



STRUCTURAL
CHEMISTRY

Volume 77 (2021)

Supporting information for article:

Zinc(II) and nickel(II) complexes of 3,5-dimethyl-1-(pyridin-2-yl)-1*H*-pyrazole: relationship between fluorescence and crystal packing

Magdalena Małecka, Joachim Kusz, Peter Mayer, Marta Sobiesiak and Elzbieta Budzisz

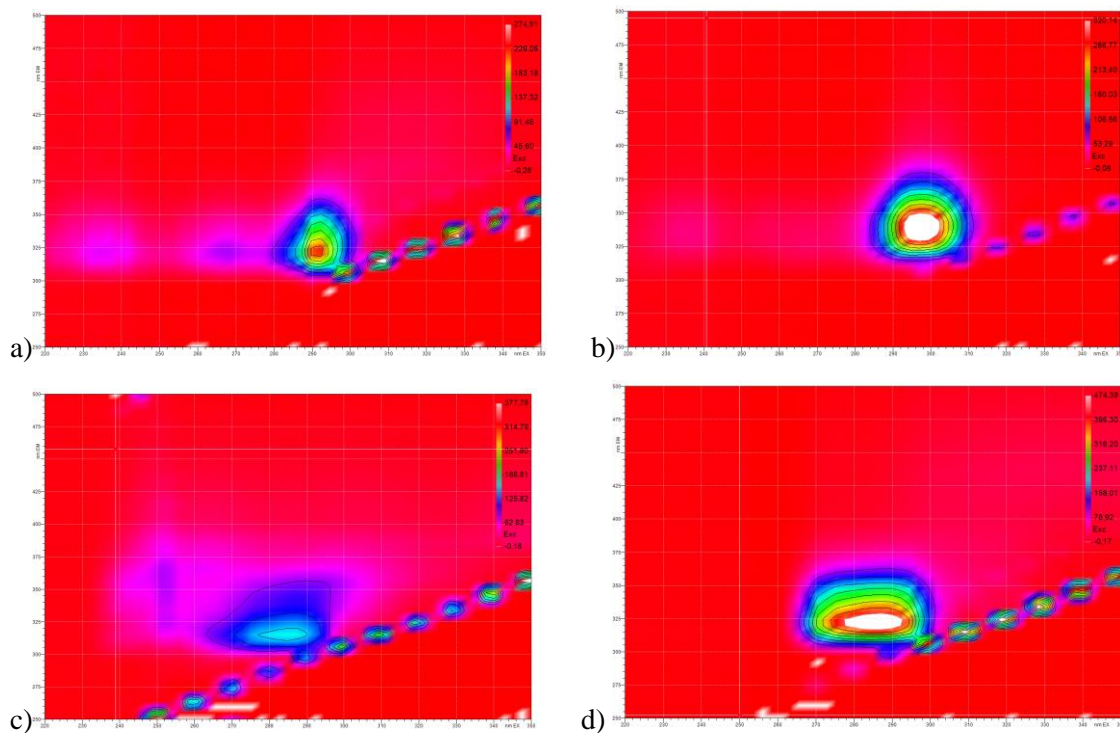


Figure S1 3D excitation and emission of L (left) i Zn(II) complex (1) (right) in methanol (a, b) and dichloromethane (c, d), respectively.

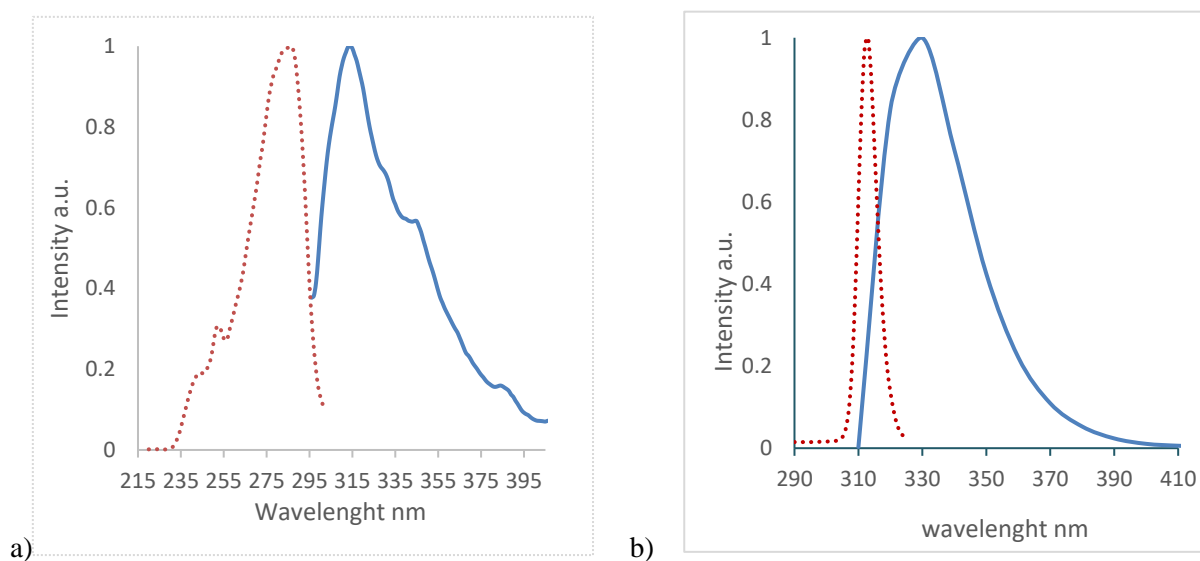


Figure S2 Excitation (dotted line) and emission (solid line) spectra of ligand L (a) and Zn(II) complex (b) in dichloromethane.

