Supplementary Material (ESI) for Dalton Transactions

Assembly of Tetra, Di and Mononuclear Molecular Cadmium Phosphonates using 2,4,6-Tri*iso*propylphenylphosphonic acid and Ancillary Ligands

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Figure S1(a): Molecular structure of **1**

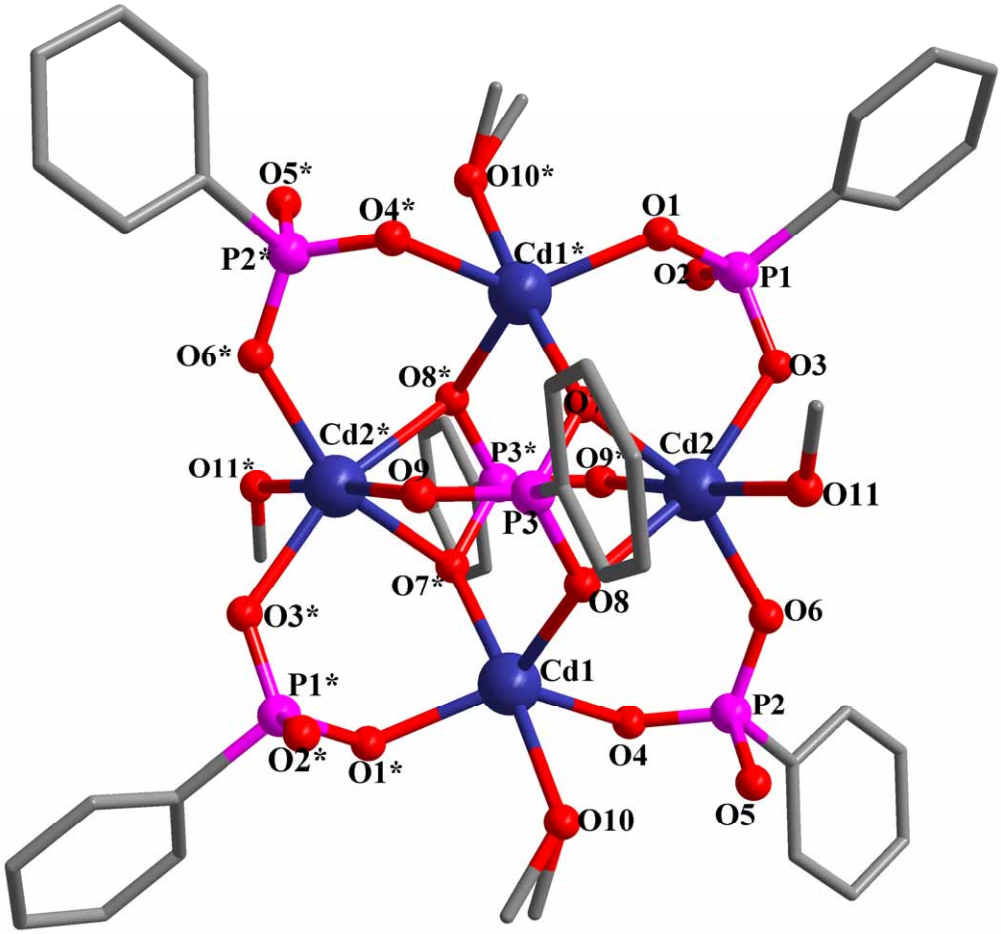

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Figure S1(b): Plane representation of **1**

