Supplement to Dalton paper

Formazanido Complexes of Heavier Group 13 Elements Aluminium, Gallium, and Indium

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NMR spectra

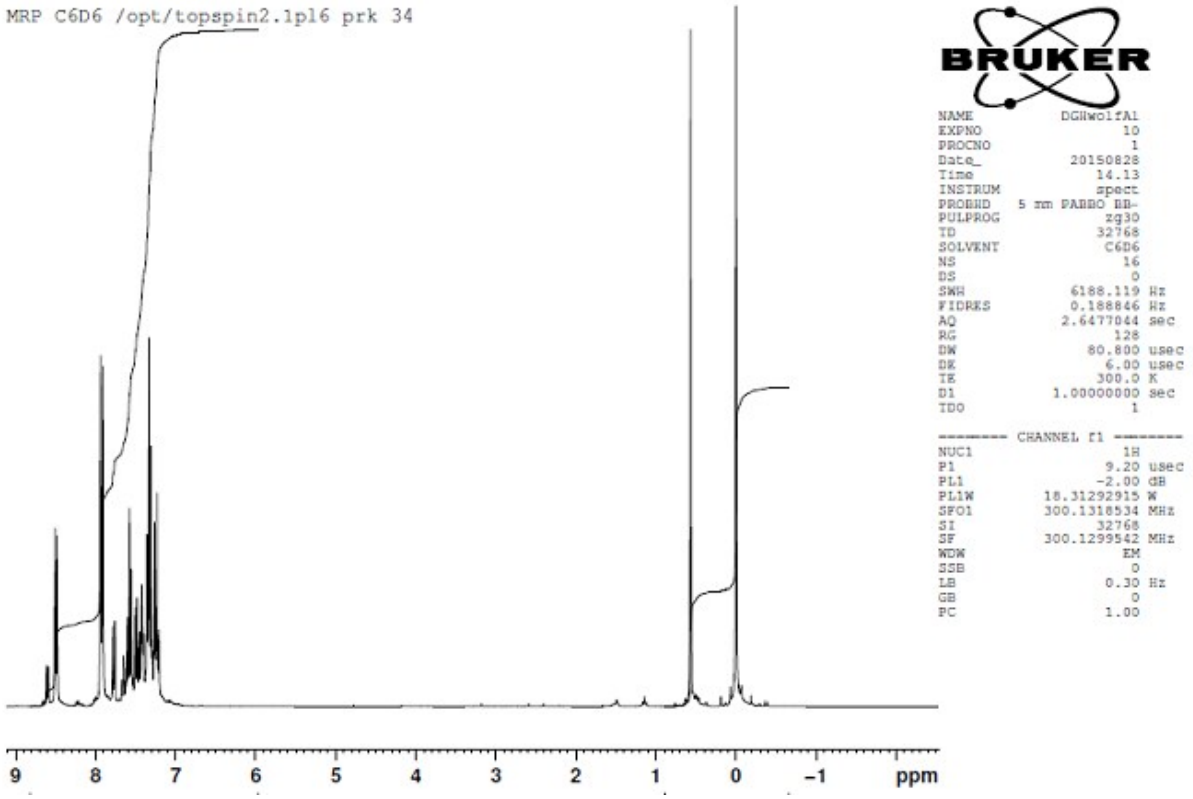

Figure S1: ^{1}H-NMR of **2** in C_6D_6.