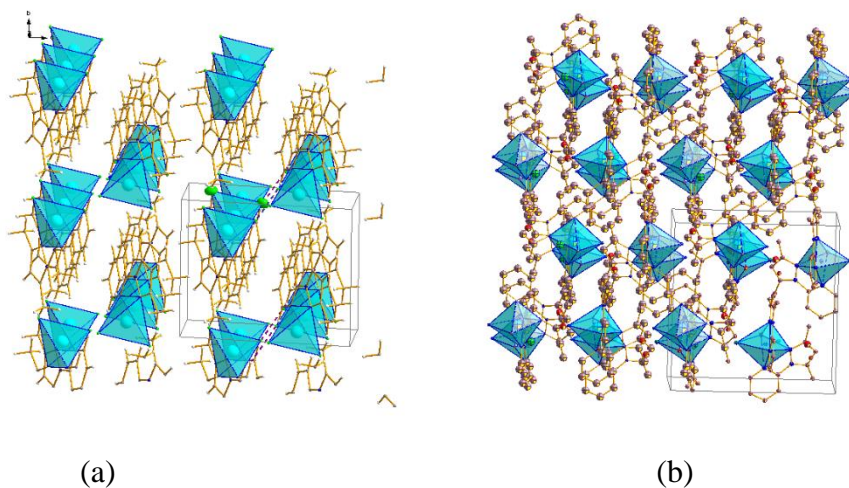
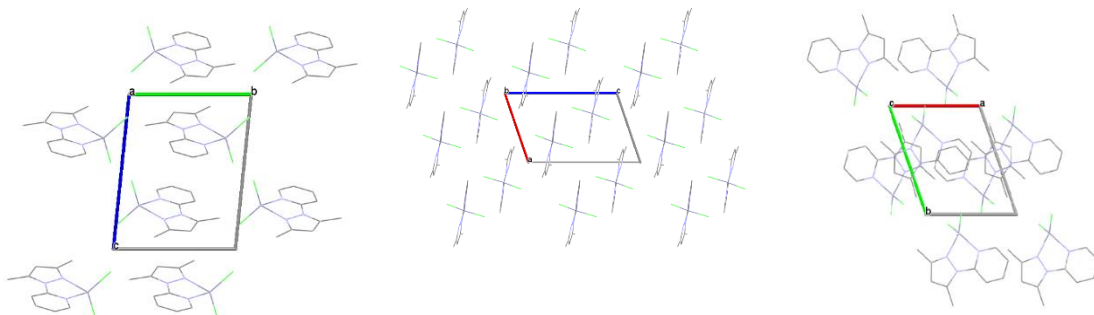
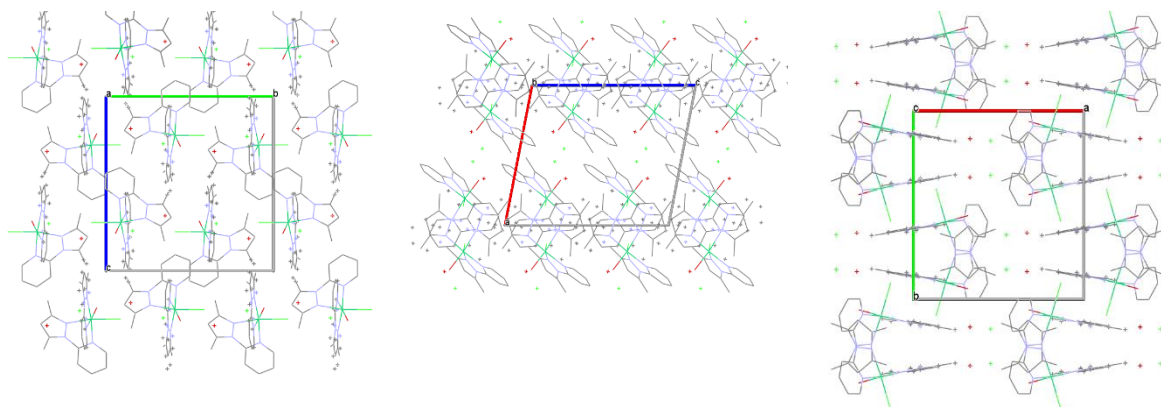


