

Unusual $\{\cdots\text{HNC}_2\text{O}\cdots\text{HC}_n\text{O}\}$, $n = 1$ or 2 , synthons predominate in the molecular packing of the one-dimensional coordination polymers, $\{\text{Cd}[\text{S}_2\text{P}(\text{OR})_2]_2(^3\text{LH}_2)\}_n$, for $R = \text{Me}$ and Et , but are precluded when $R = i\text{-Pr}$; $^3\text{LH}_2 = N,N'$ -bis(3-pyridylmethyl)oxalamide†

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ELECTRONIC SUPPLEMENTARY INFORMATION

ESI Figure 1. Measured (blue trace) and simulated (red trace) PXRD patterns for (a) **1** (b) **2** and (c) **3**.

ESI Figure 2. FT-IR spectra for (a) **1**, (b) **2** and (c) **3**.

ESI Figure 3. NMR spectra measured in DMSO- d_6 for **1**: (a) ^1H , (b) $^{13}\text{C}\{^1\text{H}\}$ and (c) $^{31}\text{P}\{^1\text{H}\}$.

ESI Figure 4. NMR spectra measured in DMSO- d_6 for **2**: (a) ^1H , (b) $^{13}\text{C}\{^1\text{H}\}$ and (c) $^{31}\text{P}\{^1\text{H}\}$.

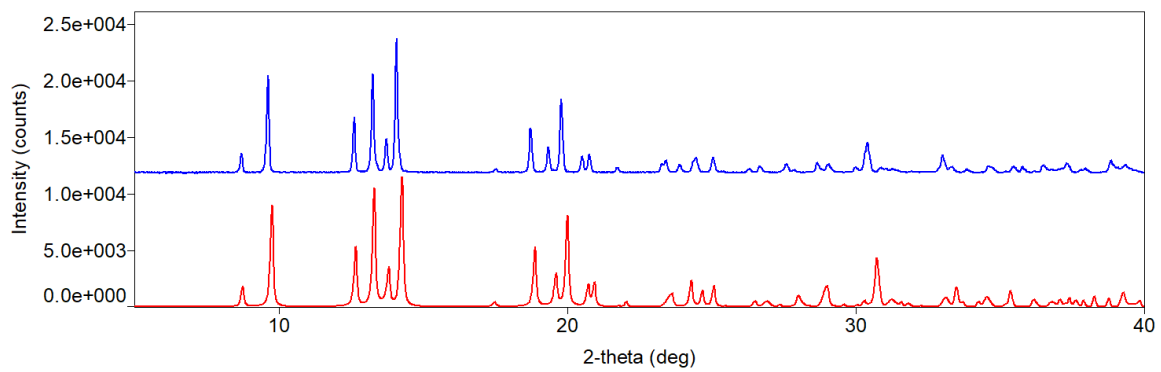
ESI Figure 5. NMR spectra measured in DMSO- d_6 for **3**: (a) ^1H , (b) $^{13}\text{C}\{^1\text{H}\}$ and (c) $^{31}\text{P}\{^1\text{H}\}$.

ESI Figure 6. Solid-state ^{13}C CP MAS spectra of (a) **1**, (b) **2** and (c) **3** measured at 25 °C. “*” denotes spinning side-bands.

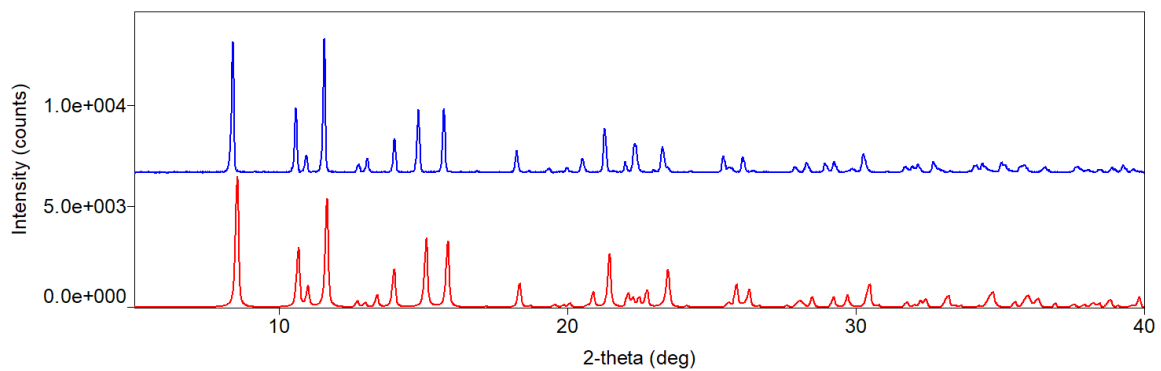
ESI Figure 7. Views of the d_{norm} -Hirshfeld surfaces for (a) **1**, (b) **2** and (c) **3** (two independent molecules), highlighting the brightest red spots owing to the covalent bonds between each repeat unit.

