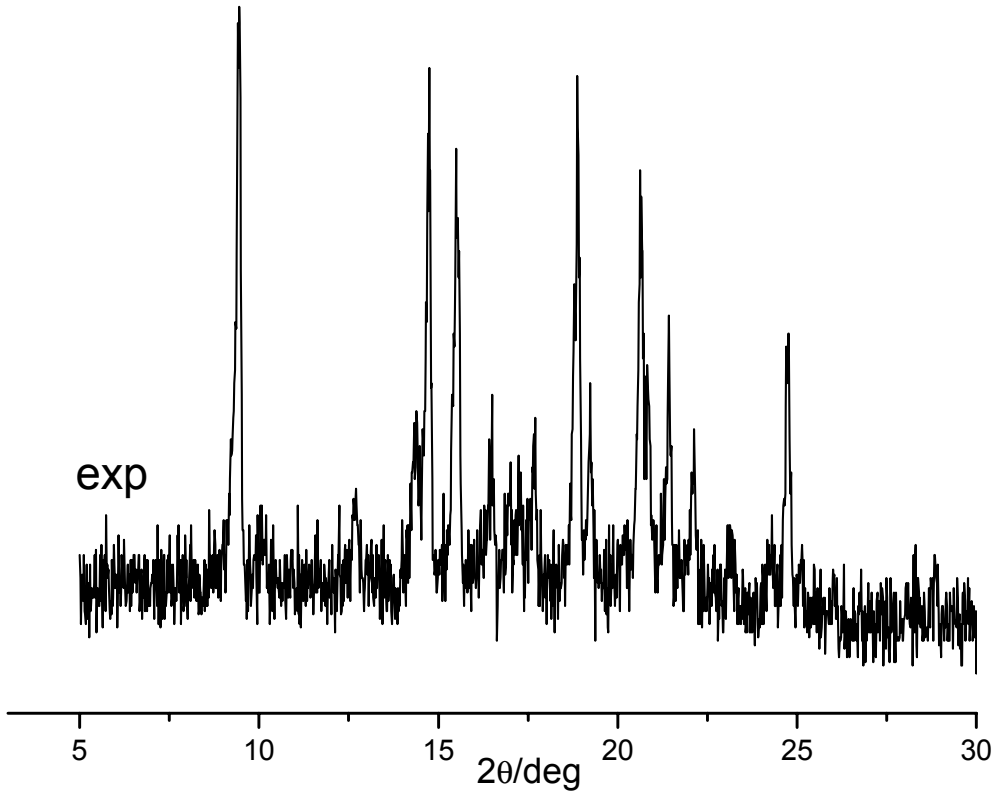
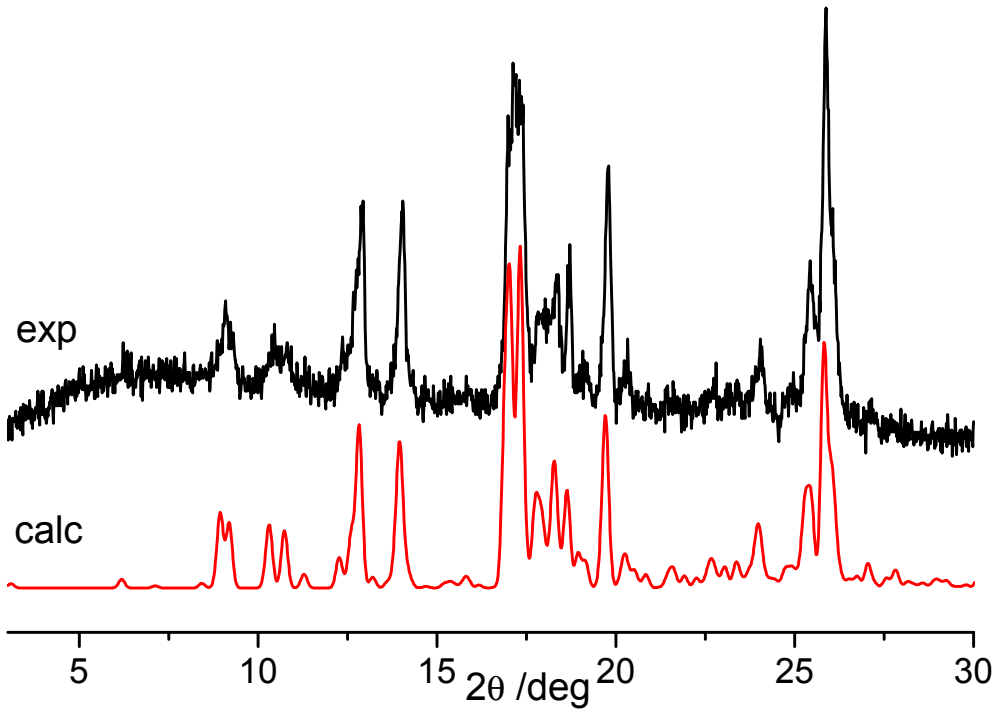
Supplementary Material (ESI) for Chemical Communications