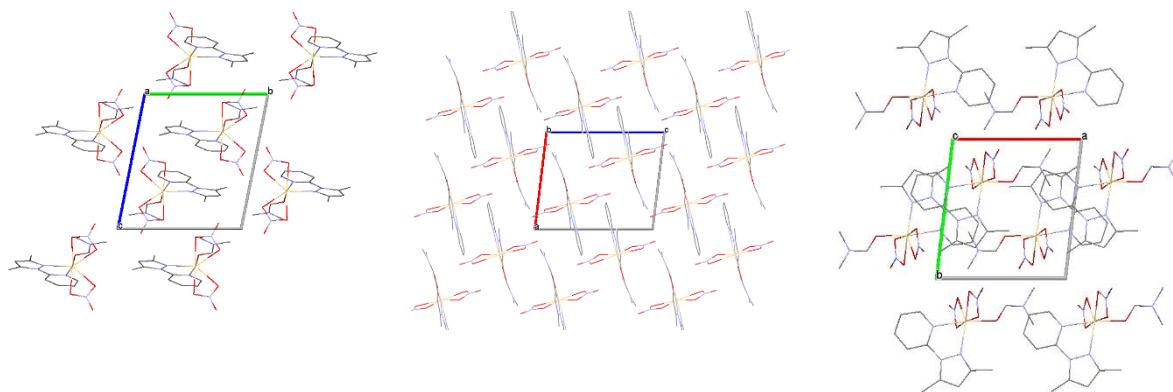
Figure S3 The crystal packing of compound 1. Both figures show polyhedron (tetrahedron) around Zn atom. The crystal packing of compound 2. Both figures show polyhedron (octahedron) around Ni atom.



compound 1



compound 2



HEWCAP

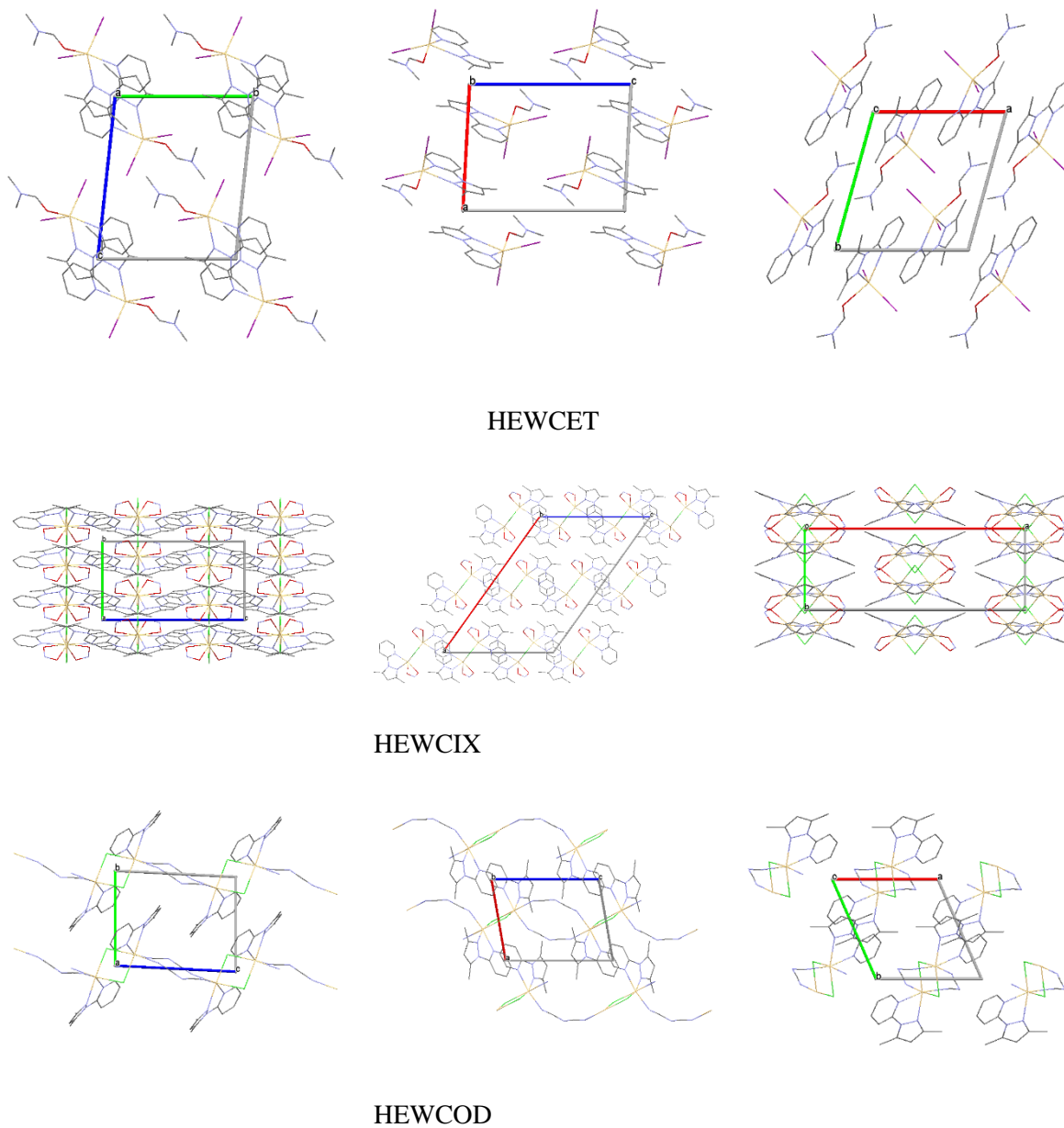
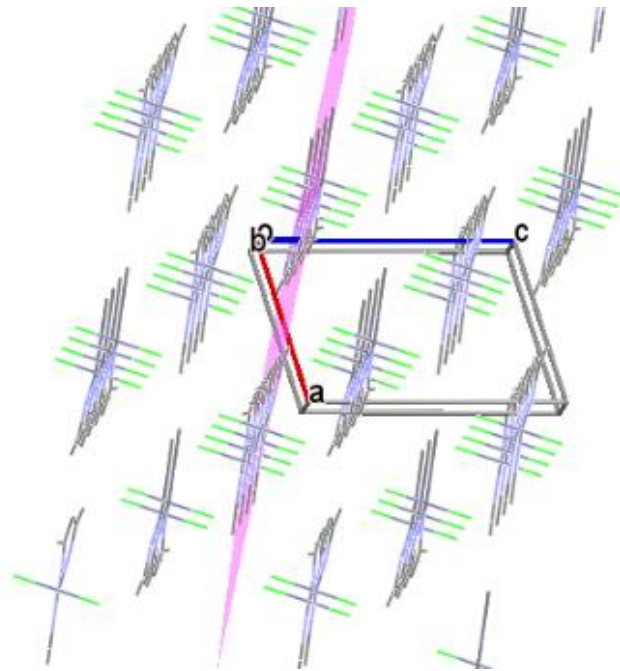
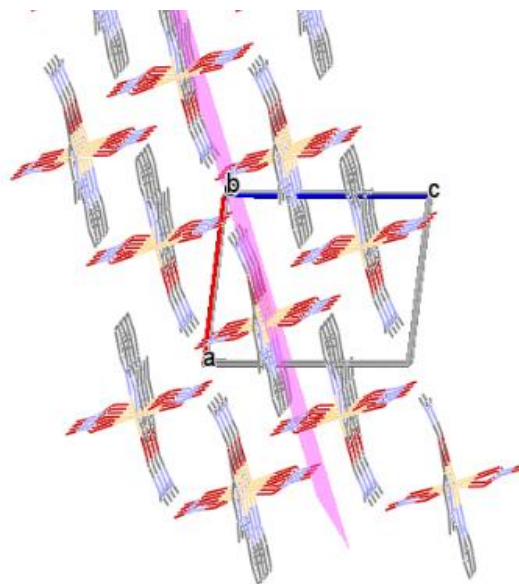


