Electronic Supplementary Information

for

N–H···O and N–H···Cl Supported 1D Chains of Heterobimetallic Cu^{II}/Ni^{II}–Sn^{IV} Cocrystals

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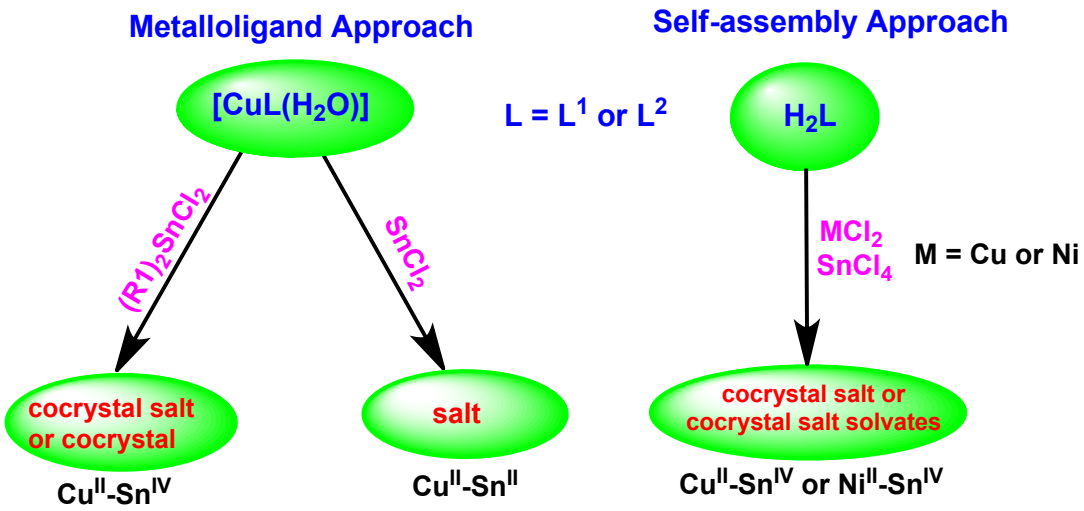
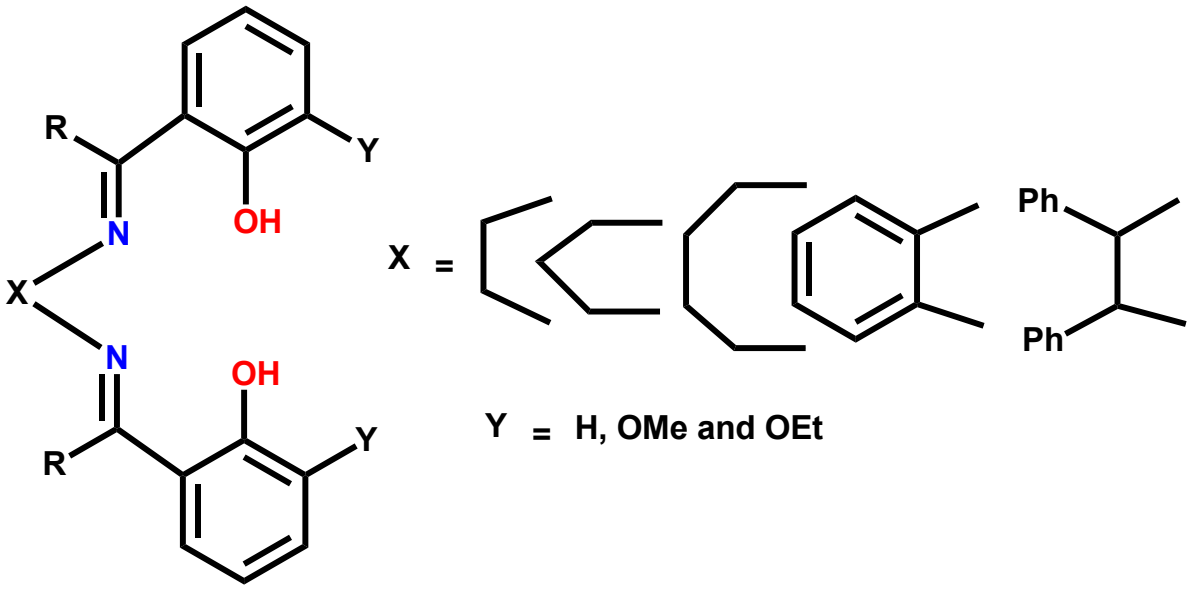


Scheme S1 Preparation of cocrystals salts, cocrystals and salts by the metalloligand and the self-assembly approaches.



