Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Probing the structural changes accompanying spin crossover in a chiral [Fe(II)(N_3O_2)($CN)_2$] macrocycle by X-ray crystallography.

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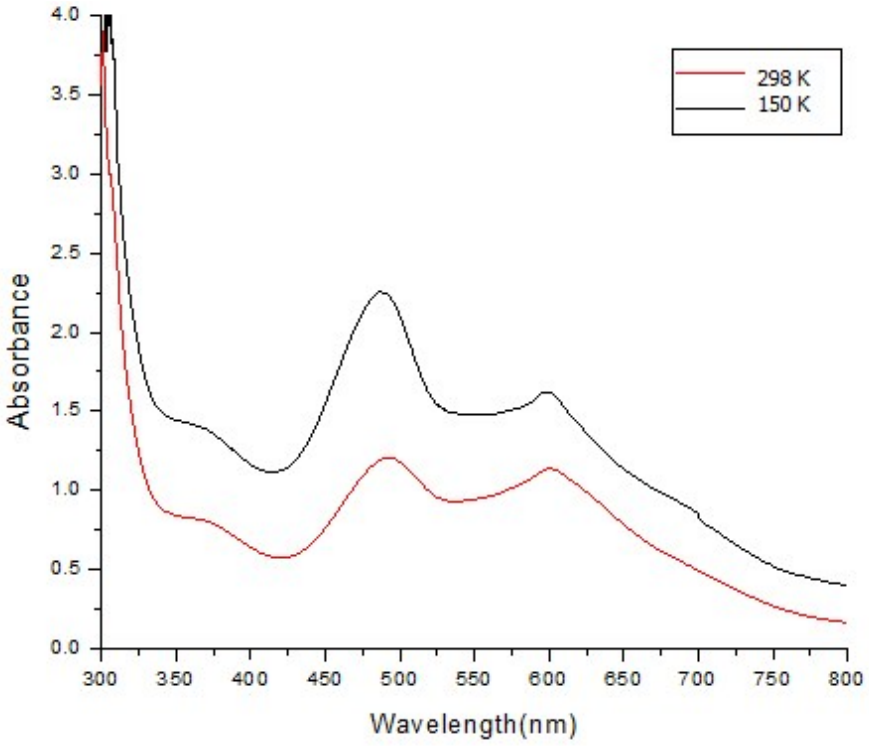
Table of Contents

S-1: UV-Vis spectroscopy



UV-Vis spectra of *S,S*-$(PhCH_2OCH_2)_2$-$[Fe(N_3O_2)(CN)_2]_2$ (**4**) at 298 K (red line) and 150 K (black line).

S-2: X-ray Crystallography

Table 1. Selected bond lengths (Å) for (**4)** at 300 K.