ESI Figure 8. Views of the d_{norm} -Hirshfeld surfaces for **3**, highlighting the weak intermolecular contacts between the Cd1- and Cd2-containing repeat units (a) C \cdots S and H \cdots H contacts and (b) C–H \cdots O contacts.

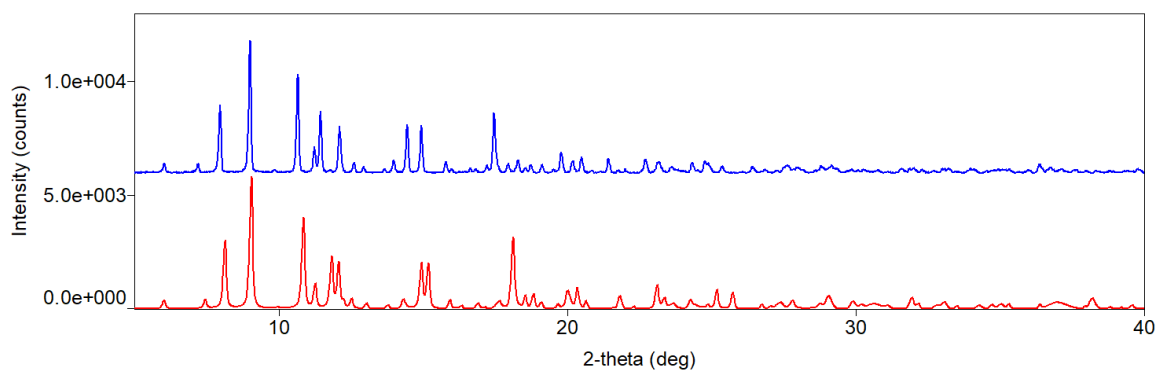
ESI Figure 9. Overall two-dimensional fingerprint plots for **1**, **2**, **3_Cd1** and **3_Cd2**, and those delineated into H \cdots H, H \cdots S/S \cdots H, H \cdots O/O \cdots H and H \cdots C/C \cdots H.



(a)

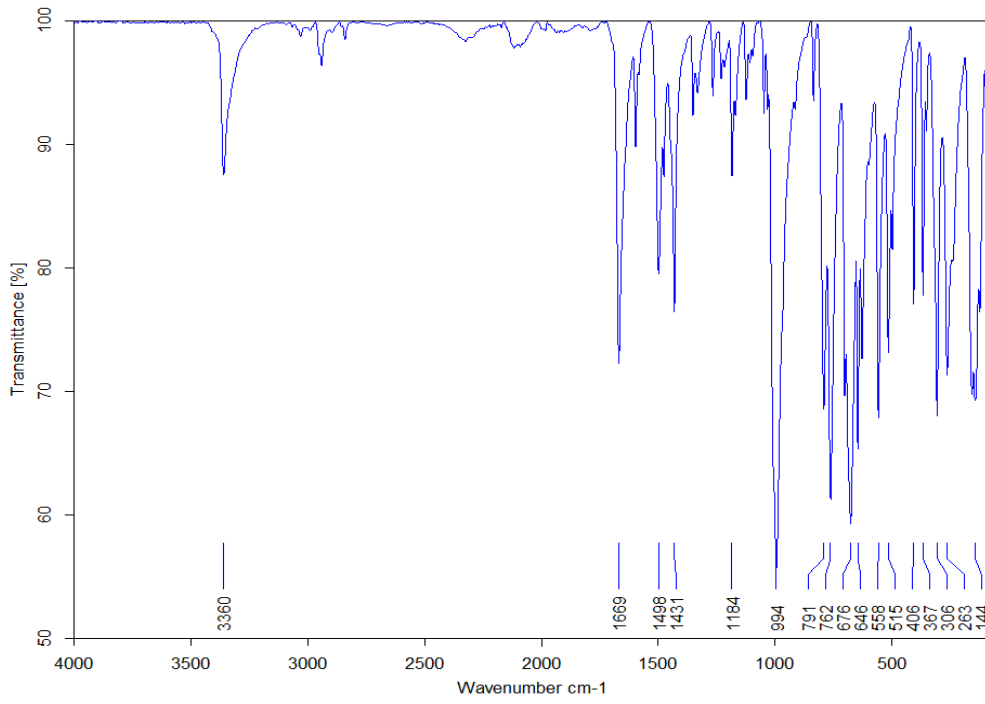


(b)

