Electronic Supplementary Material (ESI) for Dalton Transactions.


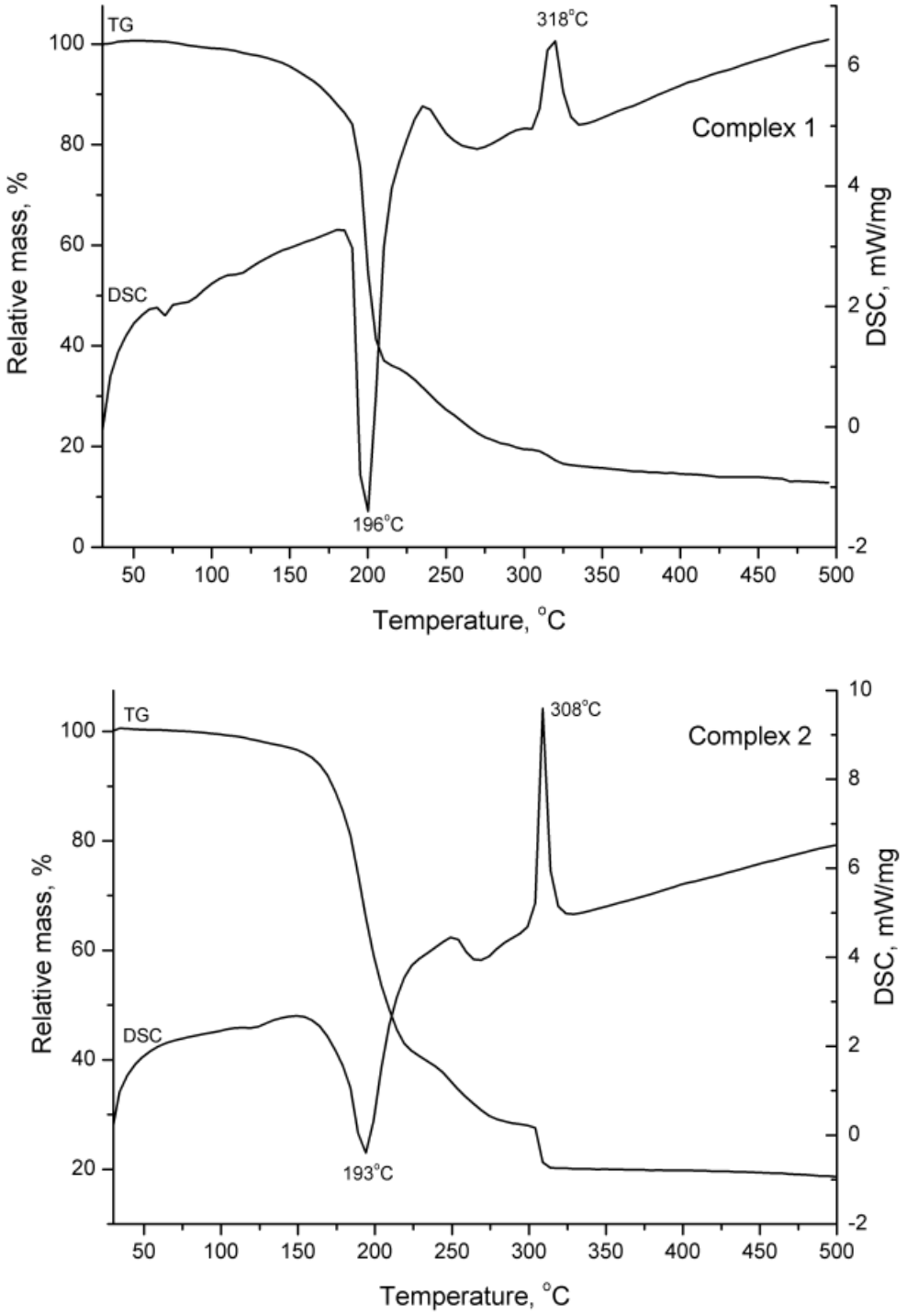


**Figure S1.** TG and DSC curves of complexes **1** (top) and **2** (bottom).

Complexes investigated show similar thermal behaviour. Their noticeable weight loss starts at about 150 °C. The first decomposition step for **1** and **2** is characterized by the endothermic peak at 196 and 193 °C, correspondingly. Further heating is accompanied by exothermic peak at 318 (**1**) and 308 °C (**2**).