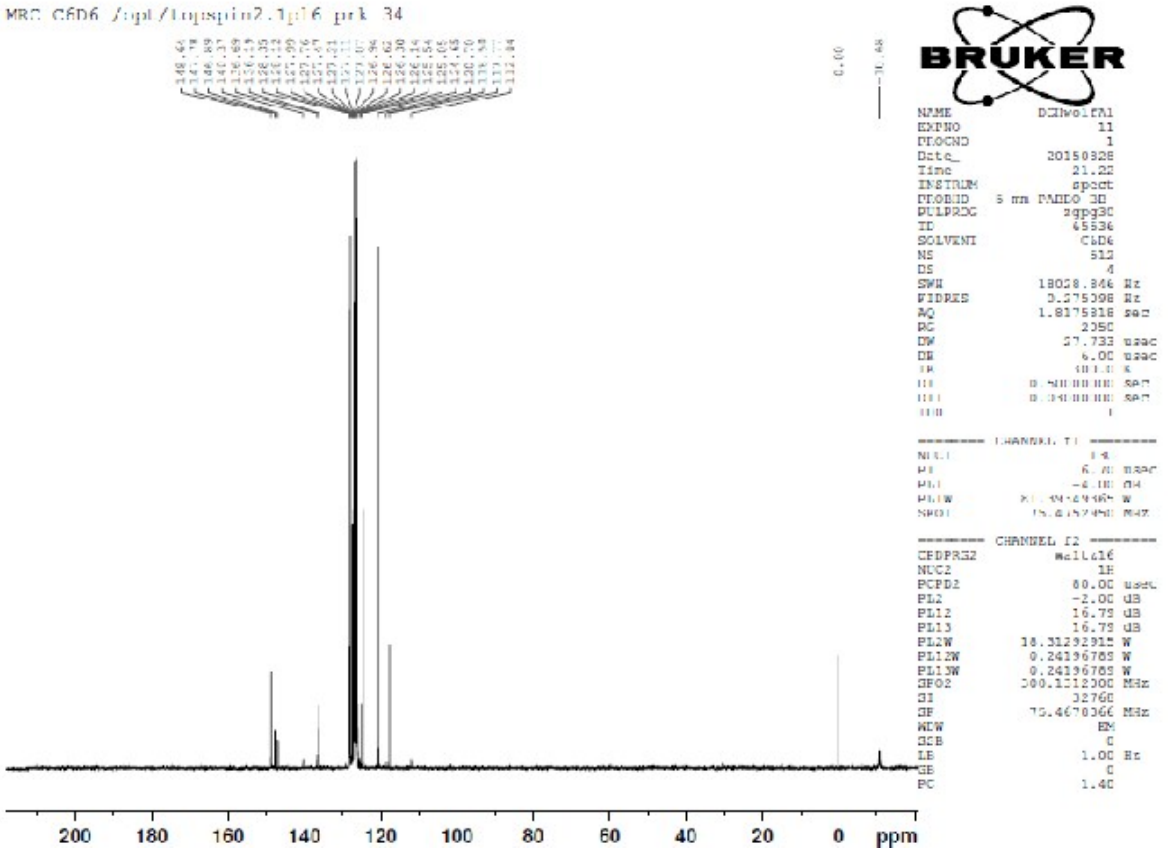

Figure S2: ^{13}C-NMR of **2** in C_6D_6.