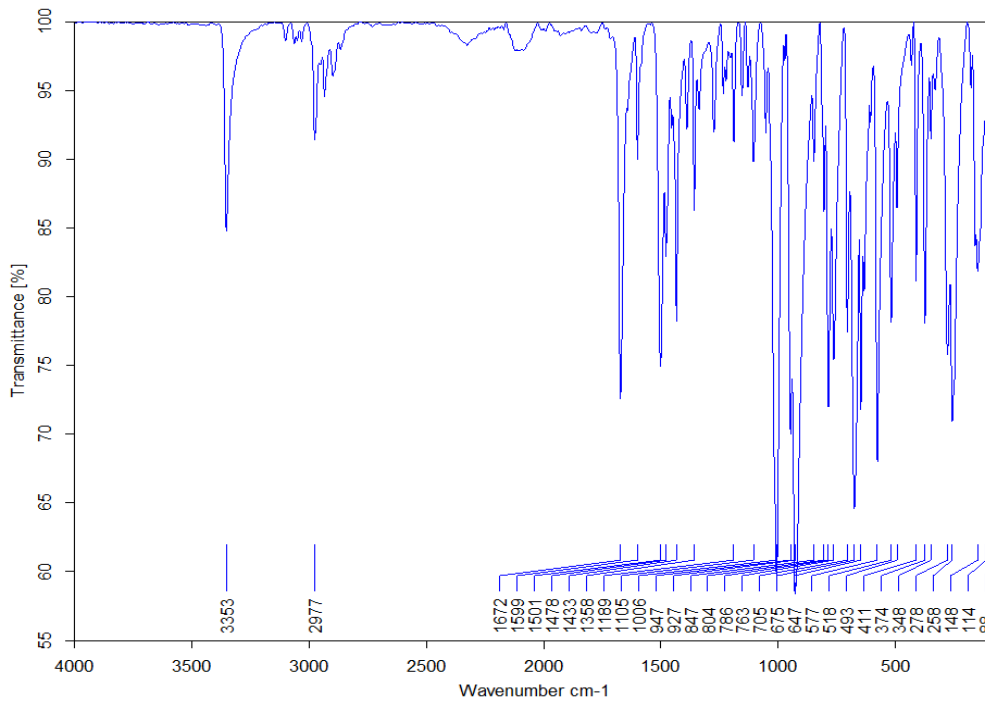


(c)

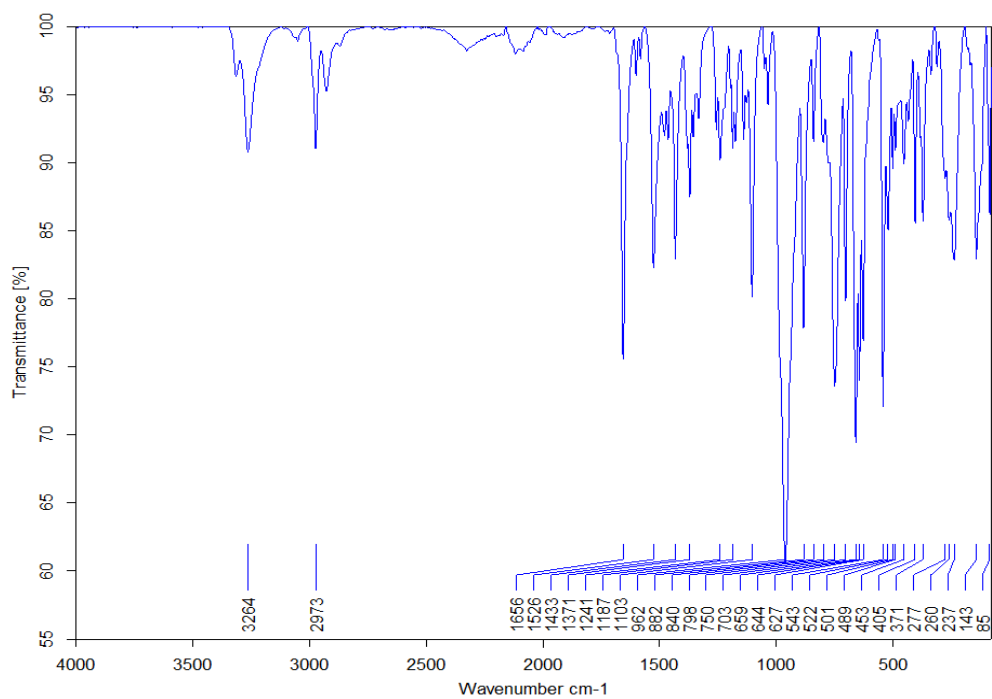
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(a)

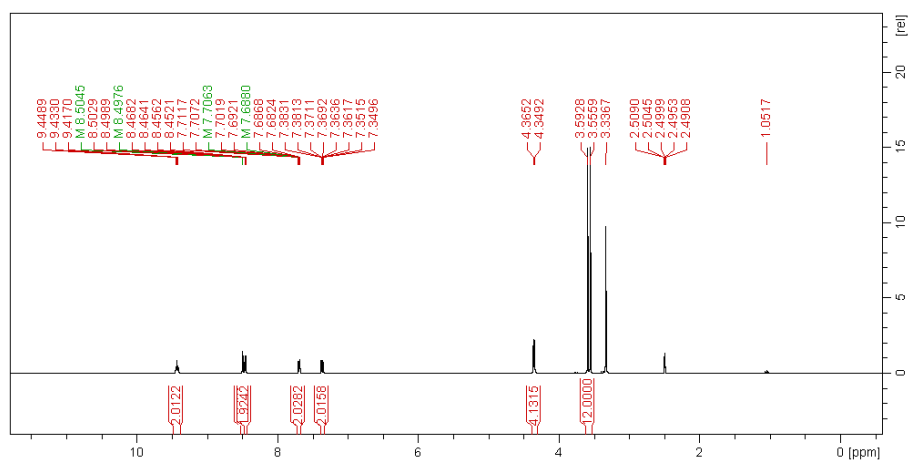


(b)

