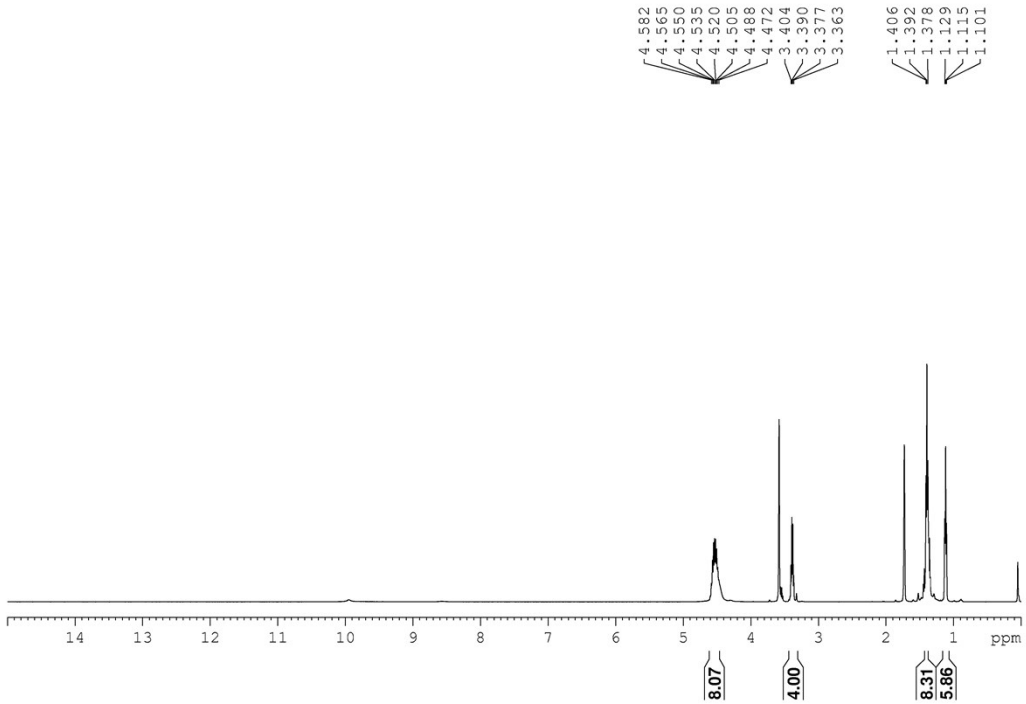

Fig. S5 ^{1}H NMR spectrum of **2** in thf-d_8

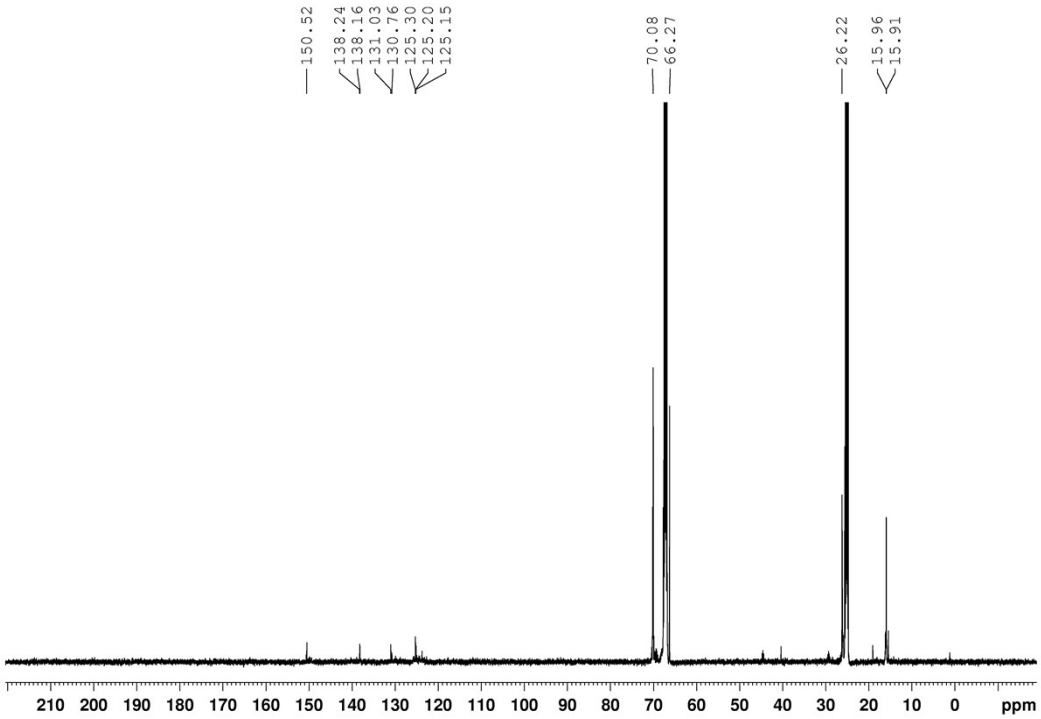

Fig. S6 ^{13}C NMR spectrum of **2** in thf-d_8

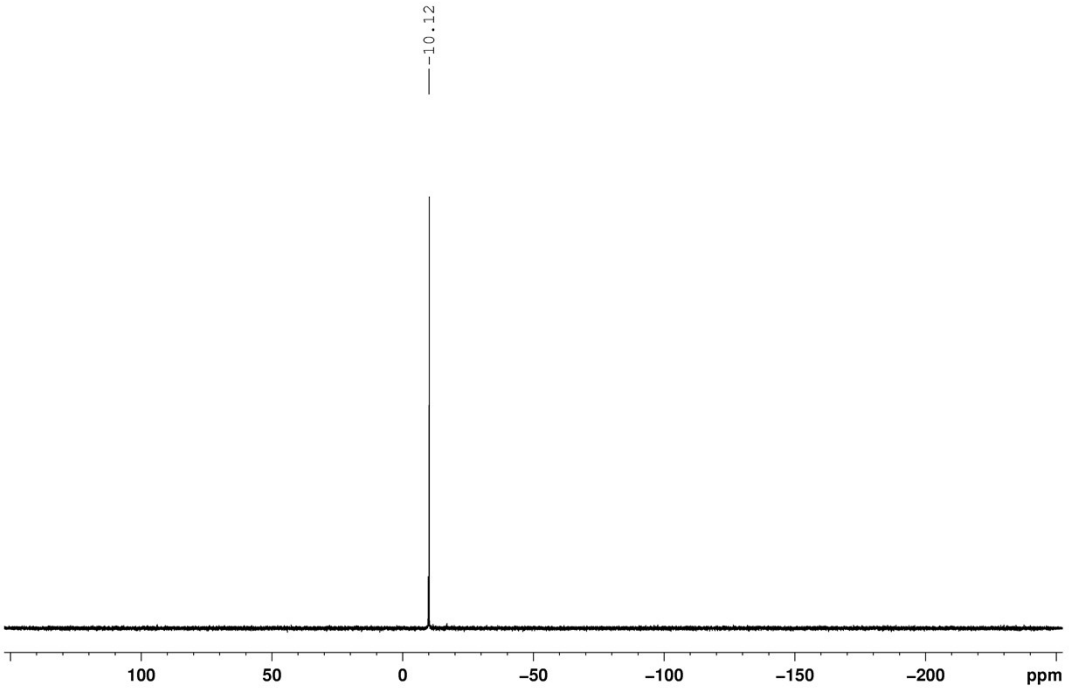

Fig. S7 ^{31}P NMR spectrum of **2** in thf-d_8

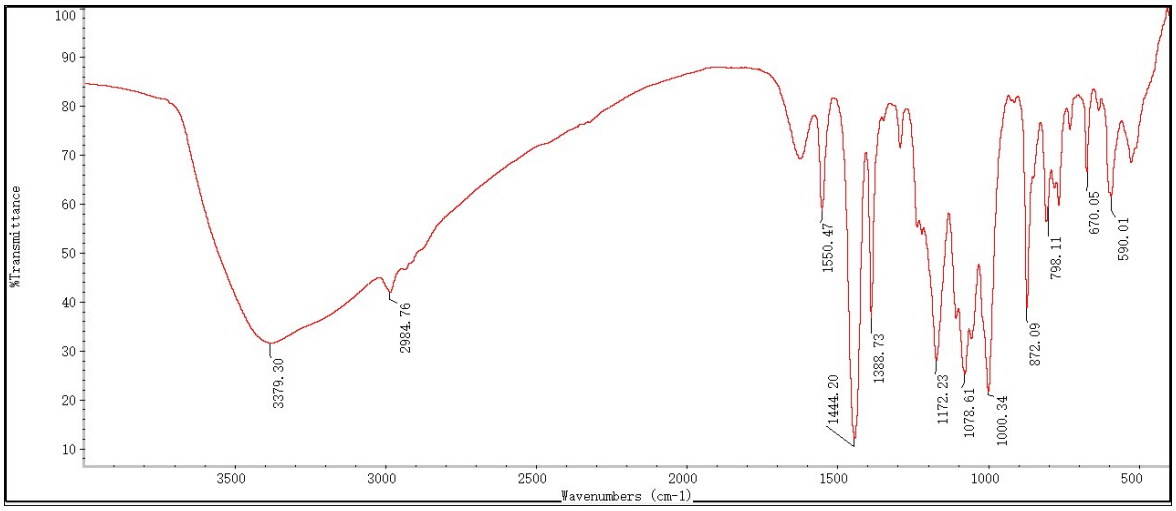

Fig. S8 FT-IR spectrum of **2** (KBr, cm^{-1})