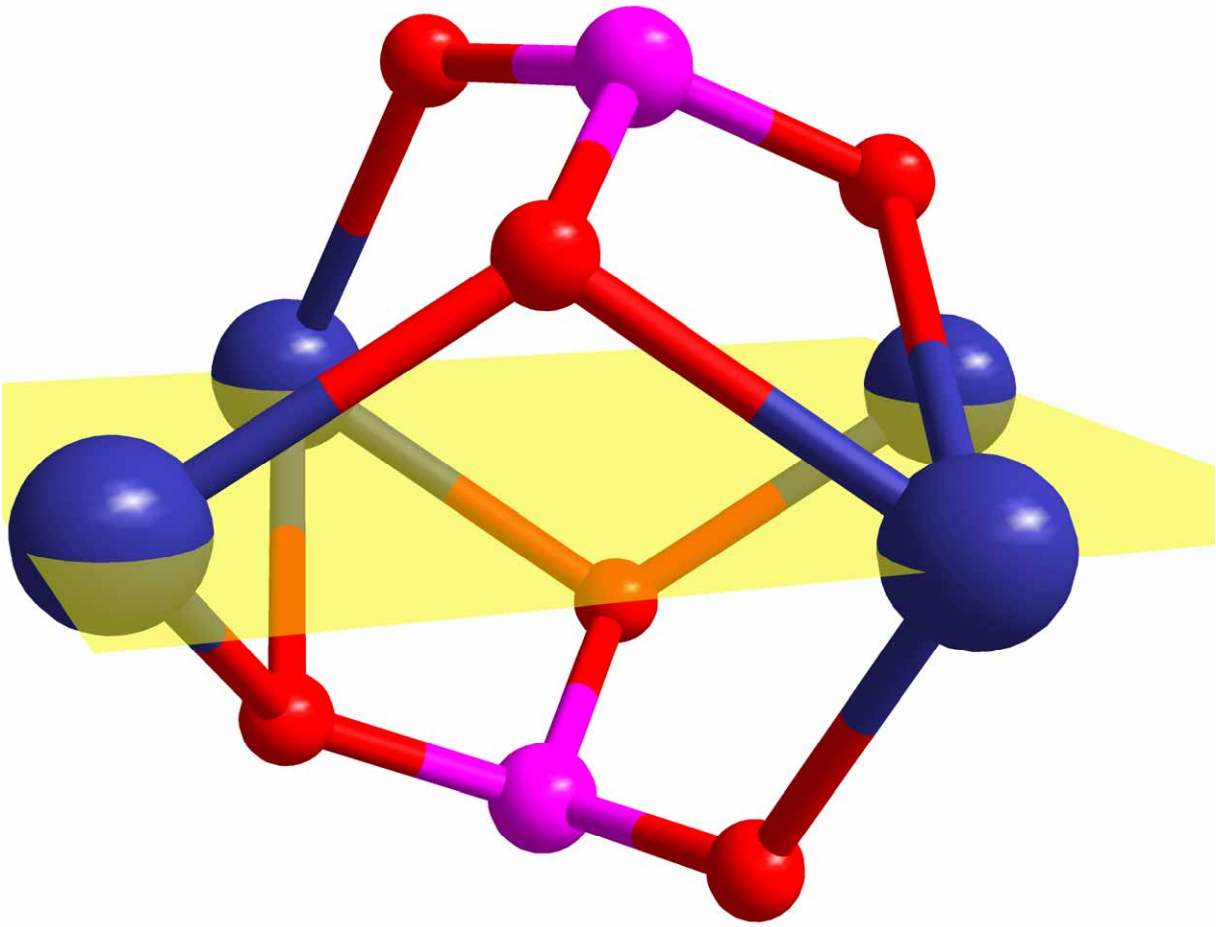

Figure S1(c): Immediate coordination environment around Cd(1) in **1**

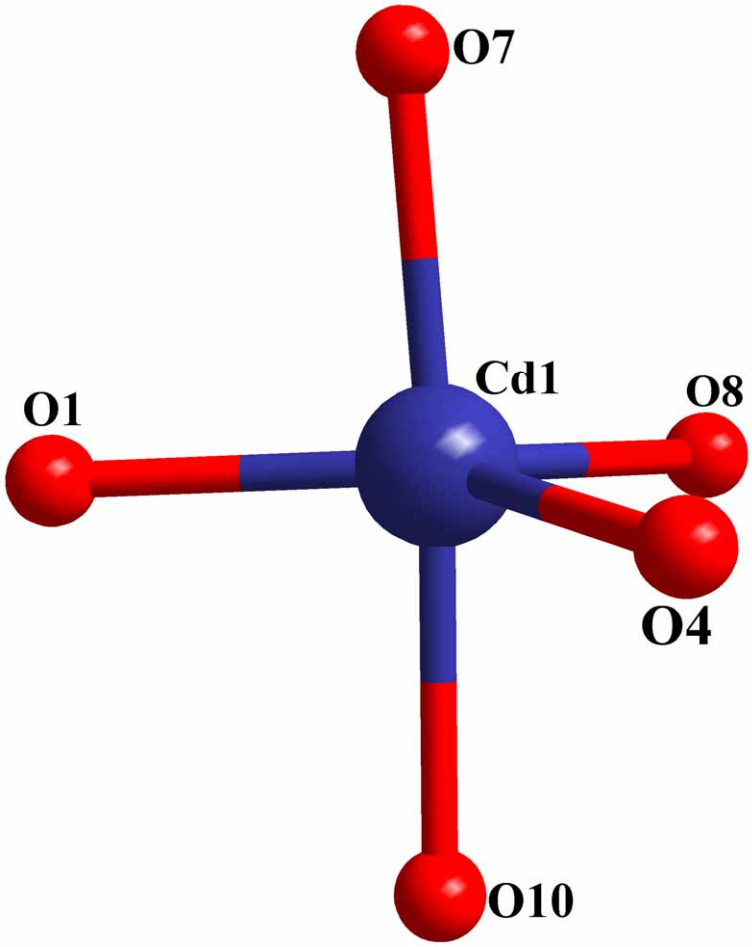

Figure S1(d): Immediate coordination environment around Cd(2) in **1**

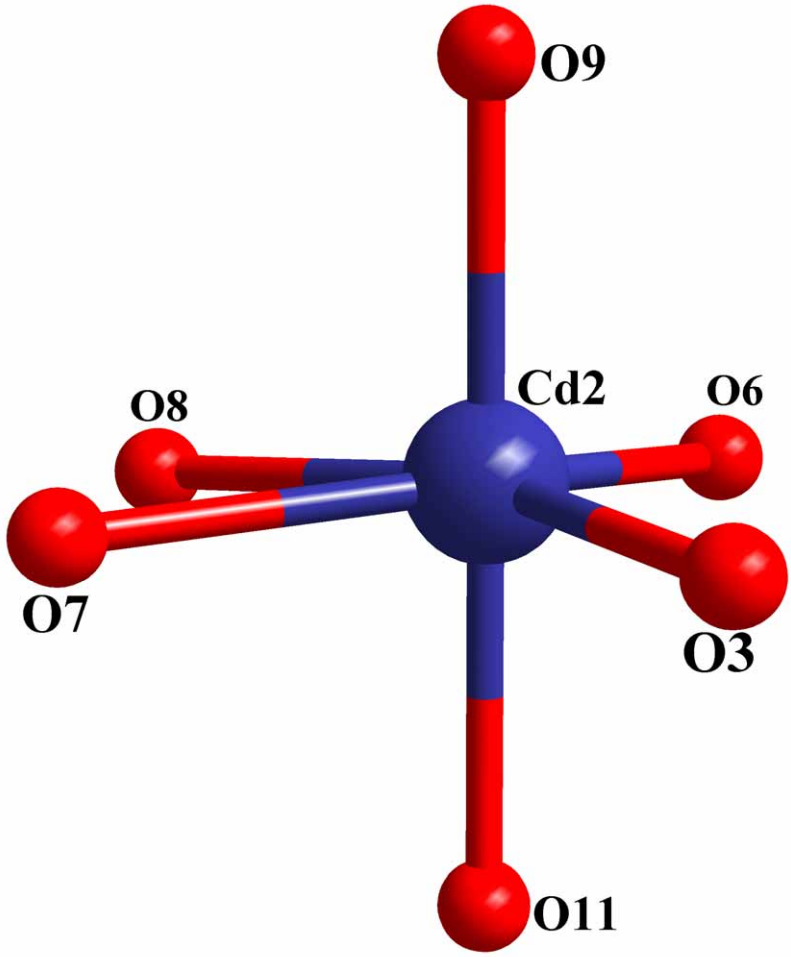

Figure S2(a): Molecular structure of **2**

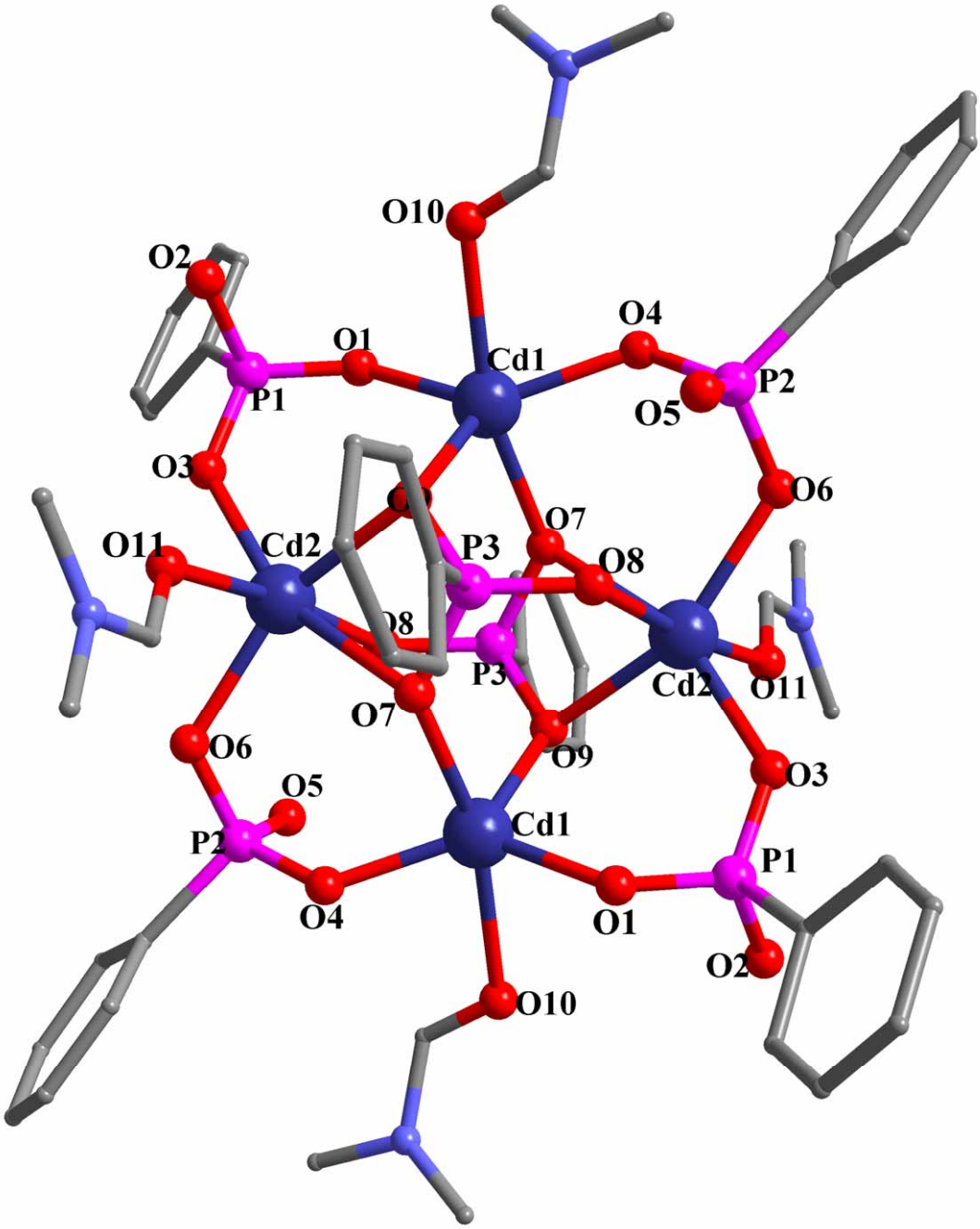

Figure S2(b): Plane representation of **2**

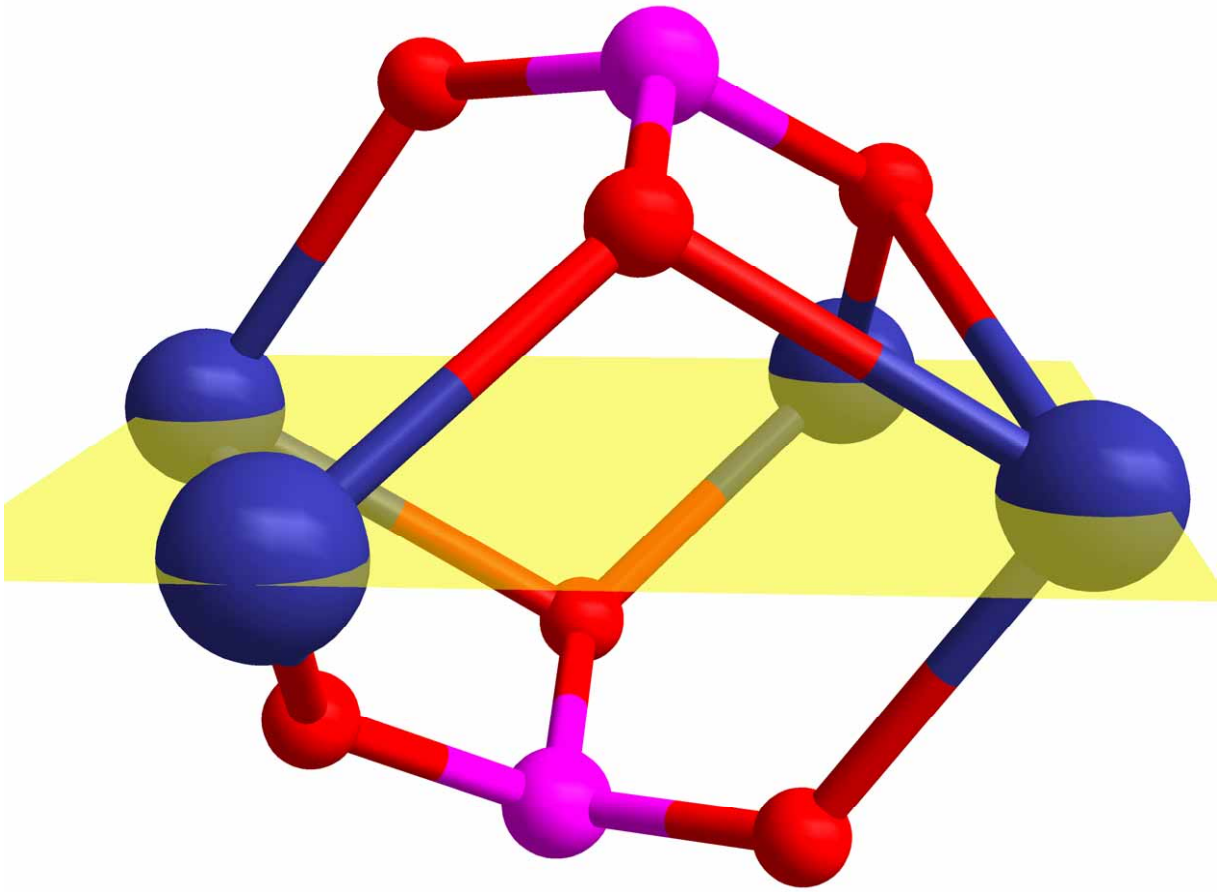