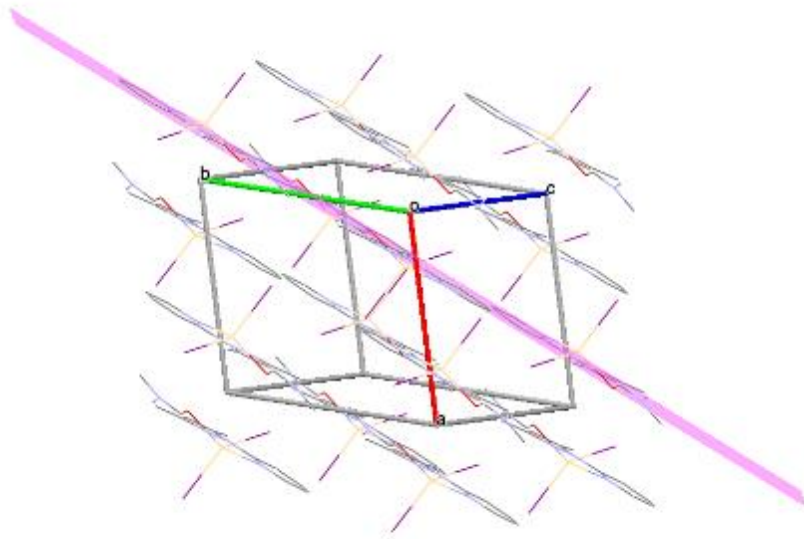
Figure S4 Molecular packing of all compounds in the unit cell in the bc, ac, ab plane, respectively. H atoms are omitted for clarity.