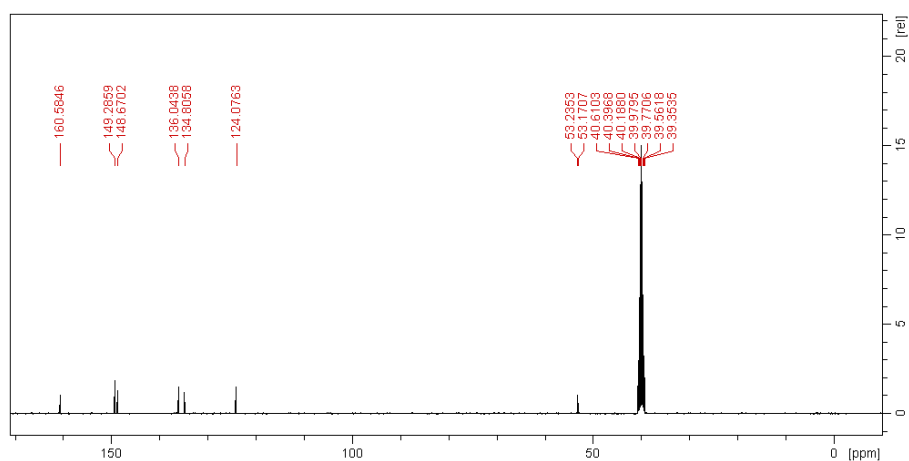


(c)

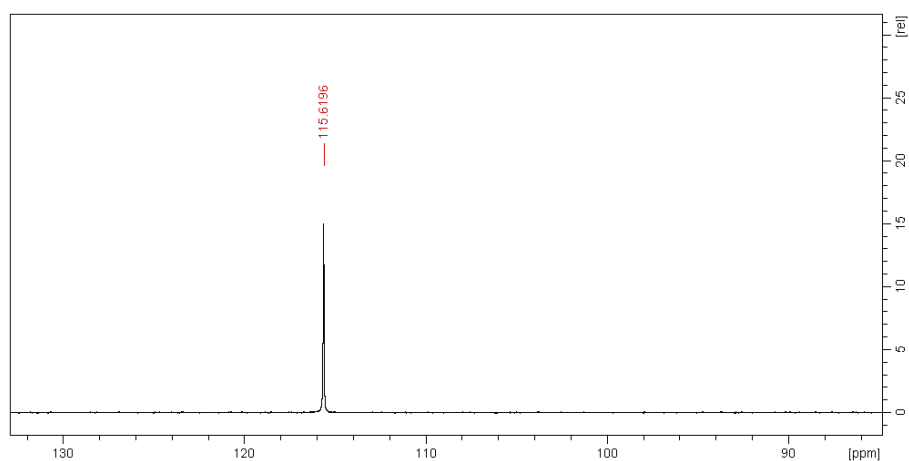
ESI Figure 2. FT-IR spectra for (a) **1**, (b) **2** and (c) **3**.



(a)

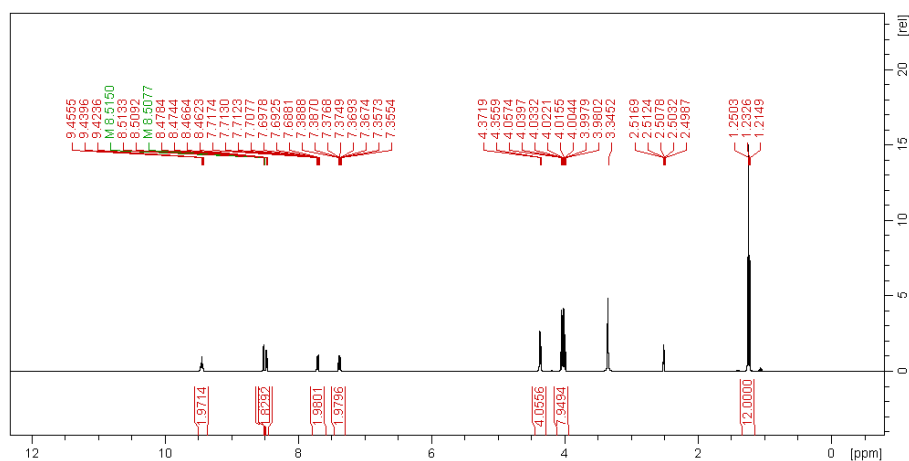


(b)

