

**Supplementary Table.**  $\pi$ - $\pi$  and C-H... $\pi$  Interactions in Complex 1

$\pi$ - $\pi$ interactions (face-to-face)					
ring(i) → ring(j)	dihedral angle (i,j), deg	slip angle (i,j), deg	distance of centroid(i) from ring(j), Å	of the (i,j) ring centroids, Å	between
R(1) → R(1) <sup>i, ii, iii, iv</sup>					
R(1) → R(2) <sup>i, ii, iii, iv</sup>	0	22.97	3.286	3.5692(13)	
R(2) → R(1) <sup>i, ii, iii, iv</sup>					
R(2) → R(2) <sup>i, ii, iii, iv</sup>					

  

C-H... $\pi$ interactions			
C-H->R(j)	H...R, Å	<C-H...R, deg	C...R, Å
C(10)-H→R(3) <sup>i, ii, iii, iv</sup>	3.3654	98.67	3.6321(16)

Symmetry code: (i) = -x, 1-y, 1-z; (ii) = -x, 1-y, 2-z; (iii) = x, 1-y, -½+z; (iv) = x, 1-y, 1/2+z;

R(i) and R(j) denote the i-th/j-th rings of tptz; R(1)= N8-C7-N8\*-C9\*-C10-C9; R(2)= C7-C8-C9-C10-C9\*-N8\* R(3)= N1-C2-N3-C4-N3\*-C2\* [\* = -x, y, 3/2-z].