Supporting information for

Selective formation of discrete versus polymeric copper organophosphates:

DNA cleavage and cytotoxic activity.

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Figure S1. FT-IR spectra of 1 and 2 (as diluted KBr discs).

Figure S2. FT-IR spectra of 3-5 (as diluted KBr discs).

Figure S3. ESI-MS spectrum of reaction mixture of **3**, inset represents the experimental and simulated isotopic pattern.

Figure S4. ESI-MS spectrum of reaction mixture of **4**, inset represents the experimental and simulated isotopic pattern.

Figure S5. ESI-MS spectrum of reaction mixture of **5**, inset represents the experimental and simulated isotopic pattern.

Figure S6. (a) Molecular fragment of **4** depicting repeating rectangular compartment (b) 1-Dimensional corner shared coordination chain.

Figure S7. (a) Molecular fragment of **5** depicting repeating rectangular compartment (b) 1-Dimensional corner shared coordination chain.

Figure S8. TGA trace of compounds 1-5.

Figure S9. X-band EPR spectra of 1 and 2 in methanol at 100K.

Figure S10. Comparison of X-band EPR spectra of 1 and 2 in methanol and the reaction mixtures EPR spectra of 3-5 at 100K.

Figure S11. ¹H NMR (500 MHz, CDCl₃) spectrum of dippH₂.

Figure S12. ¹H NMR (400 MHz, CDCl₃) spectra of halide functionalized X-dippH₂(X=Cl, Br, I) ligands.

Figure S13. ³¹P NMR (202 MHz, CDCl₃) spectrum of diPPH₂.

Figure S14. ³¹P NMR (161 MHz, CDCl₃) spectrum of X-dippH₂(X= Cl, Br, I) ligands.

Figure S15. ¹H NMR (400MHz, CDCl₃) spectrum of Pyterpy ligand.

Figure S16: ¹³C NMR spectrum of dippH₂ (CDCl₃, 125 MHz).

Figure S17: ¹³C NMR spectrum of Cl-dippH₂ (CDCl₃, 125 MHz).

Figure S18: ¹³C NMR spectrum of Br-dippH₂ (CDCl₃, 125 MHz).

Figure S19: ¹³C NMR spectrum of I-dippH₂ (CDCl₃, 125 MHz).

Figure S20: ¹³C NMR spectrum of Pyterpy (CDCl₃, 125 MHz).

Figure S21: UV-Vis spectra of dippH₂ and X-dippH₂ (X=Cl, Br, I) in acetonitrile $(1 \times 10^{-5} \text{ M})$.

Figure S22: UV-Vis spectrum of Pyterpy in CHCl₃ $(1 \times 10^{-4} \text{ M})$.

Table S1. Summary of EPR structural parameters of 1 and 2 in methanol and the reaction mixture of 3-5.
Table S2. Selected bond lengths [Å] and angles [°] of compound 2.
Table S3. Hydrogen bonds for complex 2 [Å and °].
Table S4. Selected bond lengths [Å] and angles [°] of compound 3.
Table S5. Hydrogen bonds for complex 3 [Å and °].

Table S6. Selected bond lengths [Å] and angles [°] of compound 4.**Table S7.** Hydrogen bonds for complex 4 [Å and °].

Table S8. Selected bond lengths [Å] and angles [°] of compound 5.**Table S9.** Hydrogen bonds for complex 5 [Å and °].

Table S10. Comparison of Structural Parameters of 2-5 with each other.

Table S11. Shape measures of the penta coordinate CuN_3O_2 of copper centres.

Table S12. Shape measures of hexacoordinate CuN2O4 type of copper centres



Figure S1. FT-IR spectra of 1-2 (as diluted KBr discs)



Figure S2. FT-IR spectra of 3-5 (as diluted KBr discs).



Figure S3. ESI-MS spectrum of reaction mixture of 3, inset represents the experimental and simulated isotopic pattern.



Figure S4. ESI-MS spectrum of reaction mixture of 4, inset represents the experimental and simulated isotopic pattern.



Figure S5. ESI-MS spectrum of reaction mixture of 5, inset represents the experimental and simulated isotopic pattern.



Figure S6. (a) Molecular fragment of **4** depicting repeating rectangular compartment (b) 1-Dimensional corner shared coordination chain.