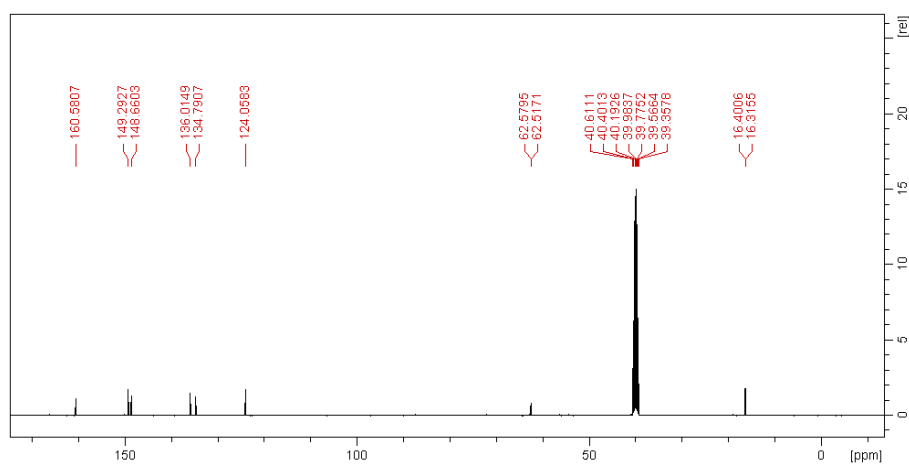


(c)

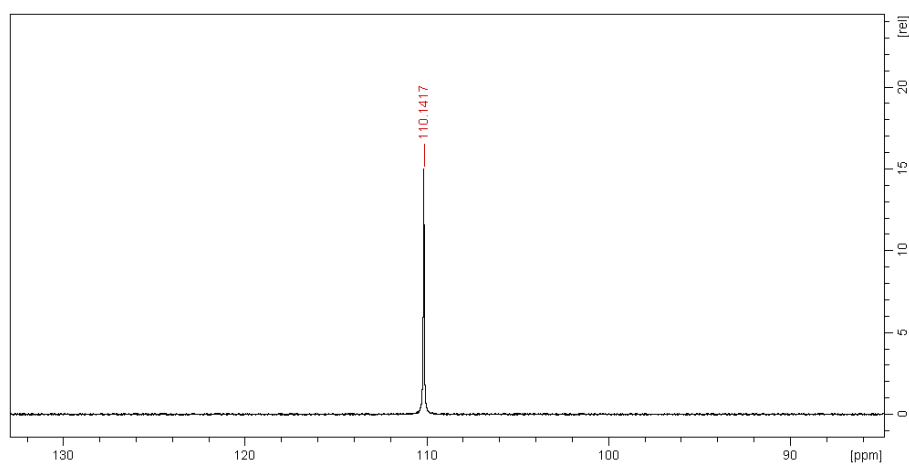
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(a)

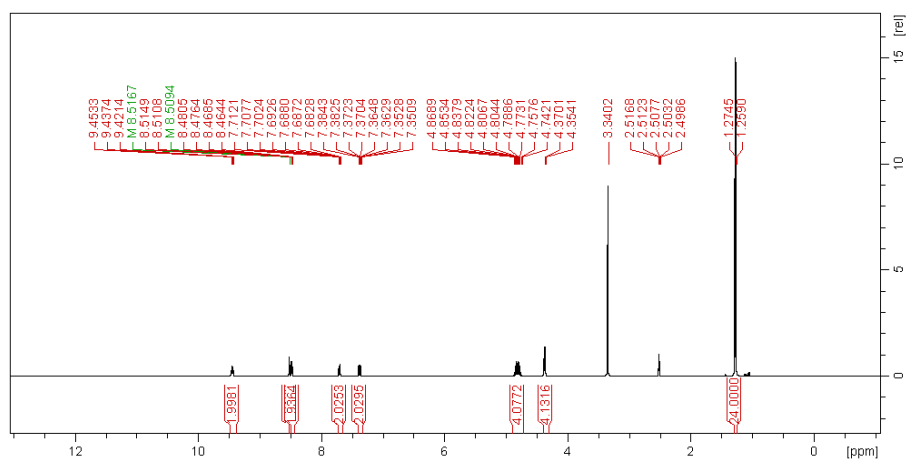


(b)

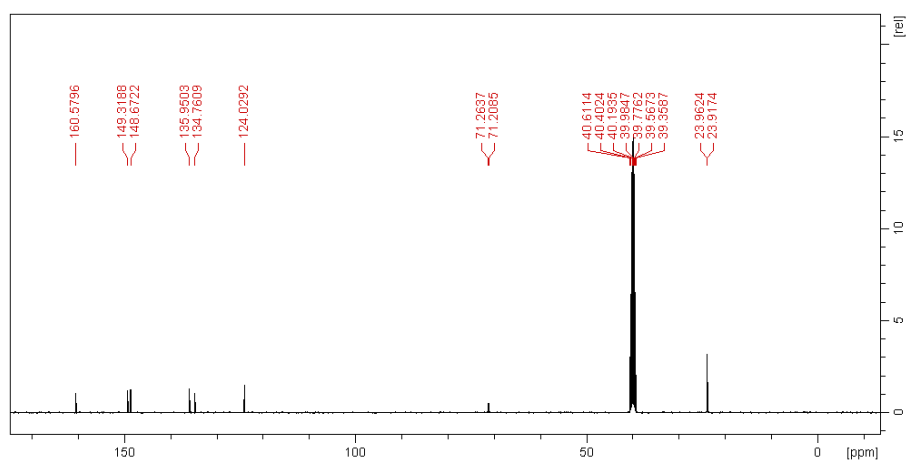


(c)