Figure S2(c): Immediate coordination environment around Cd(1) in **2**

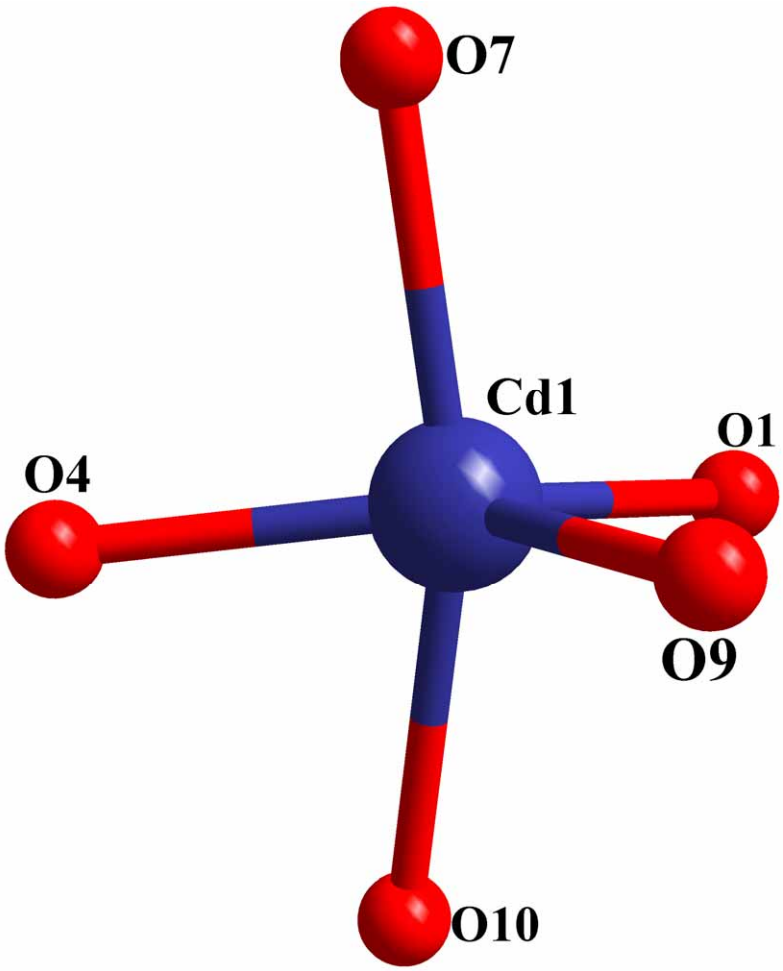

Figure S2(d): Immediate coordination environment around Cd(2) in **2**

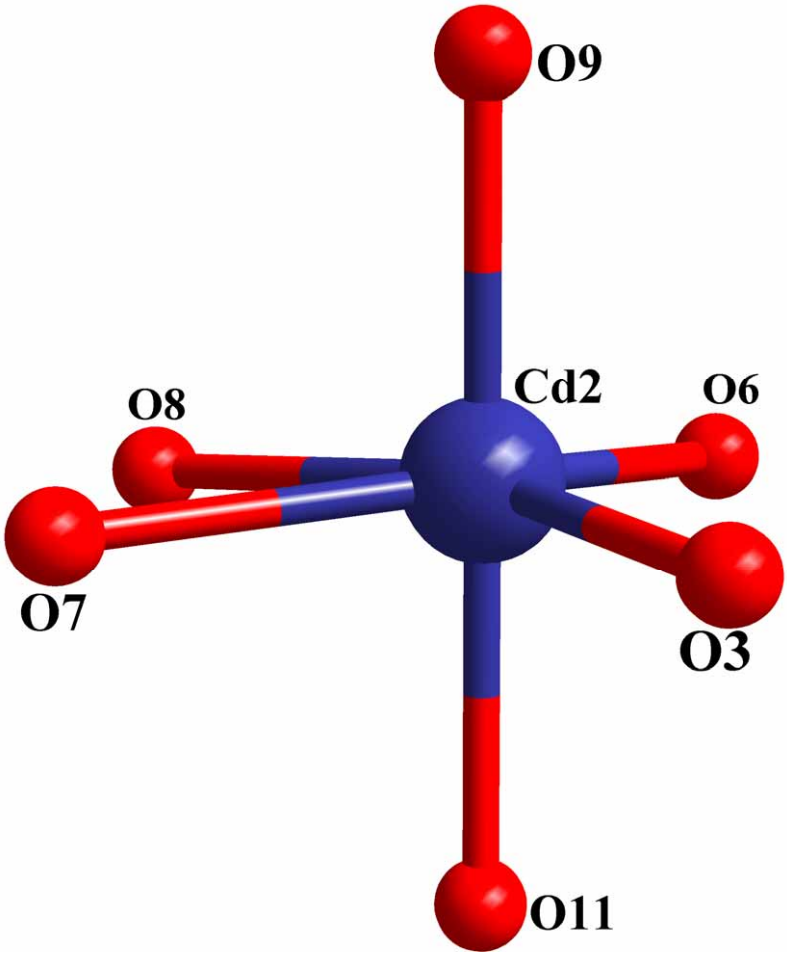

Figure S3(a): Molecular structure of **3**

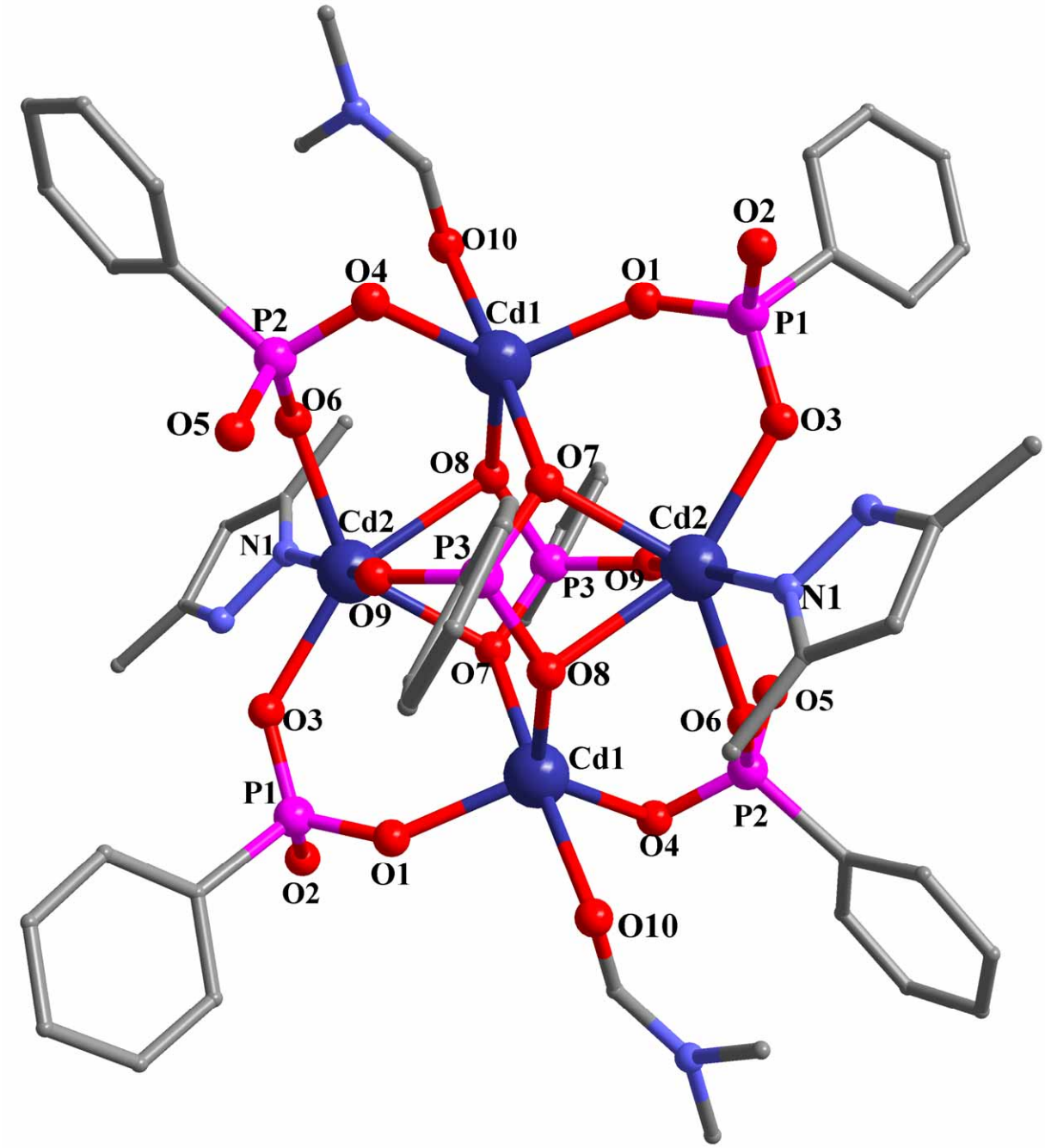

Figure S3(b): Plane representation of **3**

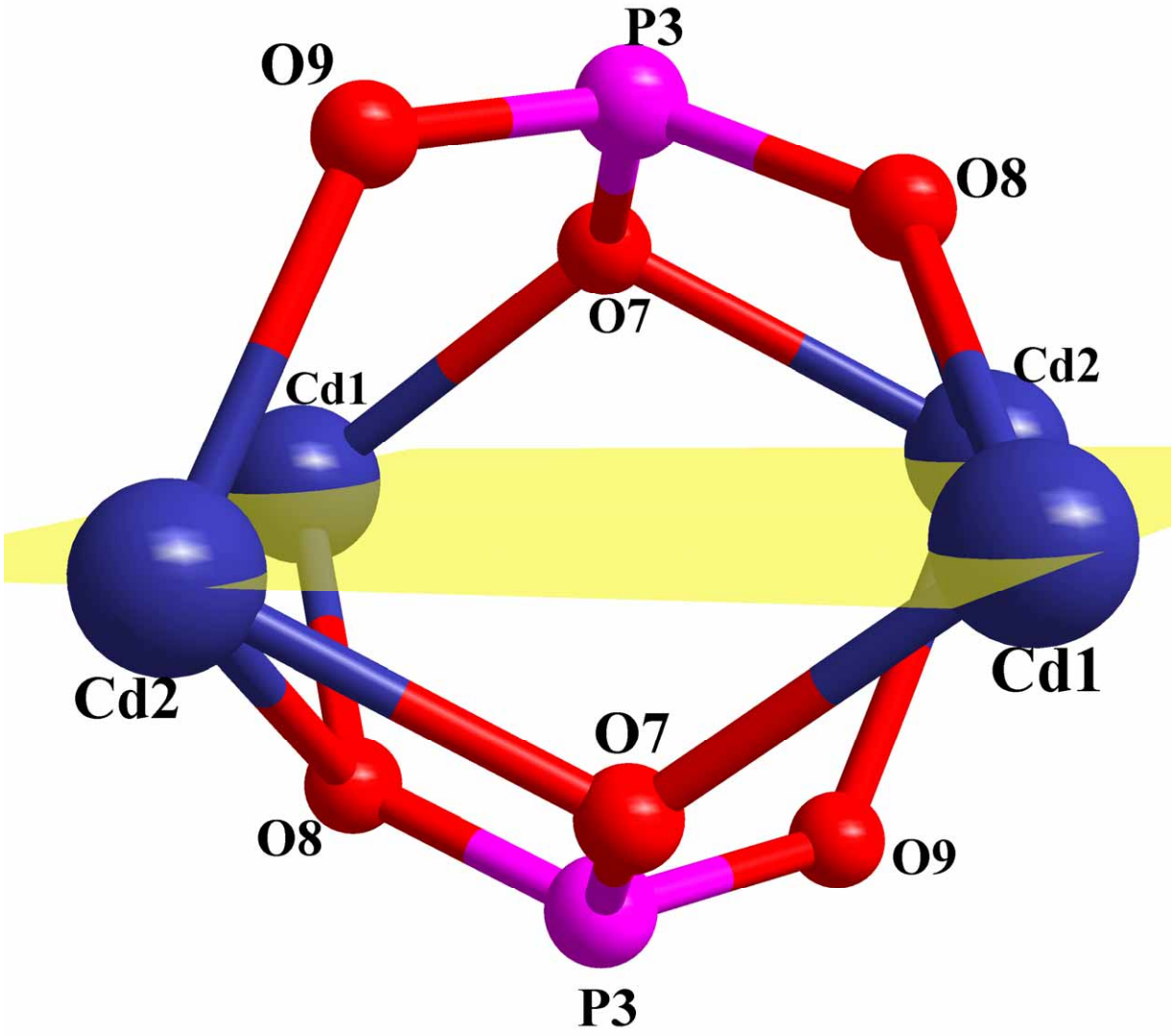

Figure S3(c): Immediate coordination environment around Cd(1) in **3**