Scheme S2. Chemical diagram of a family of related H_2L Schiff bases.

Table S1 Hydrogen bonds distances (Å) and angles (°) in **1–4**

Compounds	D–H···A	H···A	D···A	D–H···A	Symmetry
1	N3–H3C···Cl2^{i}	2.32	3.201	172.0	*i*) x, y, 1+z
	N3–H3A···O1	2.09	2.827	140.0	
	N3–H3B···O2	2.18	2.834	131.0	
	N3–H3A···O3	2.15	2.891	141.0	
	N3–H3B···O4	2.12	2.920	151.0	
2	N3–H3C···Cl3^{i}	2.44	3.259	157.0	*i*) x, 1+y, z; *ii*) 1–x, 1–y, 1–z
	N3–H3A···O1	2.01	2.760	143.0	
	N3–H3B···O2	2.13	2.803	135.0	
	N3–H3A···O3	2.13	2.856	139.0	
	N3–H3B···O4	2.12	2.880	147.0	
	O5–H5M···Cl3^{ii}	2.474	3.316	162.0	
3	N3–H3C···Cl2	2.35	3.227	166.0	
	N3–H3A···O1	2.16	2.886	137.0	
	N3–H3B···O2	2.15	2.867	137.0	
	N3–H3A···O3	2.05	2.824	143.0	
	N3–H3B···O4	2.06	2.822	142.0	
4	N3–H3A···Cl2^{i}	2.52	3.301	148.0	*i*) 1–x,1–y,–z
	N3–H3A···O1	2.27	2.840	121.0	
	N3–H3B···O2	1.97	2.788	149.0	
	N3–H3A···O3	1.95	2.815	160.0	
	N3–H3B···O4	2.12	2.795	131.0	
	O5–H5M···Cl2	2.39	3.261	171.0	

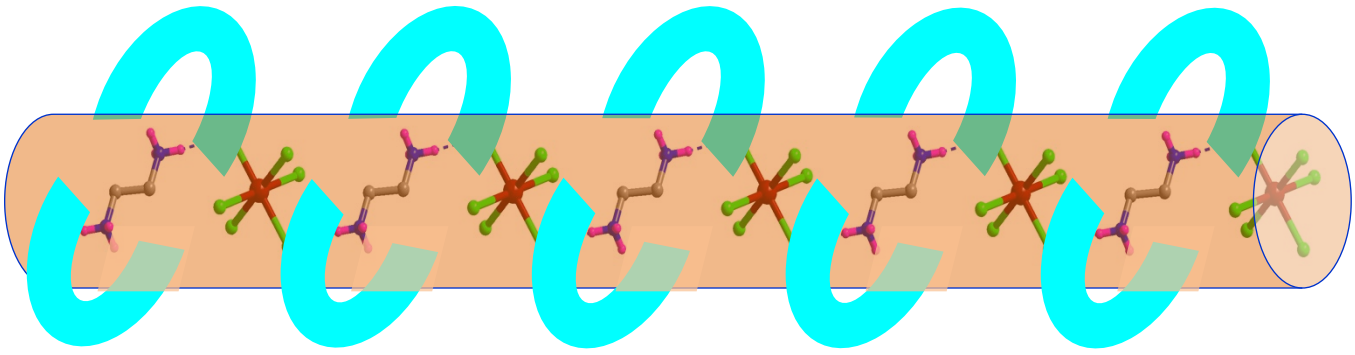


Fig. **S1** Schematic presentation of the encapsulation of a chain of $(H_2ED)^{2+}\cdot[SnCl_6]^{2-}$ species in the metallo-Schiff base pockets of [ML].