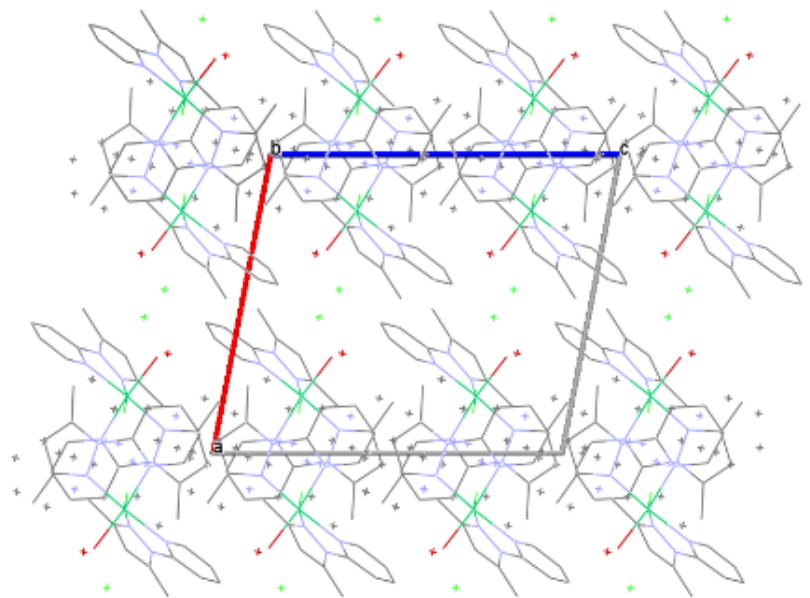
compound 1



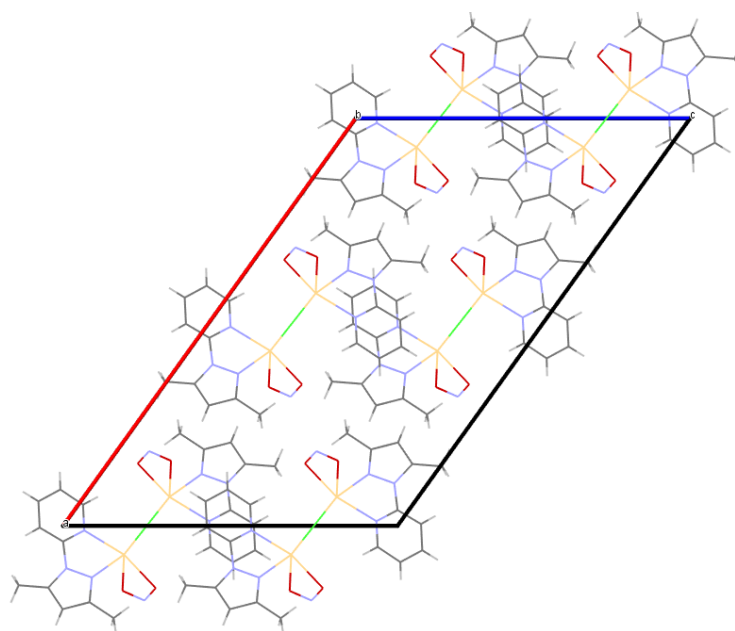
HEWCAP



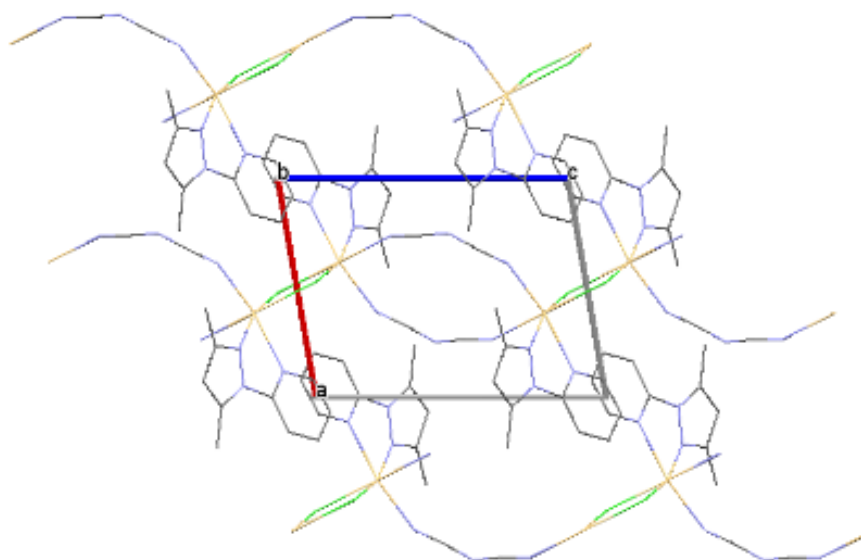
HEWCET



compound 2



HEWCIX



HEWCOD

Figure S5 Molecular packing of of compound 1, HEWCAP and HEWCET with pink plane showing the layered nature of packing (comounds with fluorescence properties). Next three figures represent the crystal packing for remaining compounds without fluorescence. The molecular packing is presented along b axis for all compounds excluding HEWCET where [0 1 1] direction is presented. H atoms are omitted for clarity.