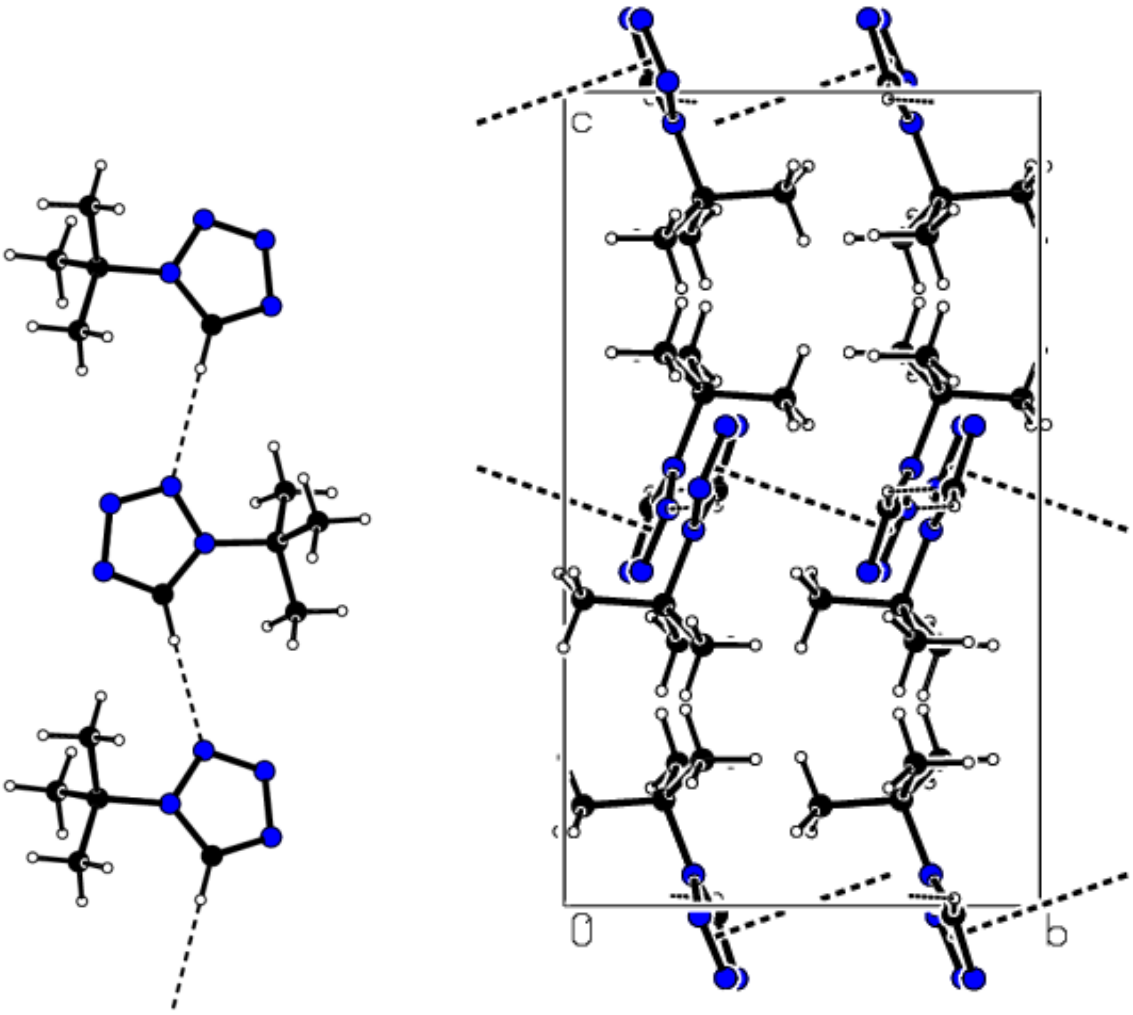


**Figure S2.** A hydrogen-bonded polymeric chain extending along the *a* axis in the crystal structure of 1-*tert*-Butyltetrazole (on the left), and crystall packing of 1-*tert*-Butyltetrazole viewed along the *a* axis, with dashed lines showing π···π interactions between the tetrazole rings (on the right).