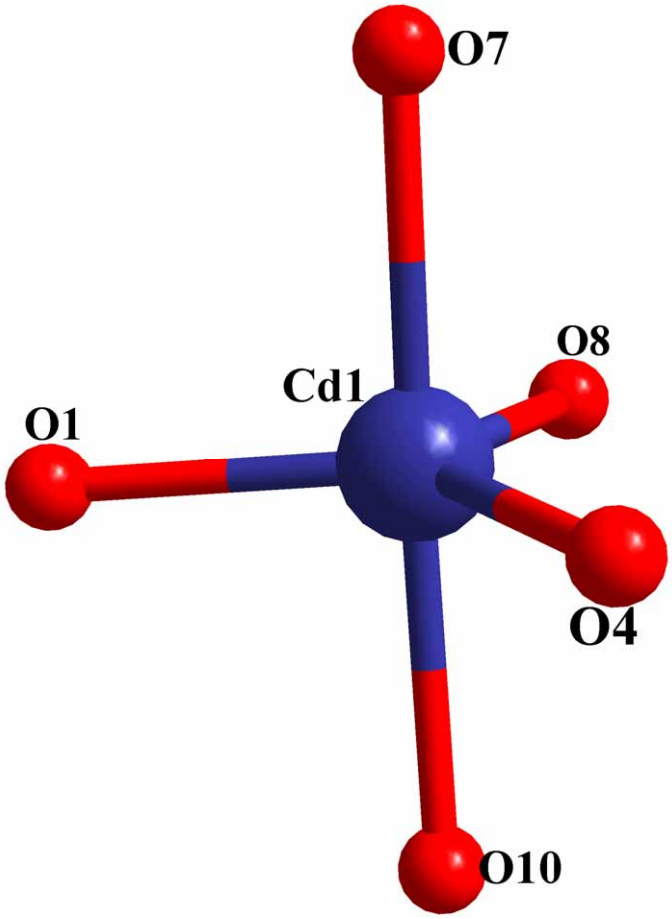

Figure S3(d): Immediate coordination environment around Cd(2) in **3**

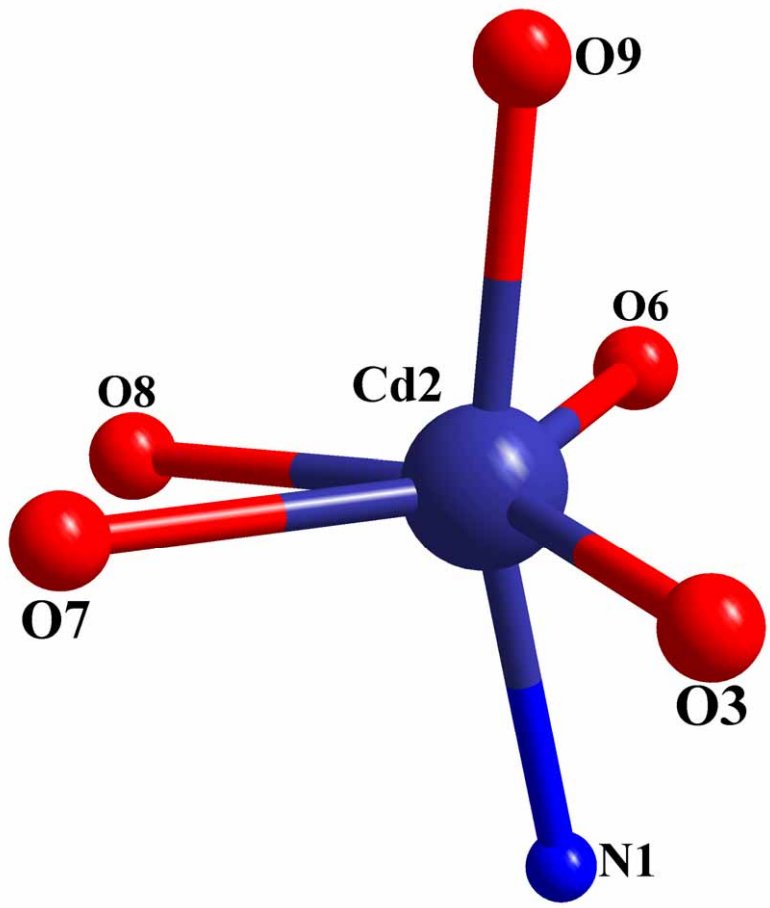

Figure S4(a): Plane representation of **4**

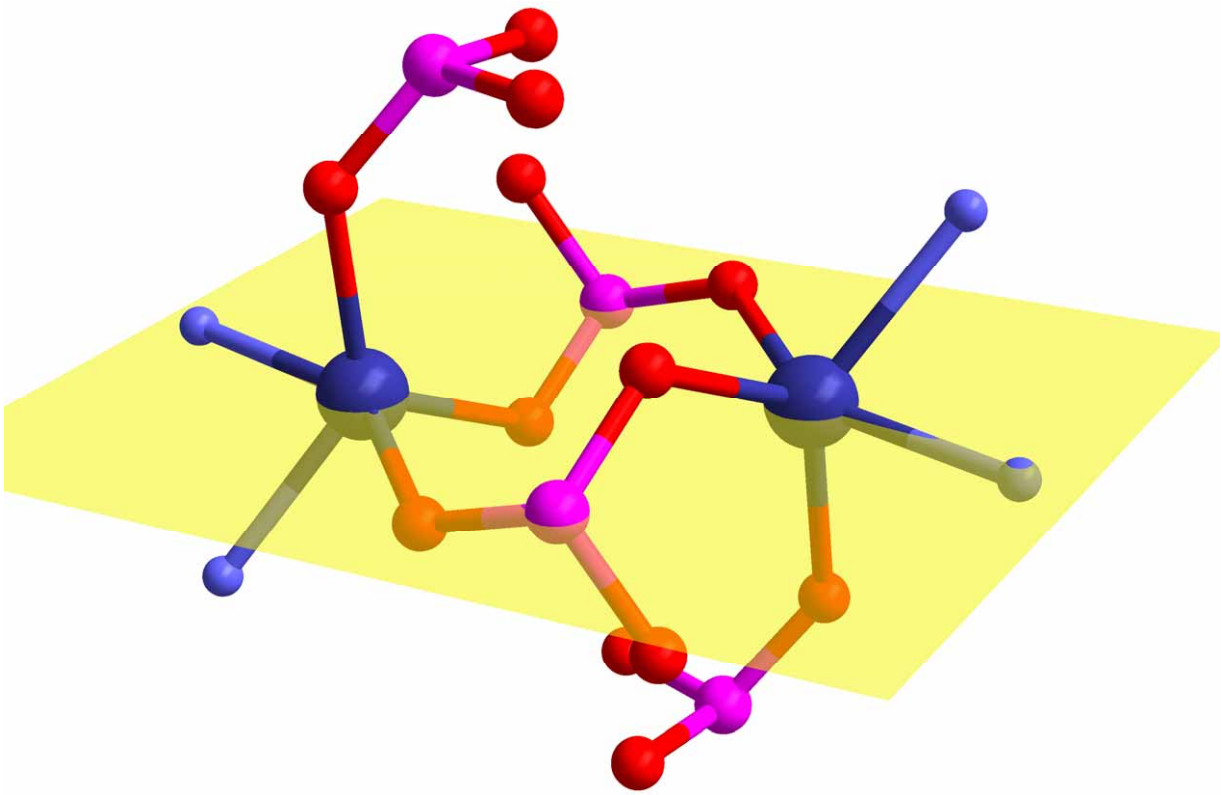

Figure S4(b): Immediate coordination environment around Cd(1) in **4**

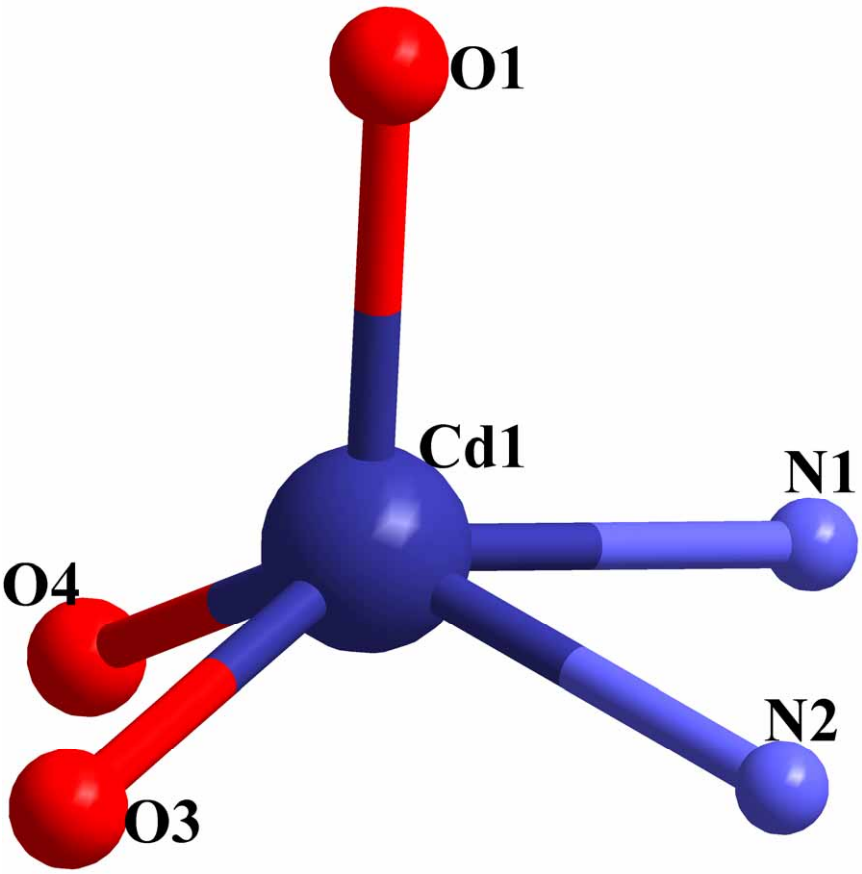

Figure S5: Immediate coordination environment around Cd(1) in **5**

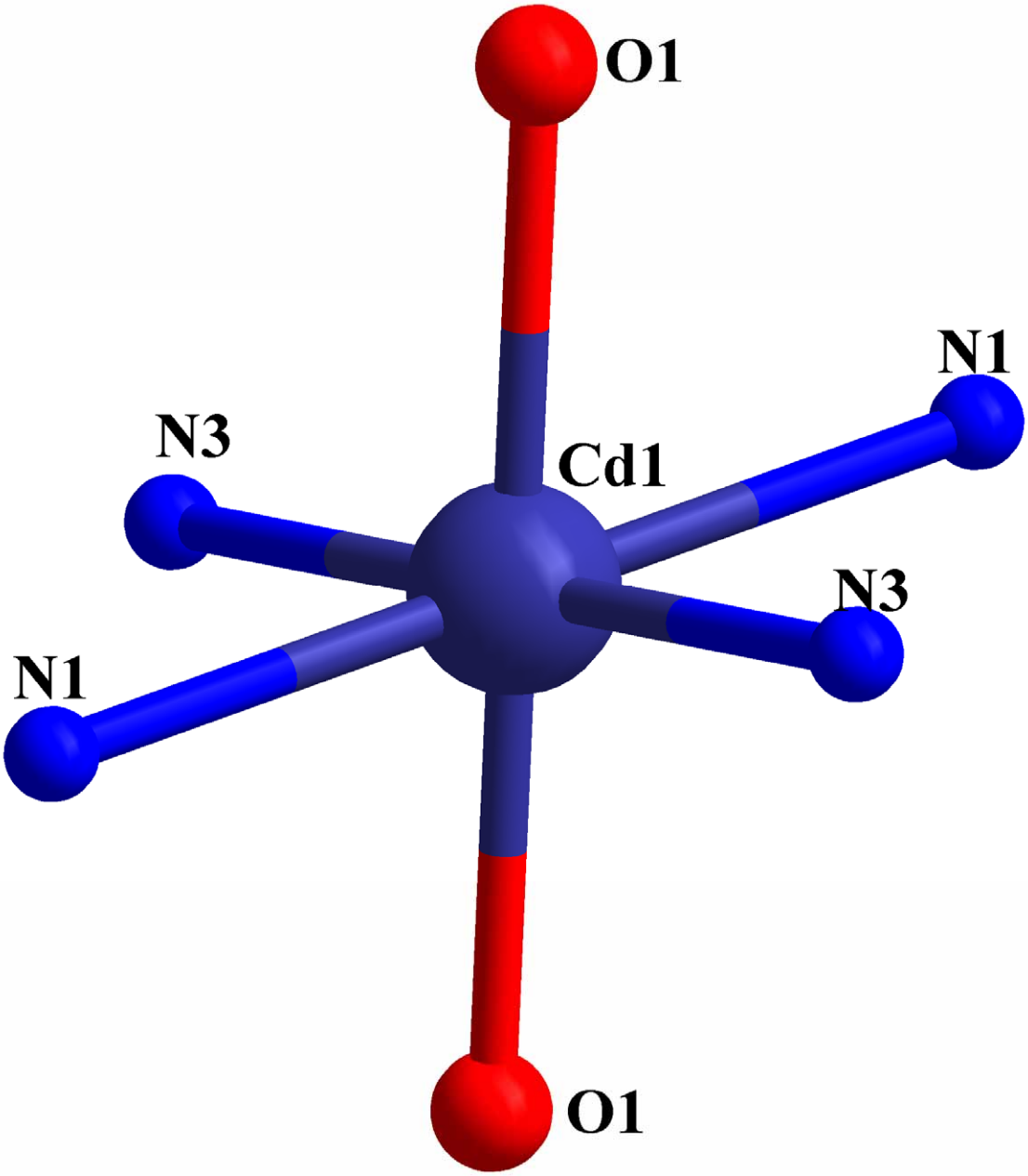