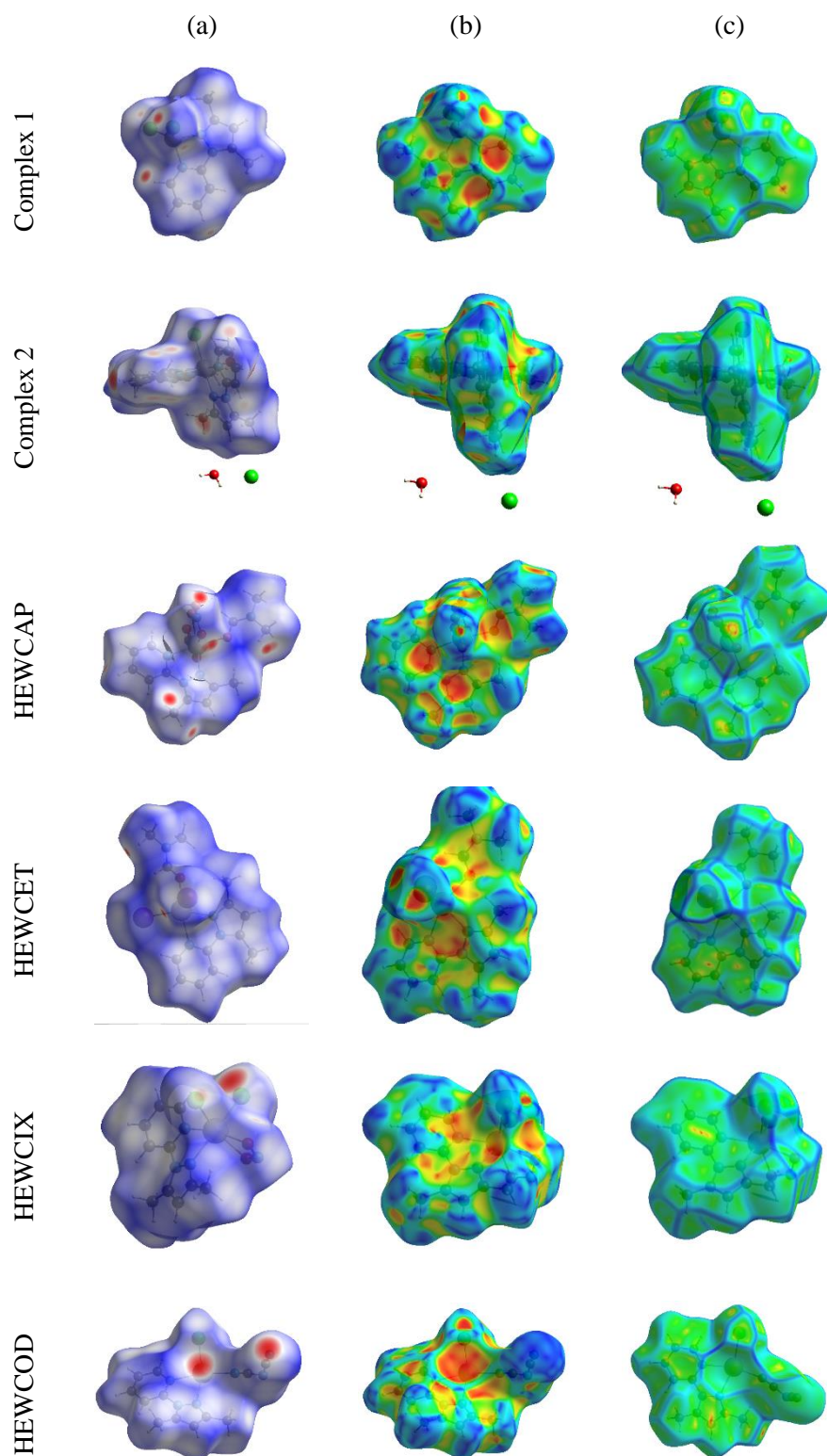
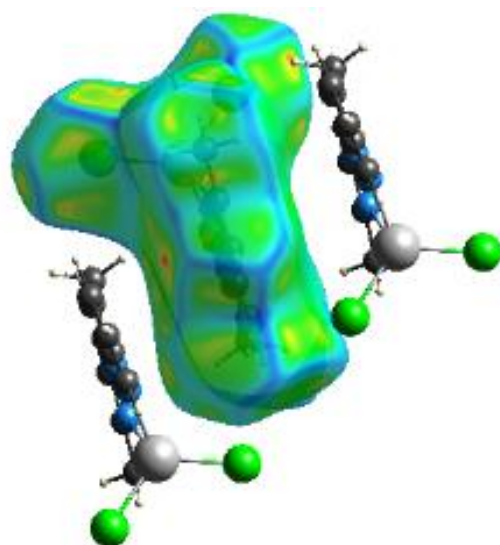
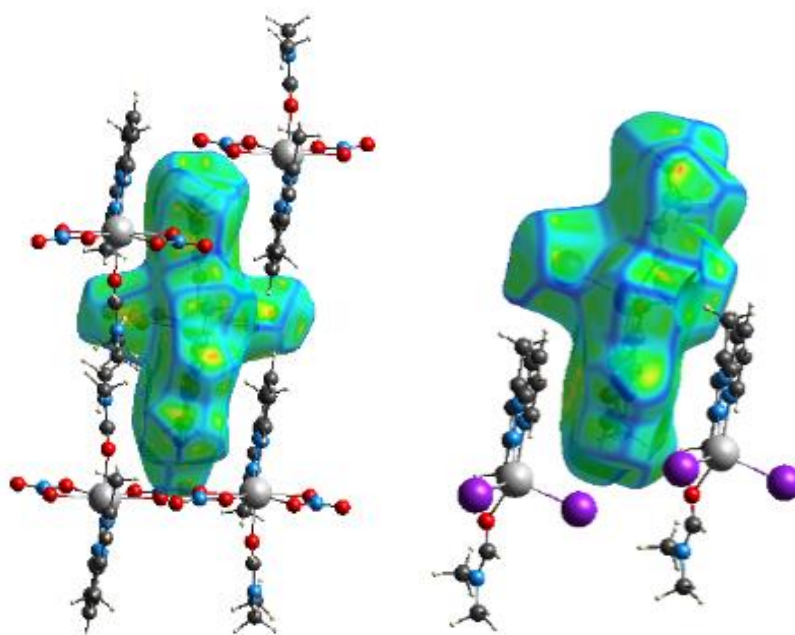