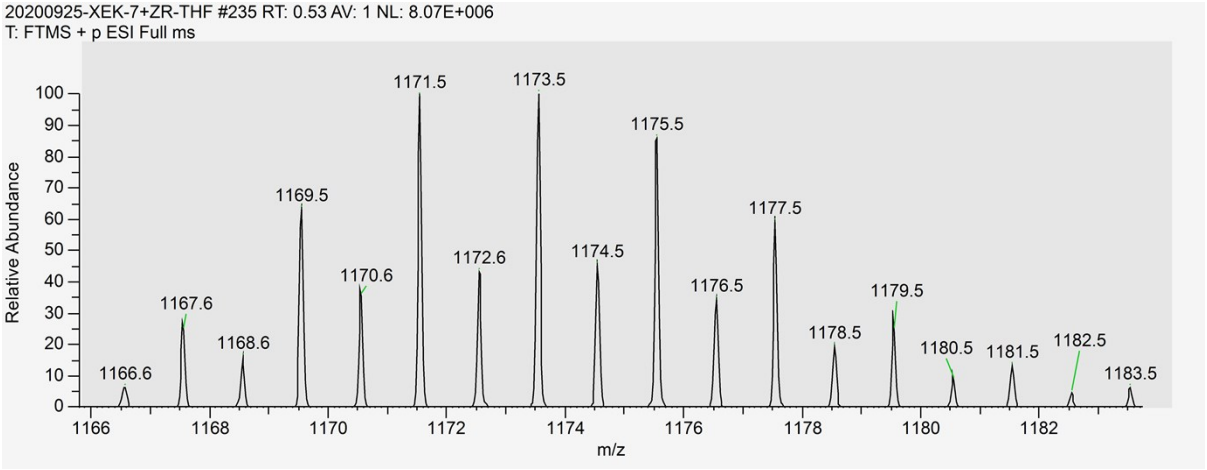

Fig. S9 ESI-MS spectrum of **2**

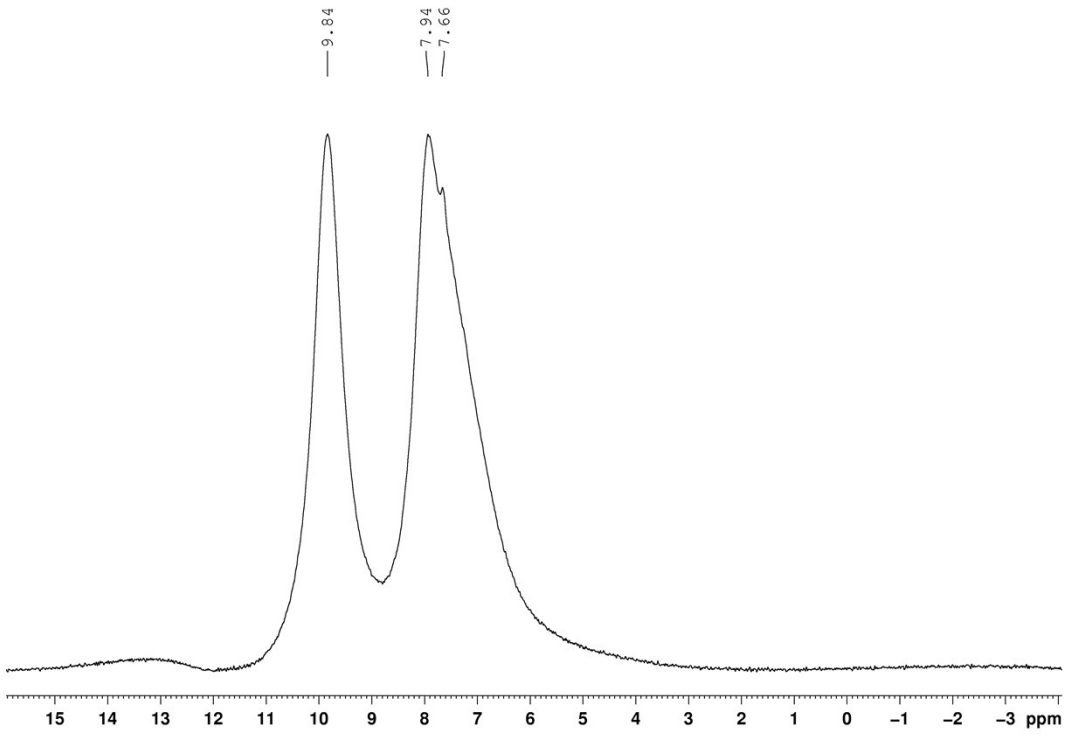

Fig. S10 Solid-state ^{1}H NMR spectrum of **3**

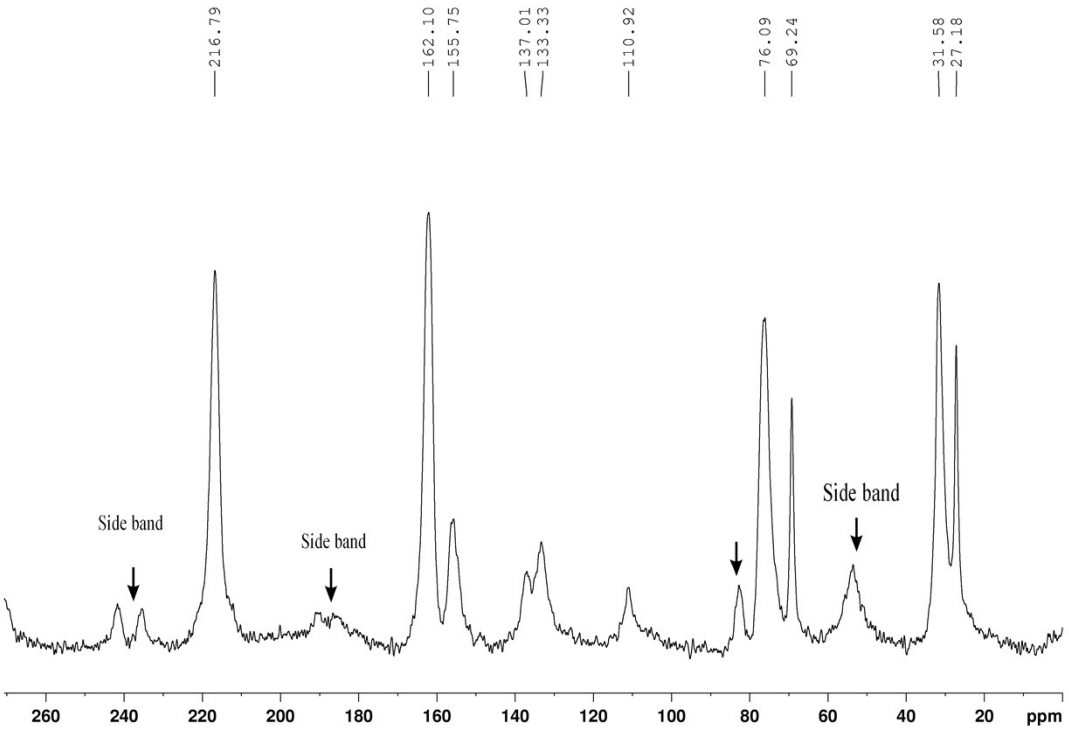

Fig. S11 Solid-state ^{13}C NMR spectrum of **3**

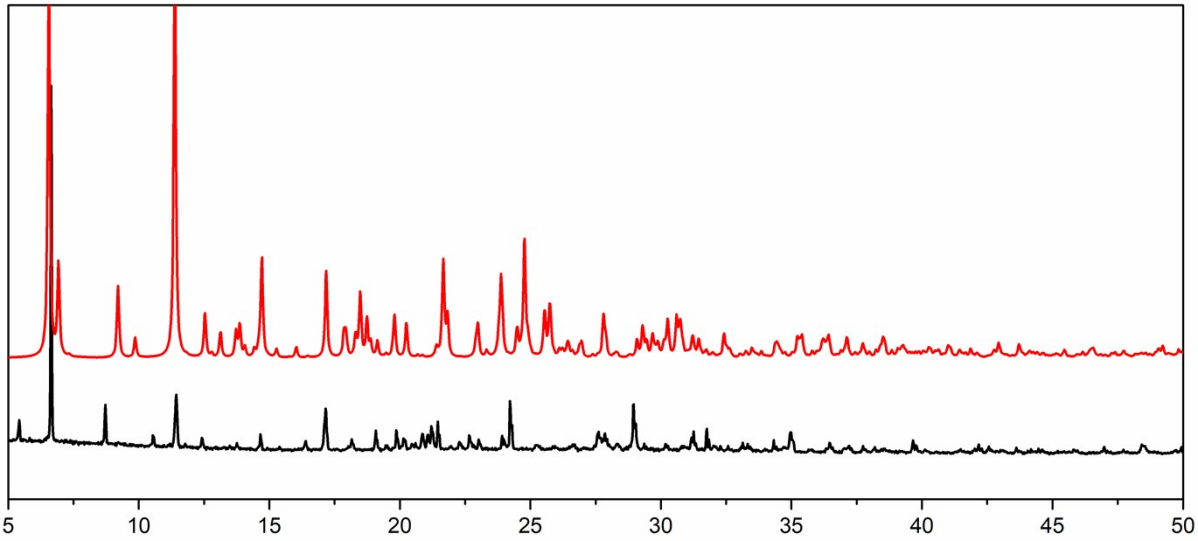

Fig. S12 Powder XRD pattern of **3** (black: experimental; red: simulated).

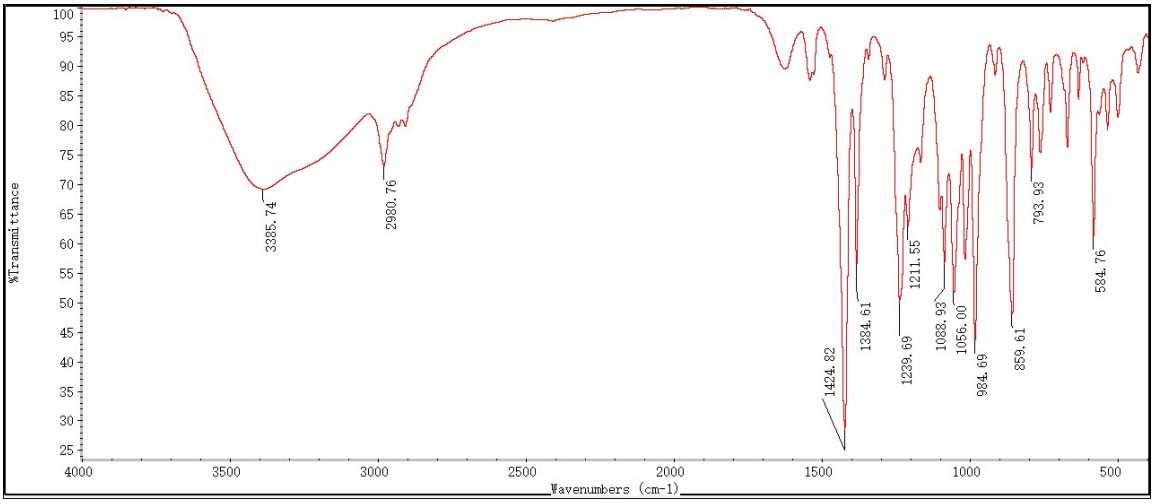

Fig. S13 FT-IR spectrum of **3** (KBr, cm^{-1})