Fe1—N2	1.835 (6)	C5—C6	1.479 (10)
Fe1—N1	1.913 (5)	C6—C7	1.538 (8)
Fe1—C32	1.957 (7)	C8—C9	1.493 (11)
Fe1—C33	1.965 (7)	C10—C11	1.502 (8)
Fe1—N3	2.042 (5)	C10—C19	1.534 (7)
Fe1—O2	2.233 (5)	C12—C13	1.518 (10)
Fe2—N7	1.844 (6)	C13—C18	1.371 (12)
Fe2—C66	1.958 (8)	C13—C14	1.393 (11)
Fe2—N8	1.967 (6)	C18—C17	1.375 (12)
Fe2—C65	1.968 (7)	C17—C16	1.372 (14)
Fe2—N6	2.041 (6)	C16—C15	1.399 (14)
Fe2—O5	2.303 (7)	C15—C14	1.369 (12)
N1—C30	1.302 (10)	C19—C20	1.523 (9)
N1—C29	1.466 (9)	C21—C22	1.507 (11)
N2—C5	1.358 (8)	C22—C23	1.389 (12)
N2—C1	1.380 (9)	C22—C27	1.391 (12)
N3—C6	1.275 (10)	C23—C24	1.372 (12)
N3—C8	1.484 (9)	C24—C25	1.368 (14)
N4—C32	1.140 (10)	C25—C26	1.364 (14)
N5—C33	1.153 (10)	C26—C27	1.399 (13)
N6—C63	1.325 (10)	C28—C29	1.521 (11)
N6—C62	1.468 (10)	C30—C31	1.515 (9)
N7—C38	1.352 (8)	C34—C35	1.402 (11)
N7—C34	1.360 (9)	C34—C63	1.447 (12)
N8—C39	1.287 (10)	C35—C36	1.380 (12)
N8—C41	1.470 (10)	C36—C37	1.397 (11)
N9—C65	1.134 (10)	C37—C38	1.388 (11)
N10—C66	1.163 (11)	C38—C39	1.481 (9)
O2—C28	1.450 (8)	C39—C40	1.492 (10)
O2—C19	1.461 (8)	C41—C42	1.490 (12)
O1—C9	1.416 (8)	C43—C52	1.505 (10)
O1—C10	1.432 (7)	C43—C44	1.530 (9)
O4—C21	1.412 (9)	C45—C46	1.493 (11)
O4—C20	1.431 (8)	C46—C51	1.387 (12)
O3—C11	1.417 (8)	C46—C47	1.393 (12)
O3—C12	1.424 (9)	C47—C48	1.370 (11)
O5—C42	1.433 (10)	C48—C49	1.381 (13)
O5—C43	1.444 (9)	C49—C50	1.350 (15)
O6—C61	1.370 (10)	C50—C51	1.402 (13)

O6—C52	1.439 (8)	C52—C53	1.527 (9)
O7—C45	1.417 (10)	C54—C55	1.495 (14)
O7—C44	1.418 (9)	C55—C60	1.380 (13)
O8—C54	1.416 (10)	C55—C56	1.390 (13)
O8—C53	1.434 (9)	C56—C57	1.372 (16)
C1—C2	1.390 (12)	C57—C58	1.382 (17)
C1—C30	1.448 (10)	C58—C59	1.352 (15)
C2—C3	1.385 (11)	C59—C60	1.395 (14)
C3—C4	1.395 (11)	C61—C62	1.509 (12)
C4—C5	1.383 (11)	C63—C64	1.467 (10)

Table 2. Selected angles (°) for (**4**) at 300 K.

N2—Fe1—N1	81.6 (3)	O3—C11—C10	108.8 (5)
N2—Fe1—C32	93.7 (3)	O3—C12—C13	112.8 (6)
N1—Fe1—C32	91.0 (3)	C18—C13—C14	119.1 (7)
N2—Fe1—C33	93.5 (3)	C18—C13—C12	120.8 (7)
N1—Fe1—C33	92.1 (3)	C14—C13—C12	120.0 (8)
C32—Fe1—C33	172.5 (3)	C13—C18—C17	120.9 (8)
N2—Fe1—N3	79.4 (3)	C16—C17—C18	120.2 (8)
N1—Fe1—N3	161.0 (3)	C17—C16—C15	119.5 (8)
C32—Fe1—N3	90.7 (2)	C14—C15—C16	119.8 (9)
C33—Fe1—N3	88.7 (3)	C15—C14—C13	120.4 (9)
N2—Fe1—O2	160.2 (2)	O2—C19—C20	111.9 (5)
N1—Fe1—O2	78.6 (2)	O2—C19—C10	108.1 (5)
C32—Fe1—O2	85.8 (2)	C20—C19—C10	117.3 (5)
C33—Fe1—O2	88.1 (2)	O4—C20—C19	107.1 (5)
N3—Fe1—O2	120.4 (2)	O4—C21—C22	109.8 (7)
N7—Fe2—C66	94.0 (3)	C23—C22—C27	119.7 (8)
N7—Fe2—N8	80.5 (3)	C23—C22—C21	121.6 (7)
C66—Fe2—N8	91.9 (3)	C27—C22—C21	118.7 (8)
N7—Fe2—C65	91.9 (3)	C24—C23—C22	119.0 (8)
C66—Fe2—C65	174.0 (4)	C25—C24—C23	122.2 (9)
N8—Fe2—C65	90.1 (3)	C26—C25—C24	118.9 (8)
N7—Fe2—N6	79.9 (3)	C25—C26—C27	120.9 (8)
C66—Fe2—N6	90.3 (3)	C22—C27—C26	119.2 (9)
N8—Fe2—N6	160.3 (3)	O2—C28—C29	107.2 (5)
C65—Fe2—N6	89.8 (3)	N1—C29—C28	107.6 (6)
N7—Fe2—O5	156.1 (2)	N1—C30—C1	113.2 (6)
C66—Fe2—O5	82.8 (3)	N1—C30—C31	126.2 (6)
N8—Fe2—O5	76.0 (3)	C1—C30—C31	120.6 (7)
C65—Fe2—O5	92.2 (3)	N4—C32—Fe1	177.4 (7)
N6—Fe2—O5	123.7 (3)	N5—C33—Fe1	177.6 (7)
C30—N1—C29	123.0 (6)	N7—C34—C35	120.1 (7)