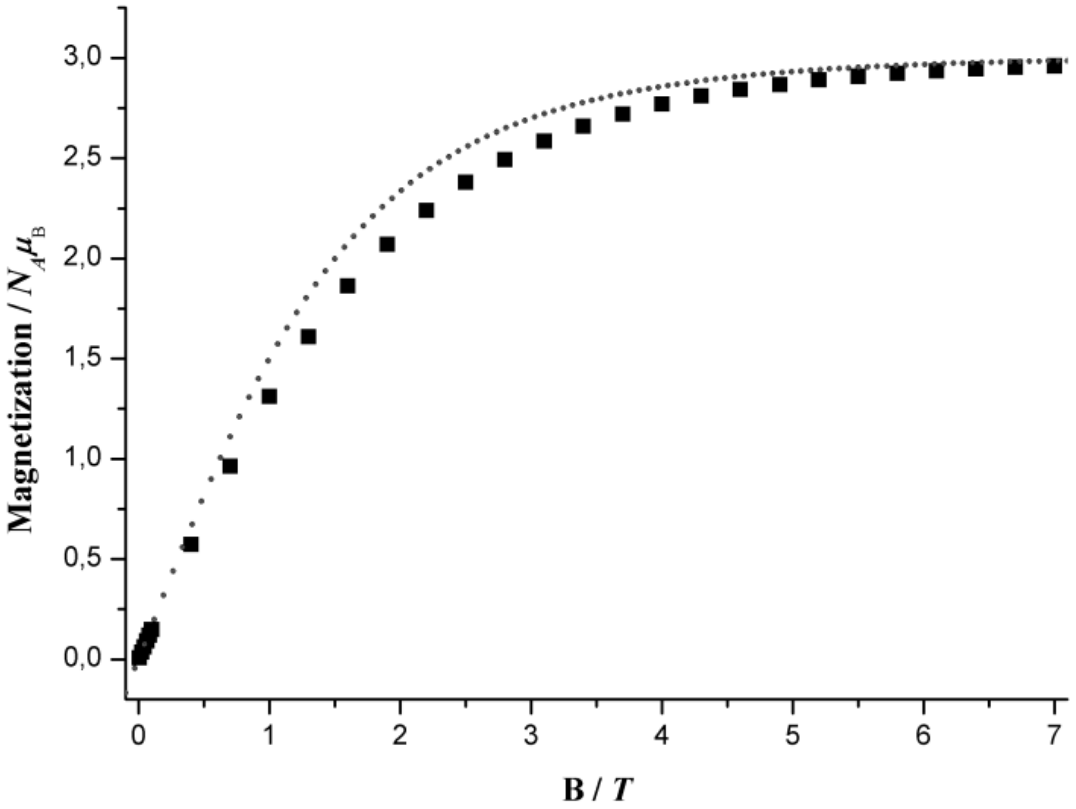


**Figure S3.** Field dependence of the magnetization of complex **2** as measured (square) and as calculated (doted).

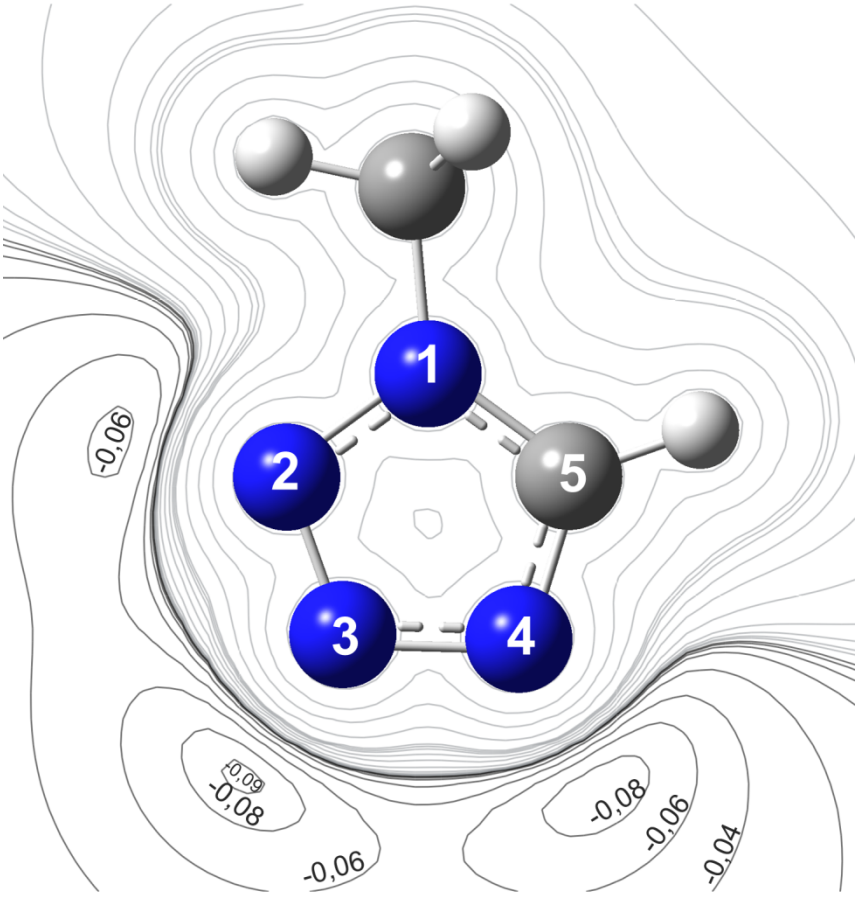


**Figure S4.** B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) calculated