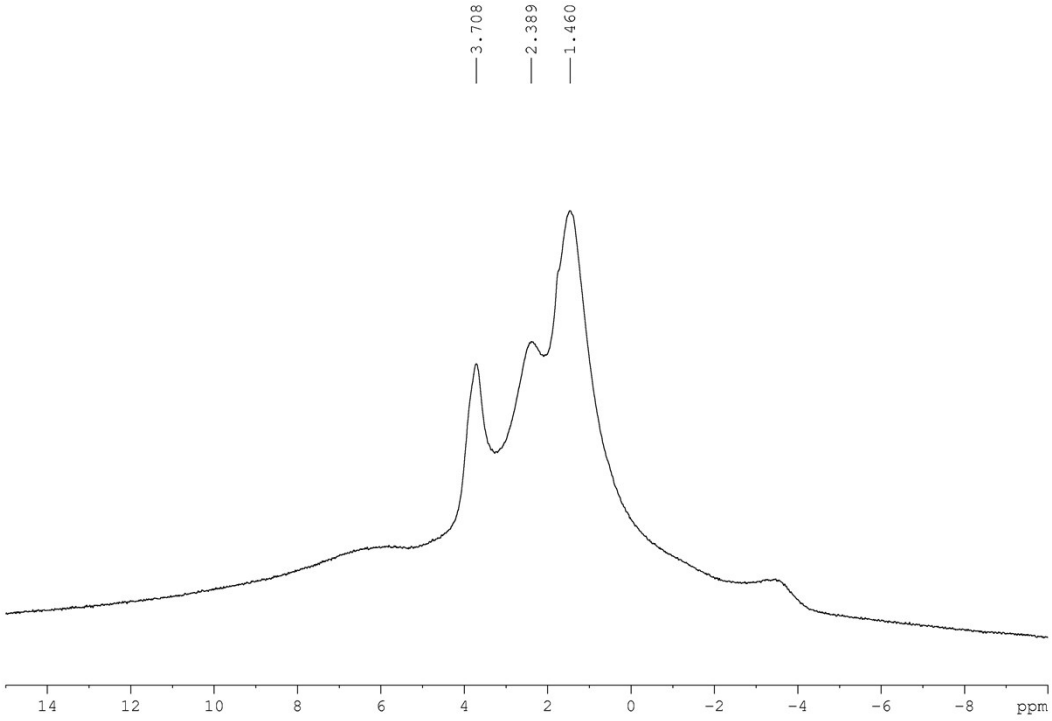

Fig. S14 Solid-state ^{1}H NMR spectrum of **4**

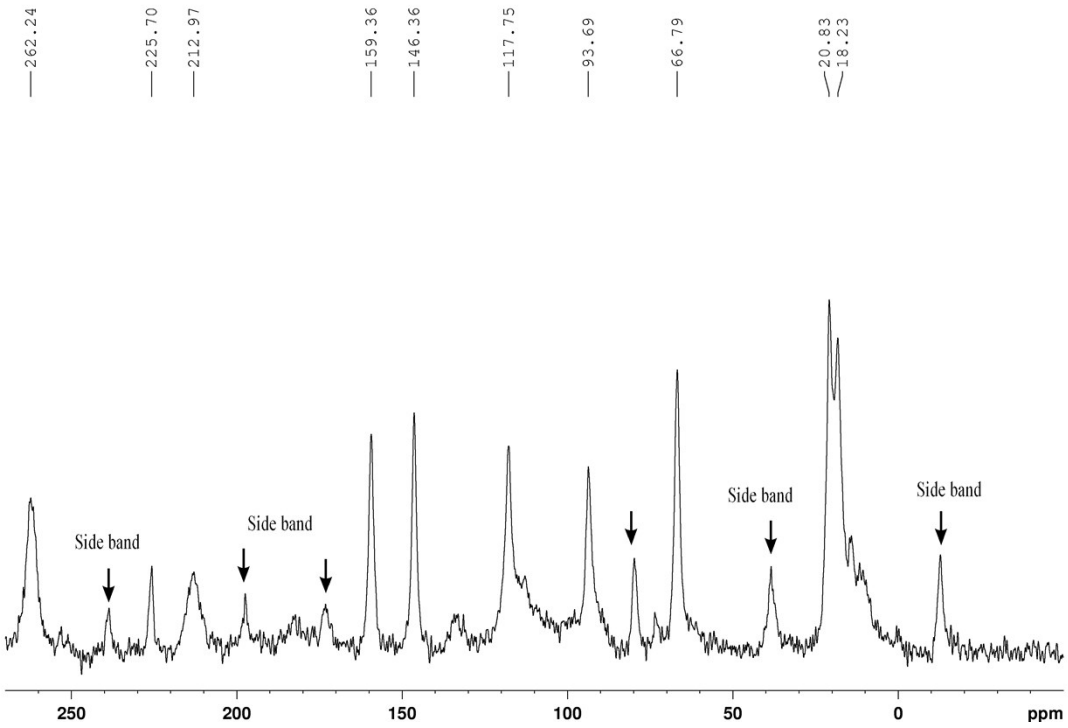

Fig. S15 Solid-state ^{13}C NMR spectrum of **4**

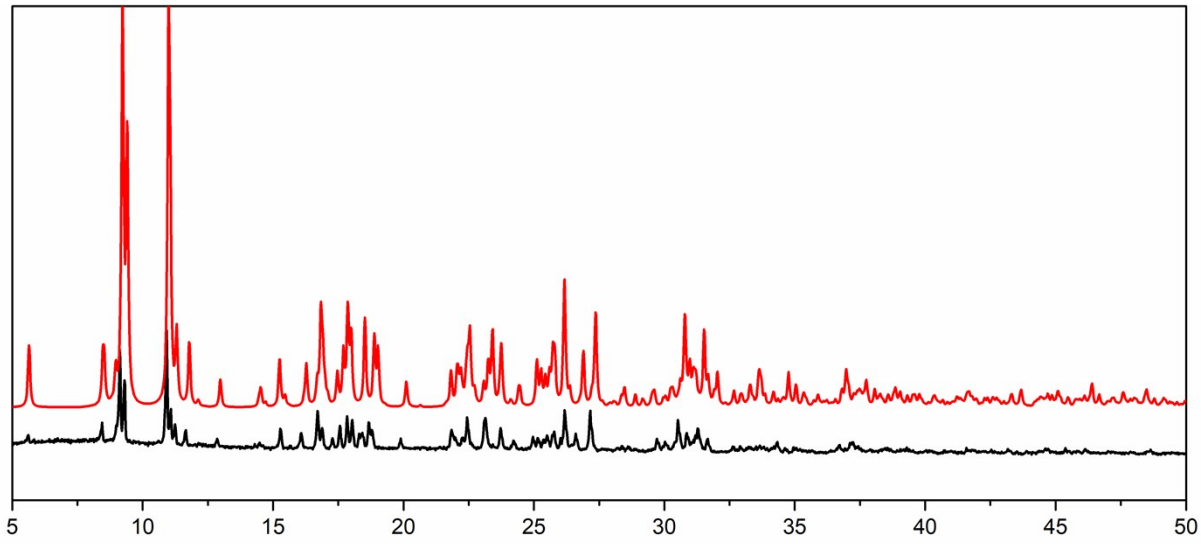