Figure S6: Infrared spectrum of **1** recorded as a KBr pellet

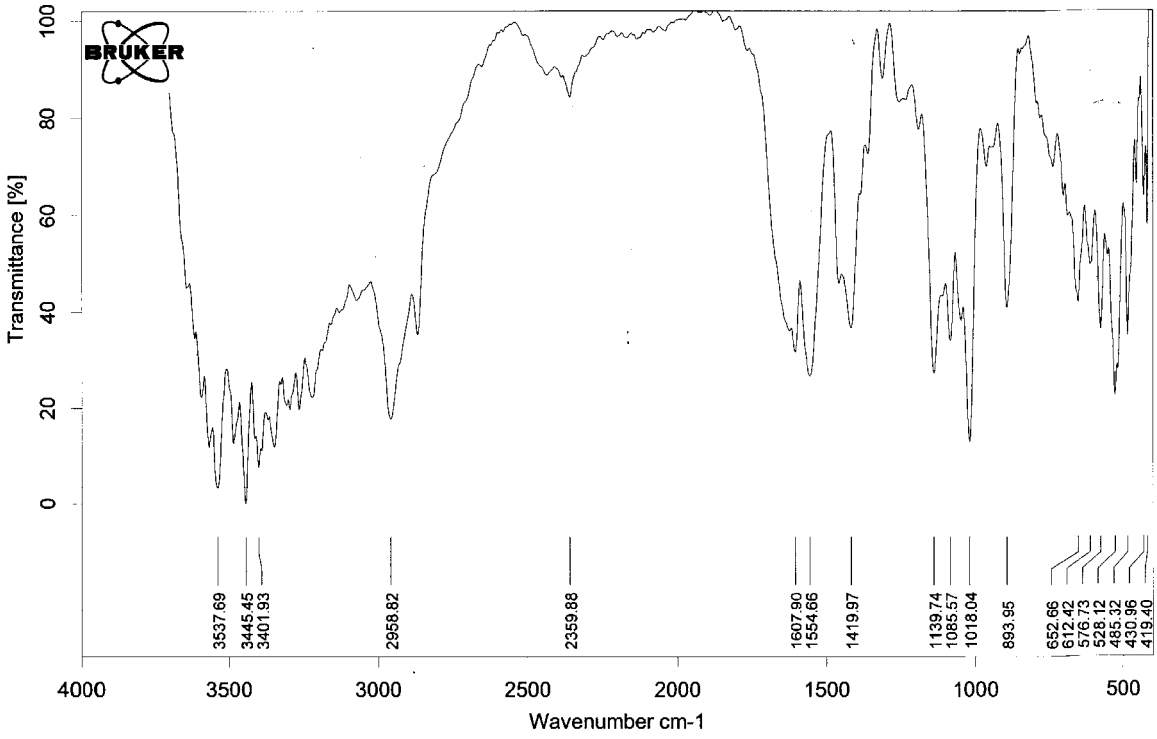

Figure S7: Infrared spectrum of **2** recorded as a KBr pellet

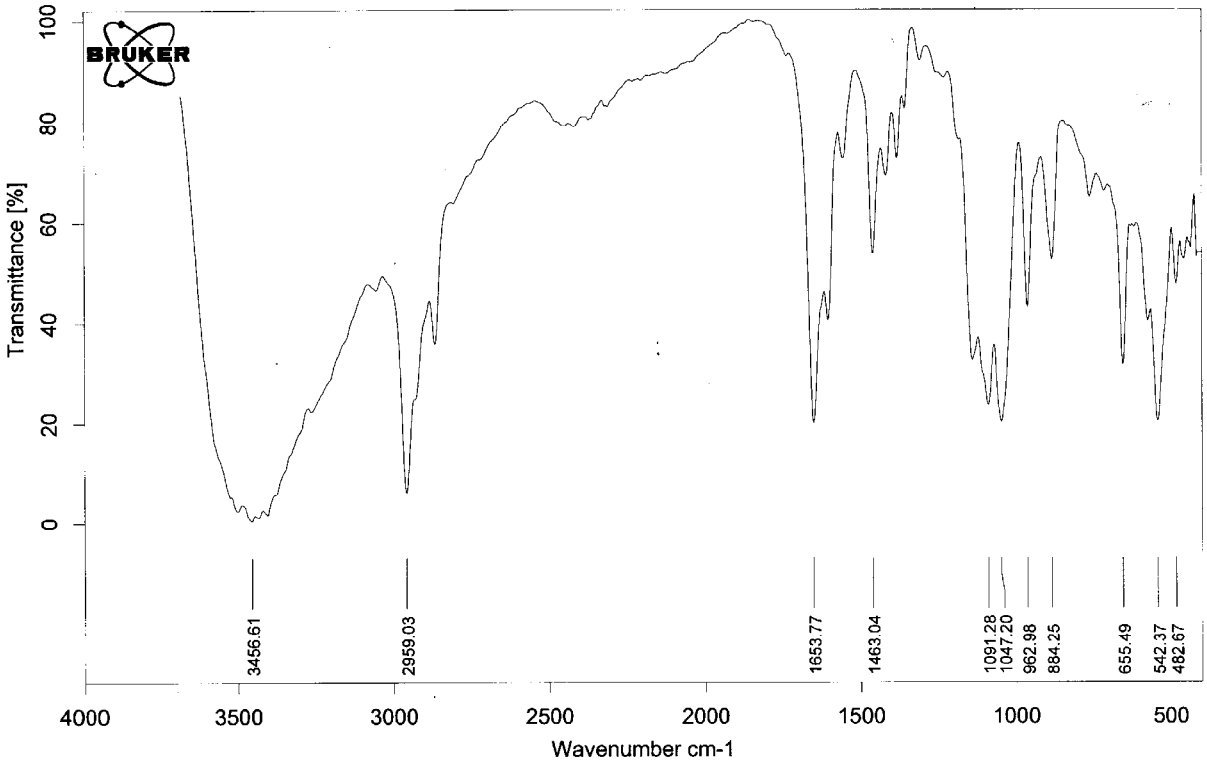

Figure S8: Infrared spectrum of **3** recorded as a KBr pellet

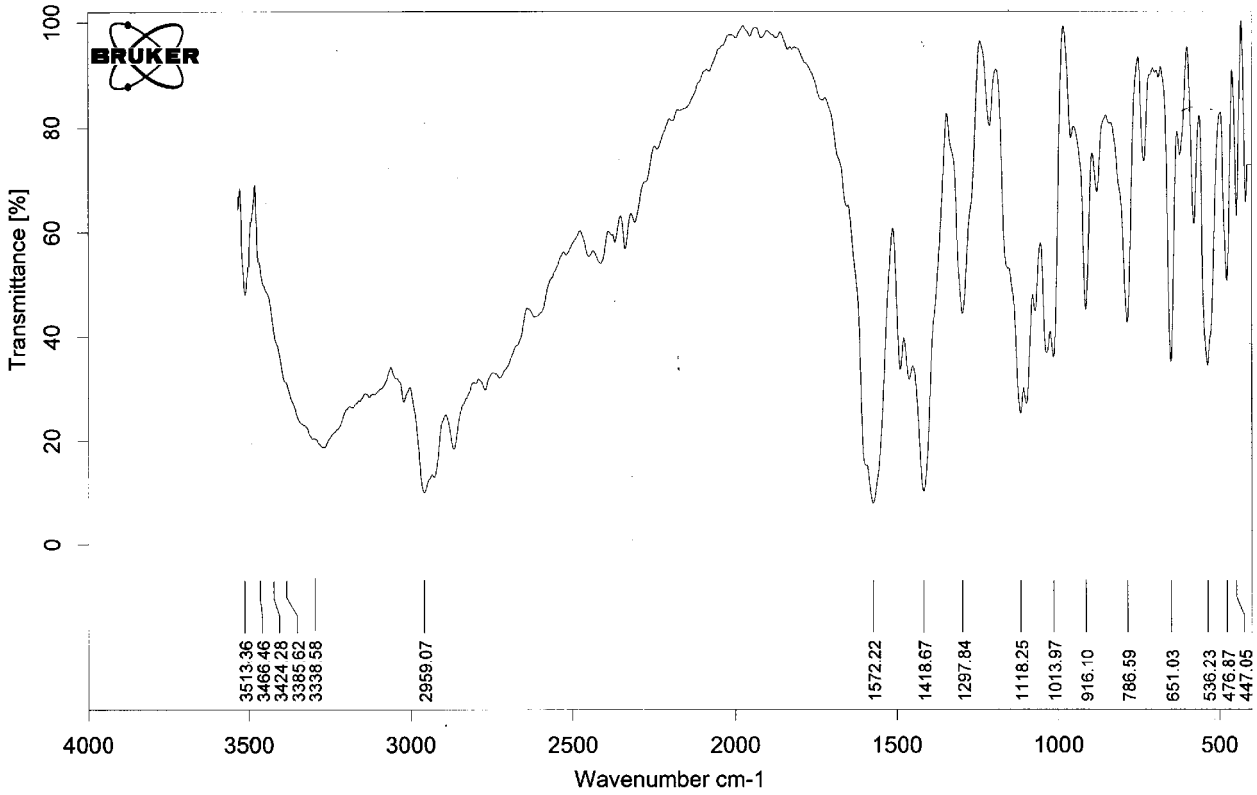

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Figure S9: Infrared spectrum of **4** recorded as a KBr pellet