Solid-state preparation of hybrid organometallic-organic macrocyclic adducts with long chain dicarboxylic acids

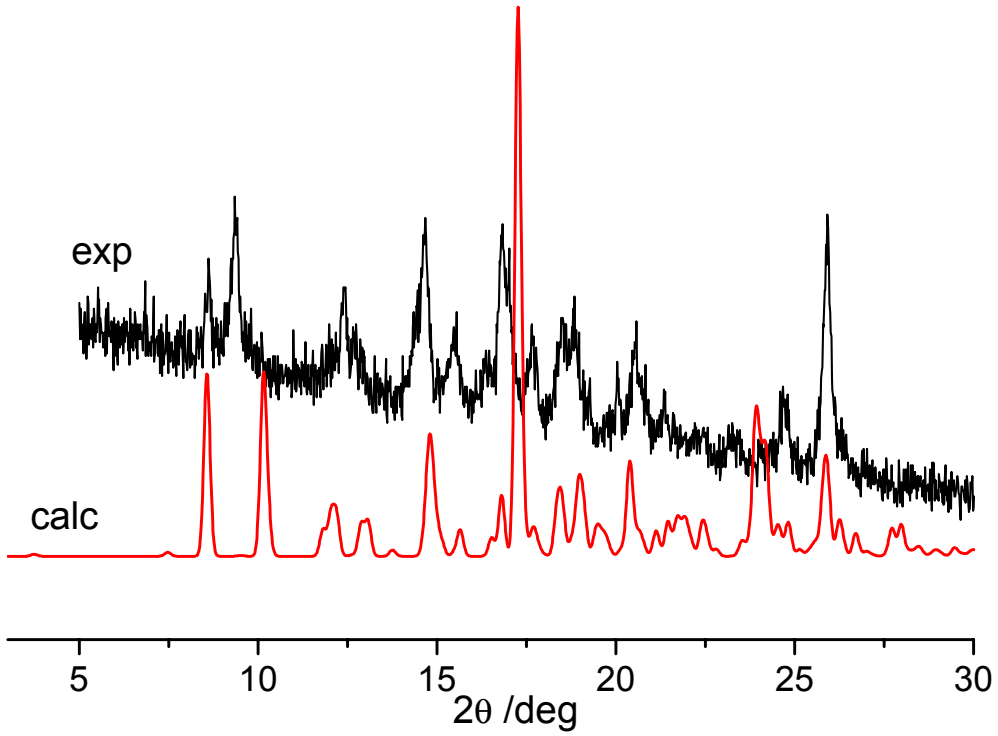
Dario Braga,* Stefano Luca Giaffreda, and Fabrizia Grepioni*



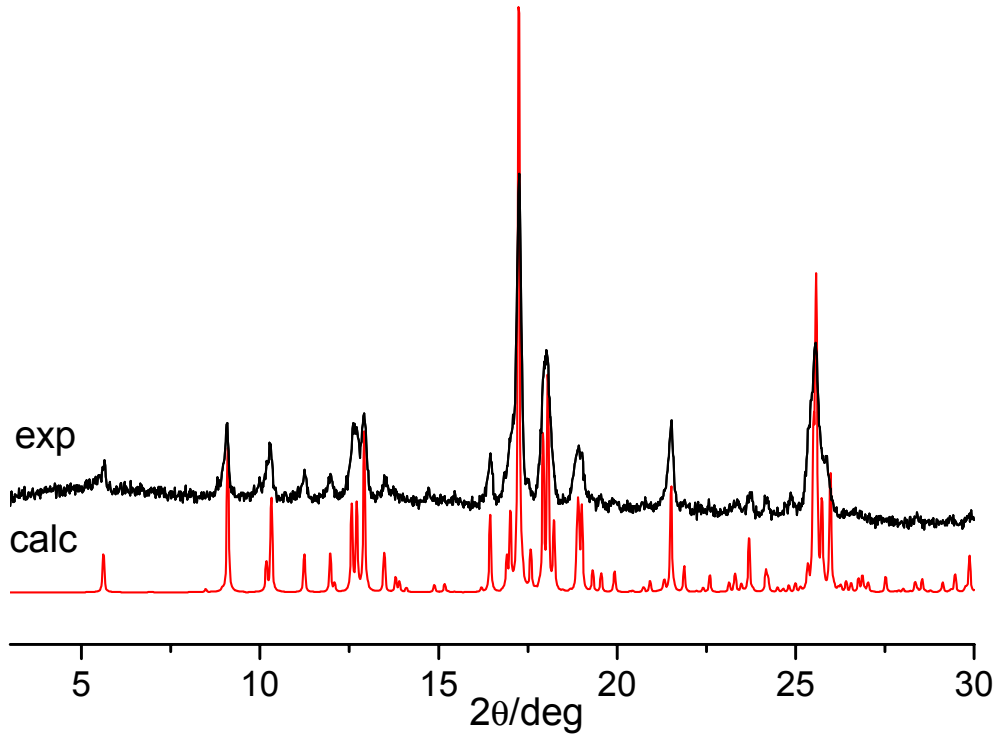
Experimental XRPD pattern for $[Fe(\eta^5\text{-}C_5H_4\text{-}C_5H_4N)_2]$