Figure S7. (a) Molecular fragment of **5** depicting repeating rectangular compartment (b) 1-Dimensional corner shared coordination chain.

Thermal decomposition studies.

The solid state thermolysis of discrete as well as polymeric copper phosphates have been reported to yield high purity meta-phosphate $[Cu(PO_3)_2]$ and pyrophosphate $[Cu_2(P_2O_7)]$ materials after combustion of labile alkyl

substituents on phosphate ligands.¹ On similar lines, the TGA study of copper phosphates **1-5** with bulkier 2,6di*iso*propylphenyl substituents on phosphate ligands, yield copper pyrophosphates in good yields.

The thermal behavior of **1-5** has been investigated in the temperature range 30–800 °C under a stream of flowing nitrogen gas at a heating rate of 10 °C min⁻¹. The thermogravimetric analysis (TGA) profiles of the copper phosphate dimers **1-2** and polymeric chains **3-5** are shown in Figure S8. The TGA traces of **1-5** shows an initial weight loss due to removal of lattice methanol molecules and on further increase in temperature the 2-3 step weight losses till around 450 °C can be attributed to the combustion of pyridine rings of pyterpy and the aryl moieties of the phosphate ligands. Finally the compounds gets transformed into to copper metaphosphates which are quite stable.



Figure S8. TGA trace of compounds 1-5

EPR Spectra of 1-5

The mass spectrometry analysis (ESI-MS) confirms the dimeric nature of **3-5** in solution state which is similar like **1** and **2**. To further probe this X-band EPR spectra of **1** and **2** after isolating them in crystalline form were recorded in methanol at 100 K and the X-band EPR spectra of reaction mixtures of **3-5** were also recorded at the same temperature. The EPR spectra of **1** and **2** (Figure S9) shows similar type of hyperfine splitting like the spectra obtained from the reaction mixtures of **3-5** (Figure S10) which clearly indicates that compounds **3-5** have similar structure in solution state like that of **1** and **2**. The polymeric compounds **3-5** after isolating them in crystalline form are not soluble in most of the solvents and hence does not show hyperfine splitting.



Figure S9. X-band EPR spectra of 1 and 2 in methanol at 100K



Figure S10. Comparision of X-band EPR spectra of 1 and 2 in methanol and the reaction mixtures EPR spectra of 3-5 at 100K.



Figure S11. ¹H NMR (500 MHz, CDCl₃) spectrum of dippH₂.



Figure S12. ¹H NMR (400 MHz, CDCl₃) spectra of halide functionalized X-dippH₂(X=Cl, Br, I) ligands.

dippH₂:¹H NMR (CDCl₃, 500 MHz): δ 8.91 (s, 2H, -OH), 7.10 (s, 2H, Ar-H), 3.34 (septet, 2H, ^{*i*}Pr-CH), 1.15 (d, 12H, ^{*i*}Pr-CH₃) ppm.

Cl-dippH₂:¹H NMR (CDCl₃, 400 MHz): δ 7.29 (s, 1H, -OH), 7.05 (s, 2H, Ar-H), 3.25 (septet, 2H, ⁱPr-CH), 1.12 (d, 12H, ⁱPr-CH₃) ppm.

Br-dippH₂: ¹H NMR (CDCl₃, 400 MHz): δ 7.05 (s, 2H, Ar-H), 5.10 (s, 1H, -OH), 3.18 (septet, 2H, ^{*i*}Pr-CH,), 1.01 (d, 12H, -CH₃) ppm.

I-dippH₂: ¹H NMR (CDCl₃, 400 MHz): δ 7.38 (s, 2H, Ar-H), 5.08 (s, 2H, -OH), 3.32 (septet, 2H, ^{*i*}Pr-CH,), 1.10 (d, 12H, CH₃) ppm.



Figure S14. ³¹P NMR (161 MHz, CDCl₃) spectrum of X-dippH₂(X= Cl, Br, I) ligands.



Figure S15. ¹H NMR (400MHz, CDCl₃) spectrum of Pyterpy ligand.