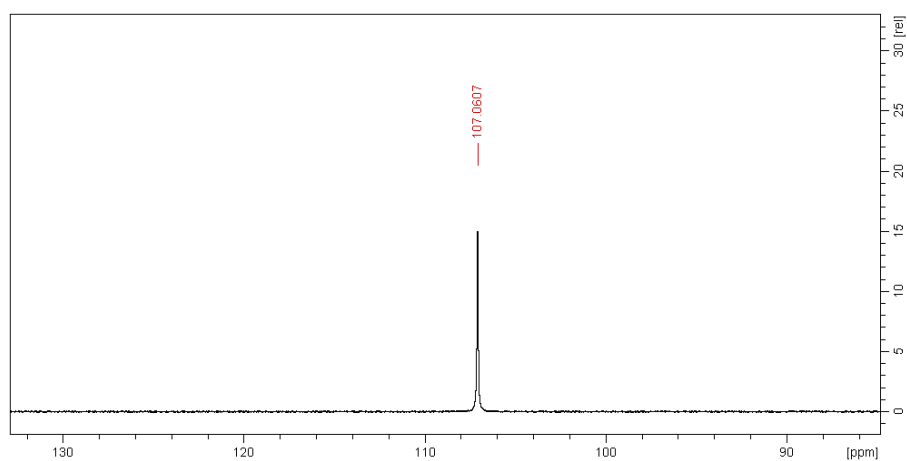
ESI Figure 4. NMR spectra measured in DMSO- d_6 for **2**: (a) ^1H , (b) $^{13}\text{C}\{^1\text{H}\}$ and (c) $^{31}\text{P}\{^1\text{H}\}$.



(a)

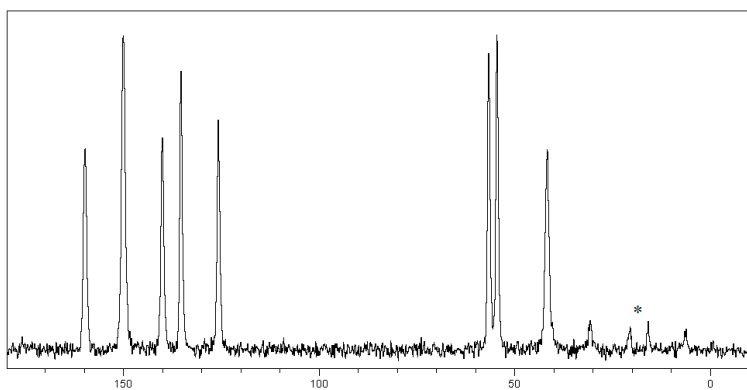


(b)

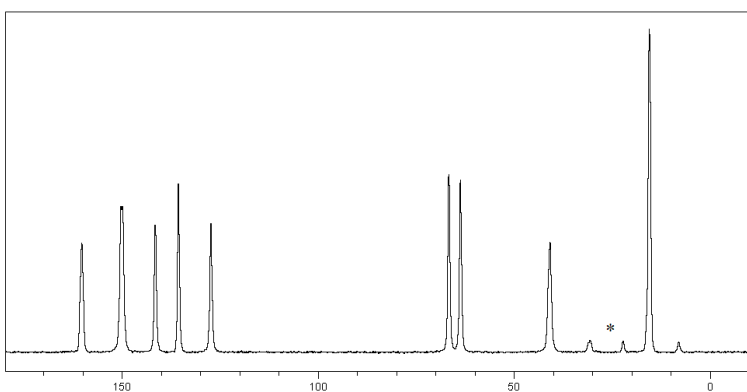


(c)

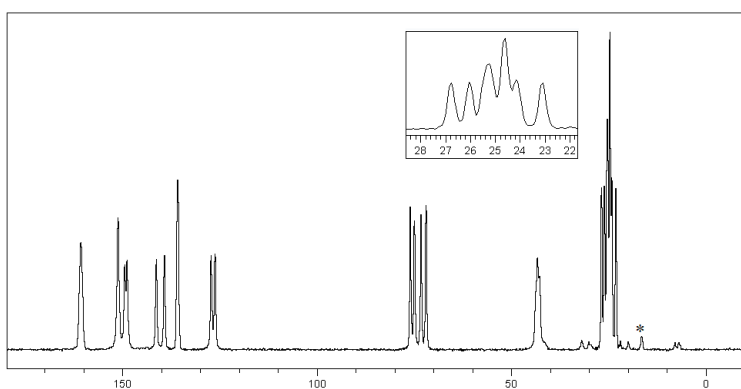
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(a)

