Electronic Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2014

SUPPORTING INFORMATION

Halide impact on emission of mononuclear copper(I) complexes with pyrazolylpyrimidine and triphenylphosphine

Katerina A. Vinogradova,[a] Victor F. Plyusnin,[b,c] Arkady S. Kupryakov,[b,c] Marianna I. Rakhmanova,[a] Natalia V. Pervukhina,[a] Dmitrii Yu. Naumov,[a] Lilia A. Sheludyakova,[a,b] Elena B. Nikolaenkova,[d] Viktor P. Krivopalov[d] and Mark B. Bushuev [*a,b]

[a] *Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, 3, Akad. Lavrentiev Ave., Novosibirsk, 630090, Russia*
E-mail: bushuev@niic.nsc.ru; Fax: +7 (383) 330-94-89

[b] *Department of Natural Sciences, Novosibirsk State University (National Research University), 2, Pirogova str., Novosibirsk, 630090, Russia*

[c] *Institute of Chemical Kinetics and Combustion, Siberian Branch of Russian Academy of Sciences, 3, Institutskaya str., Novosibirsk, 630090, Russia*

[d] *N. N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Siberian Branch of Russian Academy of Sciences, 9, Akad. Lavrentiev Ave., Novosibirsk, 630090, Russia*

Electronic Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2014

Table of contents

This journal is © The Royal Society of Chemistry 2014

Table S1. Crystal data and structure refinement for **1** – **3**.

Compound	**1**	**2**	**3**
Empirical formula	$C_{42}H_{38}ClCuN_5P$	$C_{42}H_{38}BrCuN_5P$	$C_{42}H_{38}CuIN_5P$
Formula weight	742.73	787.19	834.18
Temperature	150(2)	296(2)K	150(2) K
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$
Unit cell dimensions	*a* = 11.1677(4) Å	*a* = 11.2558(4) Å	*a* = 10.5244(3) Å
	b = 13.1184(7) Å	*b* = 13.1040(5) Å	*b* = 17.7367(7) Å
	c = 13.3150(7) Å	*c* = 13.3930(5) Å	*c* = 20.6698(9) Å
	α= 69.397(1)°	α= 69.840(1)°	
	β= 79.404(1)°	β= 79.440(1)°	β= 104.190(1)°
	γ= 82.514(1)°	γ= 82.646(1)°	
Volume	1790.2(1) $Å^3$	1818.5(1) $Å^3$	3740.7(2) $Å^3$
Z	2	2	4
Density (calculated)	1.378 Mg/m^3	1.438 Mg/m^3	1.481 Mg/m^3
Absorption coefficient	0.768 mm^{-1}	1.781 mm^{-1}	1.489 mm^{-1}
Crystal size	0.25 x 0.22 x 0.15 mm^3	0.38 x 0.25 x 0.12 mm^3	0.41 x 0.39 x 0.35 mm^3
Theta range for data collection	1.91 – 26.37°	1.66 – 26.02°	1.53 – 26.02°
Index ranges	$-13 \le h \le 8$, $-16 \le k \le 16$, $-16 \le l \le 16$	$-13 \le h \le 12$, $-16 \le k \le 14$, $-15 \le l \le 16$	$-12 \le h \le 7$, $-21 \le k \le 21$, $-24 \le l \le 25$
Reflections collected	10358	12737	21289
Independent reflections	7270 (R_{int} = 0.0149)	7157 (R_{int} = 0.0214)	6751 (R_{int} = 0.0246)
Completeness to theta = 25.50°	99.4 %	99.9 %	91.8 %
Max. and min. transmission	0.8935 and 0.8312	0.5509 and 0.8147	0.6238 and 0.5804
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	7270 / 10 / 486	7157 / 2 / 496	6751 / 0 / 451
Goodness-of-fit on F^2	1.049	1.058	1.057
Final R indices ($I>2\sigma_I$)	R_1 = 0.0330, wR_2 = 0.0756	R_1 = 0.0341, wR_2 = 0.0722	R_1 = 0.0256, wR_2 = 0.0583
R indices (all data)	R_1 = 0.0494, wR_2 = 0.0799	R_1 = 0.0504, wR_2 = 0.0762	R_1 = 0.0350, wR_2 = 0.0615
Largest diff. peak and hole	0.379 and -0.288 e/$Å^3$	0.533 and -0.396 e/$Å^3$	0.348 and -0.365 e/$Å^3$

This journal is © The Royal Society of Chemistry 2014

Table S2. Selected bond lengths (Å) and angles [°] for **1 – 3**.

Bond	d	Angle	ω
Compound **1**			
Cu(1)-N(11)	2.123(2)	N(11)-Cu(1)-N(13)	76.75(7)
Cu(1)-N(13)	2.127(2)	N(11)-Cu(1)-P(1)	113.79(5)
Cu(1)-P(1)	2.1897(6)	N(13)-Cu(1)-P(1)	110.28(5)
Cu(1)-Cl(1)	2.2752(5)	N(11)-Cu(1)-Cl(1)	114.85(5)
		N(13)-Cu(1)-Cl(1)	100.88(5)
		P(1)-Cu(1)-Cl(1)	126.67(2)
Compound **2**			
Cu(1)-N(11)	2.113(2)	N(13)-Cu(1)-N(11)	77.08(7)
Cu(1)-N(13)	2.104(2)	N(11)-Cu(1)-P(1)	115.02(6)
Cu(1)-P(1)	2.1890(7)	N(13)-Cu(1)-P(1)	110.68(7)
Cu(1)-Br(1)	2.4003(4)	N(11)-Cu(1)-Br(1)	115.18(6)
		N(13)-Cu(1)-Br(1)	100.28(7)
		P(1)-Cu(1)-Br(1)	125.31(2)
Compound **3**			
Cu(1)-N(11)	2.090(2)	N(11)-Cu(1)-N(13)	78.16(7)
Cu(1)-N(13)	2.111(2)	N(11)-Cu(1)-P(1)	124.13(5)
Cu(1)-P(1)	2.1992(6)	N(13)-Cu(1)-P(1)	113.90(6)
Cu(1)-I(1)	2.6024(3)	N(11)-Cu(1)-I(1)	109.62(5)
		N(13)-Cu(1)-I(1)	101.72(5)
		P(1)-Cu(1)-I(1)	119.43(2)