C30—N1—Fe1	116.8 (5)	N7—C34—C63	112.5 (7)
C29—N1—Fe1	120.2 (5)	C35—C34—C63	127.4 (6)
C5—N2—C1	120.9 (6)	C36—C35—C34	118.5 (7)
C5—N2—Fe1	121.5 (5)	C35—C36—C37	120.9 (8)
C1—N2—Fe1	117.6 (5)	C38—C37—C36	118.4 (7)
C6—N3—C8	117.3 (6)	N7—C38—C37	120.8 (6)
C6—N3—Fe1	114.2 (5)	N7—C38—C39	111.7 (6)
C8—N3—Fe1	128.5 (5)	C37—C38—C39	127.5 (6)
C63—N6—C62	118.1 (6)	N8—C39—C38	112.0 (6)
C63—N6—Fe2	113.9 (5)	N8—C39—C40	126.8 (7)
C62—N6—Fe2	127.9 (5)	C38—C39—C40	121.2 (7)
C38—N7—C34	121.2 (7)	N8—C41—C42	109.5 (7)
C38—N7—Fe2	118.8 (4)	O5—C42—C41	107.2 (7)
C34—N7—Fe2	120.0 (5)	O5—C43—C52	106.7 (6)
C39—N8—C41	122.8 (6)	O5—C43—C44	107.4 (6)
C39—N8—Fe2	117.0 (5)	C52—C43—C44	113.1 (5)
C41—N8—Fe2	120.2 (5)	O7—C44—C43	107.1 (5)
C28—O2—C19	112.9 (5)	O7—C45—C46	115.7 (8)
C28—O2—Fe1	106.4 (4)	C51—C46—C47	118.0 (7)
C19—O2—Fe1	132.9 (4)	C51—C46—C45	120.3 (9)
C9—O1—C10	116.7 (5)	C47—C46—C45	121.6 (8)
C21—O4—C20	112.4 (5)	C48—C47—C46	121.4 (7)
C11—O3—C12	113.5 (6)	C47—C48—C49	119.8 (8)
C42—O5—C43	116.7 (6)	C50—C49—C48	120.3 (8)
C42—O5—Fe2	106.7 (5)	C49—C50—C51	120.5 (9)
C43—O5—Fe2	134.6 (5)	C46—C51—C50	120.0 (9)
C61—O6—C52	122.3 (7)	O6—C52—C43	104.3 (6)
C45—O7—C44	115.7 (8)	O6—C52—C53	114.2 (6)
C54—O8—C53	110.0 (6)	C43—C52—C53	113.4 (6)
N2—C1—C2	119.6 (7)	O8—C53—C52	109.5 (6)
N2—C1—C30	110.7 (7)	O8—C54—C55	111.9 (8)
C2—C1—C30	129.8 (7)	C60—C55—C56	116.4 (9)
C3—C2—C1	119.7 (7)	C60—C55—C54	124.6 (8)
C2—C3—C4	119.9 (8)	C56—C55—C54	118.9 (9)
C5—C4—C3	119.3 (7)	C57—C56—C55	122.4 (10)
N2—C5—C4	120.6 (6)	C56—C57—C58	119.4 (10)
N2—C5—C6	109.5 (6)	C59—C58—C57	120.0 (10)
C4—C5—C6	129.8 (6)	C58—C59—C60	120.1 (10)
N3—C6—C5	115.3 (6)	C55—C60—C59	121.6 (10)
N3—C6—C7	126.5 (7)	O6—C61—C62	107.7 (7)
C5—C6—C7	118.3 (7)	N6—C62—C61	110.9 (6)
N3—C8—C9	110.8 (5)	N6—C63—C34	113.6 (6)
O1—C9—C8	106.3 (6)	N6—C63—C64	124.8 (7)

