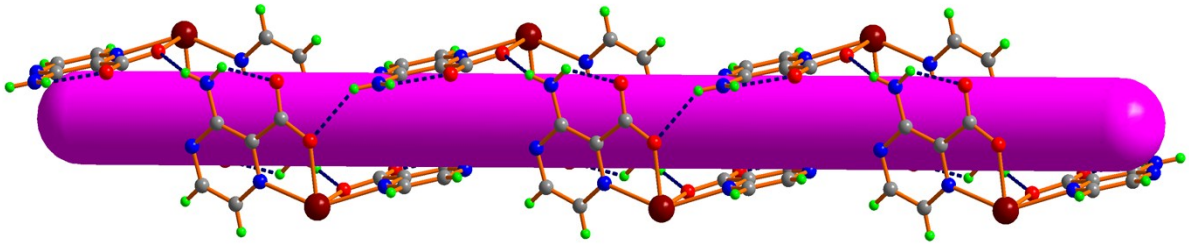
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

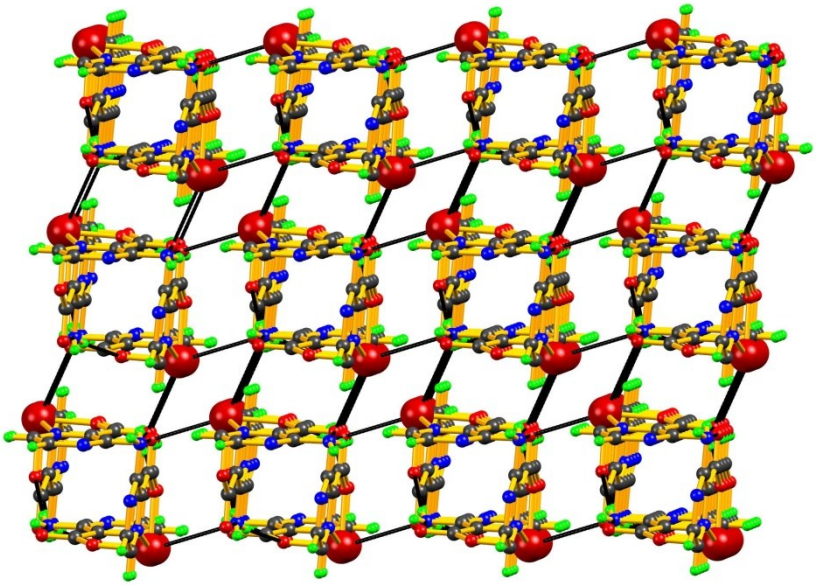
Packing polymorphism in 3-amino-2-pyrazinecarboxylate based Tin(II) complexes and their catalytic activity towards cyanosilylation of aldehydes

Anirban Karmakar*, Susanta Hazra, Guilherme M. D. M. Rúbio, M. Fátima C. Guedes da Silva and Armando J. L. Pombeiro*

[a]Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049–001, Lisbon, Portugal. E-mail: *anirbanchem@gmail.com*; *pombeiro@tecnico.ulisboa.pt.*



A



B

Figure S1 Packing diagram of complex **1**.

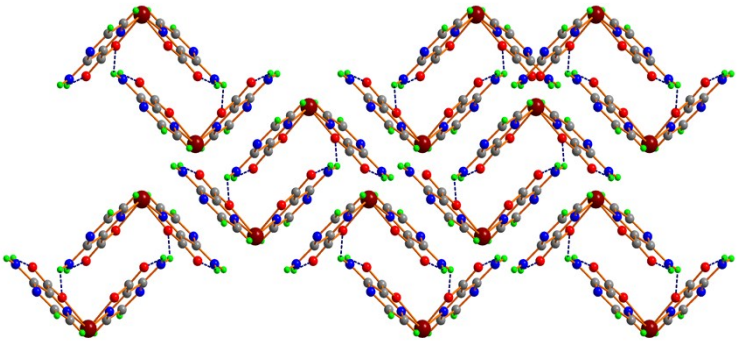


Figure S2 Packing diagram of complex **2**.

