

Table S1 Selected Bond lengths (Å), Bond angles (°) and torsional angles (°) of **6**.

Bond lengths (Å)	Experimental XRD (Å)	Bond angles (°)	Experimental XRD (°)	Torsional angles (°)	Experimental XRD (°)
N1-C2	1.3760 (1.4974)	C2-N1-C8	106.60 (101.64)	C8-N1-C2-N3	-0.83 (17.57)
N1-C8	1.3920 (1.4586)	C2-N1-C11	129.56 (113.68)	C8-N1-C2-C21	178.31 (-162.03)
N1-C11	1.4400 (1.4700)	C8-N1-C11	121.93 (113.30)	C11-N1-C2-N3	-166.19 (139.68)
N3-C2	1.3280 (1.3671)	C2-N3-C9	106.46 (105.49)	C11-N1-C2-C21	13.00 (-39.92)
N3-C9	1.3790 (1.4604)	N1-C2-N3	111.66 (113.56)	C2-N1-C8-C7	-177.06(166.13)
C2-C21	1.4600 (1.5400)	N3-C2-C21	121.90 (123.21)	C2-N1-C8-C9	0.64 (-13.73)
C7-C8	1.3820 (1.3863)	N1-C2-C21	126.44 (123.23)	C11-N1-C8-C7	-10.30 (43.76)
C8-C9	1.4040 (1.4769)	N1-C8-C7	131.52 (130.71)	C11-N1-C8-C9	167.36 (-136.10)
C14-C15	1.3820 (1.4014)	N1-C8-C9	105.57 (108.28)	C2-N1-C11-C12	-124.86 (152.30)
C15-C16	1.3920 (1.4014)	N3-C9-C4	131.18 (130.69)	C2-N1-C11-C16	59.40 (-27.70)
C21-C22	1.4050 (1.4014)	N3-C9-C8	109.43 (108.25)	N1-C2-C21-C22	19.60 (-0.22)
C24-C25	1.3810 (1.4014)	N1-C11-C12	119.43 (120.00)	N1-C2-C21-C26	-160.78 (179.78)
C25-C26	1.3890 (1.4014)	N1-C11-C16	119.08 (120.00)	N3-C2-C21-C22	-161.38 (-179.78)
C26-O26	1.3610 (1.4300)	C21-C26-O26	122.24 (120.00)	N3-C2-C21-C26	18.30 (0.22)
O26-H26	0.9700 (0.9600)			C21-C26-O26-H26	157.00 (150.00)

values within the parenthesis corresponds to theoretical values