O1—C10—C11	104.0 (4)	C34—C63—C64	121.6 (7)
O1—C10—C19	113.7 (5)	N9—C65—Fe2	176.5 (8)
C11—C10—C19	112.6 (5)	N10—C66—Fe2	178.1 (8)

Table 3. Selected bond lengths (Å) for (**4**) at 150 K.

Fe1—N2	1.835 (6)	C5—C6	1.479 (10)
Fe1—N1	1.913 (5)	C6—C7	1.538 (8)
Fe1—C32	1.957 (7)	C8—C9	1.493 (11)
Fe1—C33	1.965 (7)	C10—C11	1.502 (8)
Fe1—N3	2.042 (5)	C10—C19	1.534 (7)
Fe1—O2	2.233 (5)	C12—C13	1.518 (10)
Fe2—N7	1.844 (6)	C13—C18	1.371 (12)
Fe2—C66	1.958 (8)	C13—C14	1.393 (11)
Fe2—N8	1.967 (6)	C18—C17	1.375 (12)
Fe2—C65	1.968 (7)	C17—C16	1.372 (14)
Fe2—N6	2.041 (6)	C16—C15	1.399 (14)
Fe2—O5	2.303 (7)	C15—C14	1.369 (12)
N1—C30	1.302 (10)	C19—C20	1.523 (9)
N1—C29	1.466 (9)	C21—C22	1.507 (11)
N2—C5	1.358 (8)	C22—C23	1.389 (12)
N2—C1	1.380 (9)	C22—C27	1.391 (12)
N3—C6	1.275 (10)	C23—C24	1.372 (12)
N3—C8	1.484 (9)	C24—C25	1.368 (14)
N4—C32	1.140 (10)	C25—C26	1.364 (14)
N5—C33	1.153 (10)	C26—C27	1.399 (13)
N6—C63	1.325 (10)	C28—C29	1.521 (11)
N6—C62	1.468 (10)	C30—C31	1.515 (9)
N7—C38	1.352 (8)	C34—C35	1.402 (11)
N7—C34	1.360 (9)	C34—C63	1.447 (12)
N8—C39	1.287 (10)	C35—C36	1.380 (12)
N8—C41	1.470 (10)	C36—C37	1.397 (11)
N9—C65	1.134 (10)	C37—C38	1.388 (11)
N10—C66	1.163 (11)	C38—C39	1.481 (9)
O2—C28	1.450 (8)	C39—C40	1.492 (10)
O2—C19	1.461 (8)	C41—C42	1.490 (12)
O1—C9	1.416 (8)	C43—C52	1.505 (10)
O1—C10	1.432 (7)	C43—C44	1.530 (9)
O4—C21	1.412 (9)	C45—C46	1.493 (11)
O4—C20	1.431 (8)	C46—C51	1.387 (12)
O3—C11	1.417 (8)	C46—C47	1.393 (12)
O3—C12	1.424 (9)	C47—C48	1.370 (11)
O5—C42	1.433 (10)	C48—C49	1.381 (13)