PyterPy: ¹H NMR (CDCl₃, 400 MHz, ppm) $\delta = 8.78$ (2H, dd, Ha), 8.77 (2H, s, Hb),8.74 (2H, brdm, Hc), 8.66 (2H, d, Hd), 7.9 (2H, td, He); $\delta = 7.8$ (2H, dd, Hf), 7.7 (2H, ddd, Hg).; IR(KBr disk, cm⁻¹):1581,1563, 1538, 1470 MS (ESI) m/e: 311.15



Figure S16: ¹³C NMR spectrum of dippH₂ (CDCl₃, 125 MHz)



Figure S17: ¹³C NMR spectrum of Cl-dippH₂ (CDCl₃, 125 MHz)



Figure S18: ¹³C NMR spectrum of Br-dippH₂ (CDCl₃, 125 MHz)



Figure S19: ¹³C NMR spectrum of I-dippH₂ (CDCl₃, 125 MHz)



Figure S20: ¹³C NMR spectrum of Pyterpy (CDCl₃, 125 MHz)



Figure S21: UV-Vis spectra of dippH₂ and X-dippH₂ (X=Cl, Br, I) in acetonitrile $(1 \times 10^{-5} \text{ M})$. Summary of EPR structural parameters of UV-Visible data of dippH₂ and X-dippH₂ ligands

λmax(nm)
203, 264
203, 220, 265
202,220, 267
206,222, 263



Figure S22: UV-Vis spectrum of Pyterpy in CHCl₃ (1×10^{-5} M).

Compound	Solvent	gll	g⊥	A∥ (×10 ⁻⁴ cm ⁻¹)
1	Methanol	2.27	2.07	165
2	Methanol	2.27	2.01	162
3	Reaction Mixture	2.32	1.97	190
4	Reaction Mixture	2.25	2.06	140
5	Reaction Mixture	2.43	2.26	167

Table S1. Summary of EPR structural parameters of 1 and 2 in methanol and the reaction mixture of 3-5.

Table S2. Selected bond lengths $[{\rm \AA}]$ and angles $[^\circ]$ of compound 2

Cu(1)-O(1)	1.911(2)	O(1)-Cu(1)-N(2)	153.47(10)
Cu(1)-N(2)	1.965(2)	N(2)-Cu(1)-N(1)	78.81(10)
Cu(1)-N(3)	2.049(2)	N(3)-Cu(1)-O(3)	97.99(9)
Cu(1)-N(1)	2.055(2)	O(1)-Cu(1)-N(1)	91.94(9)
Cu(1)-Q(3)	2.121(2)	O(1)-Cu(1)-O(3)	105.28(9)
O(1)-P(1)	1 523(2)	O(3)-P(1)-O(1)	112 96(12)
O(2)-P(1)	1.656(2)	O(3)-P(1)-O(2)	106.87(11)
O(2) P(1)	1.503(2)	O(3)-P(1)-O(4)	116.42(13)
O(4) - P(1)	1.505(2)	O(4) - P(1) - O(1)	111.55(12)
O(1) Cu(1) N(3)	104.48(0)	N(2) Cu(1) O(2)	100 10(0)
N(3)-Cu(1)-N(1)	156 10(10)	N(1)-Cu(1)-O(3)	94 18(9)
	100.10(10)	1 1 1 2 4 (1) 0 (3)	> 1.10())

Table S3. Hydrogen bonds for complex 2 [Å and $^\circ]$

D-H···A	d(D-H)	d(H••••A)	d(D••••A)	<(DHA)
C(7)-H(7)O(6)	0.95	2.54	3.479(4)	169.0
C(12)-H(12)O(5)	0.95	2.57	3.508(4)	171.6
C(14)-H(14)Br(1)	0.95	3.02	3.885(3)	151.7
C(15)-H(15)O(3)	0.95	2.37	3.283(4)	160.9
C(17)-H(17)O(6)	0.95	2.49	3.323(4)	145.7
O(5)-H(5)O(4)	0.84	1.86	2.689(3)	168.0

Table S4. Selected bond lengths [Å] and angles [°] of compound 3

Cu(1)-O(5)	1.941(2)	P(2)-O(7)	1.626(2)
Cu(1)-N(1)	2.049(3)	P(1)-O(3)	1.492(2)
Cu(1)-N(3)	2.051(3)	Cu(1)-N(2)	1.943(3)
Cu(1)-O(1)	2.143(2)	P(1)-O(4)	1.615(2)
Cu(2)-O(8)	1.943(2)	O(5)-Cu(1)-N(2)	166.76(10)
Cu(2)-N(4)	2.042(3)	O(5)-Cu(1)-N(1)	103.45(11)
P(2)-O(6)	1.494(2)	N(2)-Cu(1)-N(1)	79.86(11)