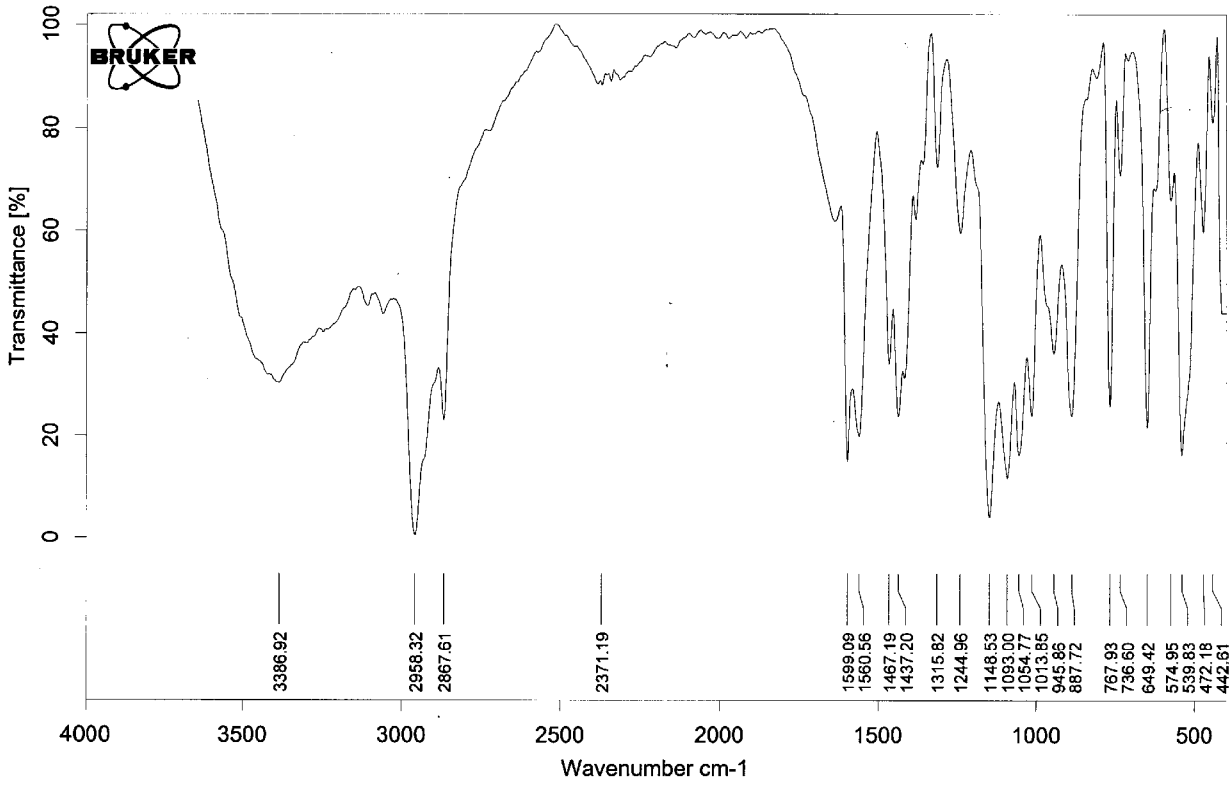


Figure S10: Infrared spectrum of **5** recorded as a KBr pellet

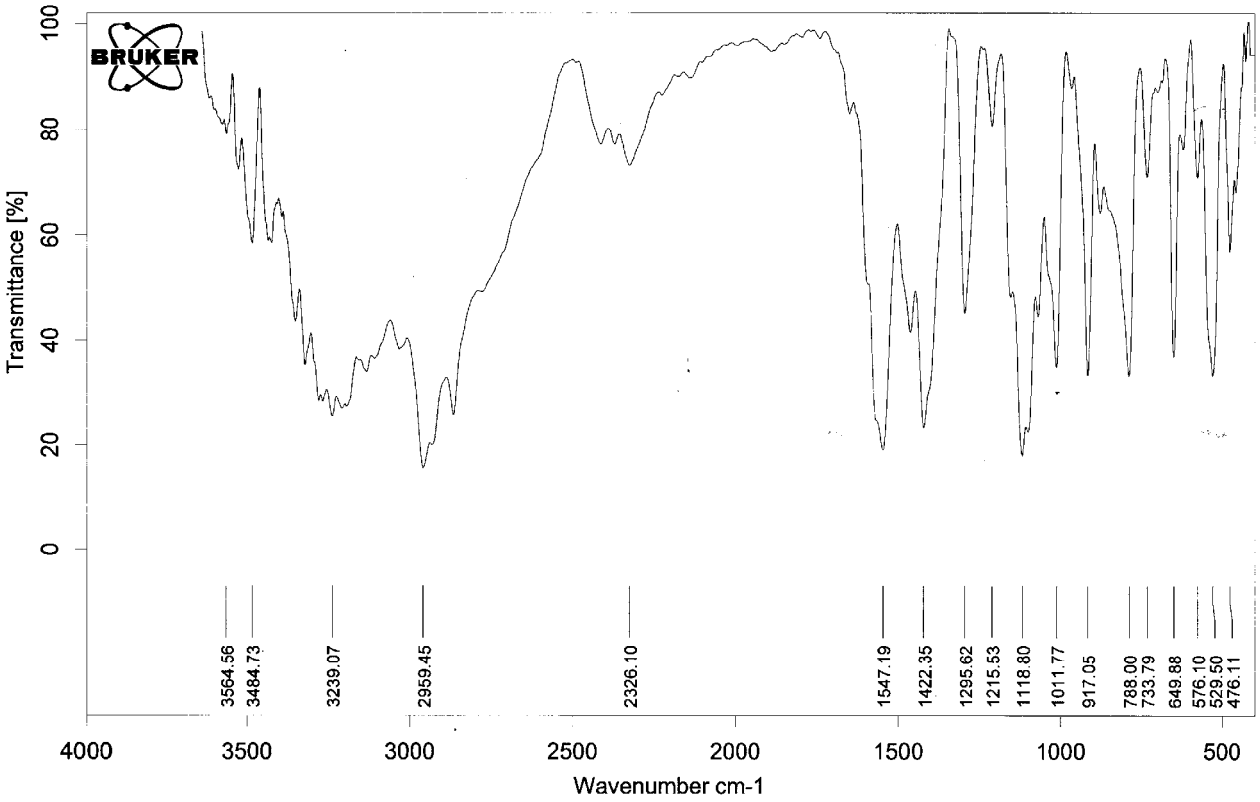


Figure S11(a) : Infrared spectrum of the char residue of **1** recorded as a KBr pellet

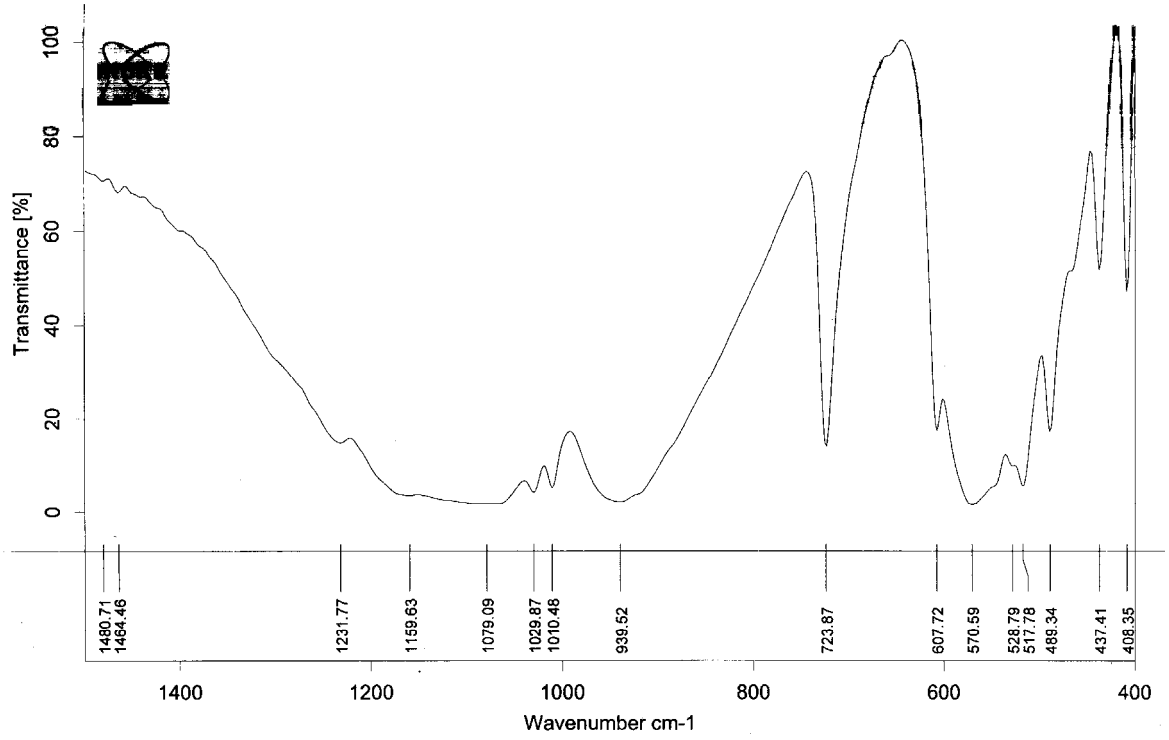


Figure S11(b) : Infrared spectrum of $Cd_2P_2O_7$[1]

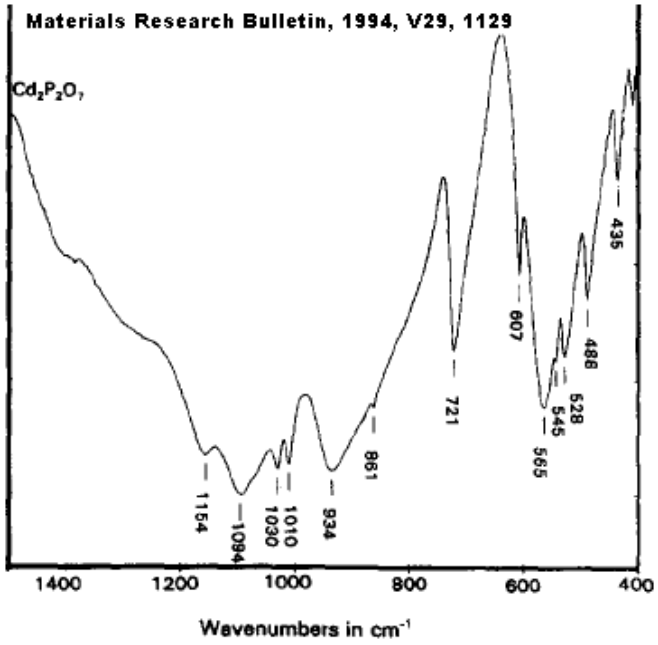
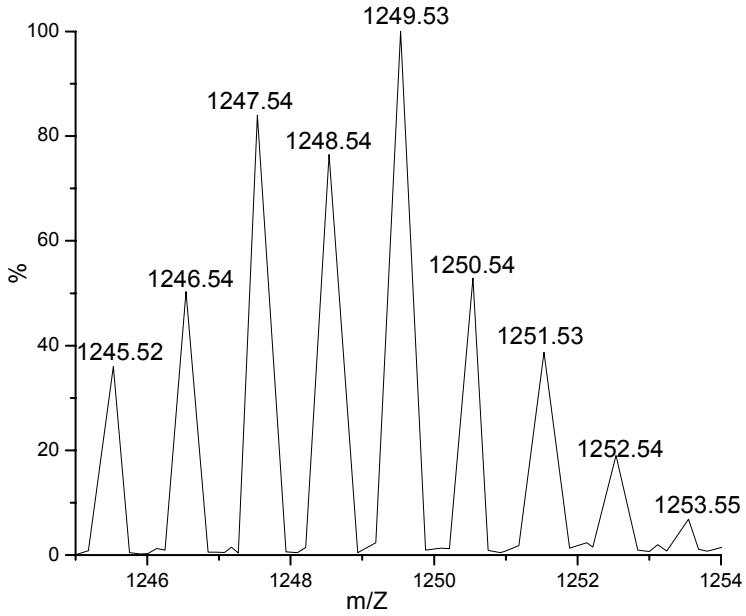
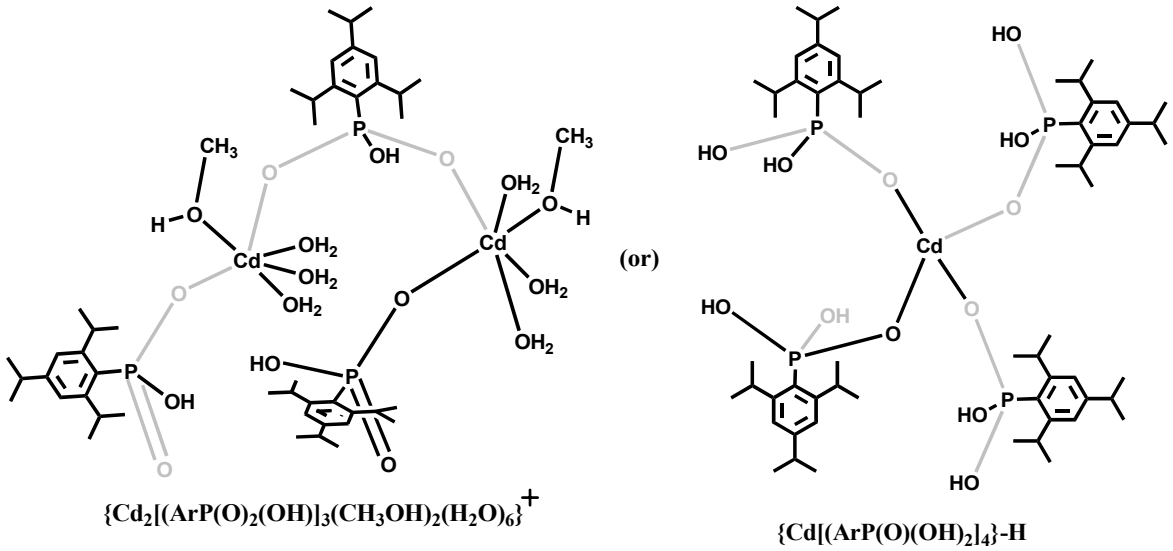


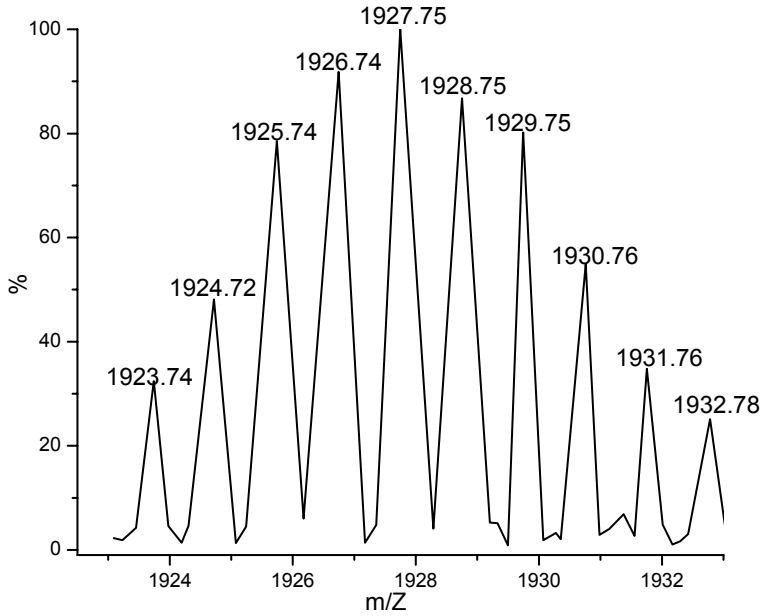
Figure S12(a): ESI-MS of **1** of fragmented species. The possible fragments are shown below.

