

Table 2: Selected angles ($^{\circ}$) for the complex $[\text{Et}_8\text{N}_4(\Delta)\text{Ni}]$, experimentally synthesized, and the corresponding model system $[\text{H}_8\text{N}_4(\Delta)\text{Ni}](\mathbf{6a})$. For the numbering of the atoms, see Scheme 1.

Parameter	Calculated	Experimental	Parameter	Calculated	Experimental
N3-Ni-N4	84.1	84.1	Ni-N4-C19	126.0	129.9
N2-Ni-N4	171.2	173.9	Ni-N4-C16	118.2	118.7
N2-Ni-N3	91.3	90.5	C16-N4-C19	107.7	107.3
N1-Ni-N4	91.3	91.1	N1-C1-C20	124.0	125.1
N1-Ni-N3	171.2	173.6	N1-C1-C2	108.6	108.5
N1-Ni-N2	92.3	94.1	C2-C1-C20	127.1	126.3
Ni-N1-C4	125.7	125.0	N1-C4-C3	108.8	107.7
Ni-N1-C1	125.6	126.7	C3-C4-C5	130.6	131.0
C1-N1-C4	108.5	108.1	N1-C4-C5	120.5	120.4
Ni-N2-C9	125.6	126.3	C4-C5-C6	112.0	109.6
Ni-N2-C6	125.7	125.2	N2-C6-C5	120.5	120.5
C6-N2-C9	108.5	108.5	C5-C6-C7	130.6	130.7
Ni-N3-C14	118.2	118.1	N2-C6-C7	108.8	108.6
Ni-N3-C11	126.0	128.9	N2-C9-C8	108.6	108.3
C11-N3-C14	107.7	108.1	C8-C9-C10	127.1	126.8
N2-C9-C10	124.0	124.7	C14-C15-C16	65.5	61.9
C9-C10-C11	117.3	113.2	C14-C16-C15	57.3	59.3
N3-C11-C10	122.6	124.0	N4-C16-C15	118.0	116.8
C10-C11-C12	126.9	126.3	N4-C16-C14	109.1	108.4
N3-C11-C12	110.3	109.6	C15-C16-C17	128.6	126.8
N3-C14-C13	107.5	106.6	C14-C16-C17	127.9	133.1
C13-C14-C16	127.9	131.2	N4-C16-C17	107.5	106.3
C13-C14-C15	128.6	127.1	N4-C19-C18	110.3	110.0
N3-C14-C16	109.1	109.3	C18-C19-C20	126.9	125.6
N3-C14-C15	118.0	117.2	N4-C19-C20	122.6	124.3
C15-C14-C16	57.3	58.8	C1-C20-C19	117.3	114.4
dihedral angles between the N_4 core and the A, B, C, and D pyrrole rings					
A	195.7	156.2	C	144.5	149.9
B	184.4	156.6	D	156.1	152.1