P(2)-O(8)	1.520(2)	O(5)-Cu(1)-N(3)	96.10(10)
P(2)-O(5)	1.541(2)	N(2)-Cu(1)-N(3)	79.04(11)
P(1)-O(1)	1.498(2)	N(1)-Cu(1)-N(3)	158.36(10)
P(1)-O(2)	1.573(3)	O(5)-Cu(1)-O(1)	97.63(9)
N(2)-Cu(1)-O(1)	94.98(10)	O(8)-Cu(2)-N(4)	93.70(11)
N(1)-Cu(1)-O(1)	93.04(10)	O(6)-P(2)-O(5)	113.50(14)
N(3)-Cu(1)-O(1)	93.49(10)	O(8)-Cu(2)-N(4)	86.30(11)
O(8)-Cu(2)-O(8)	180.00(13)	N(4)-Cu(2)-N(4)	180.00(13)
O(8)-P(2)-O(7)	106.64(13)	O(8)-P(2)-O(5)	110.24(13)
O(2)-P(1)-O(4)	99.12(13)	C(15)-N(3)-C(11)	119.0(3)
O(1)-P(1)-O(4)	108.63(13)	C(10)-N(2)-Cu(1)	119.7(2)
O(1)-P(1)-O(2)	110.26(14)	C(6)-N(2)-Cu(1)	118.2(2)
O(3)-P(1)-O(1)	116.81(13)	P(2)-O(8)-Cu(2)	137.30(14)
O(5)-P(2)-O(7)	105.07(12)	P(1)-O(1)-Cu(1)	127.54(14)
O(3)-P(1)-O(2)	109.93(14)	P(2)-O(5)-Cu(1)	132.28(13)

D-H···A	d(D-H)	d(H···A)	d(D••••A)	<(DHA)
O(2)-H(2)O(5)	0.84	1.83	2.667(3)	174.0
O(9)-H(9A)O(6)	0.84	1.94	2.735(4)	156.4
O(12)-H(12A)O(6)	0.87	1.89	2.756(3)	175.9
O(12)-H(12B)O(9)	0.87	2.07	2.907(4)	160.2
O(11)-H(11)O(3)	0.84	1.85	2.680(4)	168.9
O(10)-H(10)O(3)	0.84	2.07	2.900(4)	172.3
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 Table S5. Hydrogen bonds for complex 3 [Å and °]

Table S6. Selected bond lengths $[\text{\AA}]$ and angles $[^\circ]$ of compound 4