Figure S6 Hirshfeld surface mapped with (a) d norm, (b) shape index and curvedness(c) of the complexes 1, 2 and HEWCAP, HEWCET, HEWCIX and HEWCOD.



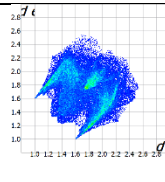
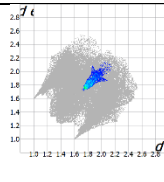
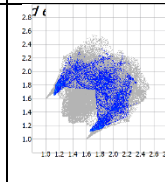
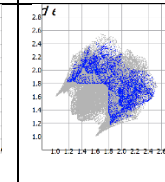
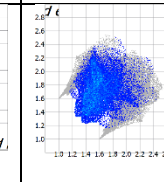
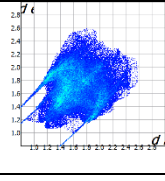
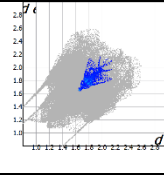
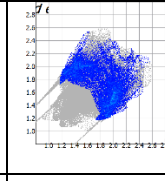
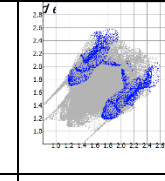
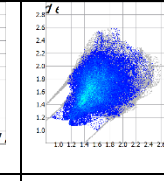
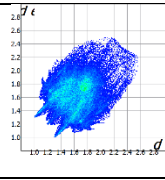
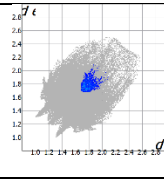
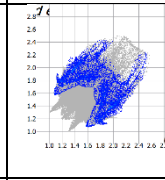
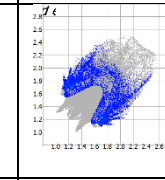
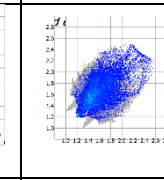
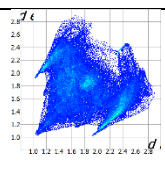
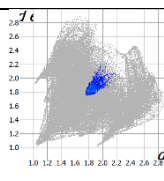
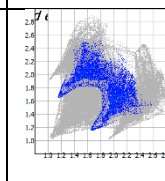
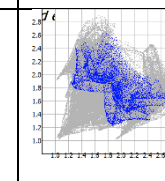
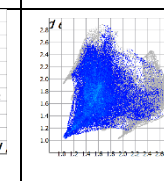
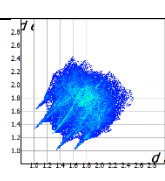
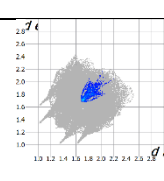
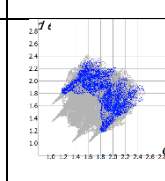
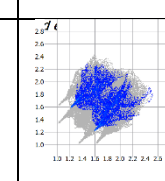
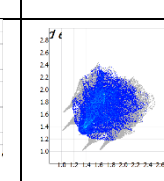
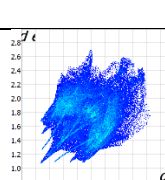
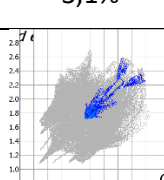
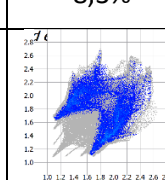
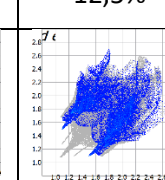
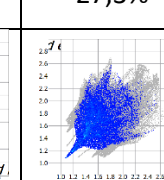
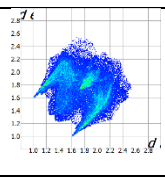
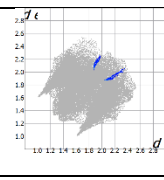
Complex 1