Fig. S16. Powder XRD pattern of **4** (black: experimental; red: simulated).

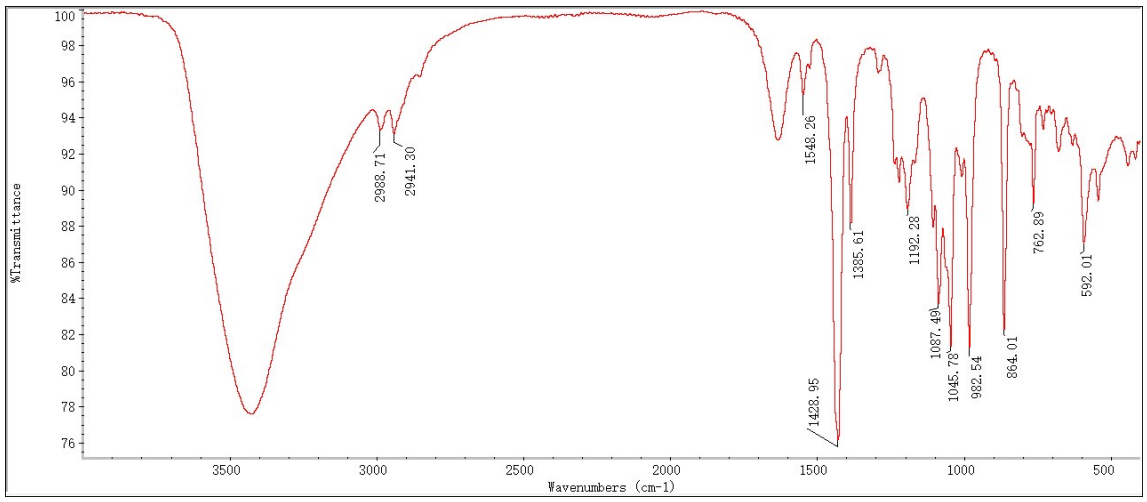

Fig. S17 FT-IR spectrum of **4** (KBr, cm^{-1})

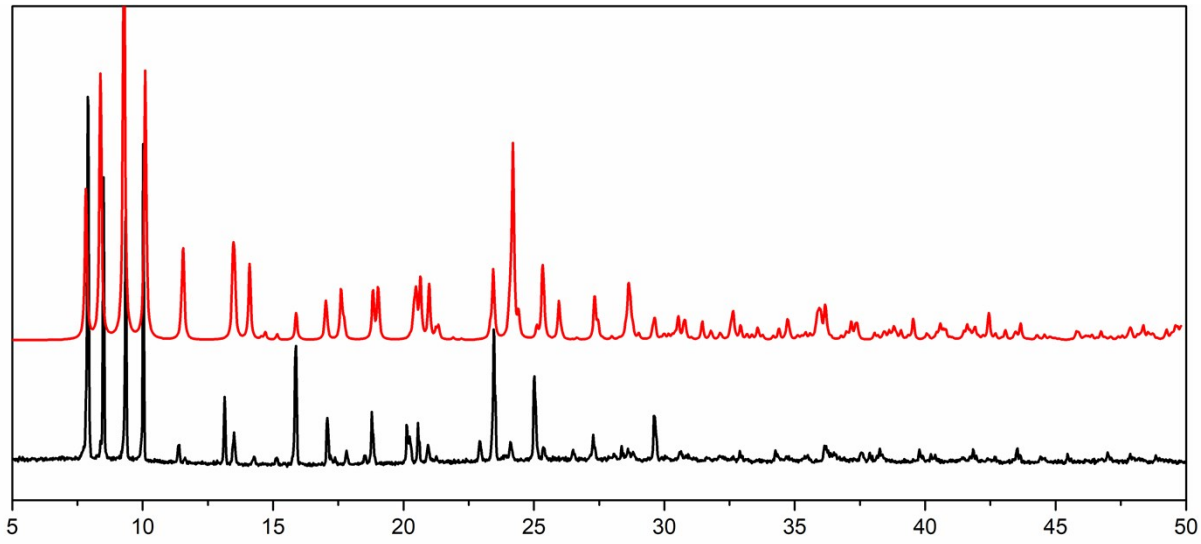

Fig. S18. Powder XRD pattern of **5** (black: experimental; red: simulated).