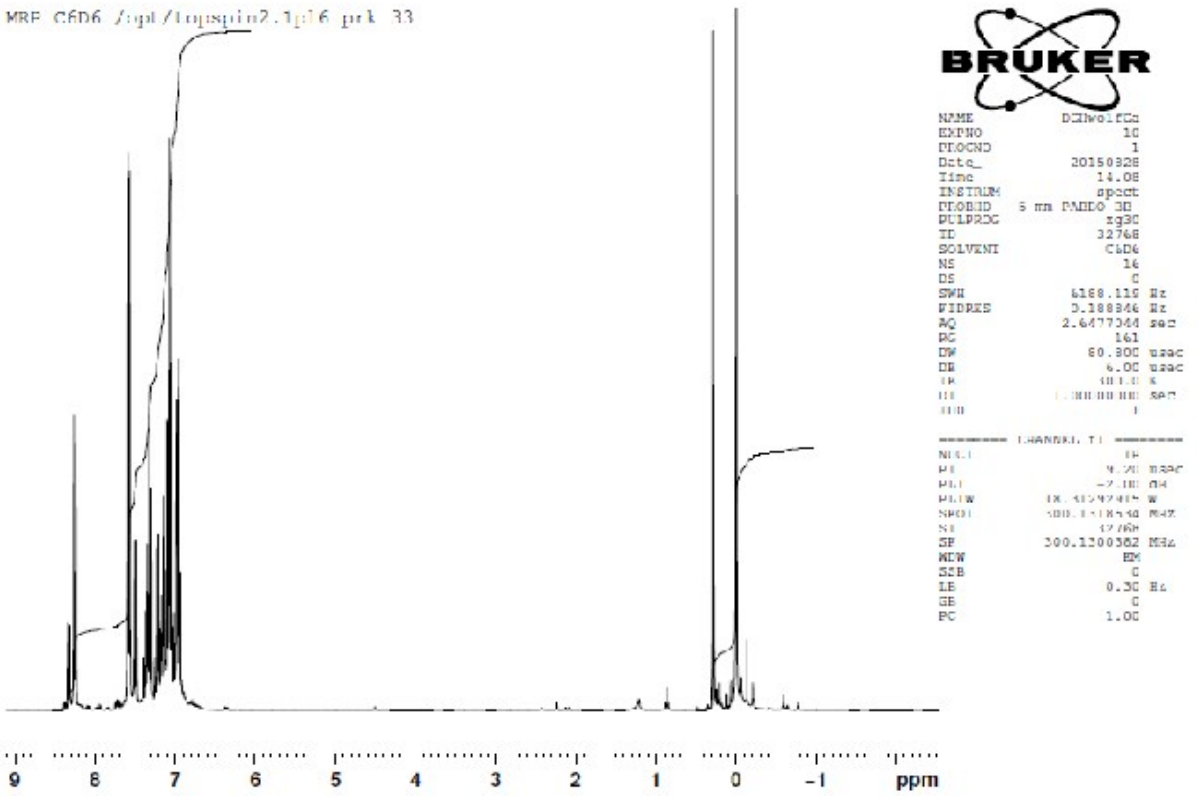

Figure S3: ^{1}H-NMR of **3** in C_6D_6.