	Cu(1)-N(2)	1.941(4)	O(1)-P(1)	1.495(3)
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Cu(1)-O(5)	1.945(3)	O(2)-P(1)	1.564(3)
Cu(1)-N(1)	2.049(3)	O(3)-P(1)	1.494(3)
Cu(1)-N(3)	2.050(3)	O(4)-P(1)	1.608(3)
Cu(2)-O(8)	1.947(3	O(5)-P(2)	1.532(3)
Cu(1)-O(1)	2.138(3)	O(6)-P(2)	1.488(3)
Cu(2)-N(43	2.046(4)	O(8)-P(2)	1.516(3)
Cu(2)-O(9)	2.533(4)	O(7)-P(2)	1.617(3)
N(2)-Cu(1)-O(5)	166.41(13)	N(3)-Cu(1)-O(1)	93.69(12)
N(2)-Cu(1)-N(1)	79.69(15)	N(1)-Cu(1)-O(1)	93.59(12)
O(5)-Cu(1)-N(1)	103.30(14)	O(8)-Cu(2)-O(8)	180.0
N(2)-Cu(1)-N(3)	79.12(15)	O(8)-Cu(2)-N(4)	93.55(13)
O(5)-Cu(1)-N(3)	96.12(14)	O(8)-Cu(2)-N(4)	86.45(13)
N(1)-Cu(1)-N(3)	158.14(15)	O(8)-Cu(2)-N(4)	93.55(13)
N(2)-Cu(1)-O(1)	95.45(14)	N(4)-Cu(2)-N(4)	180.0
O(5)-Cu(1)-O(1)	97.57(12)	C(15)-N(3)-Cu(1)	126.2(3)
C(1)-N(1)-C(5)	118.2(4)	C(15)-N(3)-C(11)	119.2(4)
C(11)-N(3)-Cu(1)	114.5(3)	C(6)-N(2)-Cu(1)	118.3(3)
C(19)-N(4)-Cu(2)	123.3(3)	C(10)-N(2)-Cu(1)	119.7(3)
C(18)-N(4)-Cu(2)	119.5(3)	C(10)-N(2)-C(6)	121.7(4)
P(1)-O(1)-Cu(1)	127.78(17)	C(1)-N(1)-Cu(1)	127.9(3)
P(1)-O(2)-H(2)	109.5	C(5)-N(1)-Cu(1)	113.7(3)
P(2)-O(5)-Cu(1)	131.79(17)	Cu(2)-O(9)-H(9A)	110.8
P(2)-O(8)-Cu(2)	136.87(19)	O(3)-P(1)-O(1)	116.71(18)
Cu(2)-O(9)-H(9B)	110.1	O(1)-P(1)-O(2)	110.20(17)
O(3)-P(1)-O(2)	110.03(19)	O(1)-P(1)-O(4)	109.18(18)
O(3)-P(1)-O(4)	110.24(16)	O(6)-P(2)-O(8)	114.19(17)
O(2)-P(1)-O(4)	99.04(17)	O(8)-P(2)-O(5)	110.45(18)
O(6)-P(2)-O(5)	113.33(17)	O(8)-P(2)-O(7)	106.25(16)

D-H···A	d(D-H)	d(H•••A)	d(D••••A)	<(DHA)
O(2)-H(2)O(5)	0.84	1.82	2.662(4)	175.5
O(11)-H(11)O(3)	0.84	2.06	2.897(5)	173.7
O(10)-H(10)O(3)	0.84	1.84	2.674(4)	169.5
O(9)-H(9A)O(12)	0.89	2.37	2.915(6)	119.3
O(9)-H(9B)O(6)	0.89	1.97	2.736(4)	143.7
O(12)-H(12A)O(6)	0.84	1.95	2.732(5)	154.0

Table S7. Hydrogen bonds for complex 4 [Å and °]

Cu(1)-N(2)	1.954(6)	P(2)-O(8)	1.518(5)
Cu(1)-N(3)	2.046(7)	P(2)-O(6)	1.544(5)
Cu(1)-N(1)	2.055(7)	P(2)-O(5)	1.621(5)
Cu(1)-O(2)	2.149(5)	O(6)-Cu(1)-N(1)	103.0(2)
Cu(2)-N(4)	2.037(6)	N(2)-Cu(1)-N(1)	80.0(3)
Cu(2)-O(8)	1.943(5)	N(3)-Cu(1)-N(1)	158.2(3)
P(1)-O(3)	1.500(6)	O(6)-Cu(1)-O(2)	97.6(2)
P(1)-O(2)	1.508(6)	N(2)-Cu(1)-O(2)	95.9(2)
P(1)-O(4)	1.583(6)	N(3)-Cu(1)-O(2)	93.3(2)
P(1)-O(1)	1.616(6)	N(1)-Cu(1)-O(2)	93.8(2)
P(2)-O(7)	1.509(6)	O(8)-Cu(2)-N(4)	86.0(2)
O(6)-Cu(1)-N(2)	166.0(2)	O(8)-Cu(2)-N(4)	94.0(2)
O(6)-Cu(1)-N(3)	96.5(2)	O(8)-Cu(2)-O(8)	180.00(14)
N(2)-Cu(1)-N(3)	78.8(3)	O(8)-Cu(2)-N(4)	94.0(2)
N(4)-Cu(2)-N(4)	180.0(3)	O(3)-P(1)-O(2)	116.3(3)
O(3)-P(1)-O(4)	109.9(3)	O(2)-P(1)-O(4)	109.5(3)
O(3)-P(1)-O(1)	110.6(3)	O(2)-P(1)-O(1)	109.8(3)
O(4)-P(1)-O(1)	99.3(3)	O(7)-P(2)-O(8)	114.1(3)
O(7)-P(2)-O(6)	113.6(3)	O(8)-P(2)-O(6)	110.6(3)
O(7)-P(2)-O(5)	106.0(3)	O(8)-P(2)-O(5)	105.9(3)
O(6)-P(2)-O(5)	105.7(3)	C(32)-O(1)-P(1)	125.6(5)
P(1)-O(2)-Cu(1)	128.1(3)	C(21)-O(5)-P(2)	124.1(5)
P(2)-O(6)-Cu(1)	131.9(3)	P(2)-O(8)-Cu(2)	137.3(3)
C(1)-N(1)-C(5)	118.0(7)	C(1)-N(1)-Cu(1)	128.6(5)
C(5)-N(1)-Cu(1)	113.3(5)	O(8)-Cu(2)-N(4)	86.0(2)