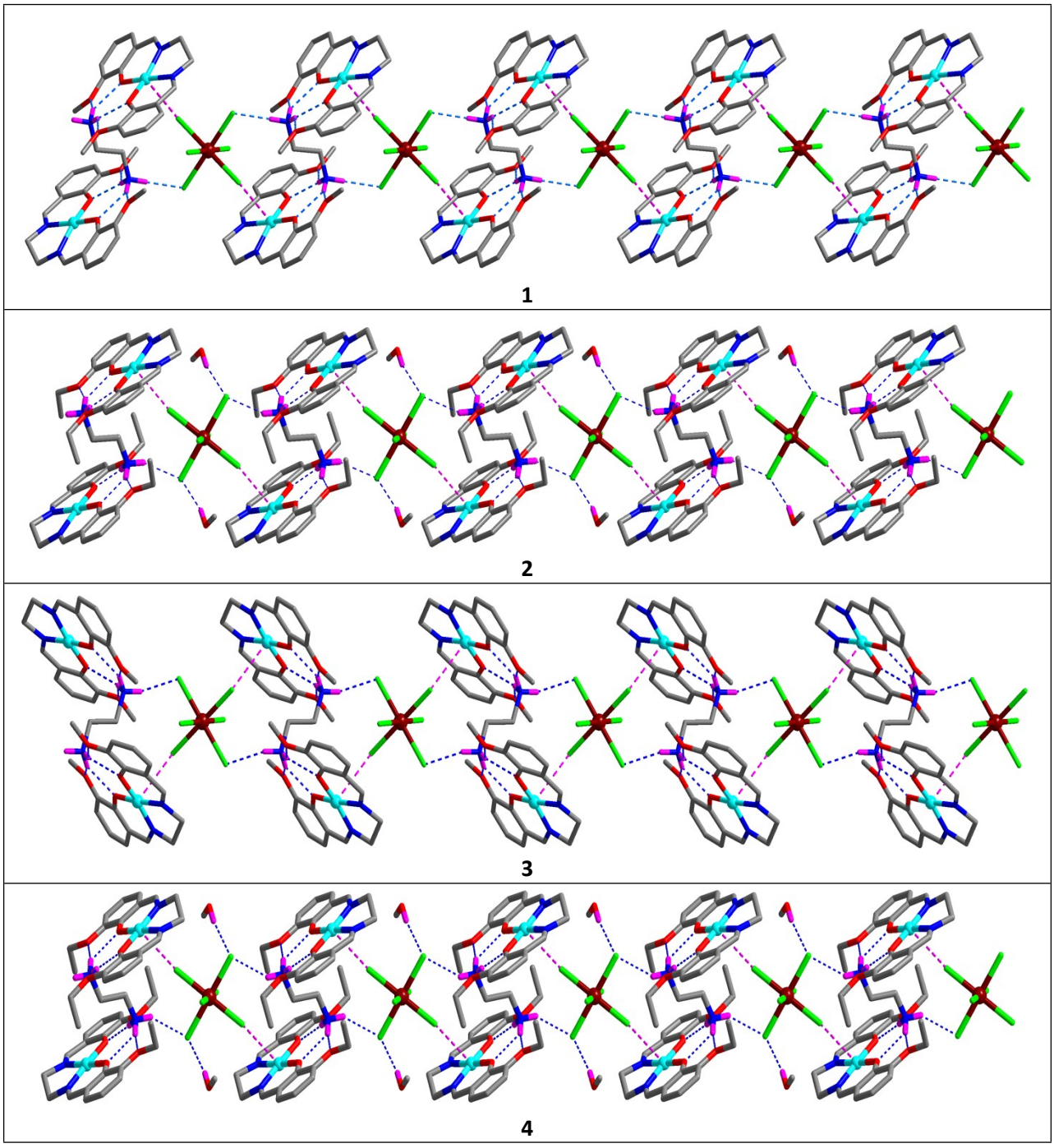


Fig. S2 Supramolecular 1D chain in **2–4** supported by non-covalent interactions.