This journal is © The Royal Society of Chemistry 2014

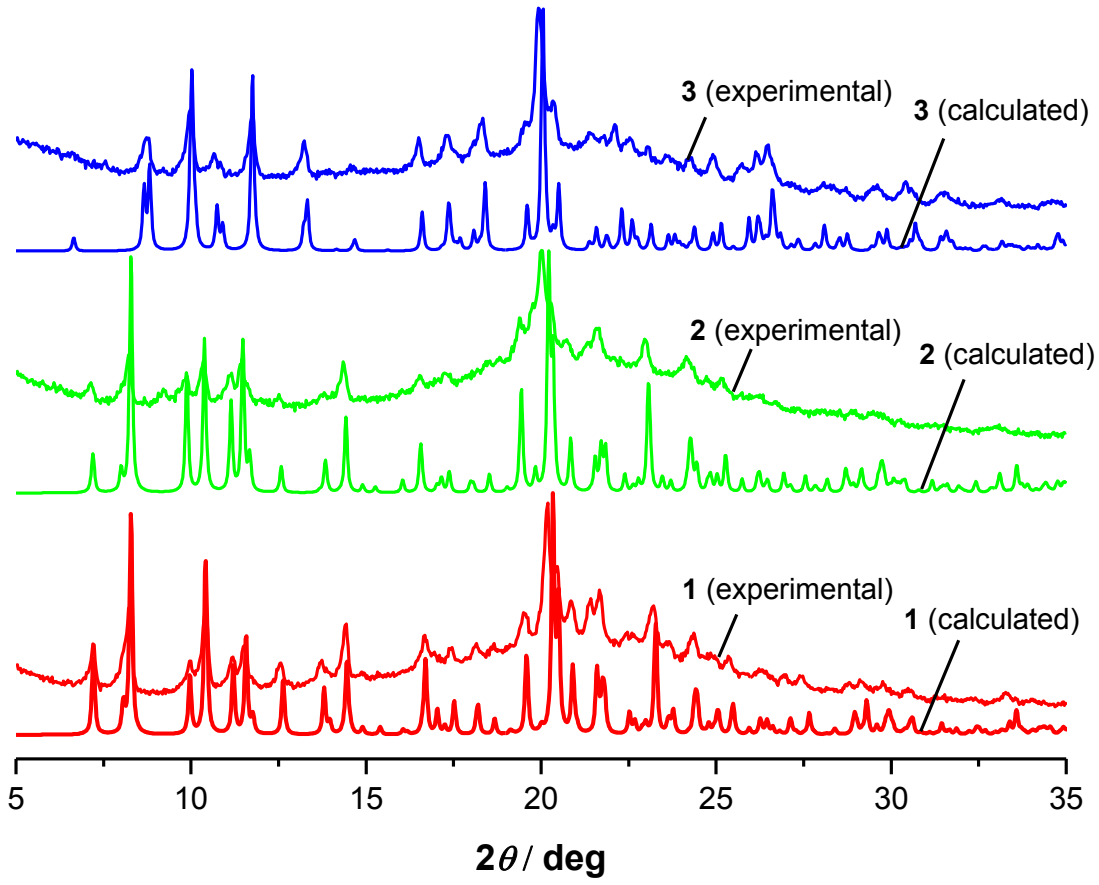

Fig. S1. X-ray powder patterns for **1**, **2** and **3**.