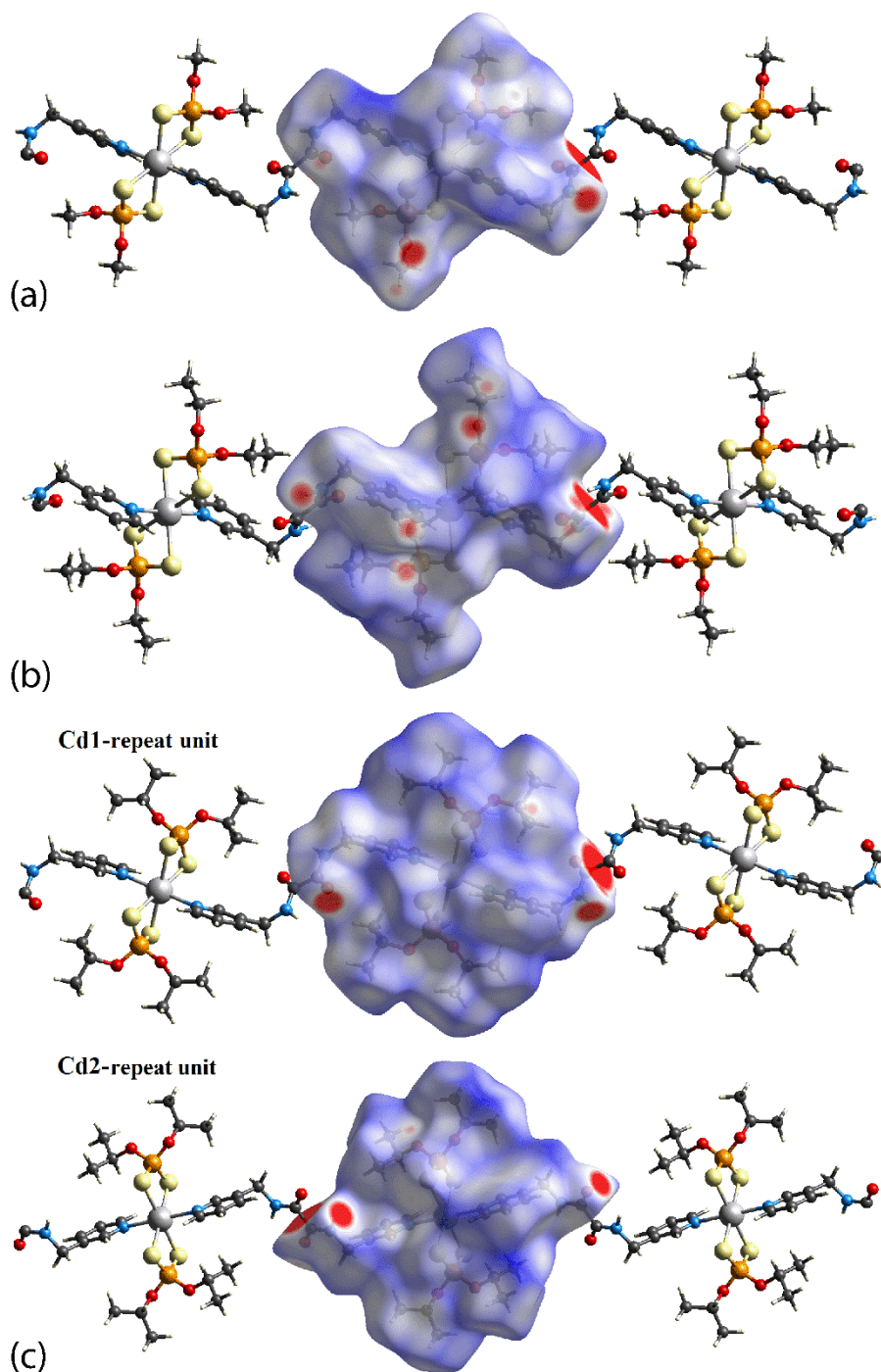


(b)