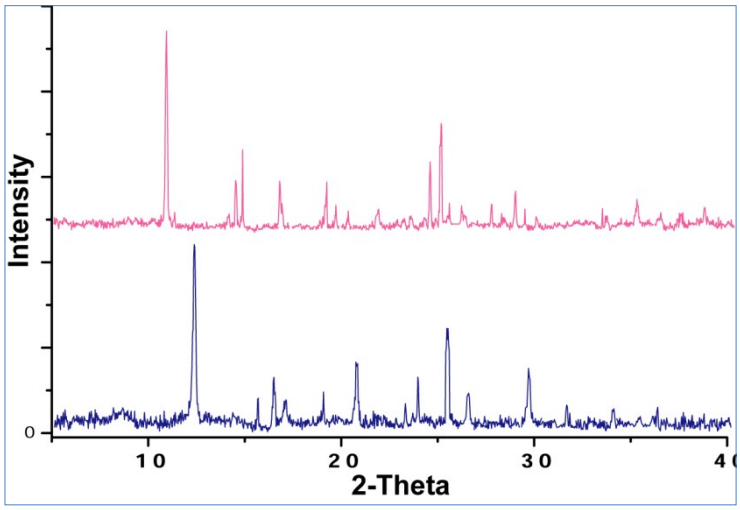
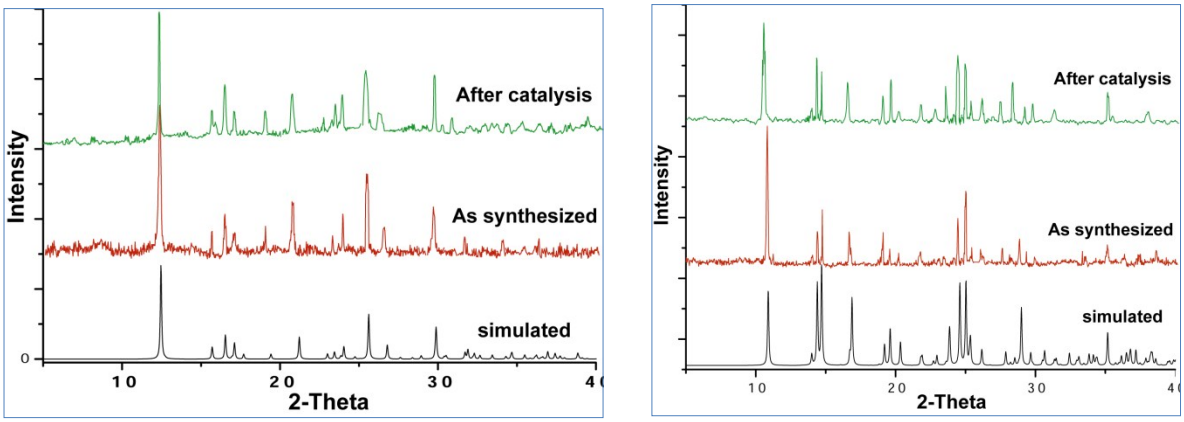


Figure S3 Powder XRD diffractograms of **1** and **2** (the blue and pink curves refer to complexes **1** and **2**, respectively).



A B

Figure S4 Powder XRD diffractograms of **1** (A) and **2** (B) (the red and green curves refer to before and after the catalysis reaction and the black curve is the theoretical one).