This journal is © The Royal Society of Chemistry 2014

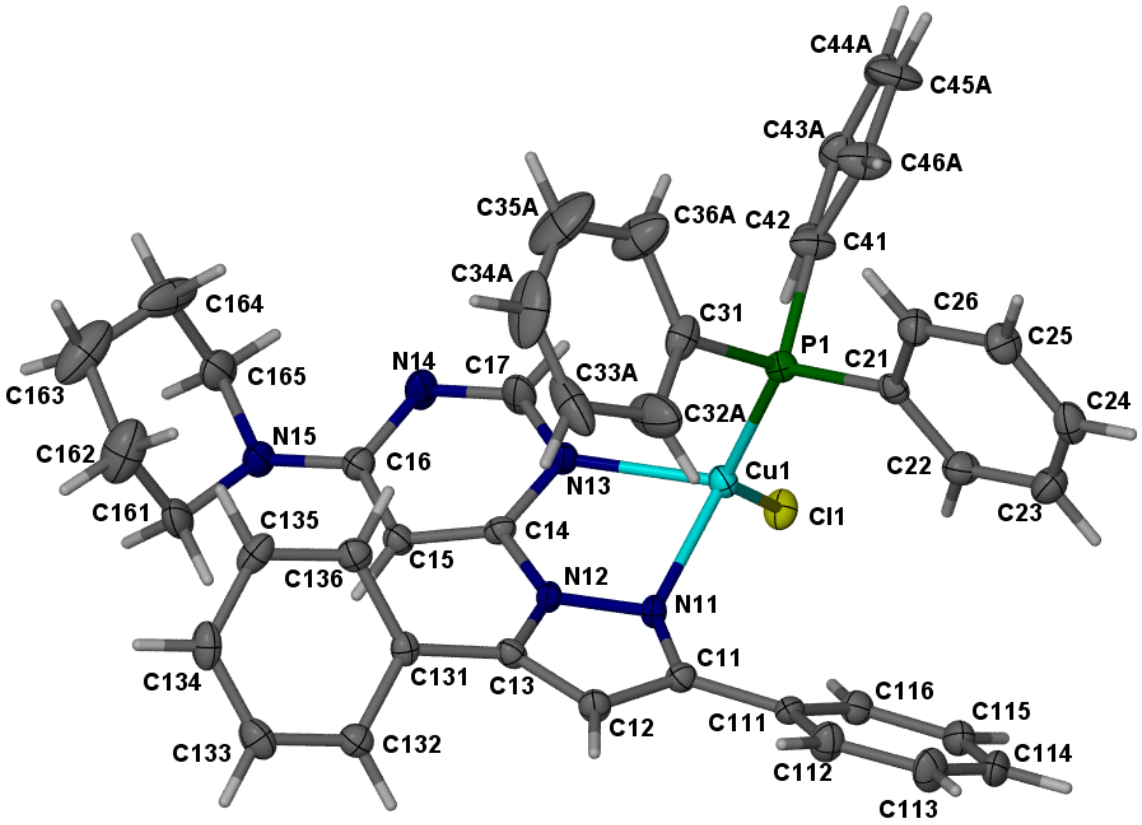

Fig. S2. Molecular structure of **1**.

This journal is © The Royal Society of Chemistry 2014

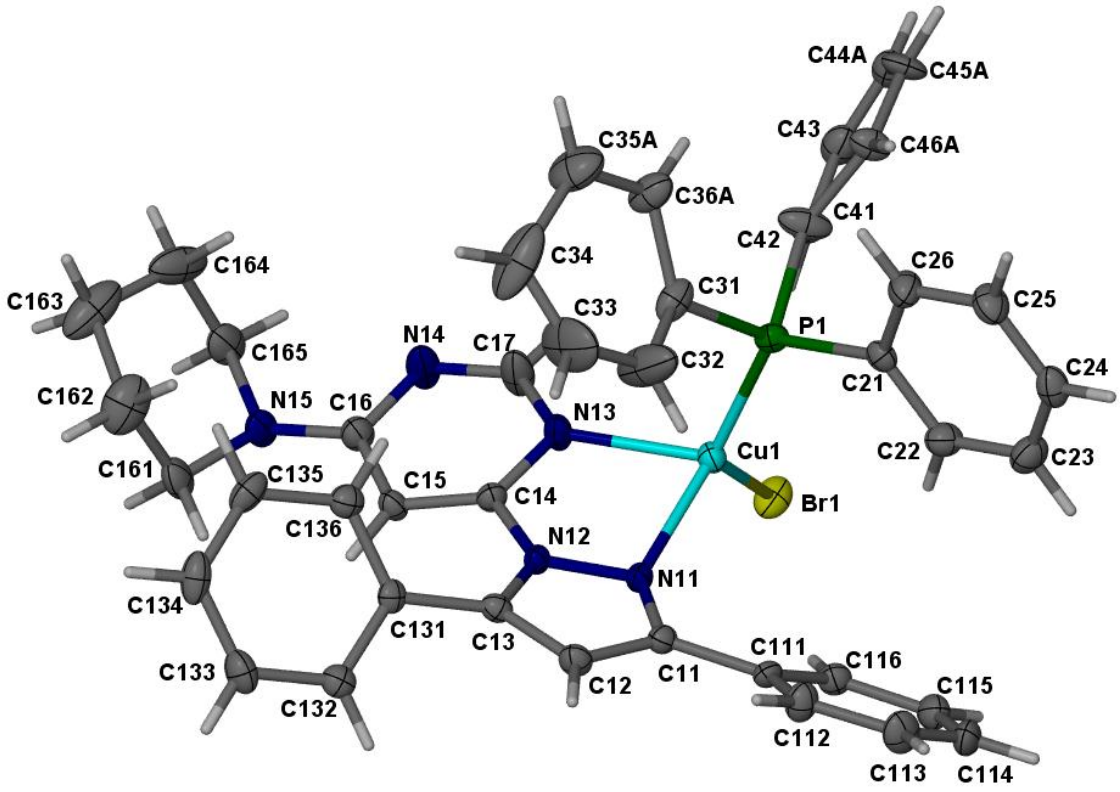

Fig. S3. Molecular structure of **2**.