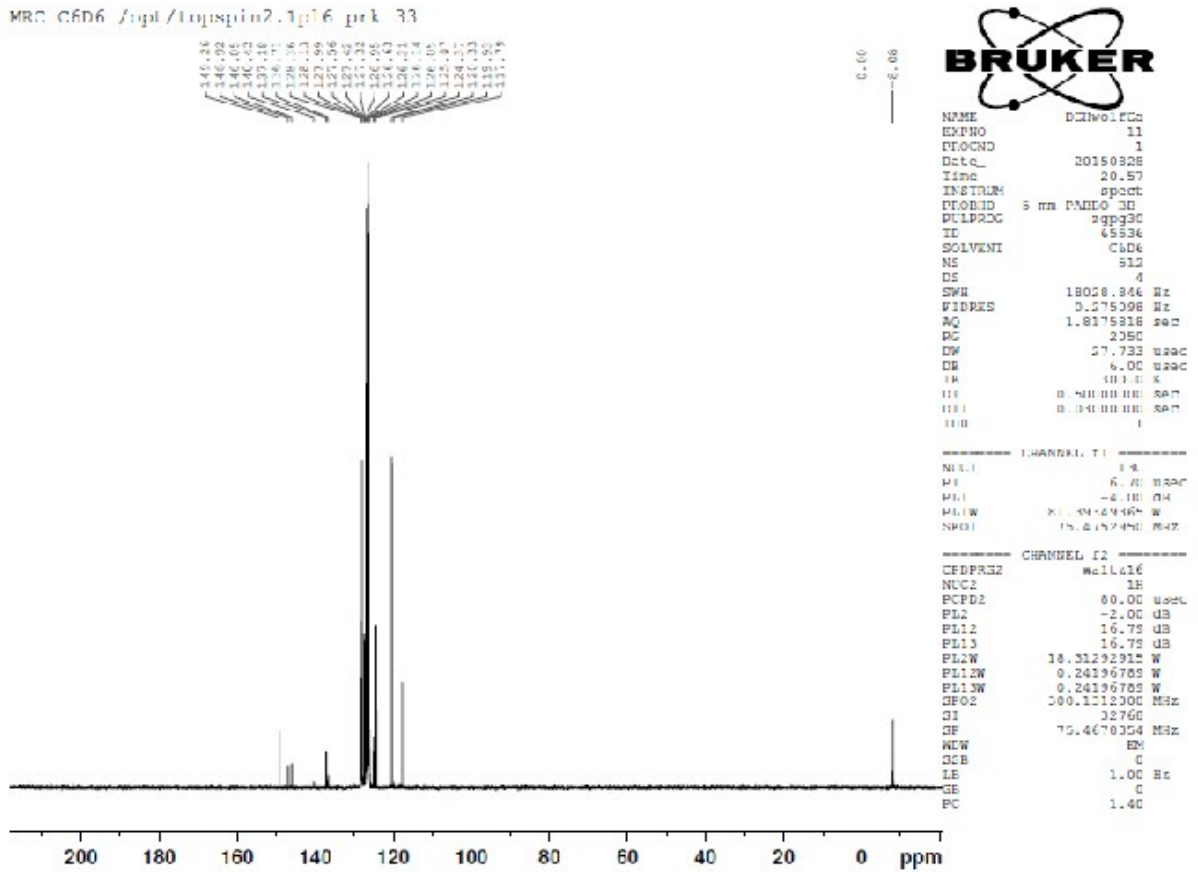

Figure S4: ^{13}C-NMR of **3** in C_6D_6.

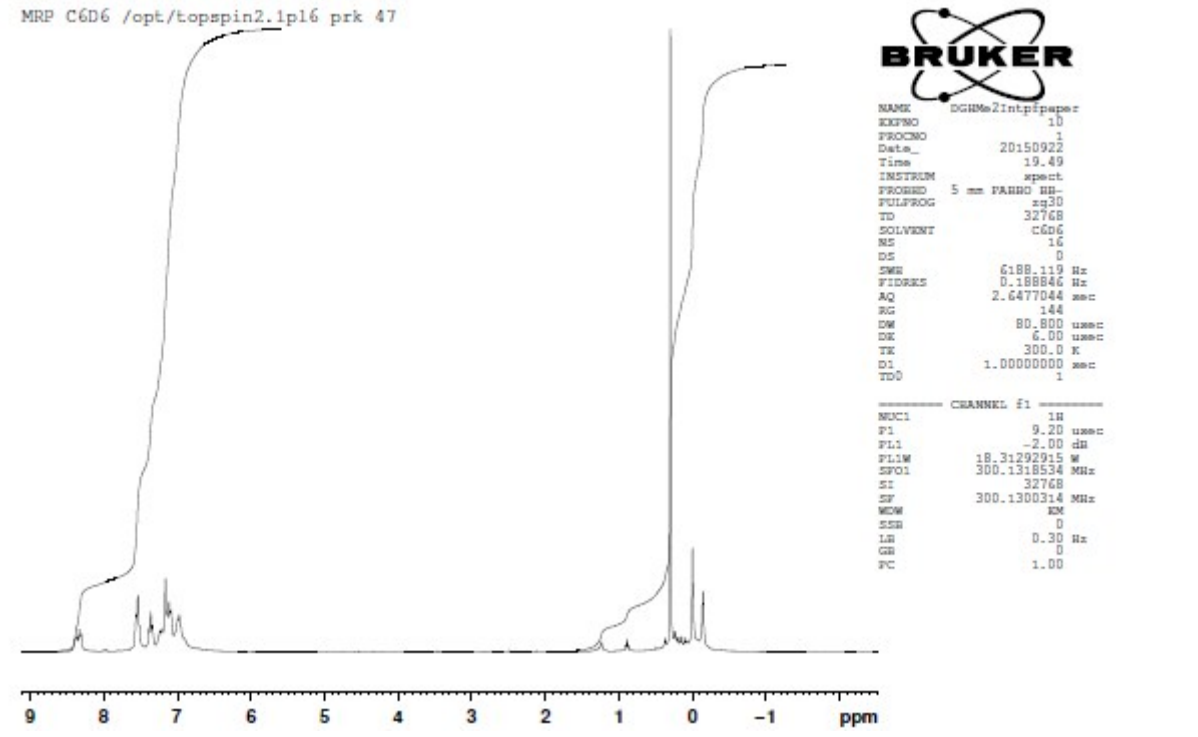

Figure S5: ^{1}H-NMR of **4** in C_6D_6.