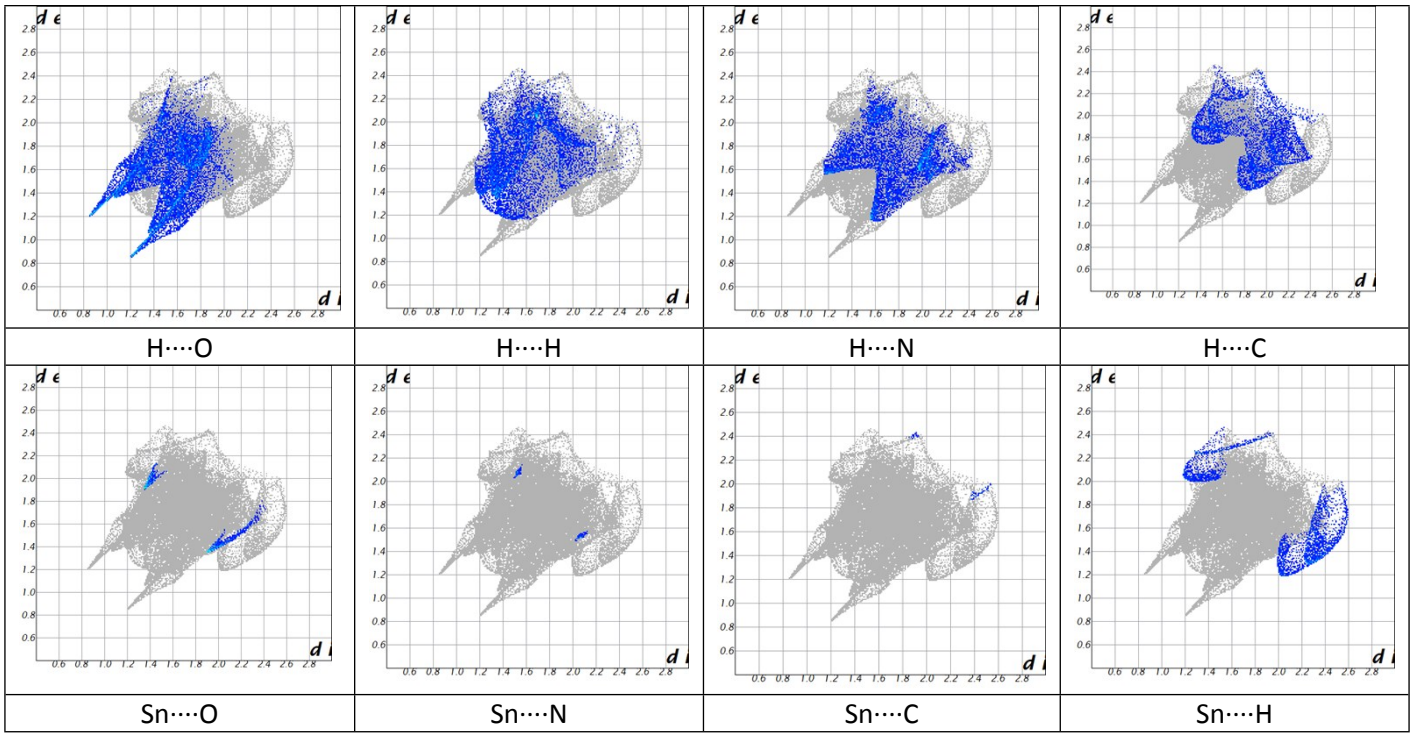


Figure S5 2D fingerprint plots of **1**, exhibiting different intermolecular interactions.