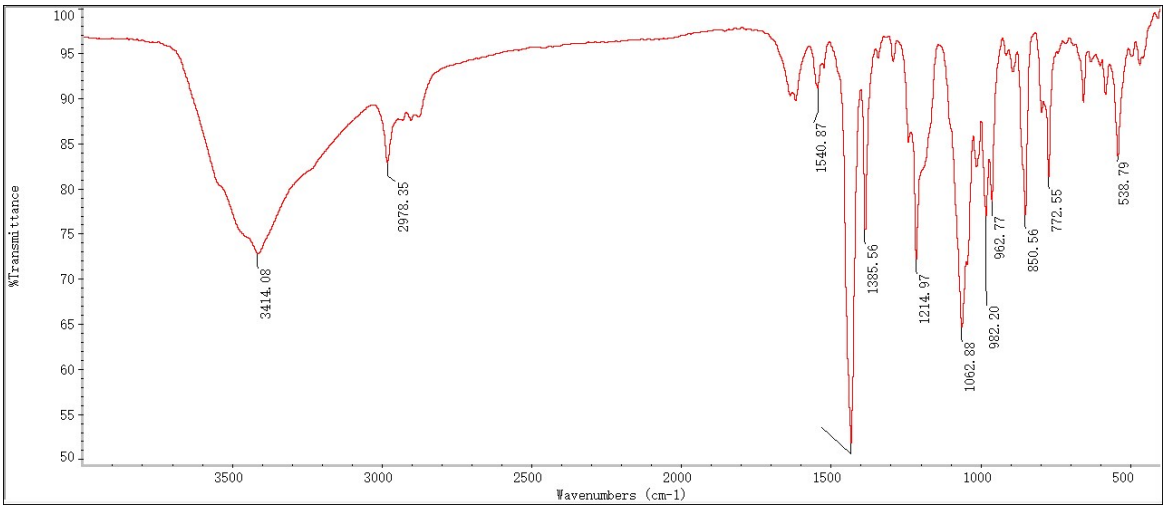

Fig. S19 FT-IR spectrum of **5** (KBr, cm^{-1})

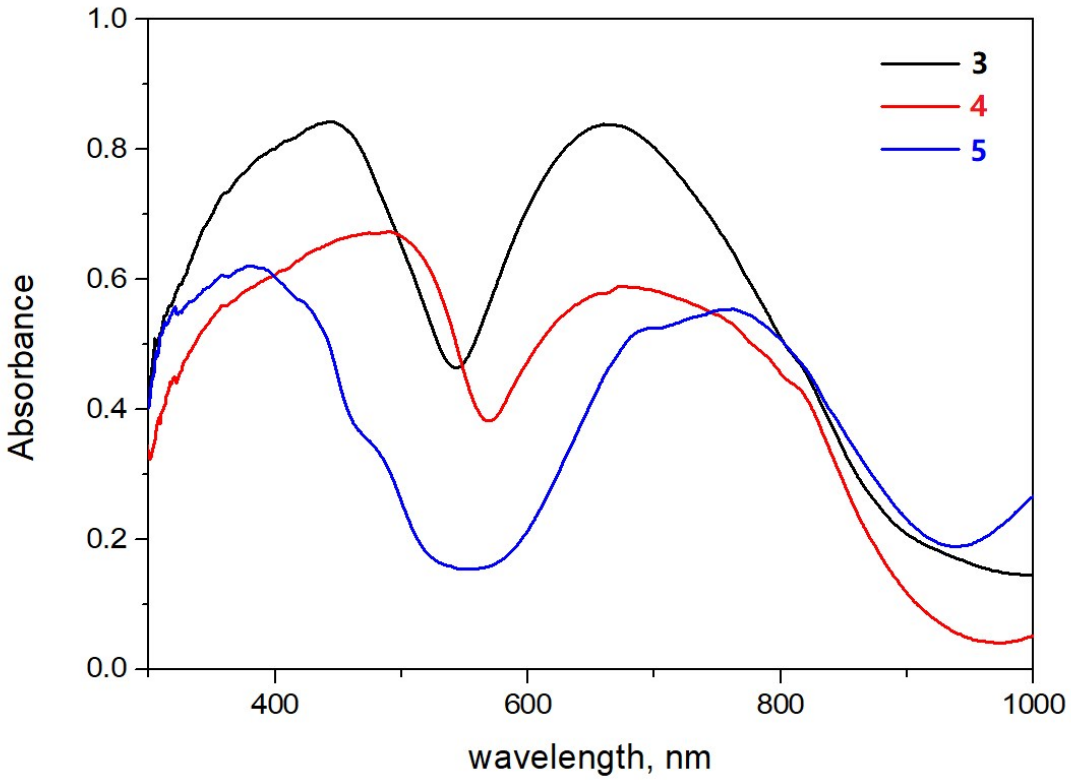

Fig. S20. Solid-state UV-Vis-NIR spectra of complexes **3** (black), **4** (red) and **5** (blue) at room temperature

Computational details

Geometry optimizations were performed using the hybrid B3LYP density functional augmented with the D3BJ version of Grimme's empirical dispersion correction implemented in Gaussian 16.[S3, S4] The Def2-SVP basis set was employed for all the atoms. Frequency calculations were carried out at the same level of theory to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide the thermal corrections of Gibbs free energy.

The single-point energy calculations were performed at the B3LYP-D3BJ/Def2-TZVP level of theory for solution-phase. All the solution phase calculations were on the basis of the gas-phase geometry. The SMD method was used with the corresponding solvent (THF), and the Bondi radii were chosen as the atomic radii to define the molecular cavity.[S5] The Gibbs free energy corrections from frequency calculations were added to the single-point energies to obtain the Gibbs free energy in solution. All the energies reported correspond to the reference state of 1 mol/L, 298K. Optimized structures are visualized by CYL-View program.[S6]

Table. S2 Energy of Intermediates and Transition States.

Species	Thermal Corrections of Gibbs Free Energies (Hartree)	Solvation Energies (Hartree)
1	0.208213	-3025.237886
NiI_2 (triplet)	-0.023813	-2104.088119
THF	0.088298	-232.565429
IN1	0.313058	-5361.970225
TS1	0.307888	-5361.934839

IN2	0.247923	-4984.887807
CH_3CH_2I	0.036841	-377.076188
TS2	0.357489	-5217.431617
IN3	0.303953	-4840.369778
5 (triplet)	0.633569	-9680.856935
5 (singlet)	0.632035	-9680.753465

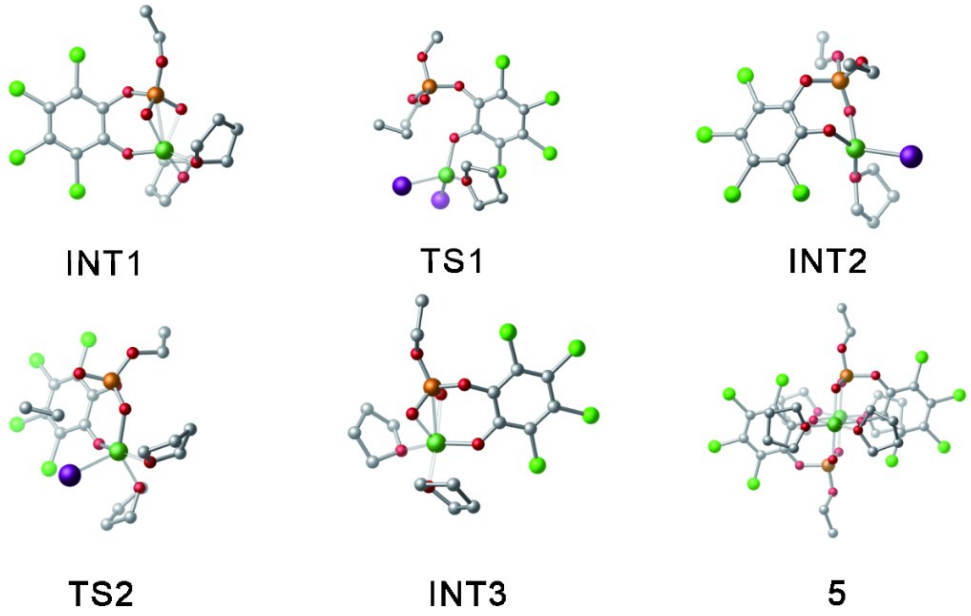

Fig. S21 3D-structures of optimized intermediates and transition states. Hydrogen atoms are omitted for clarity.