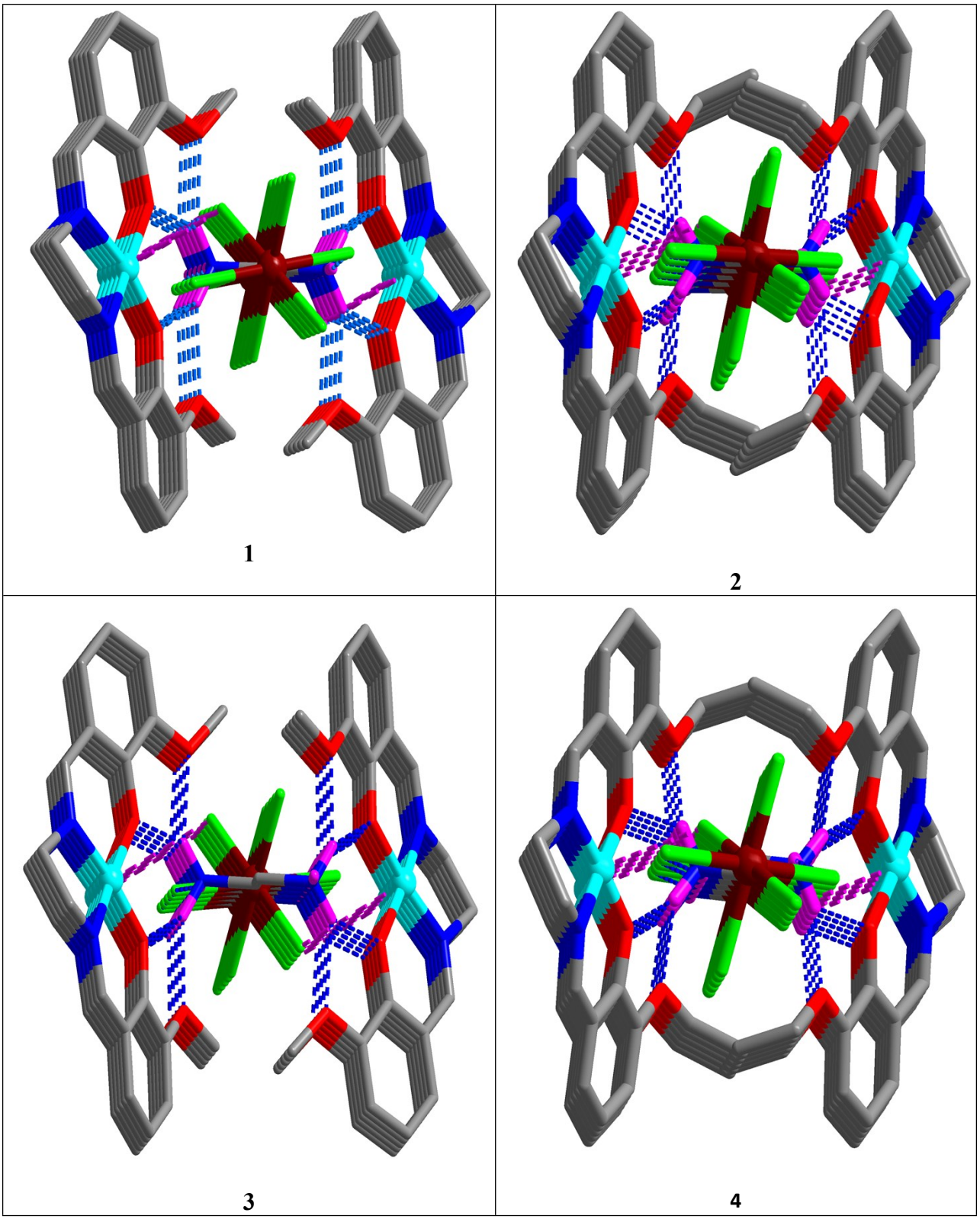


Fig. S3 Entrapping of 1D chains of $(H_2ED)^{2+}\cdot[SnCl_6]^{2-}$ adducts by mononuclear complexes in **1**–**4**. Methanol molecules in **2** and **4** are omitted for clarity.