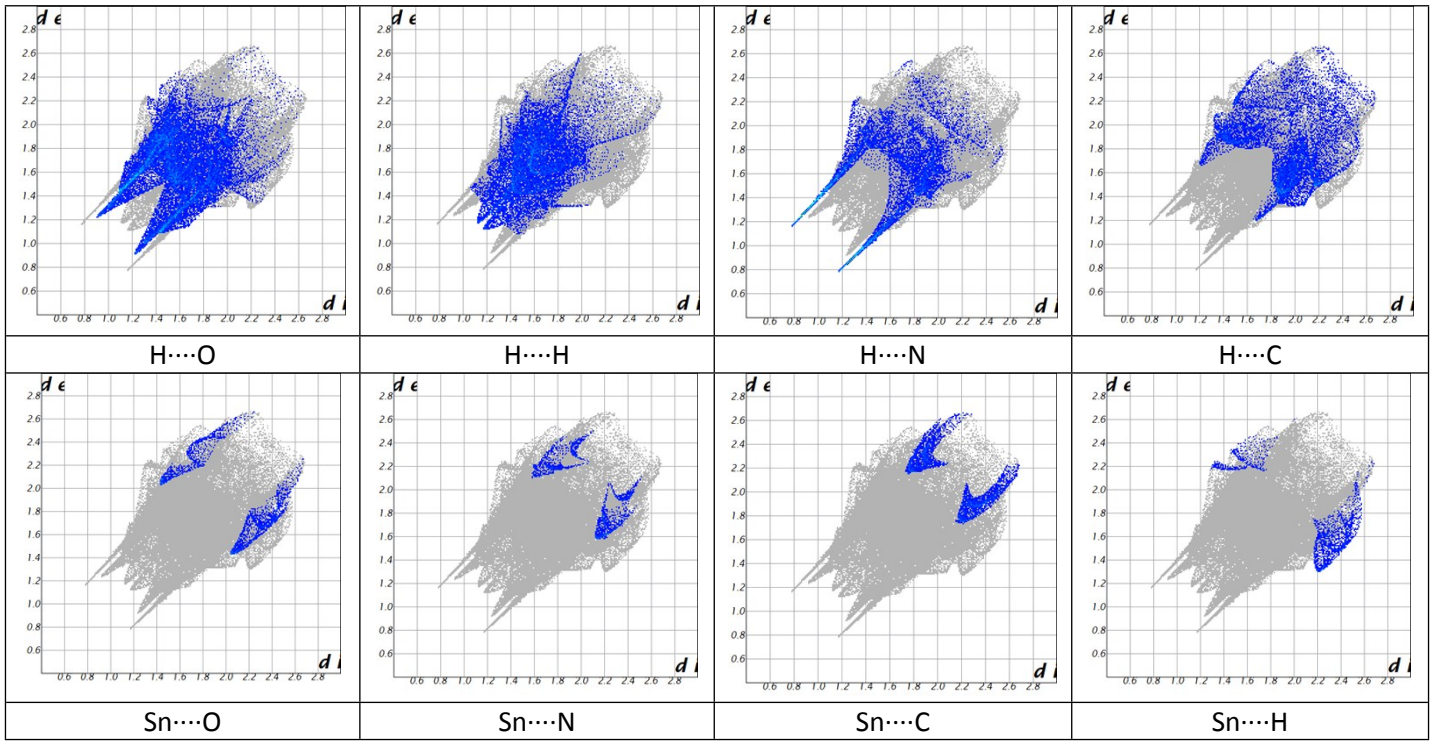


Figure S6 2D fingerprint plots of **2**, exhibiting different intermolecular interactions.

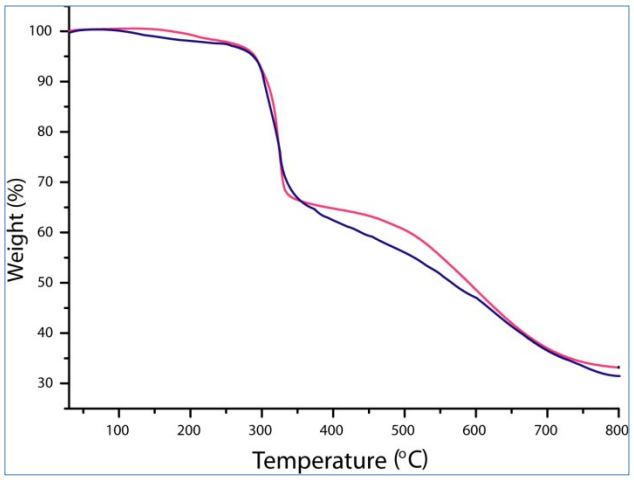


Figure S7 Thermogravimetric curves for **1** (red curve) and **2** (blue curve).