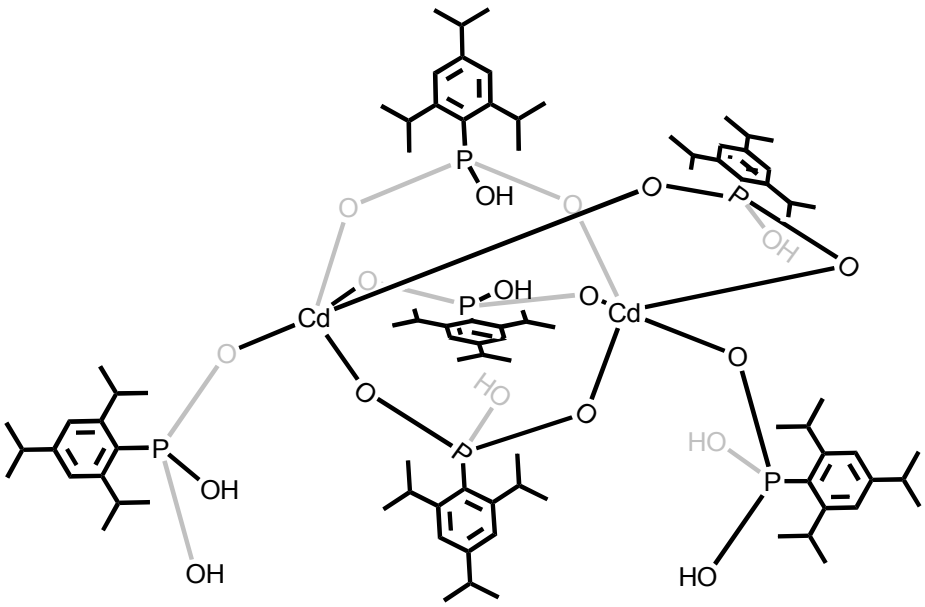




$\{Cd_2[(ArP(O)_2(OH)]_3(CH_3OH)_2(H_2O)_6\}^+$ $\{Cd[(ArP(O)(OH)_2]_4\}$-H

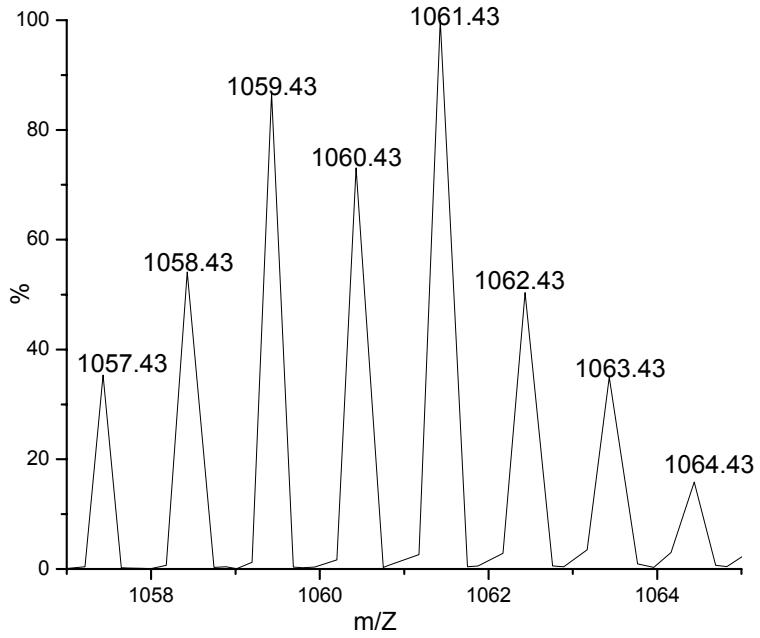
Figure S12(b): ESI-MS of **1** of fragmented species. The possible fragments are shown below.

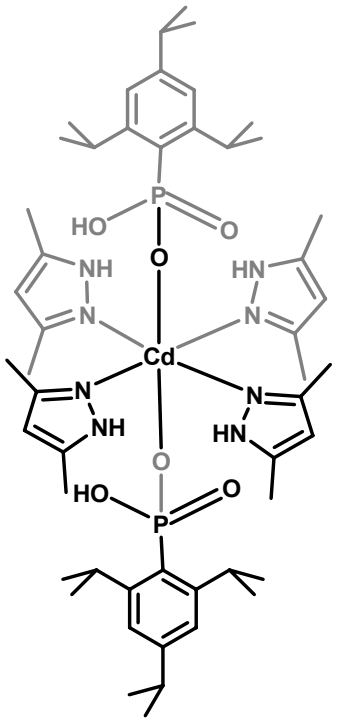




$\{Cd_2[(ArP(O)_2(OH)]_4[(ArPO(OH)_2]_2\}$-H

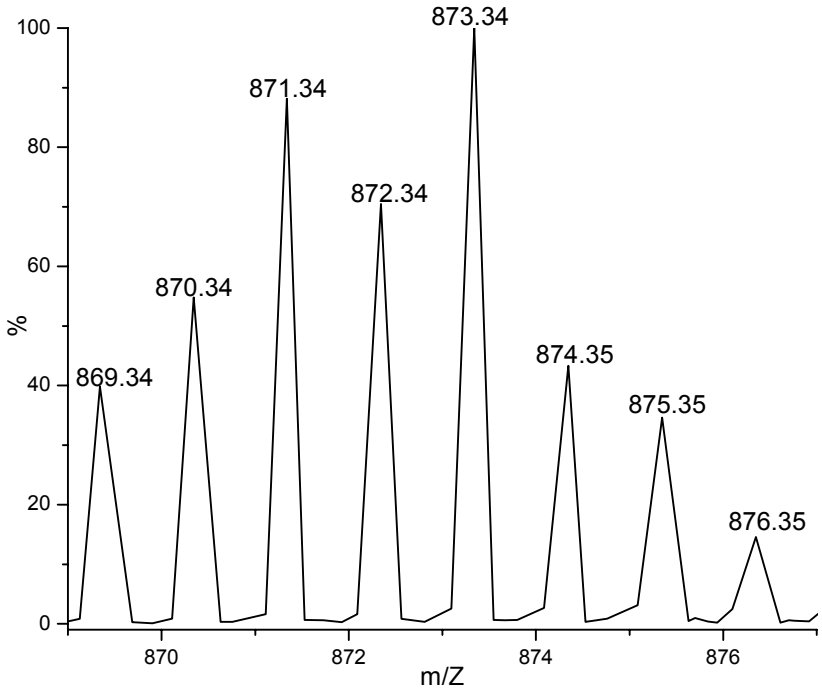
Figure S13(a): ESI-MS of **5** shows parent ion peak $[M-H]^+$

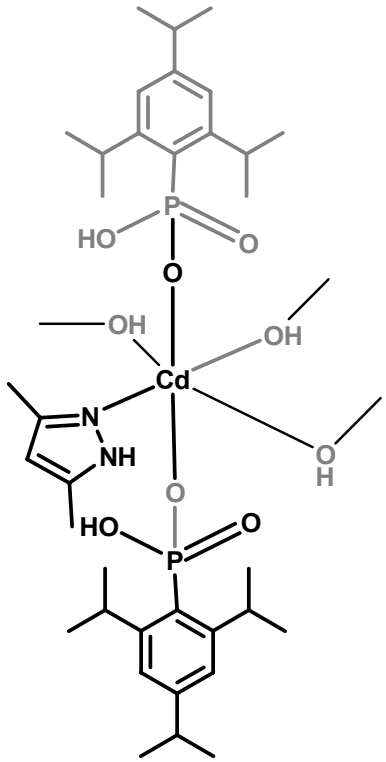




{Cd[(ArP(O)$_2$(OH)]$_2$[(DMPZH)]$_4$}-H

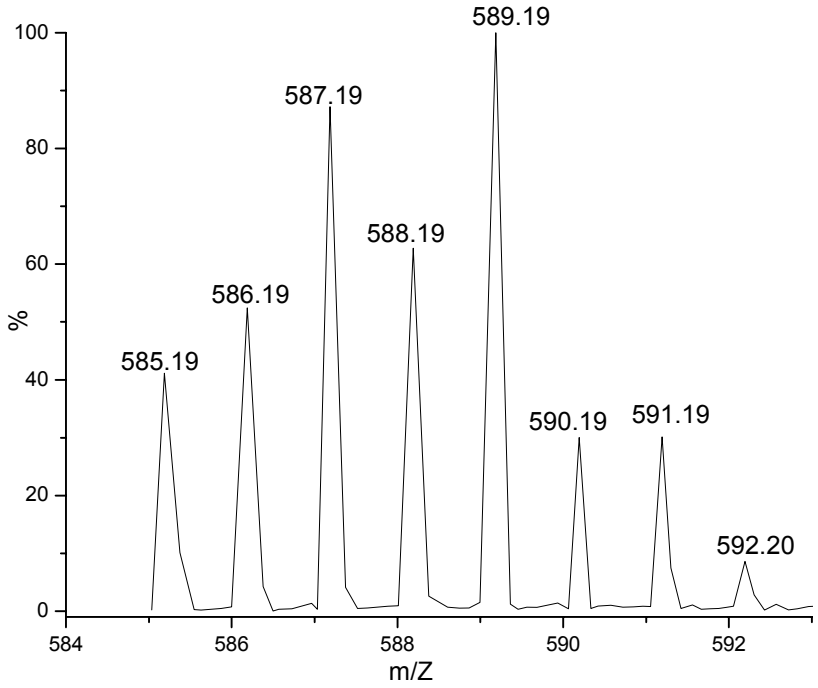
Figure S13(b): ESI-MS of **5** of fragmented species. The possible fragments are shown below.