Table S8. Selected bond lengths $[\text{\AA}]$ and angles $[^\circ]$ of compound 5

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(1)-H(1)O(7)	0.95	2.42	3.323(9)	158.9
C(4)-H(4)O(11)	0.95	2.41	3.361(10)	174.2
C(7)-H(7)O(11)	0.95	2.65	3.574(10)	164.4
C(9)-H(9)O(10)	0.95	2.41	3.342(10)	168.6
C(18)-H(18)O(10)	0.95	2.33	3.268(10)	170.4

O(10)-H(10)O(3)	0.84	1.89	2.691(9)	158.4	
O(9)-H(9A)O(7)	0.84	1.95	2.735(9)	154.1	
C(46)-H(46C)O(7)	0.98	2.65	3.157(12)	112.4	
O(11)-H(11)O(3)	0.84	2.05	2.887(9)	176.1	
O(12)-H(12A)O(9)	0.87	2.14	2.921(10)	149.8	
O(12)-H(12B)O(7)	0.87	1.93	2.758(8)	158.2	

Table S9. Hydrogen bonds for complex 5 [Å and °]

Table S10. Comparison of Structural Parameters of 2-5 with each other.

Compound	Formula	Crystal	Space	Cu–N	Cu–O	Р-О	Cu–Cu	Р-Р
		System	group					
2	$C_{68}H_{74} Br_2Cu_2N_8O_{12}P_2$	Triclinic	P -1	2.023	2.016	1.560	4.449	4.808
3	$C_{94}H_{122}Cl_4Cu_3N_8O_{24}P_4$	Triclinic	P -1	2.021	2.009	1.544	5.003	4.844
4	$C_{94}H_{122}Br_4Cu_3N_8O_{24}P_4$	Triclinic	P -1	2.021	2.012	1.539	4.994	4.842
5	$C_{94}H_{122}I_4Cu_3N_8O_{24}P_4$	Triclinic	P -1	2.021	2.013	1.549	5.022	4.874

Table S11. Shape measures of the penta coordinate CuN₃O₂ of copper centres.

Structure [ML5]	2	3	4	5
PP-5	30.491	29.594	29.605	29.731
vOC-5	2.153	1.370	1.394	1.408
TBPY-5	4.294	5.812	5.814	5.709
SPY-5	1.167	1.432	1.408	1.391
JTBPY-5	6.554	7.666	7.708	7.657

Label	Symmetry	Shape
PP-5	$D_{5\mathrm{h}}$	Pentagon
vOC-5	C _{4v}	Vacant octahedron
TBPY-5	D_{3h}	Trigonal bipyramid
SPY-5	$C_{4\mathrm{v}}$	Spherical square pyramid
JTBPY-5	C_{2v}	Johnson trigonal bipyramid J12

Table S12. Shape measures of hexacoordinate CuN_2O_4 type of copper centres

Structure ML ₆	3	4	5
HP-6	31.068	31.002	30.900
PPY-6	28.497	28.464	28.447
OC-6	1.583	1.498	1.713
TPR-6	17.213	17.150	17.247
JPPY-6	30.857	30.855	28.447

Label	Symmetry	Shape
HP-6	D6h	Hexagon
PPY-6	C5v	Pentagonal pyramid
OC-6	Oh	Octahedron
TPR-6	D3h	Trigonal prism

JPPY-6	C5v	Johnson pentagonal
		pyramid

References:

(1) Murugavel, R.; Walawalkar, M. G.; Dan, M.; Roesky, H. W.; Rao, C. N. R. Acc. Chem. Res. 2004, 37,763.