Cartesian coordinates:

INT1

0 3

P	-0.03652400	2.18398000	-0.12404200
Cl	-4.53900400	1.41615700	-1.47325800
Cl	-5.72584400	-1.14234600	0.01437800
Cl	-0.92463100	-1.74546800	2.59781500
Cl	-3.91785300	-2.72646800	2.05824800
O	-0.25226300	0.68466300	0.86973800

O	0.12142900	3.40141600	-1.18665300
O	-1.64206100	1.95795700	-0.61016100
O	0.23859500	3.08678600	1.15848800
O	1.19700500	1.33151300	-0.78983500
C	-1.50873100	0.22116400	0.86086900
C	-2.31823600	0.93682900	-0.01437900
C	-1.99202400	-0.88762200	1.54415800
C	-3.61731900	0.54358500	-0.29858000
C	-4.12016700	-0.59894400	0.36386100
C	-3.31317600	-1.30453200	1.27923500
C	-0.68587600	4.58900600	-1.16294700
C	0.32155500	2.75549700	2.57431400
C	2.31239300	1.91889700	-1.55902600
C	1.41999300	3.59748100	3.17883800
C	-1.63561000	4.61556600	-2.34462900
C	2.05977500	1.79608000	-3.03982300
H	-1.23129500	4.65560300	-0.20894200
H	0.01772200	5.43561300	-1.19697700
H	-0.66526800	2.98289400	3.00717800
H	0.53733100	1.68788200	2.68922900
H	2.42825600	2.95697800	-1.23098800
H	3.17874500	1.32867100	-1.23455900
H	2.38930600	3.32096600	2.73846700
H	1.23937400	4.67171300	3.02181000
H	1.47151800	3.40335000	4.26144400
H	-1.07976600	4.52843200	-3.29091300
H	-2.35866100	3.79018500	-2.28310400
H	-2.18954100	5.56779100	-2.35847300
H	1.97333600	0.73846000	-3.32734600
H	1.15328600	2.34526200	-3.32959600

H	2.91771000	2.22176500	-3.58395500
O	-0.18822000	-1.46667900	-0.90991100
C	-0.42757100	-2.89339000	-0.75252400
H	-1.13767500	-3.01903100	0.07741100
H	0.52710600	-3.37458700	-0.49785200
C	-1.00023100	-3.35390700	-2.08947300
H	-1.71308700	-4.18211800	-1.97103000
H	-0.18586200	-3.68519800	-2.75183400
C	-1.63856400	-2.07323600	-2.64198000
H	-1.78423500	-2.09423500	-3.73142100
H	-2.61399100	-1.87927400	-2.16578100
C	-0.62413300	-1.02530900	-2.21584300
H	0.25167700	-1.00216000	-2.88406100
H	-1.03537800	-0.01316400	-2.11670000
Ni	1.47652200	-0.59995800	0.01425100
I	3.05267300	-1.82325200	-1.67316300
I	2.96149600	-0.06291400	2.03413900

TS1

0 3

P	1.89868700	2.66735700	-0.39862600
Cl	5.01874700	0.02918300	-0.30323800
Cl	4.77635900	-3.08949500	0.17959400
Cl	-0.51693500	-2.75603600	-1.10129400
Cl	1.98279900	-4.49007300	-0.28333500
O	-0.01450100	0.19628600	-0.76483500
O	2.96985200	3.75039300	-0.84166300
O	2.50999400	1.32525900	-1.03858800
O	0.59292300	3.10080100	-1.16208600
O	1.64773600	2.58081400	1.09359400
C	1.03194300	-0.56747200	-0.71435500

C	2.33770500	-0.00324100	-0.69813800
C	0.99650000	-1.99291900	-0.70694800
C	3.47625200	-0.76396900	-0.42535300
C	3.38198000	-2.15543200	-0.25260000
C	2.12889900	-2.76637000	-0.42951200
C	4.39908500	3.62359500	-0.63036800
C	0.18741300	2.72123700	-2.50809000
C	-0.27590900	2.51798800	1.57662800
C	-1.32094600	2.74761700	-2.56501200
C	4.77069400	3.56643000	0.83740700
C	-0.56261600	3.97356700	1.70423200
H	4.74480700	2.72864800	-1.16794200
H	4.81904300	4.51326300	-1.11879300
H	0.64852900	3.44369300	-3.19944500
H	0.57443500	1.71559900	-2.71426100
H	-0.44557700	1.96618900	0.66528000
H	-0.05654600	1.93659400	2.46842400
H	-1.75197700	2.01333000	-1.87098500
H	-1.71021400	3.74667200	-2.31768900
H	-1.65459900	2.48515000	-3.58060300
H	4.36622900	4.43380100	1.38009100
H	4.39259200	2.64933500	1.31143600
H	5.86759200	3.57186500	0.93491200
H	0.32023200	4.47201900	2.13367300
H	-0.80035200	4.42060300	0.73119400
H	-1.40174700	4.13916000	2.39390600
O	-0.95826500	-1.36807200	1.49795800
C	-1.58088100	-2.52172400	2.08072200
H	-2.13715900	-3.03286300	1.28540000
H	-2.28686200	-2.18658900	2.86064700

C	-0.40339500	-3.31524100	2.65111300
H	-0.02234500	-4.01524000	1.89502100
H	-0.69445400	-3.89388300	3.53893500
C	0.66409200	-2.23098800	2.95970800
H	0.87740600	-2.14377600	4.03452500
H	1.60836300	-2.46358000	2.44877200
C	0.05047400	-0.93043900	2.41505700
H	-0.43340100	-0.33638000	3.20983900
H	0.75322600	-0.29303400	1.86639900
Ni	-1.80859700	-0.40371700	-0.11615000
I	-2.92007100	1.39378100	1.57223600
I	-3.76904100	-0.85542900	-1.65447200

INT2

0 3

Ni	1.32069900	-0.32124100	0.06142400
P	-0.17154000	2.41392600	-0.03876400
Cl	-4.28890100	1.54123900	-0.35330500
Cl	-0.33139500	-3.00162200	1.36848500
Cl	-3.26713100	-3.76021900	0.43150500
Cl	-5.27712800	-1.46932100	-0.39292400
O	0.11089800	-0.08425500	1.56158200
O	0.56096900	1.32178200	-0.79312400
O	0.59588000	3.24625300	1.04311800
O	1.55507300	-1.32370800	-1.68306500
O	-1.55196000	1.88473300	0.64496300
O	-0.64014900	3.58567300	-0.99756100
C	-1.97095700	0.57229900	0.65103200
C	-1.38466100	3.28806500	-2.20277300
H	-2.30811600	2.75616500	-1.92443600
H	-0.77377300	2.62431700	-2.83525500

C	-1.07289700	-0.42103400	1.11802700
C	-3.67779700	-1.08128700	0.14932200
C	-2.78516600	-2.09828800	0.53601900
C	-3.24928000	0.25901400	0.18925300
C	2.81673400	-2.90383100	-2.90685200
H	2.15050700	-3.24369400	-3.71631400
H	3.61525400	-3.64969400	-2.78685800
C	-1.49989400	-1.76886800	0.98789000
C	-1.69141700	4.59682500	-2.89308500
H	-0.76398200	5.12931000	-3.15191400
H	-2.29605000	5.24545800	-2.24188700
H	-2.25677500	4.40612200	-3.81833400
C	3.34546200	-1.49307500	-3.19754300
H	4.20646700	-1.26582000	-2.55000700
H	3.64218100	-1.34581500	-4.24591200
C	2.03330900	-2.69607900	-1.61556800
H	1.15898900	-3.35080300	-1.49636400
H	2.67874400	-2.78300400	-0.72705100
C	2.16505100	-0.62024300	-2.79905300
H	2.43935000	0.38427300	-2.45290400
H	1.41119700	-0.53706800	-3.59927900
C	1.26517300	2.75630300	2.24594700
H	1.77572300	1.81385100	2.01287700
H	2.02483200	3.52349200	2.44613100
C	0.29155100	2.60773200	3.39182500
H	-0.42119100	1.79771500	3.19116900
H	0.85184400	2.34772700	4.30368200
H	-0.25477000	3.54601200	3.57229200
I	3.77270900	-0.11156600	0.77045400