MESP contour map for 1-methyltetrazole. One hydrogen atom is not shown for clarity.

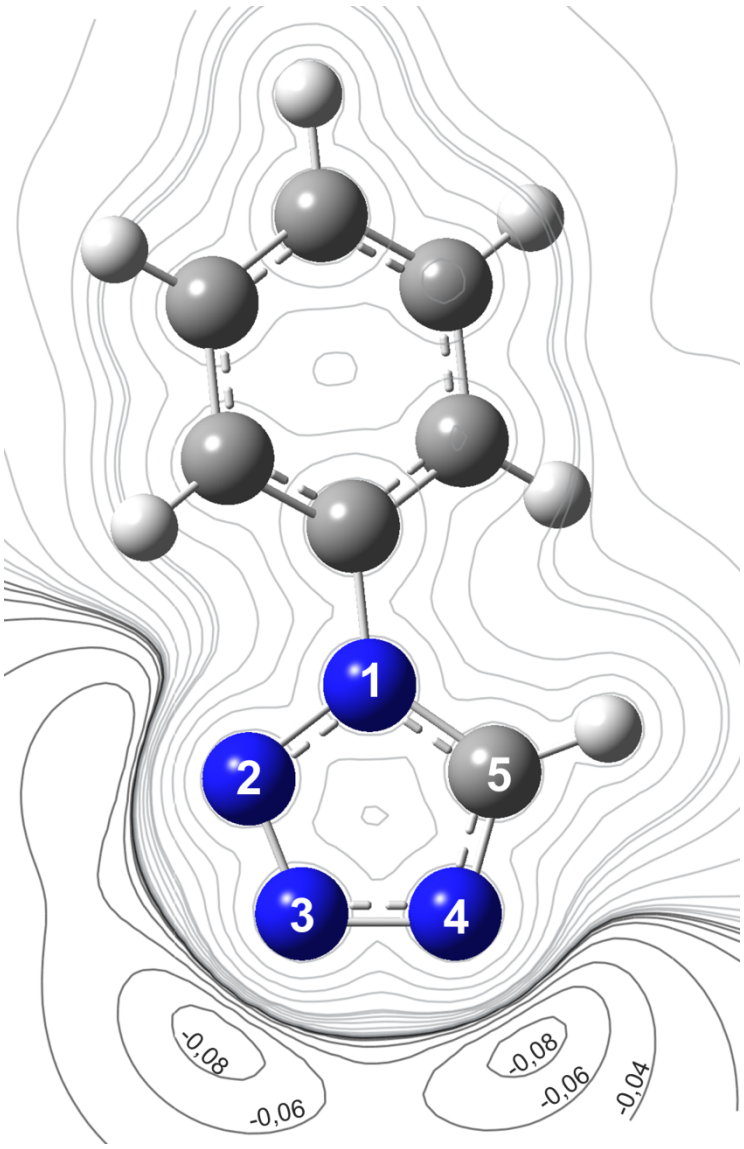


**Figure S5.** B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) calculated MESP contour map for 1-phenyltetrazole.