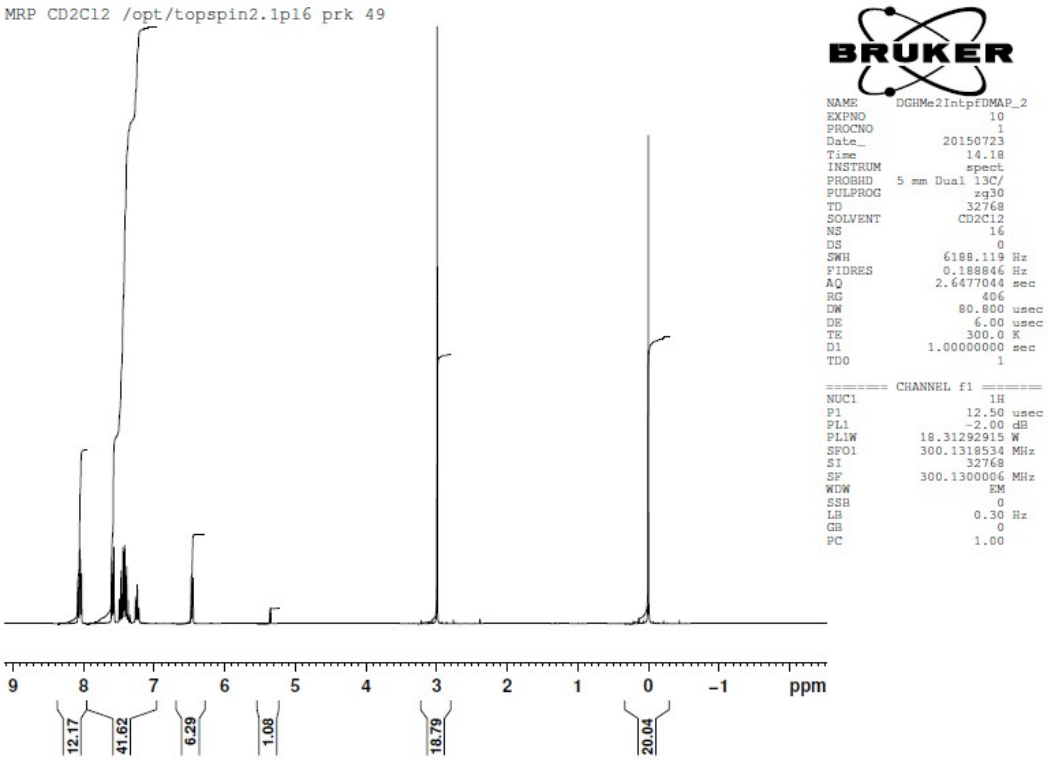

Figure S6: ^{1}H-NMR of **5** in CD_2Cl_2.