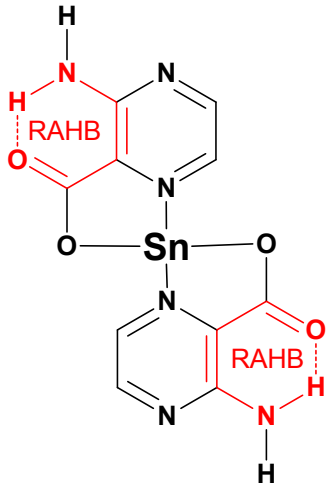
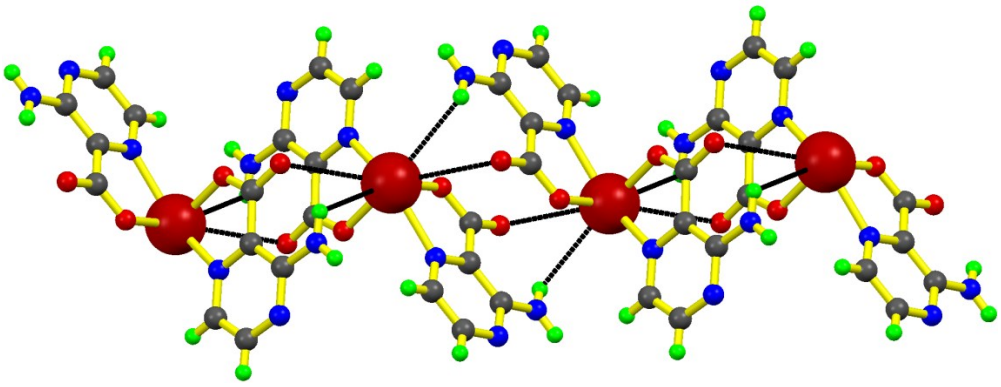
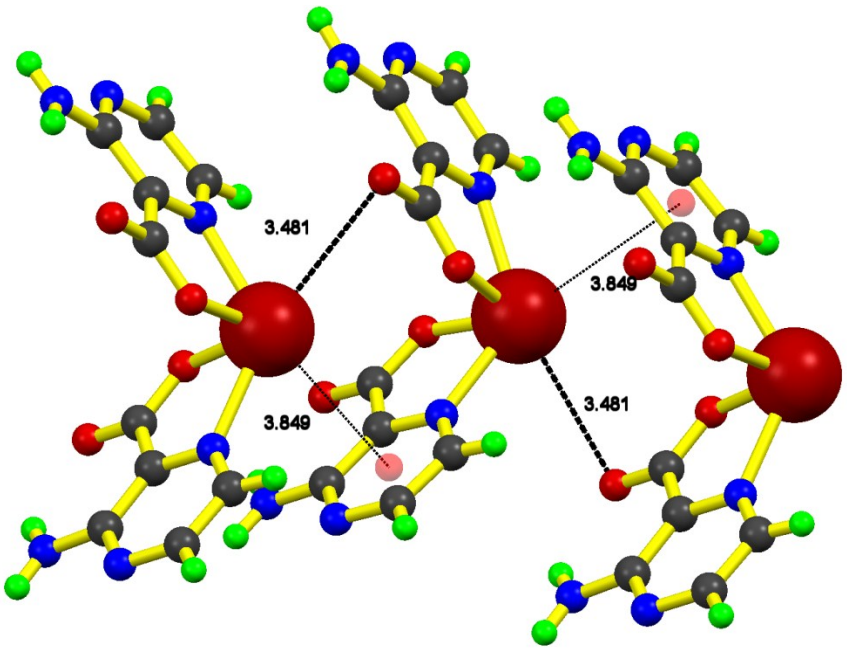


Figure S8 Schematic representation of intramolecular resonance assisted hydrogen bond (RAHB) in complex **1** and **2**.