This journal is © The Royal Society of Chemistry 2014

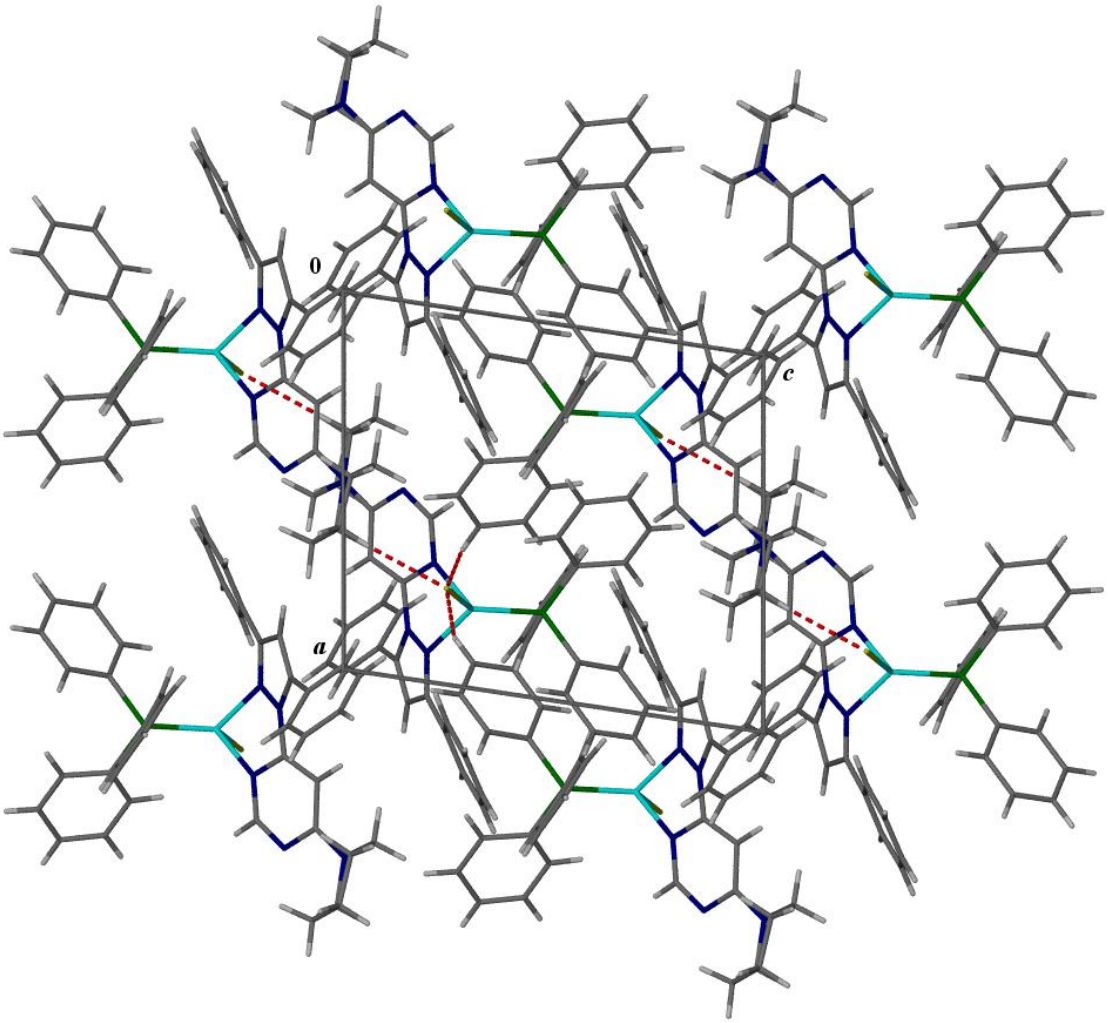

Fig. S4. Packing diagram of **1**.

This journal is © The Royal Society of Chemistry 2014

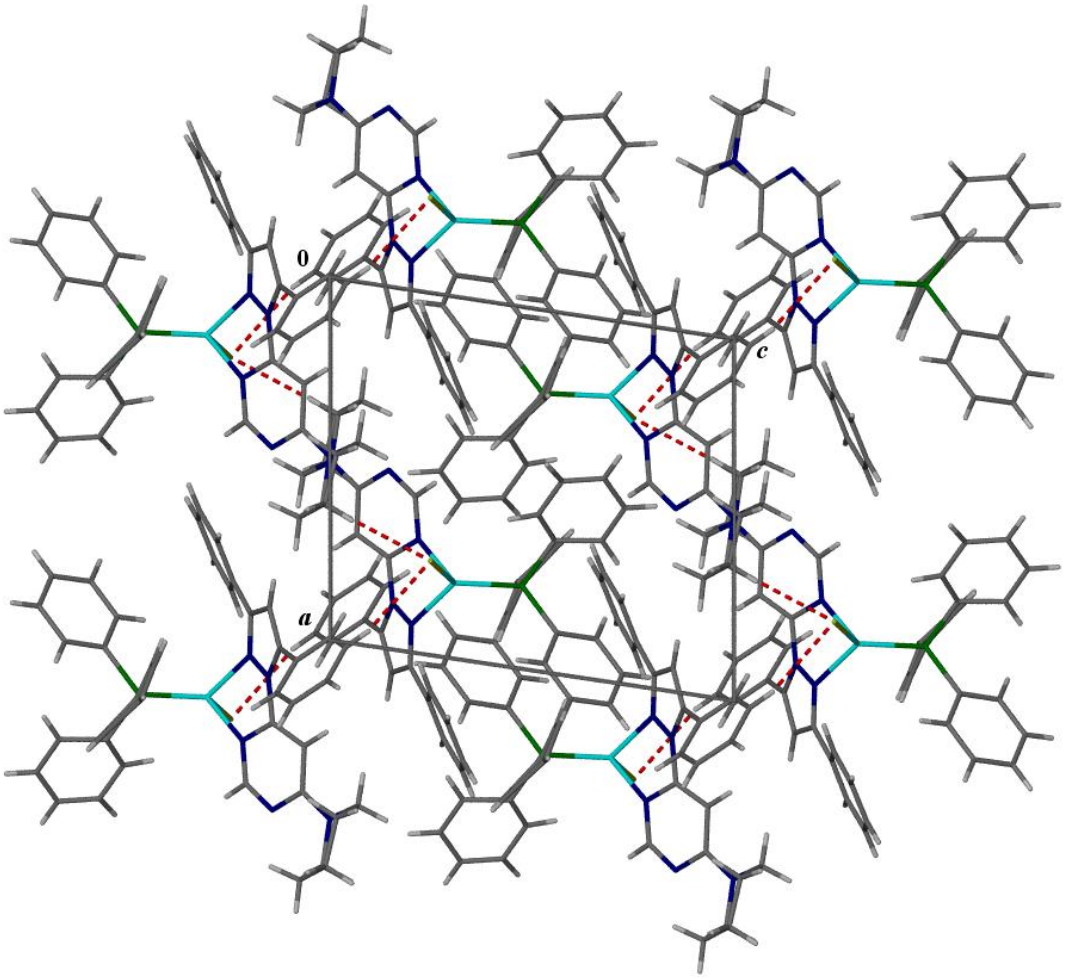

Fig. S5. Packing diagram of **2**.