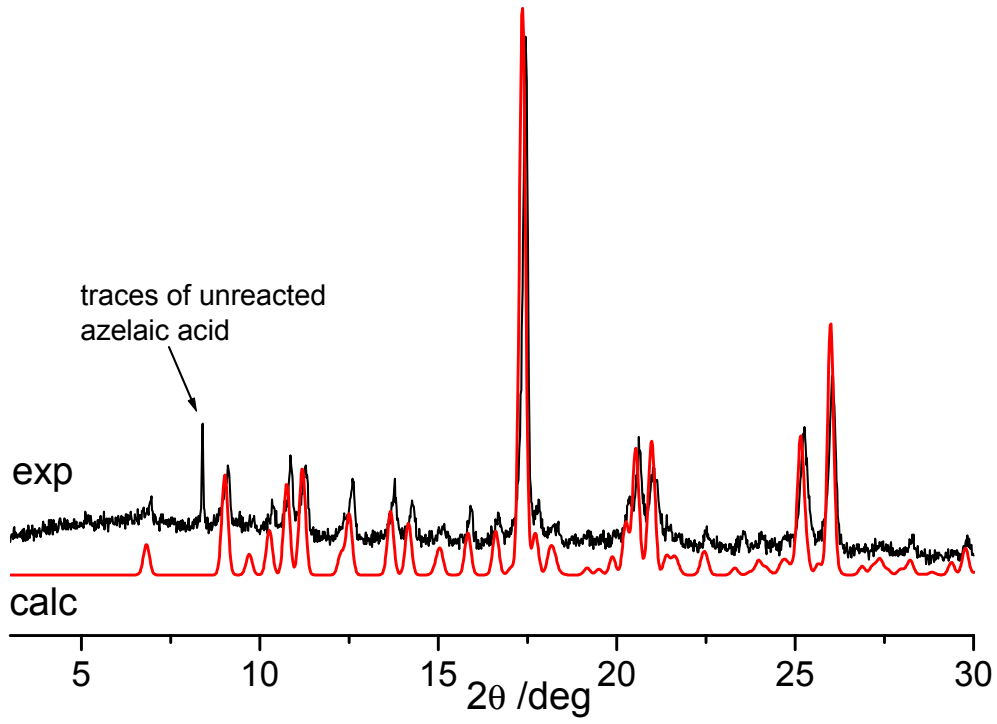
Comparison between experimental and calculated XRPD patterns for **1·adipic(4)**