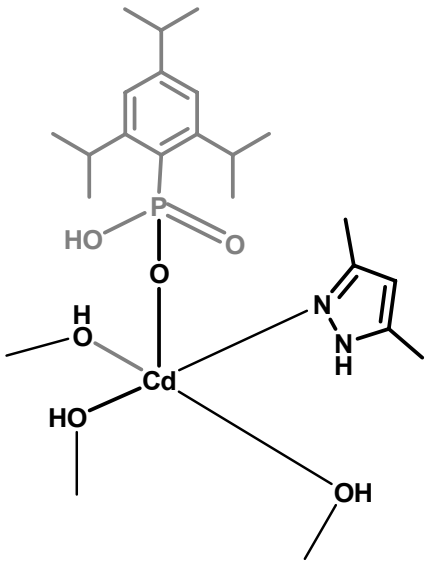




{Cd[(ArP(O)$_2$(OH)]$_2$(DMPZH)(MeOH)$_3$}-H

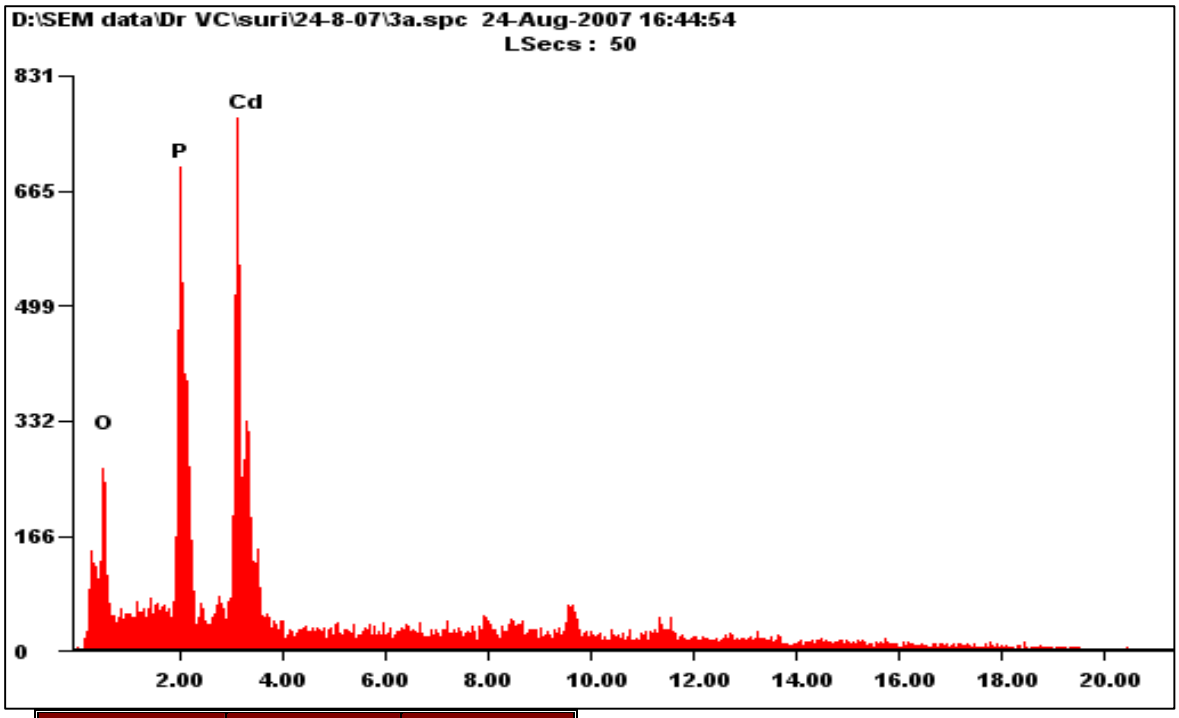
Figure S13(c): ESI-MS of **5** of fragmented species. The possible fragments are shown below.





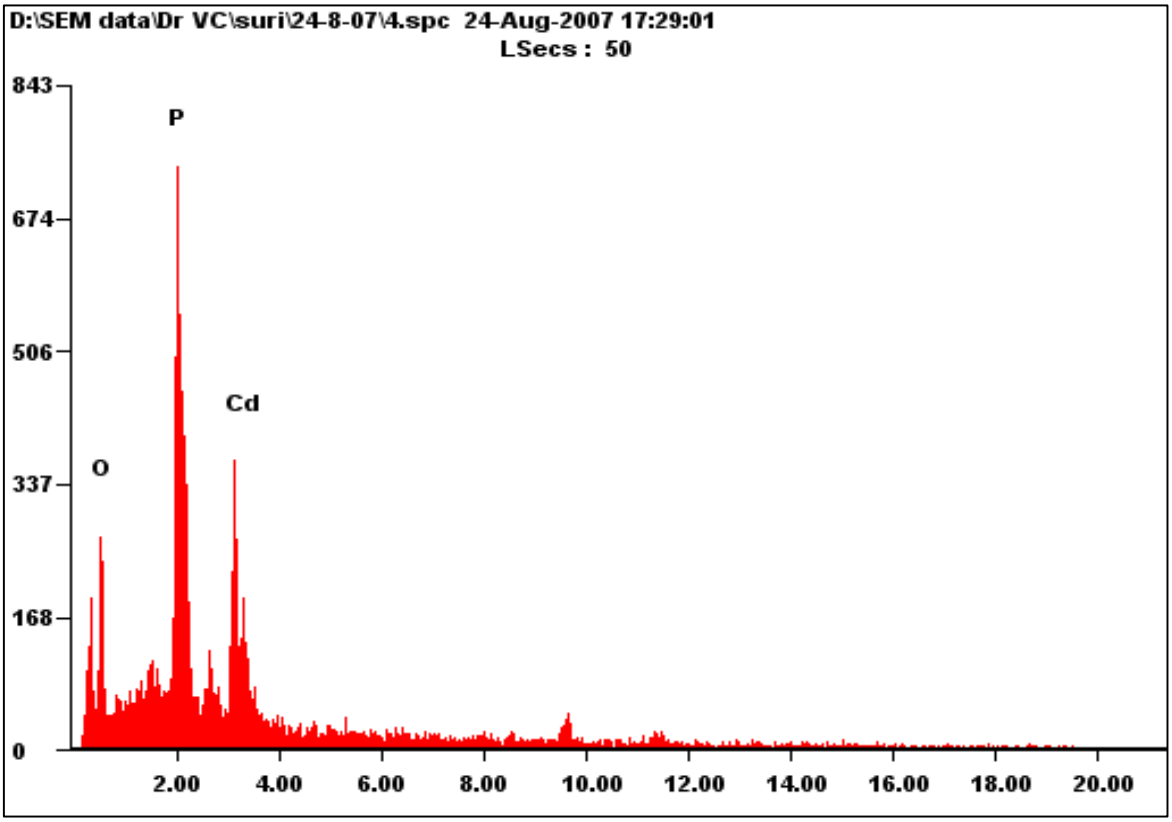
{Cd[(ArP(O)$_2$(OH)](DMPZH)(MeOH)$_3$}

Figure S14(a): EDX analysis of char residue obtained from **1**



Element	*Wt %*	*At %*
O K	29.01	64.24
P K	16.15	18.48
CdL	54.83	17.28

Figure S14(b): EDX analysis of char residue obtained from **4**



Element	*Wt %*	*At %*
O K	28.70	64.05
P K	16.22	18.69
CdL	55.08	17.26

Figure S15: SEM picture of the char residue obtained in the TGA of **1**

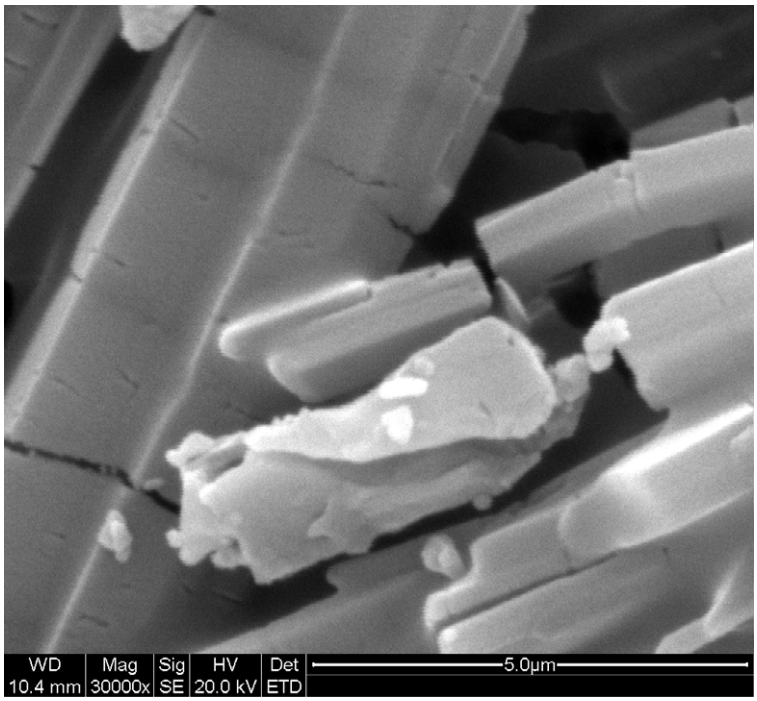


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Table S1(a): Selected bond distance data (Å) for **1** and **2**

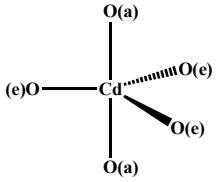
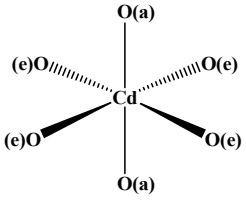
Bond distances Å				
Geometry	**1**		**2**	
	Cd(1)-O(7) Cd(1)-O(10) Cd(1)-O(1) Cd(1)-O(4) Cd(1)-O(8)*	2.260(3) 2.365(3) 2.154(3) 2.183(3) 2.206(3)	Cd(1)-O(7) Cd(1)-O(10) Cd(1)-O(1) Cd(1)-O(4) Cd(1)-O(9)*	2.270(5) 2.424(8) 2.094(6) 2.068(6) 2.171(5)
	Cd(2)-O(9) Cd(2)-O(11) Cd(2)-O(3)* Cd(2)-O(6) Cd(2)-O(7)* Cd(2)-O(8)*	2.263(3) 2.356(4) 2.235(3) 2.181(3) 2.358(3) 2.441(3)	Cd(2)-O(8)* Cd(2)-O(11) Cd(2)-O(3)* Cd(2)-O(6) Cd(2)-O(7) Cd(2)-O(9)	2.286(4) 2.310(5) 2.180(5) 2.210(5) 2.509(5) 2.347(5)

Table S1(b): Selected bond angle data (°) for **1** and **2**

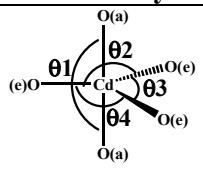
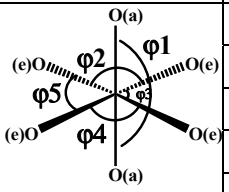
Bond angles °				
Geometry	**1**		**2**	
	O(7)-Cd(1)-O(10)	175.67(12)	O(7)-Cd(1)-O(10)	163.3(2)
	O(1)-Cd(1)-O(8)*	129.90(12)	O(4)-Cd(1)-O(1)	135.4(2)
	O(4)-Cd(1)-O(8)*	99.14(12)	O(1)-Cd(1)-O(9)*	100.1(2)
	O(1)-Cd(1)-O(4)	129.76(13)	O(4)-Cd(1)-O(9)*	122.7(2)
	O(9)-Cd(2)-O(11)	176.68(14)	O(8)*-Cd(2)-O(11)	173.84(18)
	O(6)-Cd(2)-O(8)*	91.49(12)	O(6)-Cd(2)-O(7)	92.21(18)
	O(6)-Cd(2)-O(3)*	108.71(13)	O(3)*-Cd(2)-O(6)	111.0(2)
	O(3)*-Cd(2)-O(7)*	97.68(12)	O(3)*-Cd(2)-O(9)	96.67(18)
	O(7)*-Cd(2)-O(8)*	61.14(10)	O(9)-Cd(2)-O(7)	59.81(15)

Table S2: Comparison of Infrared spectral data of char residue obtained from **1** with that of **$Cd_2P_2O_7$**[1]

TGA residue of **1**	**$Cd_2P_2O_7$**	Stretching vibration ν
1160 (s) 1079 (s)	1154 (s) 1094 (vs)	PO_3 (asym)
1030 (s) 1010 (s)	1030 (s) 1010 (s)	PO_3 (sym)
940 (s)	934 (s) 861 (sh)	POP (asym)
724 (m)	721 (m)	POP (sym)

TGA residue of **1**	**$Cd_2P_2O_7$**	Bending vibration δ
608 (m) 571 (s) 546 (sh)	607 (m) 565 (s) 545 (sh)	PO_3 (asym)
529 (m) 518 (m) 489 (m) 437 (w) 408 (w)	528 (m) 488 (m) 435 (w) 409 (vw)	PO_3 (sym)

References

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(1) D. D. Waal and C. Hutter, *Mater. Res. Bull.* 1994, **29**, 1129.