This journal is © The Royal Society of Chemistry 2014

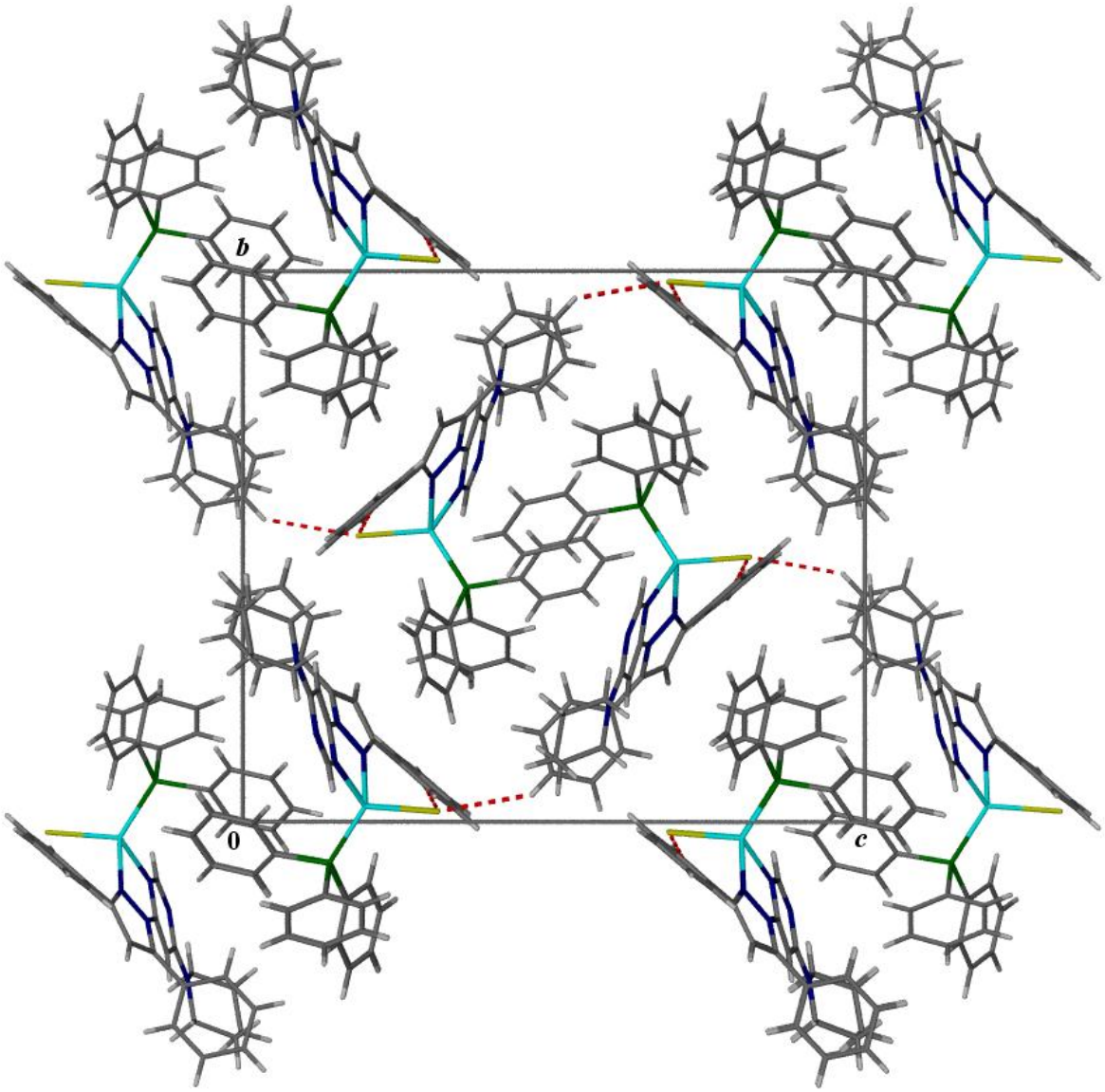

Fig. S6. Packing diagram of **3**.