TS2

0 3

Ni	1.64615500	-0.09313100	-0.37500600
P	-0.17661500	2.30801300	0.62908800
Cl	-3.93396400	2.63928500	-0.22692400
Cl	-1.62355000	-3.17930600	-0.42662200
Cl	-4.73183400	-2.75212100	-0.04705500
Cl	-5.91246600	0.17395100	0.03492700
O	-0.14255500	-0.69388600	-0.82553600
O	1.22371200	1.74226400	0.31483800
O	-0.81925900	1.88393500	1.93323600
O	3.62421200	0.61909600	-0.43824500
O	2.32912100	-1.15504400	-2.08698200
O	-1.13643700	1.89441300	-0.65543000
O	-0.13592000	3.90195600	0.52079300
C	-1.97435700	0.80973900	-0.54608900
C	0.16378800	4.56707400	-0.71965600
H	0.68728800	3.87360600	-1.39872600
H	0.86540600	5.37744400	-0.46694500
C	-1.40833400	-0.49085800	-0.61579300
C	-4.21229700	-0.08234800	-0.19973700
C	-3.68065000	-1.38398100	-0.24252100
C	-3.33959900	1.01091900	-0.33286900
C	3.08785600	-2.35745900	-1.86833300
H	3.60271800	-2.25959700	-0.90525300
H	3.83830200	-2.45033600	-2.67479100
C	4.16932800	2.87411000	-0.85126200
H	3.25683700	3.38088400	-0.50348600
H	4.72460800	3.54824700	-1.51925000
C	-2.30636700	-1.57877500	-0.43649700
C	-1.10238600	5.10799100	-1.35378800

H	-1.61375600	5.79479200	-0.66248200
H	-1.79078900	4.28710000	-1.59727900
H	-0.85845500	5.65860600	-2.27660500
C	4.98723500	2.38381300	0.34903700
H	6.00826600	2.11038000	0.03609500
H	5.06603300	3.12725400	1.15506800
C	1.40170500	-1.45276000	-3.15455800
H	1.91558200	-1.24234700	-4.10813400
H	0.54524800	-0.78219700	-3.03131800
C	1.04849000	-2.94411800	-3.00601600
H	1.17323700	-3.47000500	-3.96422300
H	0.01254400	-3.07206200	-2.66987800
C	2.03546700	-3.45847700	-1.93197200
H	1.52910800	-3.52898200	-0.95862400
H	2.46890400	-4.43949100	-2.17385500
C	3.79357500	1.56100500	-1.52248000
H	2.85638400	1.60791200	-2.09472300
H	4.58878100	1.18501200	-2.18813000
C	4.20226200	1.15051600	0.78363400
H	4.80884800	0.35861000	1.24228000
H	3.37737700	1.41539100	1.45924700
C	0.07363600	-0.01612700	2.46856900
H	-0.21486600	-0.30499700	1.46946700
H	0.92788500	0.63142300	2.60299000
C	-0.72911600	-0.48847400	3.61346900
H	-1.18889400	-1.46530400	3.41009300
H	-0.15546500	-0.51827200	4.54948400
H	-1.54324700	0.24991900	3.73018100
I	2.08104600	-1.79035600	1.75884700

INT3

0 3

Ni	1.77908000	-0.71708900	0.36454500
P	0.98533300	1.65684900	-0.12334900
Cl	-2.95107900	2.75226900	-0.68390900
Cl	-1.91417400	-3.25055200	0.78163000
Cl	-4.83892200	-2.06799500	1.03398900
Cl	-5.36770700	0.95974300	0.30610100
O	0.04792300	-1.34100300	-0.15523600
O	2.11792200	0.97637300	-0.91575100
O	0.91881200	1.09931100	1.29548700
O	3.49659700	-0.63116200	1.55790000
O	2.63236800	-2.21772900	-0.87371600
O	-0.42490000	1.34836200	-0.90896400
O	1.07405500	3.24629200	-0.13365500
C	-1.41676600	0.54430700	-0.39931700
C	0.63957600	4.07844100	-1.23061900
H	-0.06379300	3.51368500	-1.85933400
H	1.52895800	4.33008500	-1.83081700
C	-1.13809900	-0.80421200	-0.04772900
C	-3.77464800	0.28573100	0.16748600
C	-3.53283000	-1.05956700	0.49577300
C	-2.70114700	1.07977300	-0.27021500
C	1.93373400	-3.48880500	-0.83519600
H	1.38028500	-3.53189300	0.11069200
H	2.69270500	-4.28784600	-0.85771500
C	4.98308600	0.94247900	0.64908600
H	4.49830500	1.26346500	-0.28198500
H	6.05374400	1.18711500	0.59955200
C	-2.23859200	-1.58573700	0.38729500
C	-0.02386500	5.31259300	-0.66025400

H	0.66472300	5.85816000	0.00271000
H	-0.91658300	5.02749800	-0.08450200
H	-0.33185700	5.98562900	-1.47597800
C	4.26690800	1.59159100	1.86283100
H	4.96869300	2.08333300	2.55183100
H	3.53863900	2.34262200	1.52921100
C	2.70600400	-1.81620400	-2.26335500
H	3.54386900	-2.36315900	-2.73202300
H	2.89749200	-0.73661300	-2.28218700
C	1.35525800	-2.22170500	-2.83806800
H	1.39486800	-2.36520400	-3.92733400
H	0.62290900	-1.43749600	-2.60661200
C	1.01120600	-3.51648100	-2.06851800
H	-0.04072400	-3.52476300	-1.75836800
H	1.20651800	-4.41314500	-2.67561700
C	4.75457300	-0.55585800	0.85517300
H	4.65761300	-1.15141500	-0.05922800
H	5.52897700	-1.00875200	1.49914800
C	3.55099100	0.42105000	2.55386800
H	4.12579500	0.03044100	3.41002600
H	2.52208700	0.64718100	2.85073800

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0 5

Ni	-0.27347500	-0.04076900	1.49170500
P	-1.00674400	-2.45517100	-0.30241000
Cl	-5.45011600	-2.66224000	-0.49221700
Cl	-2.65166500	2.91871200	-0.01166400
Cl	-5.79538600	2.74969400	0.08855900
Cl	-7.21500800	-0.05829400	-0.13687000
O	-1.33536000	0.28918600	-0.24946000

O	-0.74885300	-2.02312000	1.13999400
O	-0.18854400	-1.95812800	-1.48088100
O	0.85592100	-0.44961300	3.17876400
O	-1.97604800	0.27732600	2.60838000
O	-2.62058500	-2.16785900	-0.62930700
O	-1.03097600	-4.05409000	-0.40031200
C	-3.30780000	-1.01625800	-0.43543800
C	-1.78027200	-4.82509500	0.55096600
H	-2.85021500	-4.57982300	0.44184100
H	-1.46733600	-4.54210700	1.56962900
C	-2.64301700	0.23042000	-0.29298700
C	-5.48769300	0.06230200	-0.23829400
C	-4.85079500	1.30838400	-0.12886300
C	-4.70524000	-1.09593100	-0.38756800
C	-2.27332400	1.49527300	3.30110500
H	-1.84088300	2.31287700	2.71474100
H	-1.79014900	1.46392500	4.29554800
C	2.76706100	-0.20364100	4.54001100
H	2.41273100	-0.40098000	5.56506300
H	3.71685000	0.34598900	4.60814700
C	-3.45025400	1.38392600	-0.16077700
C	-1.52023300	-6.29085900	0.27940500
H	-0.44895500	-6.52085700	0.38494400
H	-1.83077300	-6.55695700	-0.74237600
H	-2.08460700	-6.91479500	0.99007000
C	2.87836800	-1.51429500	3.75106600
H	3.50651800	-1.37505500	2.85869800
H	3.29971400	-2.34314400	4.33787200
C	-2.86624200	-0.72752900	3.09934500
H	-2.47246900	-1.11653200	4.05659600