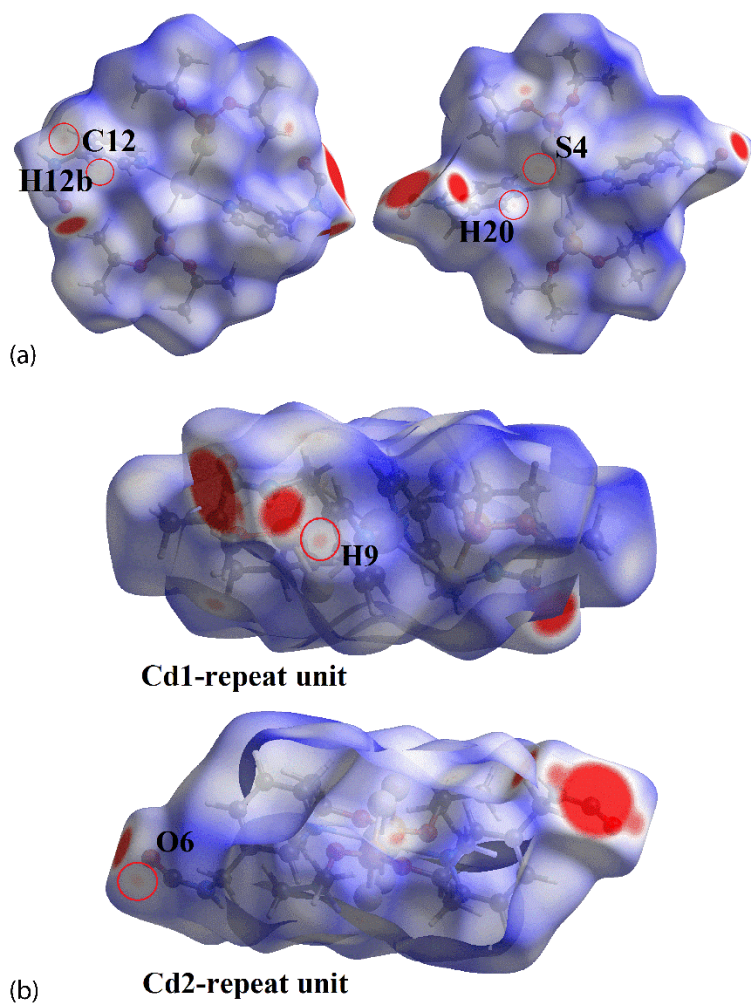


(c)

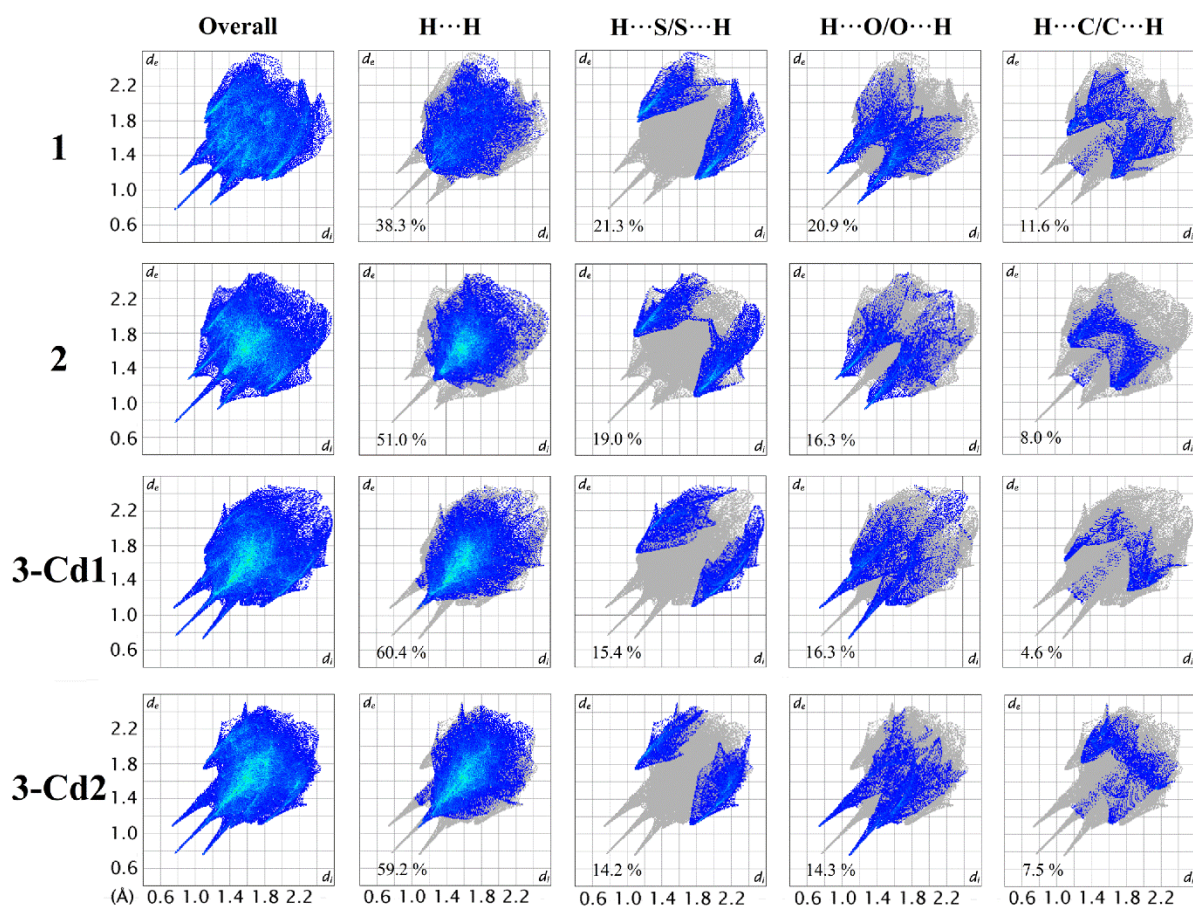
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