This journal is © The Royal Society of Chemistry 2014

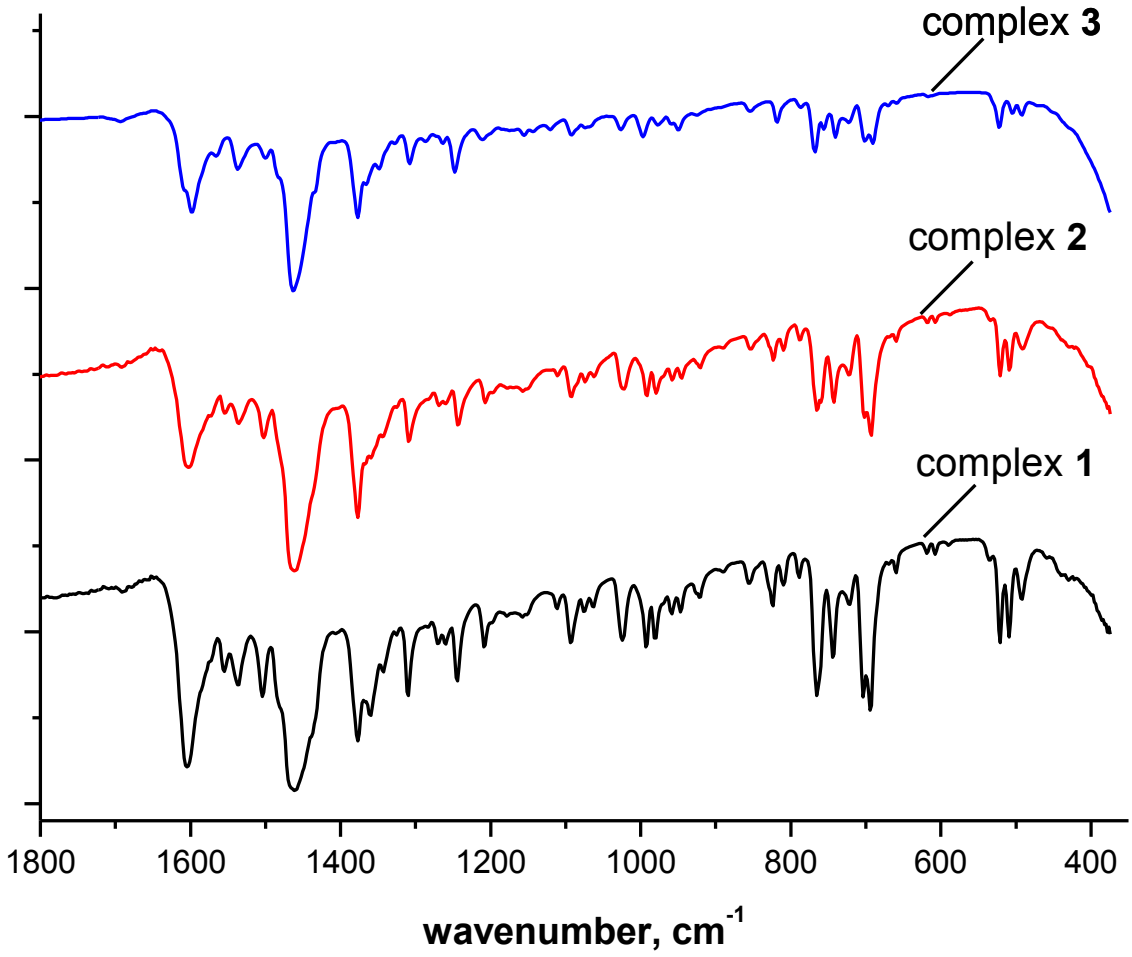

Fig. S7. IR spectra of **1**, **2** and **3** (1800 – 400 cm^{-1}, Nujol).

This journal is © The Royal Society of Chemistry 2014

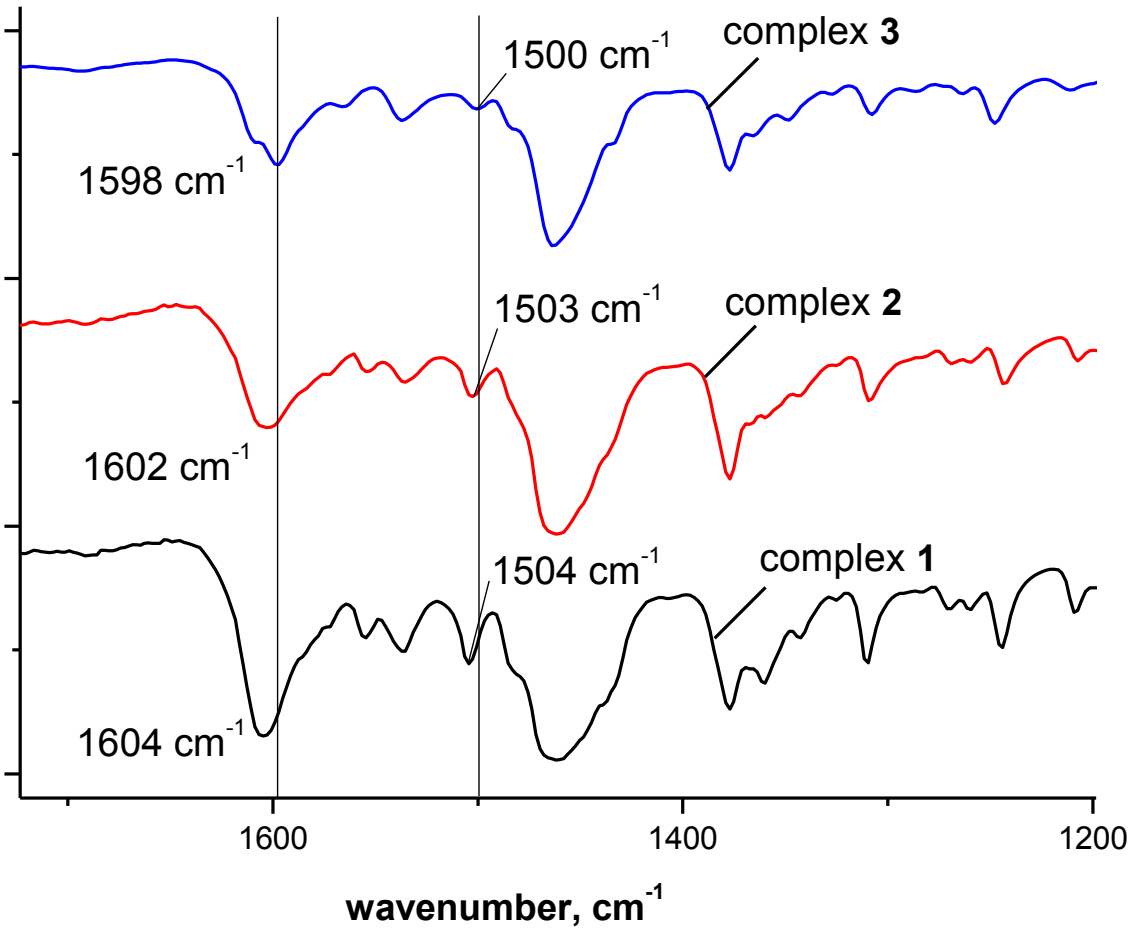

Fig. S8. IR spectra of **1**, **2** and **3** (1700 – 1200 cm^{-1}, Nujol).