H	-2.87659800	-1.54210600	2.36693000
C	-4.20245200	0.00566100	3.28678500
H	-4.73768000	-0.36513400	4.17270800
H	-4.85533100	-0.14866600	2.41750200
C	-3.80342500	1.50129100	3.41334200
H	-4.24652300	2.09184800	2.60054300
H	-4.13154500	1.94590400	4.36386700
C	1.71679900	0.56655800	3.74568100
H	1.09697800	1.24202500	4.35240200
H	2.15490600	1.15223900	2.92677000
C	1.43241500	-1.76792300	3.34327900
H	1.30916000	-2.31119200	2.39992400
H	0.86729800	-2.29166600	4.13353700
Ni	0.27345400	0.04087900	-1.49257100
P	1.00678800	2.45526400	0.30162600
Cl	5.45027100	2.66192300	0.49365500
Cl	2.65143100	-2.91867500	0.01117000
Cl	5.79522400	-2.75003500	-0.08715200
Cl	7.21507300	0.05774900	0.13952200
O	1.33528800	-0.28903400	0.24857700
O	0.74897100	2.02323900	-1.14079600
O	0.18852700	1.95820500	1.48004700
O	-0.85611400	0.44979800	-3.17945200
O	1.97590900	-0.27712600	-2.60945200
O	2.62060100	2.16793100	0.62860800
O	1.03105700	4.05417100	0.39956700
C	3.30778100	1.01623200	0.43531300
C	1.78046900	4.82519600	-0.55160900
H	2.85040000	4.57994400	-0.44232400
H	1.46768100	4.54219800	-1.57031500

C	2.64293300	-0.23039300	0.29258700
C	5.48767100	-0.06262300	0.23965100
C	4.85068800	-1.30861500	0.12973600
C	4.70526300	1.09571500	0.38841600
C	2.27383200	-1.49527900	-3.30153300
H	1.84115200	-2.31273700	-2.71514000
H	1.79127500	-1.46437500	-4.29628700
C	-2.76759900	0.20398700	-4.54024600
H	-2.41348800	0.40140300	-5.56536200
H	-3.71742200	-0.34560200	-4.60822400
C	3.45011000	-1.38397900	0.16077200
C	1.52035800	6.29095200	-0.28008400
H	0.44909200	6.52092800	-0.38578100
H	1.83074200	6.55705400	0.74174400
H	2.08482500	6.91490300	-0.99066200
C	-2.87865100	1.51458400	-3.75117200
H	-3.50650300	1.37526800	-2.85860200
H	-3.30018700	2.34349100	-4.33776100
C	2.86646900	0.72763500	-3.09992100
H	2.47357300	1.11626600	-4.05768900
H	2.87602600	1.54245900	-2.36776800
C	4.20288800	-0.00552100	-3.28585200
H	4.73914400	0.36527800	-4.17115100
H	4.85474300	0.14882400	-2.41580700
C	3.80402700	-1.50115600	-3.41283900
H	4.24672000	-2.09181400	-2.59989400
H	4.13271900	-1.94559200	-4.36325100
C	-1.71719000	-0.56631000	-3.74621400
H	-1.09754300	-1.24179600	-4.35308900
H	-2.15514300	-1.15198000	-2.92721300

C	-1.43256200	1.76813700	-3.34385100
H	-1.30895300	2.31144100	-2.40056200
H	-0.86768400	2.29179600	-4.13434000

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Ni	0.69277800	-0.60808700	1.16665600
P	1.18705100	2.21004300	0.51128900
Cl	5.45247800	2.90603200	-0.17995200
Cl	3.16757800	-2.87301500	-0.97369300
Cl	6.30313000	-2.41848600	-1.02098600
Cl	7.45419200	0.49000400	-0.60538700
O	1.64128200	-0.42689200	-0.43042300
O	1.20708400	1.16841900	1.64234300
O	0.07563600	2.24634700	-0.52497900
O	-0.36288700	-0.68486900	2.79454000
O	2.31028700	-1.71964500	2.73026800
O	2.65148900	2.15011400	-0.25510000
O	1.25618200	3.67253700	1.14238700
C	3.47551600	1.06852400	-0.35003600
C	2.26507400	4.00587600	2.11402100
H	3.25734400	3.77693900	1.69267200
H	2.11616200	3.37866600	3.00830700
C	2.93570800	-0.23826400	-0.46408400
C	5.74337100	0.21344400	-0.58822700
C	5.22667400	-1.08088400	-0.76544300
C	4.85569100	1.28656900	-0.38212200
C	3.08663800	-2.90905100	2.60881600
H	2.76499700	-3.41949300	1.69251900
H	2.88403700	-3.57039700	3.47293500
C	-1.69817700	-1.49246100	4.54258300

H	-1.05357100	-1.39828500	5.43188800
H	-2.50069700	-2.20701200	4.77579500
C	3.84139300	-1.29567600	-0.71259300
C	2.13367300	5.47709700	2.43932700
H	1.13499000	5.69931700	2.84490600
H	2.28424400	6.08759400	1.53627800
H	2.88836900	5.76644100	3.18715800
C	-2.21405500	-0.11448000	4.10943700
H	-3.05802200	-0.22311900	3.40946000
H	-2.54457100	0.51599300	4.94740000
C	3.08626000	-0.77747400	3.45762200
H	3.05177000	-1.01147200	4.54170600
H	2.65028200	0.21545600	3.28899500
C	4.50106000	-0.94969600	2.90167900
H	5.27915900	-0.61847900	3.60490600
H	4.60824700	-0.36115200	1.98011200
C	4.56839100	-2.46285300	2.59139000
H	5.04283100	-2.65805400	1.62093900
H	5.14701900	-3.00556000	3.35394700
C	-0.88378100	-1.92288900	3.32868700
H	-0.02607700	-2.57015100	3.55062800
H	-1.50804500	-2.39830700	2.56017900
C	-1.00837900	0.46937000	3.38579600
H	-1.25794100	1.16915900	2.58320800
H	-0.29204700	0.94281700	4.07631000
Ni	-0.69271500	0.60815900	-1.16600300
P	-1.18691300	-2.21001300	-0.51071800
Cl	-5.45244300	-2.90613600	0.17927200
Cl	-3.16795600	2.87300700	0.97352200
Cl	-6.30351200	2.41840300	1.01975300

Cl	-7.45435700	-0.49013400	0.60387300
O	-1.64140100	0.42685700	0.43095000
O	-1.20687100	-1.16838800	-1.64176800
O	-0.07565500	-2.24624700	0.52572200
O	0.36313200	0.68510300	-2.79376600
O	-2.31024000	1.71938500	-2.72963200
O	-2.65145900	-2.15014800	0.25548400
O	-1.25584900	-3.67251300	-1.14182200
C	-3.47557500	-1.06858400	0.35004700
C	-2.26452300	-4.00590400	-2.11366600
H	-3.25688400	-3.77684200	-1.69260400
H	-2.11533400	-3.37882100	-3.00799600
C	-2.93584400	0.23822000	0.46420700
C	-5.74353500	-0.21354000	0.58733500
C	-5.22693200	1.08081400	0.76466100
C	-4.85575900	-1.28665600	0.38161400
C	-3.08647800	2.90893500	-2.60894000
H	-2.76514300	3.41967900	-1.69270500
H	-2.88345100	3.56992800	-3.47322800
C	1.69792100	1.49279800	-4.54212300
H	1.05300900	1.39880700	-5.43122700
H	2.50043700	2.20729800	-4.77550600
C	-3.84164000	1.29564100	0.71229500
C	-2.13314900	-5.47717700	-2.43874500
H	-1.13437300	-5.69952600	-2.84402300
H	-2.28401200	-6.08754400	-1.53565600
H	-2.88766400	-5.76656100	-3.18674200
C	2.21379900	0.11469900	-4.10934400
H	3.05802200	0.22314200	-3.40964300
H	2.54395800	-0.51568500	-4.94751500

C	-3.08593100	0.77719800	-3.45725700
H	-3.05077600	1.01099700	-4.54136200
H	-2.65019400	-0.21576300	-3.28820800
C	-4.50104100	0.94972000	-2.90217000
H	-5.27876500	0.61865900	-3.60588700
H	-4.60894700	0.36119700	-1.98067500
C	-4.56828100	2.46290200	-2.59193200
H	-5.04294900	2.65815900	-1.62159900
H	-5.14664800	3.00567400	-3.35463900
C	0.88396400	1.92314000	-3.32790200
H	0.02626300	2.57052400	-3.54948200
H	1.50853200	2.39839500	-2.55953300
C	1.00830600	-0.46912700	-3.38537600
H	1.25805200	-1.16903400	-2.58294800
H	0.29170100	-0.94243500	-4.07569700

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