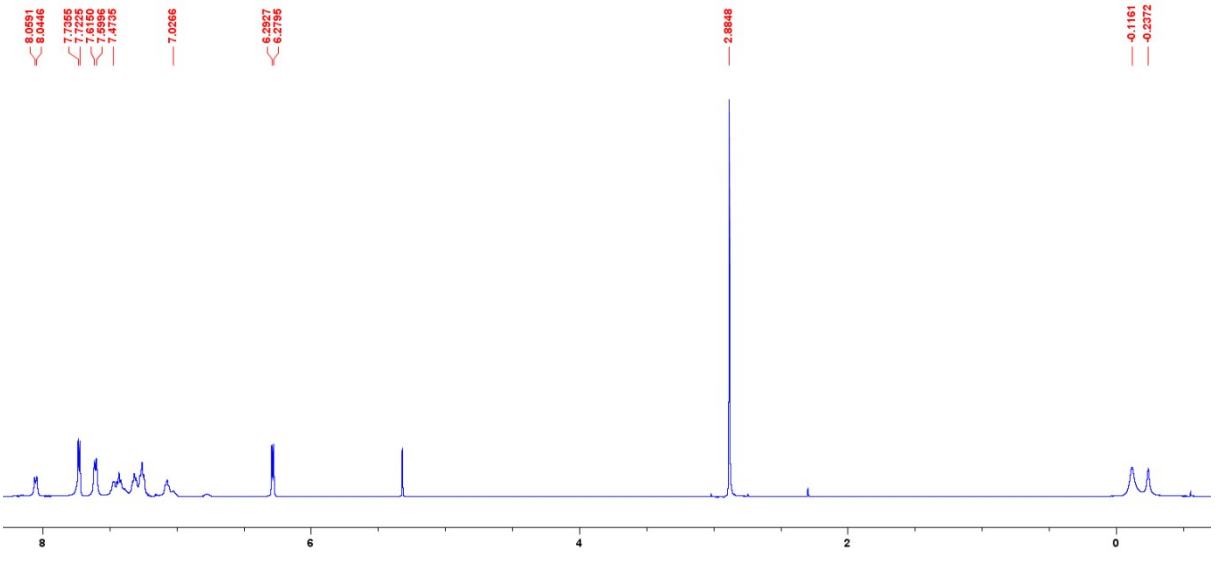

Figure S7: vt-^{1}H-NMR of **5** in CD_2Cl_2.

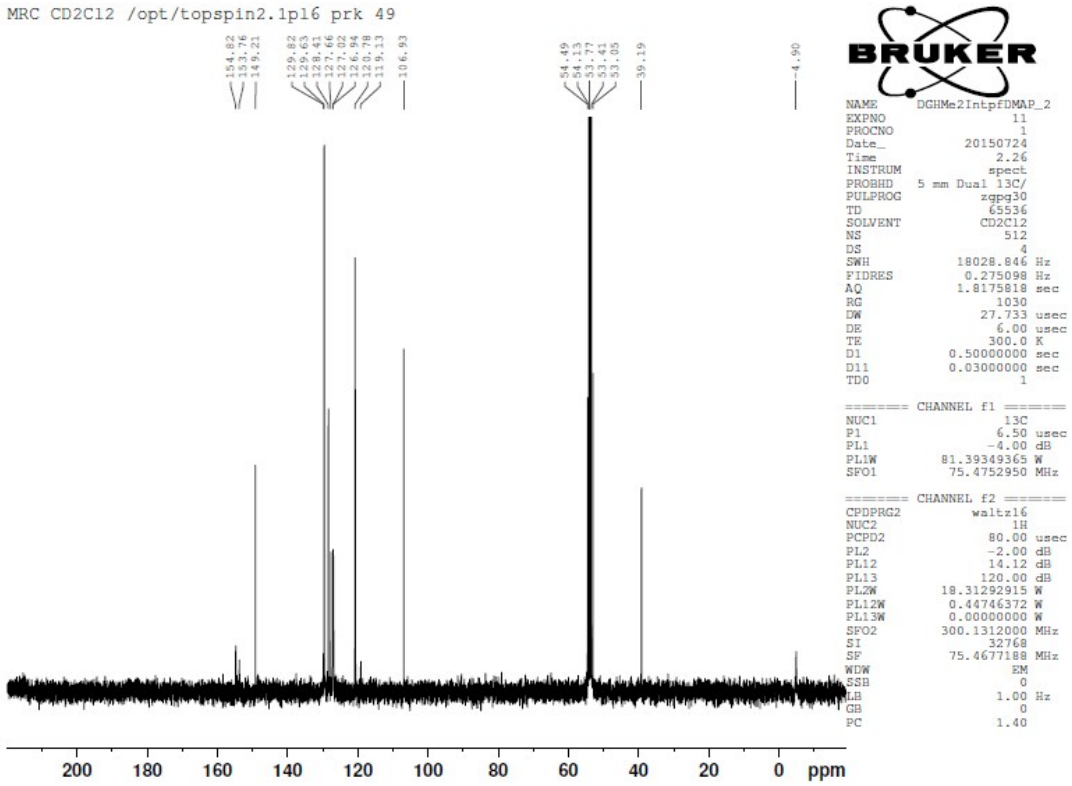

Figure S8: ^{13}C-NMR of **5** in C_6D_6.

