Electronic Supporting Information (ESI)

Insights on the Binding Ability of a New Nucleobase Analog: 7-amine-1,2,4-triazole[1,5-*a*]pyrimidine. Synthesis and Magnetic Study of the First Copper(II) Complexes

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Figure S1. ORTEP representation of the asymmetric unit of the 7atp ligand (**1**). Thermal ellipsoids are drawn at the 50% probability level.

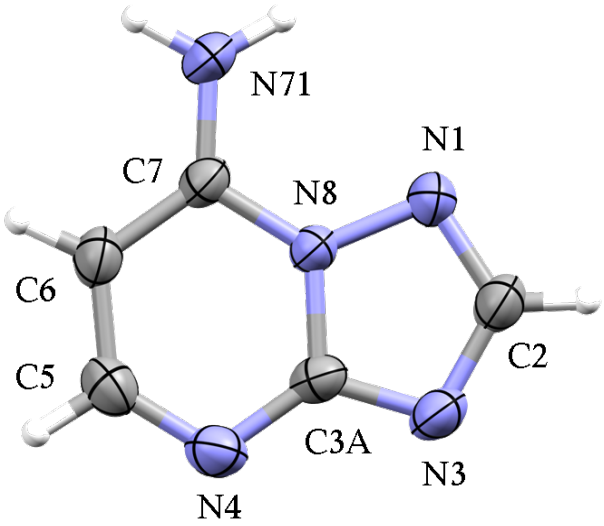

Table S1 Experimental (X-Ray) and calculated (B3LYP/6-31+G**) bonds distances and angles for compound **1** (7atp).

Distance (Å)	X-Ray	DFT	Angle (º)	X-Ray	DFT
N1-C2	1.3208(19)	1.337	N1-C2-N3	117.30(13)	117.0
N3-C2	1.3458(19)	1.350	C3A-N3-C2	103.17(12)	103.5
N3-C3A	1.3340(18)	1.337	N3-C3A-N4	128.81(13)	130.3
N4-C3A	1.3391(19)	1.342	N3-C3A-N8	108.43(13)	107.9
N4-C5	1.3317(19)	1.329	N4-C3A-N8	122.76(12)	121.8
C6-C5	1.374(2)	1.410	C5-N4-C3A	113.76(12)	115.2

C7-C6	1.393(2)	1.392	N4-C5-C6	126.39(13)	125.8
C7-N71	1.3132(19)	1.354	C5-C6-C7	119.85(13)	118.7
N8-C7	1.3641(16)	1.363	N8-C7-C6	113.55(12)	115.1
N8-N1	1.3736(16)	1.363	N71-C7-C6	127.14(13)	128.0
N8-C3A	1.3795(17)	1.400	N71-C7-N8	119.31(13)	116.9
			C7-N8-N1	125.99(11)	126.0
			C7-N8-C3A	123.67(12)	123.4
			N1-N8-C3A	110.28(11)	110.6
			C2-N1-N8	100.82(11)	100.9