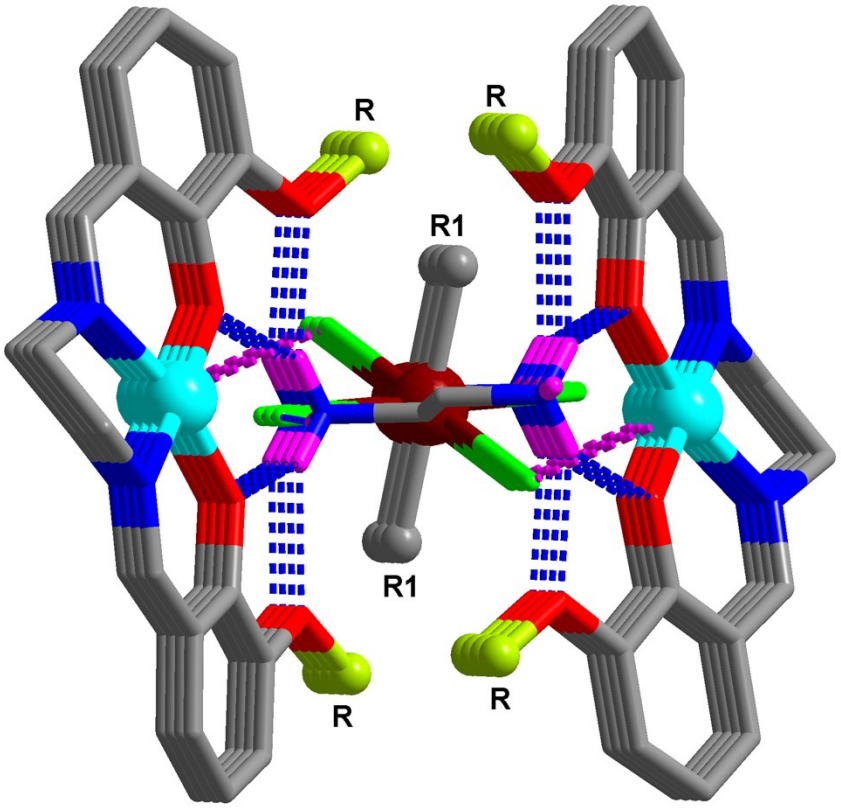


Fig. S4 Entrapping of 1D chain of $(H_2ED)^{2+}\cdot[(R1)_2SnCl_4]^{2-}$ adducts by the mononuclear [CuL] complexes in $(H_2ED)^{2+}\cdot 2[CuL]\cdot[(R1)_2SnCl_4]^{2-}$ (L = L^1, R = Me, R1 = Me, Et, *n*-Bu and Ph; L = L^2, R = Et, R1 = Ph; ED = 1,2-ethylenediamine; excluding the solvent of crystallization). (Reference 9c of the main text).

Table S2 Crystallographic data for **1–4**

	1	**2**	**3**	**4**
Formula	$C_{38}H_{46}Cl_6Cu_2N_6O_8Sn$	$C_{44}H_{62}Cl_6Cu_2N_6O_{10}Sn$	$C_{38}H_{46}Cl_6Ni_2N_6O_8Sn$	$C_{44}H_{62}Cl_6Ni_2N_6O_{10}Sn$
FW	1173.28	1293.46	1163.62	1283.80
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1
a/Å	10.466(4)	10.5572(4)	10.4892(12)	10.3172(4)
b/Å	11.006(5)	11.5990(4)	10.9238(12)	11.7507(5)
c/Å	11.089(4)	12.9106(5)	11.1384(12)	12.8219(6)
α/°	80.040(15)	112.4350(10)	90.216(4)	114.355(2)
β/°	62.536(18)	111.101(2)	117.436(4)	108.037(2)
γ/°	79.168(15)	96.452(2)	99.734(4)	96.323(2)
V/Å^3	1107.7(8)	1304.86(9)	1111.5(2)	1294.78(10)
Z	1	1	1	1
T/K	298(2)	150(2)	298(2)	150(2)
θ/°	2.266 – 26.478	2.475 – 25.744	2.229 – 25.692	2.246 – 25.723
μ (Mo Kα)/mm^{-1}	1.930	1.650	1.814	1.568
ρ_{calcd}/g cm^{-3}	1.759	1.646	1.738	1.646
F(000)	590	658	588	656
Index ranges	$-13<h<13$	$-12<h<12$	$-12<h<12$	$-12<h<12$
	$-13<k<13$	$-14<k<14$	$-13<k<13$	$-14<k<14$
	$-13<l<13$	$-15<l<15$	$-13<l<13$	$-15<l<15$
Rfs. collected	17669	22907	18140	23394
Rfs. unique/observed	4531/ 3256	4949/3918	4215/2855	4879/4091
R_{int}	0.0732	0.0488	0.0842	0.0312
R_1[a]/ wR_2[b] [I > 2σ(I)]	0.0507/0.1106	0.0292/0.0637	0.0509/0.1094	0.0267/0.0577
R_1[a]/ wR_2[b] [for all F_o^2]	0.0815/0.1237	0.0466/0.0696	0.0930/0.1265	0.0388/0.0629
GOF on F^2	1.026	1.019	1.033	1.058