This journal is © The Royal Society of Chemistry 2014

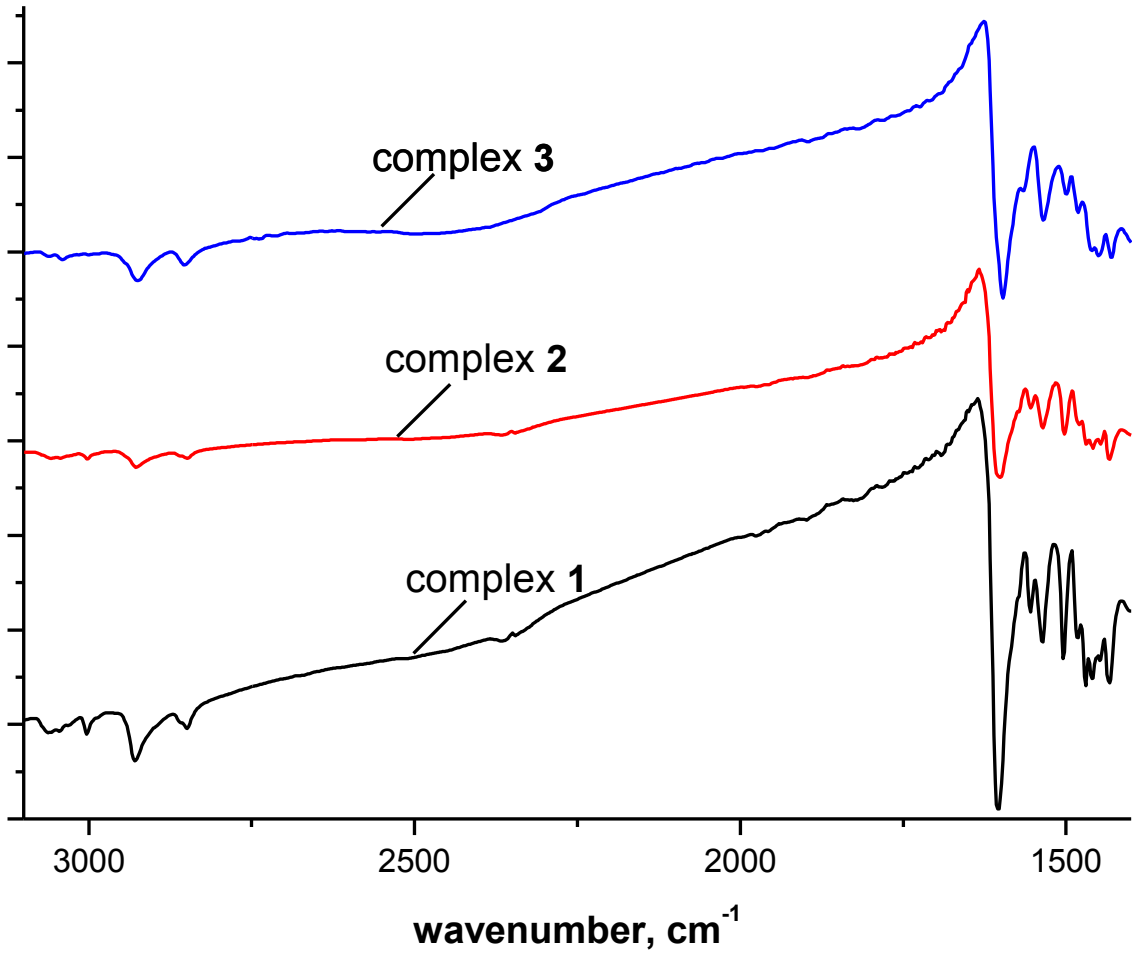

Fig. S9. IR spectra of **1**, **2** and **3** (3100 – 1400 cm^{-1}, fluorinated oil).