HEWCAP

HEWCET

Figure S7 Hirshfeld surface of the complex 1, HEWCAP and HEWCET mapped with curvedness with surrounding molecules, showing layered structure features

		C...C	C...H	N...H	H...H	Cl...H
Complex 1						
		4,6%	10%	6,7%	33,4%	40,3%
Complex 2						
		2,4%	20,1%	3,7%	55,6%	14,7%
HEWCAP						
		2,2%	11%	9%	27%	
HEWCET						
		2,2%	10,7%	6%	42,1%	
HEWCIX						
		3,1%	8,3%	12,5%	27,3%	20%
HEWCOD						
		3,3%	21,8%	24%	22,4%	11,8%
		M...Cl	N...N	O...H	I...H	M...N
Complex 1						
		0,6%				

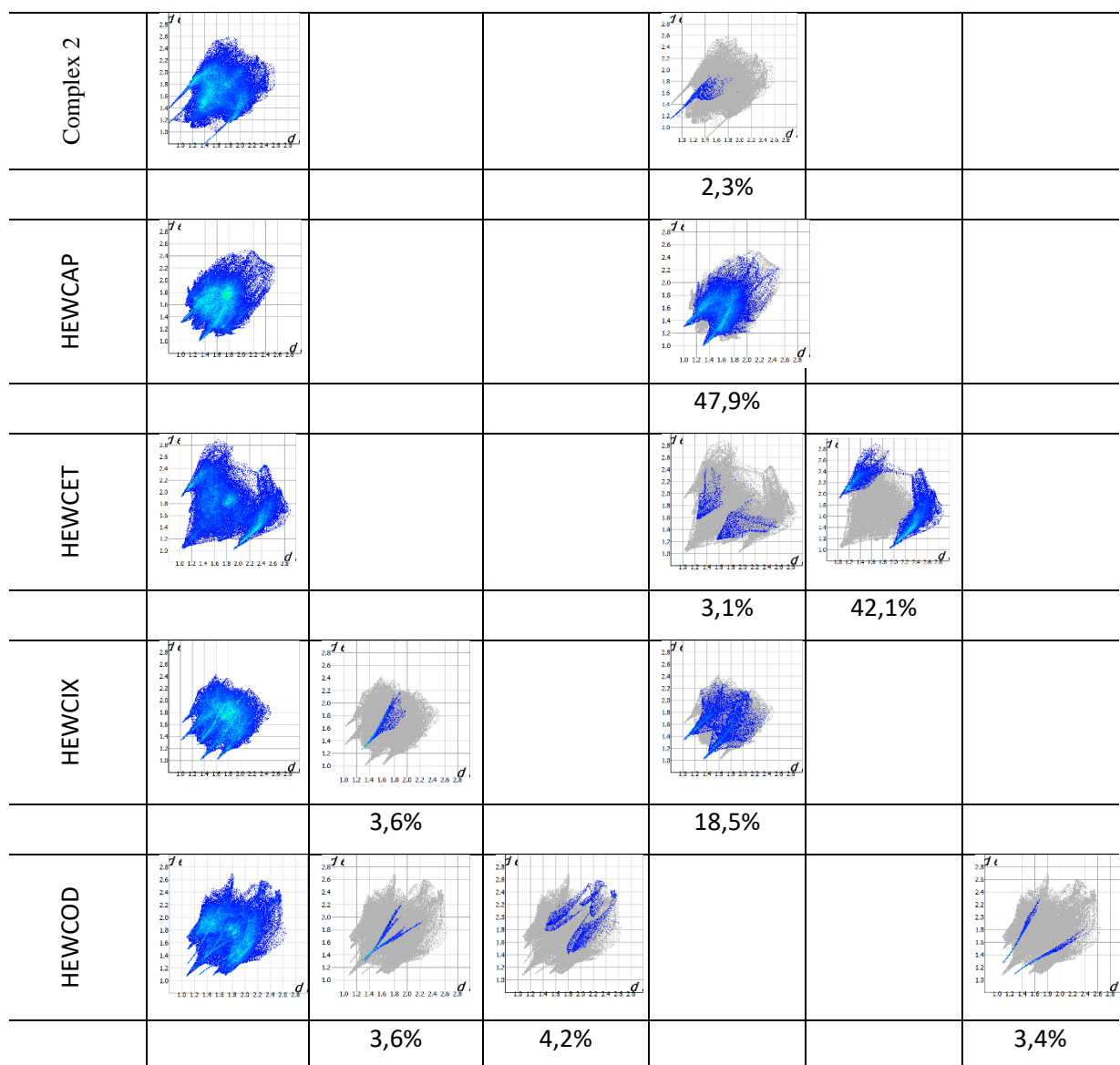


Figure S8 Fingerprint plots of examined compounds and HEWCAP, HEWCET, HEWCIX and HEWCOD