O5—C43	1.444 (9)	C49—C50	1.350 (15)
O6—C61	1.370 (10)	C50—C51	1.402 (13)
O6—C52	1.439 (8)	C52—C53	1.527 (9)
O7—C45	1.417 (10)	C54—C55	1.495 (14)
O7—C44	1.418 (9)	C55—C60	1.380 (13)
O8—C54	1.416 (10)	C55—C56	1.390 (13)
O8—C53	1.434 (9)	C56—C57	1.372 (16)
C1—C2	1.390 (12)	C57—C58	1.382 (17)
C1—C30	1.448 (10)	C58—C59	1.352 (15)
C2—C3	1.385 (11)	C59—C60	1.395 (14)
C3—C4	1.395 (11)	C61—C62	1.509 (12)
C4—C5	1.383 (11)	C63—C64	1.467 (10)

Table 4. Selected bond angles (°) for (**4**) at 100 K

N2—Fe1—N1	81.6 (3)	O3—C11—C10	108.8 (5)
N2—Fe1—C32	93.7 (3)	O3—C12—C13	112.8 (6)
N1—Fe1—C32	91.0 (3)	C18—C13—C14	119.1 (7)
N2—Fe1—C33	93.5 (3)	C18—C13—C12	120.8 (7)
N1—Fe1—C33	92.1 (3)	C14—C13—C12	120.0 (8)
C32—Fe1—C33	172.5 (3)	C13—C18—C17	120.9 (8)
N2—Fe1—N3	79.4 (3)	C16—C17—C18	120.2 (8)
N1—Fe1—N3	161.0 (3)	C17—C16—C15	119.5 (8)
C32—Fe1—N3	90.7 (2)	C14—C15—C16	119.8 (9)
C33—Fe1—N3	88.7 (3)	C15—C14—C13	120.4 (9)
N2—Fe1—O2	160.2 (2)	O2—C19—C20	111.9 (5)
N1—Fe1—O2	78.6 (2)	O2—C19—C10	108.1 (5)
C32—Fe1—O2	85.8 (2)	C20—C19—C10	117.3 (5)
C33—Fe1—O2	88.1 (2)	O4—C20—C19	107.1 (5)
N3—Fe1—O2	120.4 (2)	O4—C21—C22	109.8 (7)
N7—Fe2—C66	94.0 (3)	C23—C22—C27	119.7 (8)
N7—Fe2—N8	80.5 (3)	C23—C22—C21	121.6 (7)
C66—Fe2—N8	91.9 (3)	C27—C22—C21	118.7 (8)
N7—Fe2—C65	91.9 (3)	C24—C23—C22	119.0 (8)
C66—Fe2—C65	174.0 (4)	C25—C24—C23	122.2 (9)
N8—Fe2—C65	90.1 (3)	C26—C25—C24	118.9 (8)
N7—Fe2—N6	79.9 (3)	C25—C26—C27	120.9 (8)
C66—Fe2—N6	90.3 (3)	C22—C27—C26	119.2 (9)
N8—Fe2—N6	160.3 (3)	O2—C28—C29	107.2 (5)
C65—Fe2—N6	89.8 (3)	N1—C29—C28	107.6 (6)
N7—Fe2—O5	156.1 (2)	N1—C30—C1	113.2 (6)
C66—Fe2—O5	82.8 (3)	N1—C30—C31	126.2 (6)
N8—Fe2—O5	76.0 (3)	C1—C30—C31	120.6 (7)
C65—Fe2—O5	92.2 (3)	N4—C32—Fe1	177.4 (7)