This journal is © The Royal Society of Chemistry 2014

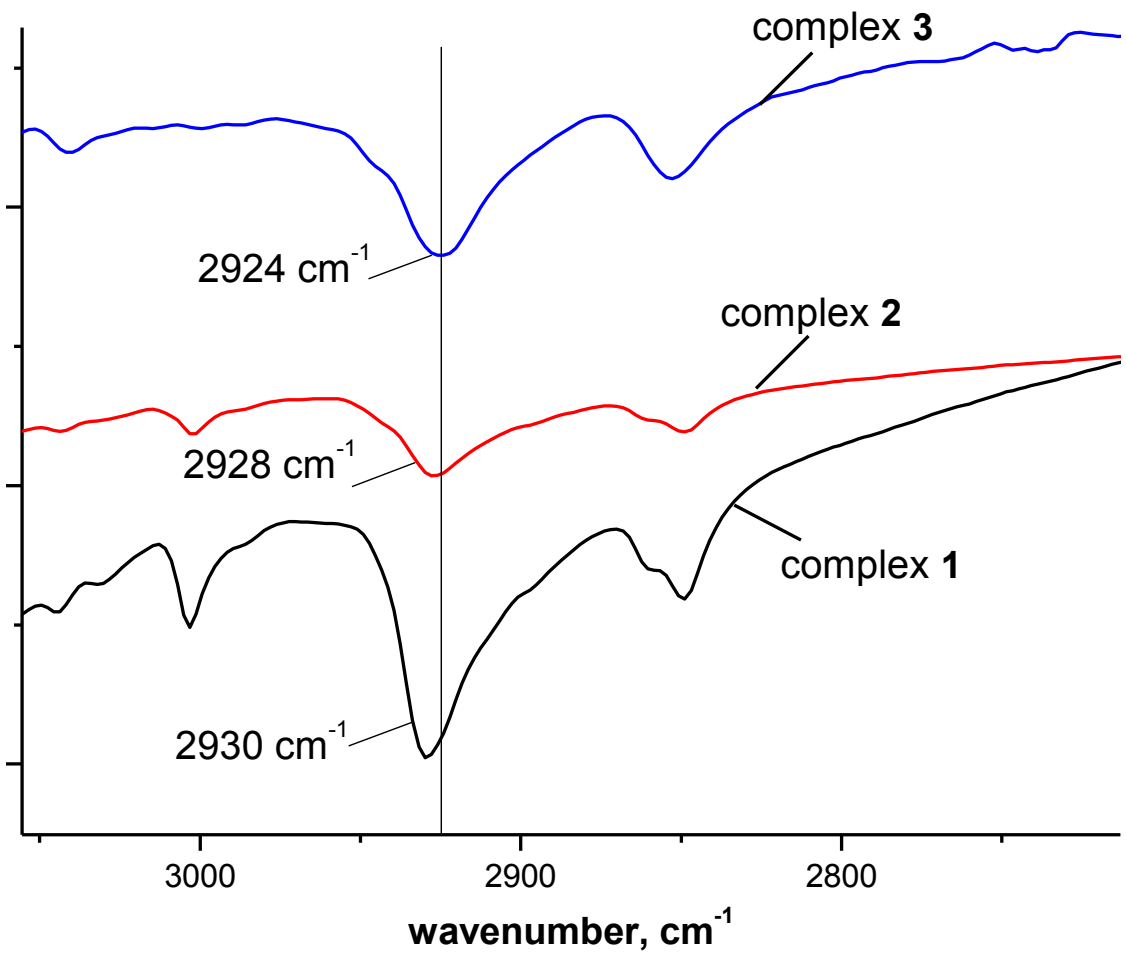

Fig. S10. IR spectra of **1**, **2** and **3** (3100 – 2700 cm^{-1}, fluorinated oil).

This journal is © The Royal Society of Chemistry 2014

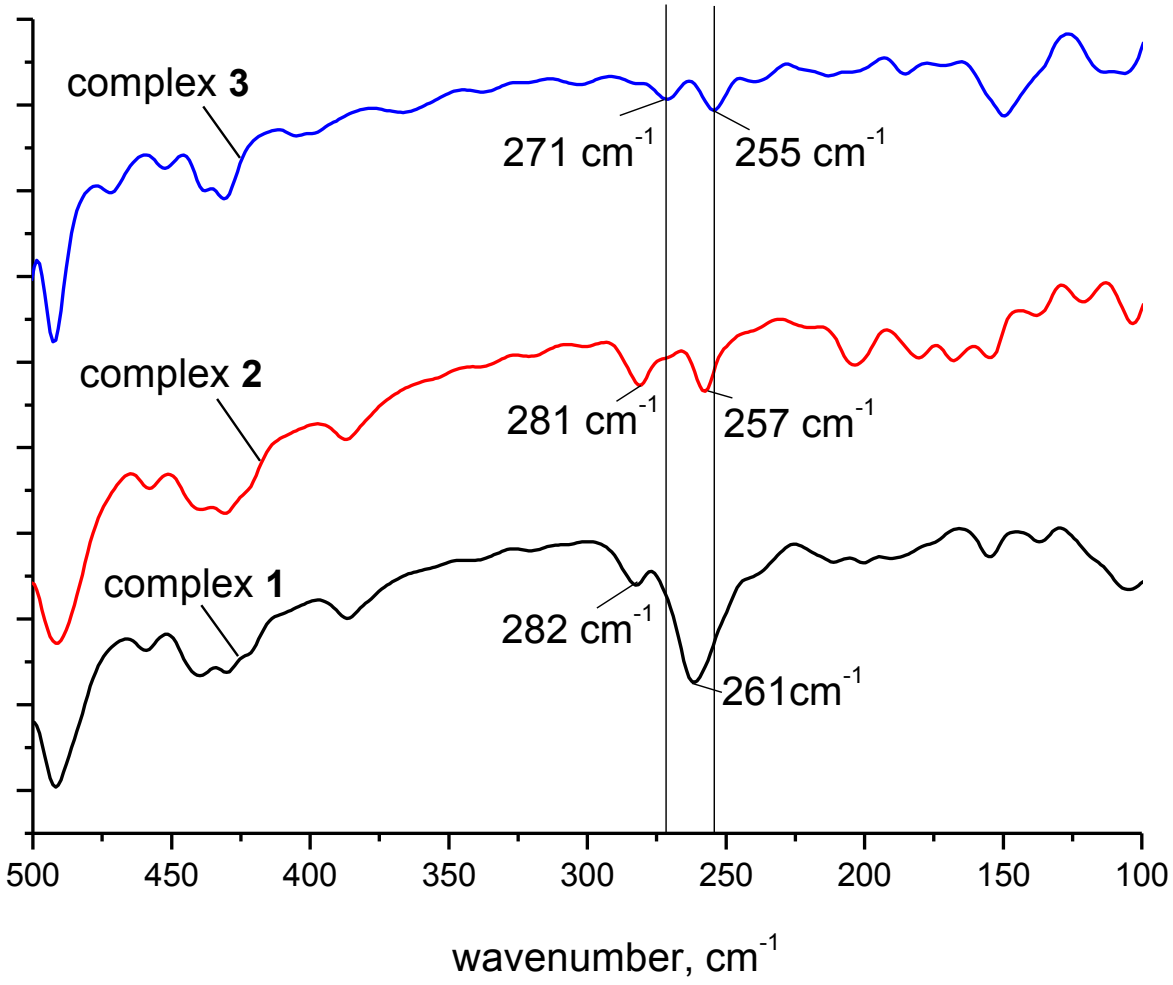

Fig. S11. Far IR spectra of **1**, **2** and **3**.