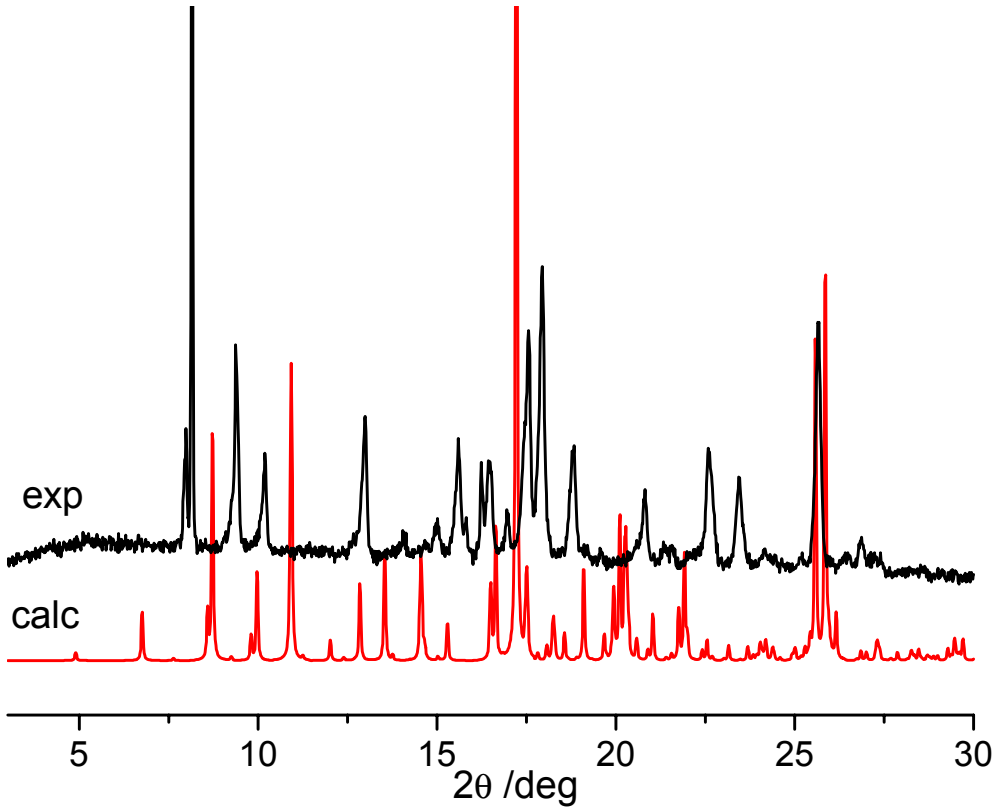
Comparison between experimental and calculated XRPD patterns for **1· pimelic(5)**



Comparison between experimental and calculated XRPD patterns for **1· suberic(6)**



Comparison between experimental and calculated XRPD patterns for **1·azelaic(7)**



Comparison between experimental and calculated XRPD patterns for **1· sebacic(8)**

Table 1. Relevant hydrogen bonding parameters for all compounds

Compound	O-H···N contact	O-H (Å)	H···N (Å)	O···N (Å)	O-H···N (deg)
1·adipic(4)	O(10) -- H(110).. N(6)	0.95(12)	1.84(12)	2.667(12)	145(11)
	O(11) -- H(111).. N(8)	1.06	1.54	2.598(12)	175
	O(14) -- H(140).. N(5)	0.99(11)	1.70(12)	2.667(12)	164(13)
	O(15) -- H(150).. N(7)	1.14(12)	1.68(12)	2.667(12)	141(10)
	O(2) -- H(200).. N(1)	1.02(12)	1.70(12)	2.630(12)	149(10)
	O(3) -- H(300).. N(3)	0.90(15)	1.79(15)	2.601(12)	149(14)
	O(5) -- H(500).. N(2)	0.96(11)	1.77(11)	2.647(12)	150(9)
	O(8) -- H(800).. N(4)	1.17(11)	1.55(11)	2.672(12)	157(9)
1·pimelic(5)	O(2) -- H(200).. N(4)	0.82	1.82	2.632(7)	175
	O(3) -- H(300).. N(1)	1.21	1.57	2.772(11)	169
	O(5) -- H(500).. N(2)	1.20	1.43	2.617(7)	169
	O(8) -- H(800).. N(3)	0.96	1.69	2.648(7)	173
1·suberic(6)	O(1) -- H(100).. N(4)	1.22(18)	1.48(19)	2.632(18)	155(15)
	O(3) -- H(300).. N(1)	1.10(10)	1.56(9)	2.644(16)	168(10)
	O(5) -- H(500).. N(3)	1.26	1.40	2.610(16)	158
	O(8) -- H(800).. N(2)	1.34(19)	1.32(18)	2.630(16)	161(11)
1·azelaic(7)	O(3) -- H(100).. N(2)	0.85(4)	1.80(4)	2.646(3)	171(3)
	O(1) -- H(300).. N(1)	0.87(4)	1.76(4)	2.628(3)	171(4)
1·sebacic(8)	O(2) -- H(200).. N(2)	1.09(11)	1.57(11)	2.644(10)	167(7)
	O(3) -- H(300).. N(3)	0.97(15)	1.68(14)	2.638(11)	170(16)
	O(6) -- H(600).. N(4)	0.97(15)	1.73(16)	2.612(12)	150(13)
	O(7) -- H(700).. N(1)	1.12(18)	1.50(17)	2.607(10)	170(10)