XRD Analyses:

Table S1 Crystallographic details and **CCDC numbers**

Compound (**CCDC Number**)	**1** (1414630)	**2** (1414631)	**3** (1414632)	**5** (1414633)
Empirical formula	$C_{19}H_{16}N_4$	$C_{21}H_{21}AlN_4$	$C_{21}H_{21}GaN_4$	$C_{28}H_{31}InN_6$
Formula weight / g mol^{-1}	300.36	356.40	399.14	566.40
Temperature / K	100	100	100	100
Wavelength / Å	0.71073 (Mo-K$_\alpha$)	0.71073 (Mo-K$_\alpha$)	0.71073 (Mo-K$_\alpha$)	0.71073 (Mo-K$_\alpha$)
Crystal system	monoclinic	orthorhombic	orthorhombic	monoclinic
Space group	$P2_1$ (4)	*Pcan* (60)	*Pcan* (60)	$P2_1/c$ (14)
a / Å	5.5221(9)	7.1385(3)	7.1467(3)	16.9585(8)
b / Å	14.646(2)	12.8158(5)	12.7892(5)	10.4646(5)
c / Å	9.6251(15)	40.238(2)	40.302(2)	15.2020(7)
α / °	90	90	90	90
β / °	97.844(6)	90	90	104.804(2)
γ / °	90	90	90	90
Volume /Å^3	771.16(20)	3681.20(28)	3681.20(28)	2608.25(20)
Z	2	8	8	4
Density (calculated) / Mg m^{-3}	1.29345	1.28606	1.44029	1.44226
Colour and habit	dark red plate	dark blue needle	violet plate	dark red block
Crystal size / mm^3	0.25×0.23×0.04	0.44×0.06×0.06	0.27×0.14×0.03	0.21×0.16×0.12
Absorption coefficient / mm^{-1}	0.080	0.122	1.507	0.934
No. of reflexes measured	11094	16826	16804	81787
No. of independent reflexes	3402	3888	3781	6269
R_{int}	0.0676	0.0862	0.1017	0.0311
R_1 ($I > 2\sigma(I)$)	0.0575	0.0411	0.0425	0.0185
wR_2 ($I > 2\sigma(I)$)	0.1403	0.0742	0.0692	0.0442
R_1 (all data)	0.0916	0.0982	0.0857	0.0232
wR_2 (all data)	0.1582	0.0848	0.0775	0.0462
Goodness of fit on F^2	1.028	0.763	0.894	1.058

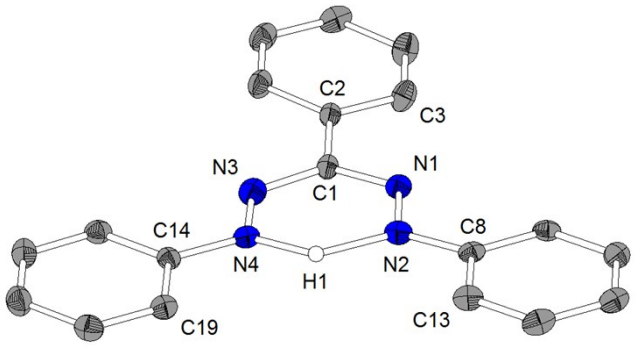

Fig. S9 Molecular structure of Htpf (**1**): Hydrogen atoms with the exception of the amino proton have been omitted for clarity. **Selected bond lengths /Å:** N2 – H1: 1.45(2), N4 – H1: 1.30(2), C1 – N1: 1.346(4), C1 – N3: 1.383(4), N1 – N2: 1.327(3), N2 – N4: 2.522(4), N3 – N4: 1.289(3). **Selected angles /°:** C1 – N1 – N2 – C8: 0.9(2), C1 – N3 – N4 – C14: 2.5(3), C3 – C2 – C1 – N1: 8.8(4).