A



B

Figure S9 (A) Sn···H(N) contacts in compound **1**. (B) Sn···π and Sn···O contacts in compound **2**.

Table S1: Crystal data and structure refinement details for complexes 1 and 2		
Identification name	**Complex 1**	**Complex 2**
Formulae	$C_{10}H_8N_6O_4Sn$	$C_{10}H_8N_6O_4Sn$
Mol. wt.	394.91	394.91
Crystal system	Monoclinic	Monoclinic
Space group	C2/c	$P2_1/c$
Temperature /K	296	296
Wavelength /Å	0.71073	0.71073
a /Å	12.9289(13)	8.2366(4)
b /Å	9.1305(9)	9.4181(4)
c /Å	11.9805(19)	16.5098(8)
α/°	90	90
β/°	119.297(3)	100.057(2)
γ/°	90	90
V/ $Å^3$	1233.4(3)	1261.04(10)
Z	4	4
Density/Mgm^{-3}	2.127	2.080
Abs. Coeff. /mm^{-1}	2.101	2.055
F(000)	768	768
Refl. collected	12182	25306
Refl. unique	1261	2594
Max. 2θ/°	26.391	26.400
Ranges (h, k, l)	-16<= h <=16	-10 <= h <=10

	-11 <= k <=11 -14 <= l <= 14	-11 <= k <=11 -20 <= l <= 20
Complete to 2θ (%)	99.6	99.9
Refl. with I > 2σ(I)	1151	2028
Data/ Restraints/Parameters	1261/ 0 / 104	2594/0/ 206
Goof (F^2)	1.118	1.104
R1 [I > 2s(I)]	0.0246	0.0281
wR2 [I > 2s(I)]	0.0573	0.0591
R1 [all data]	0.0292	0.0460
wR2 [all data]	0.0591	0.0647

Table S2: Hydrogen bond geometry (Å, °) in complexes 1 and 2

Compound	D-H---A	D···H (Å)	H···A (Å)	D···A (Å)	<D–H···A(°)
Complex 1	N3-H2N····O2	0.81(4)	2.13(4)	2.754(4)	135(3)
	N-H1N····O1	0.79(4)	2.29(4)	3.073(4)	168(4)
	C5-H5····O2	0.93	2.55	3.255(4)	133.2
Complex 2	N6-H4N····N2	0.88(4)	2.08(4)	2.959(5)	175(3)
	N3-H1N····N5	0.80(5)	2.28(5)	3.079(5)	176(4)
	N6-H3N····O2	0.79(4)	2.45(4)	2.998(4)	127(4)
	N6-H3N····O4	0.79(4)	2.12(4)	2.746(4)	136(4)
	N3-H2N····O2	0.85(4)	2.18(4)	2.773(5)	127(3)
	N3-H2N····O4	0.85(4)	2.26(4)	2.891(4)	131(3)

Table S3: Selected bond distances (Å) and angles (°) for complexes 1 and 2	
Complex 1	Sn1–O1, 2.155(2); Sn1–N1, 2.400(2). <O1–Sn1–O1' 88.64(11); <O1–Sn1–N1 71.01(8); <O1'–Sn1–N1 79.37(8); <N1–Sn1–N1' 138.25(11).
Complex 2	Sn1–O3 2.134(2); Sn1–O1 2.136(2); Sn1–N1 2.386(3); Sn1–N4 2.443(3). <O3–Sn1–O1 97.28(10); <O3–Sn1–N1 74.92(9); <O1–Sn1–N1 71.21(9); <O3–Sn1–N4 70.35(9); <O1–Sn1–N4 75.30(9); <N1–Sn1–N4 127.33(9).