N6—Fe2—O5	123.7 (3)	N5—C33—Fe1	177.6 (7)
C30—N1—C29	123.0 (6)	N7—C34—C35	120.1 (7)
C30—N1—Fe1	116.8 (5)	N7—C34—C63	112.5 (7)
C29—N1—Fe1	120.2 (5)	C35—C34—C63	127.4 (6)
C5—N2—C1	120.9 (6)	C36—C35—C34	118.5 (7)
C5—N2—Fe1	121.5 (5)	C35—C36—C37	120.9 (8)
C1—N2—Fe1	117.6 (5)	C38—C37—C36	118.4 (7)
C6—N3—C8	117.3 (6)	N7—C38—C37	120.8 (6)
C6—N3—Fe1	114.2 (5)	N7—C38—C39	111.7 (6)
C8—N3—Fe1	128.5 (5)	C37—C38—C39	127.5 (6)
C63—N6—C62	118.1 (6)	N8—C39—C38	112.0 (6)
C63—N6—Fe2	113.9 (5)	N8—C39—C40	126.8 (7)
C62—N6—Fe2	127.9 (5)	C38—C39—C40	121.2 (7)
C38—N7—C34	121.2 (7)	N8—C41—C42	109.5 (7)
C38—N7—Fe2	118.8 (4)	O5—C42—C41	107.2 (7)
C34—N7—Fe2	120.0 (5)	O5—C43—C52	106.7 (6)
C39—N8—C41	122.8 (6)	O5—C43—C44	107.4 (6)
C39—N8—Fe2	117.0 (5)	C52—C43—C44	113.1 (5)
C41—N8—Fe2	120.2 (5)	O7—C44—C43	107.1 (5)
C28—O2—C19	112.9 (5)	O7—C45—C46	115.7 (8)
C28—O2—Fe1	106.4 (4)	C51—C46—C47	118.0 (7)
C19—O2—Fe1	132.9 (4)	C51—C46—C45	120.3 (9)
C9—O1—C10	116.7 (5)	C47—C46—C45	121.6 (8)
C21—O4—C20	112.4 (5)	C48—C47—C46	121.4 (7)
C11—O3—C12	113.5 (6)	C47—C48—C49	119.8 (8)
C42—O5—C43	116.7 (6)	C50—C49—C48	120.3 (8)
C42—O5—Fe2	106.7 (5)	C49—C50—C51	120.5 (9)
C43—O5—Fe2	134.6 (5)	C46—C51—C50	120.0 (9)
C61—O6—C52	122.3 (7)	O6—C52—C43	104.3 (6)
C45—O7—C44	115.7 (8)	O6—C52—C53	114.2 (6)
C54—O8—C53	110.0 (6)	C43—C52—C53	113.4 (6)
N2—C1—C2	119.6 (7)	O8—C53—C52	109.5 (6)
N2—C1—C30	110.7 (7)	O8—C54—C55	111.9 (8)
C2—C1—C30	129.8 (7)	C60—C55—C56	116.4 (9)
C3—C2—C1	119.7 (7)	C60—C55—C54	124.6 (8)
C2—C3—C4	119.9 (8)	C56—C55—C54	118.9 (9)
C5—C4—C3	119.3 (7)	C57—C56—C55	122.4 (10)
N2—C5—C4	120.6 (6)	C56—C57—C58	119.4 (10)
N2—C5—C6	109.5 (6)	C59—C58—C57	120.0 (10)
C4—C5—C6	129.8 (6)	C58—C59—C60	120.1 (10)
N3—C6—C5	115.3 (6)	C55—C60—C59	121.6 (10)
N3—C6—C7	126.5 (7)	O6—C61—C62	107.7 (7)
C5—C6—C7	118.3 (7)	N6—C62—C61	110.9 (6)

N3—C8—C9	110.8 (5)	N6—C63—C34	113.6 (6)
O1—C9—C8	106.3 (6)	N6—C63—C64	124.8 (7)
O1—C10—C11	104.0 (4)	C34—C63—C64	121.6 (7)
O1—C10—C19	113.7 (5)	N9—C65—Fe2	176.5 (8)
C11—C10—C19	112.6 (5)	N10—C66—Fe2	178.1 (8)