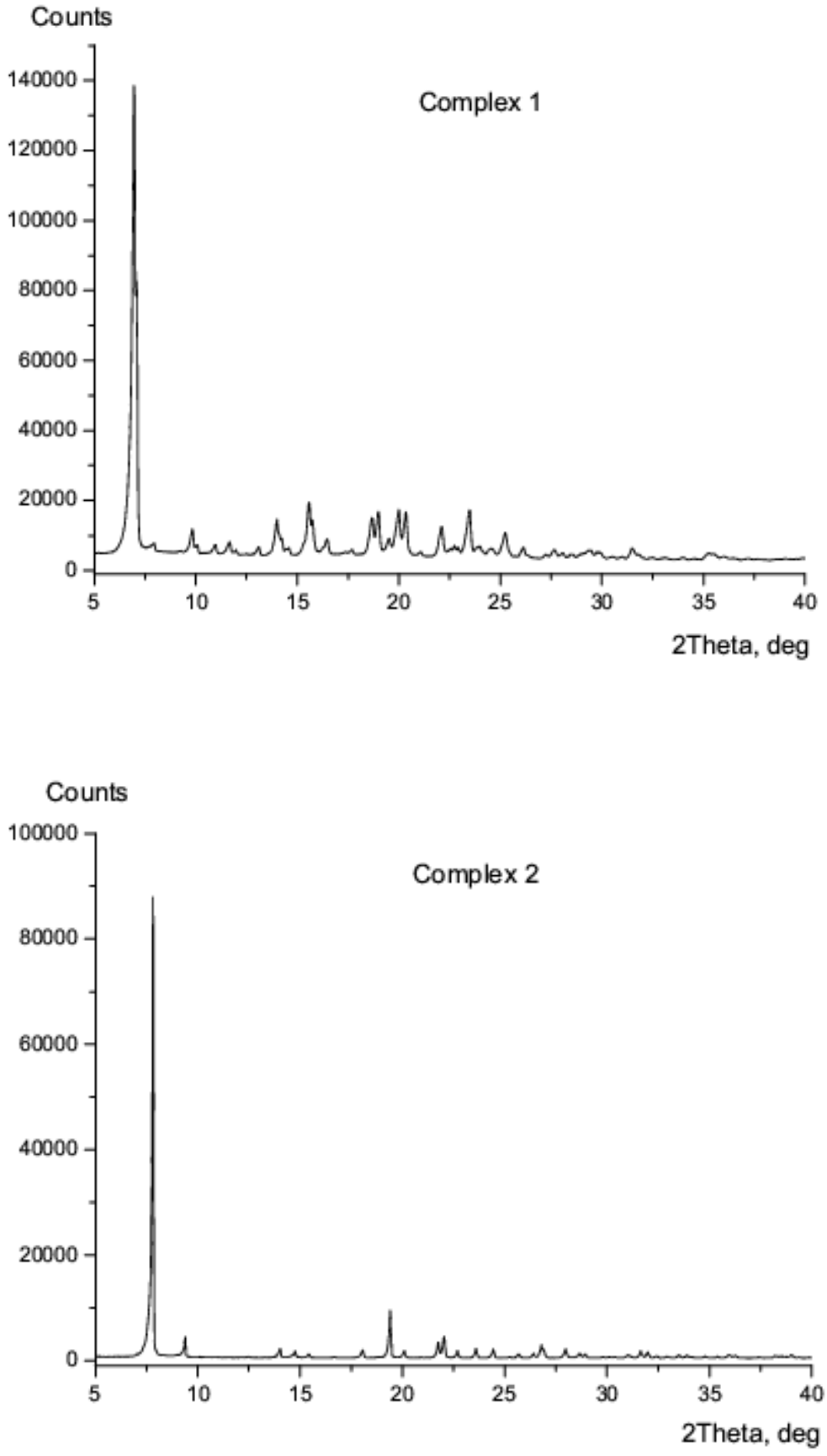


**Figure S6.** X-ray powder diffraction patterns of complexes **1** (top) and **2** (bottom) registered at 296 K using CuKα radiation.