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Supporting Information

for

Mononuclear iron(II) complexes containing a tripodal and macrocyclic nitrogen ligand: synthesis, reactivity and application in cyclohexane oxidation catalysis

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1. Crystallographic data

Table S1. Selected geometric parameters (Å,°) of complex **2**

C1—C2	1.463(16)	C20—C21	1.376(16)
C1—N1	1.491(16)	C21—C22	1.412(13)
C2—N2	1.348(15)	C21—N5	1.418(15)
C2—C3	1.386(14)	C22—C23	1.400(17)
C3—C4	1.390(17)	C23—C24	1.389(16)
C4—C5	1.330(18)	C24—C25	1.398(14)
C5—C6	1.404(14)	C25—C26	1.467(16)
C6—N2	1.353(15)	C26—N6	1.337(13)
C6—C7	1.473(16)	C26—C27	1.395(15)
C7—C8	1.389(14)	C27—C28	1.359(16)
C7—C12	1.405(14)	C28—C29	1.383(15)
C8—C9	1.384(16)	C29—C30	1.410(16)
C9—C10	1.385(15)	C30—N6	1.352(15)
C10—C11	1.399(16)	C30—C31	1.482(15)
C11—C12	1.392(16)	C31—N1	1.473(13)
C11—N3	1.424(13)	C32—N1	1.473(17)
C13—O1	1.223(15)	C32—C33	1.534(14)
C13—N3	1.335(16)	C33—N7	1.342(15)
C13—C14	1.500(13)	C33—C34	1.368(15)
C14—N4	1.338(16)	C34—C35	1.331(16)
C14—C15	1.353(18)	C35—C36	1.398(18)
C15—C16	1.422(15)	C36—C37	1.371(15)
C16—C17	1.399(18)	C37—N7	1.334(12)
C17—C18	1.391(16)	N1—Fe1	2.240(17)
C18—N4	1.342(12)	N2—Fe1	2.299(9)
C18—C19	1.515(18)	N7—Fe1	2.154(21)
C19—O2	1.195(13)	Fe1—Cl2	2.308(27)
C19—N5	1.361(14)	Fe1—Cl1	2.366(3)
C20—C25	1.375(17)		
C2—C1—N1	115.47(80)	N6—C26—C27	121.22(87)
N2—C2—C3	121.23(93)	N6—C26—C25	116.44(84)
N2—C2—C1	116.82(84)	C27—C26—C25	122.28(87)
C3—C2—C1	121.94(93)	C28—C27—C26	120.76(89)
C2—C3—C4	118.17(92)	C27—C28—C29	118.20(94)
C5—C4—C3	120.47(103)	C28—C29—C30	119.74(89)
C4—C5—C6	120.56(97)	N6—C30—C29	120.50(94)
N2—C6—C5	119.29(87)	N6—C30—C31	117.75(85)
N2—C6—C7	117.86(90)	C29—C30—C31	121.74(91)
C5—C6—C7	122.39(90)	N1—C31—C30	115.77(79)
C8—C7—C12	119.31(88)	N1—C32—C33	112.28(76)
C8—C7—C6	119.86(91)	N7—C33—C34	123.10(87)
C12—C7—C6	120.82(87)	N7—C33—C32	114.60(81)
C9—C8—C7	120.78(99)	C34—C33—C32	122.23(87)
C8—C9—C10	119.79(98)	C35—C34—C33	119.15(97)
C9—C10—C11	120.50(97)	C34—C35—C36	120.22(102)
C12—C11—C10	119.40(99)	C37—C36—C35	116.99(94)
C12—C11—N3	118.07(87)	N7—C37—C36	123.73(90)
C10—C11—N3	122.31(88)	C31—N1—C32	108.95(71)
C11—C12—C7	120.05(89)	C31—N1—C1	107.52(71)

O1—C13—N3	123.90(91)	C32—N1—C1	110.73(67)
O1—C13—C14	121.70(87)	C31—N1—Fe1	117.00(56)
N3—C13—C14	114.35(83)	C32—N1—Fe1	110.58(52)
N4—C14—C15	123.80(96)	C1—N1—Fe1	101.77(54)
N4—C14—C13	117.73(84)	C2—N2—C6	120.26(85)
C15—C14—C13	118.45(89)	C2—N2—Fe1	109.77(64)
C14—C15—C16	120.03(98)	C6—N2—Fe1	129.37(64)
C17—C16—C15	115.75(95)	C13—N3—C11	128.11(83)
C18—C17—C16	120.34(89)	C14—N4—C18	117.97(81)
N4—C18—C17	122.09(81)	C19—N5—C21	126.60(76)
N4—C18—C19	119.69(80)	C26—N6—C30	119.42(84)
C17—C18—C19	118.21(85)	C37—N7—C33	116.79(82)
O2—C19—N5	125.32(96)	C37—N7—Fe1	122.62(62)
O2—C19—C18	120.50(92)	C33—N7—Fe1	117.07(61)
N5—C19—C18	113.92(82)	N7—Fe1—N1	77.52(28)
C25—C20—C21	121.83(90)	N7—Fe1—N2	76.86(27)
C20—C21—C22	120.60(88)	N1—Fe1—N2	78.20(29)
C20—C21—N5	118.11(83)	N7—Fe1—Cl2	167.94(22)
C22—C21—N5	120.95(83)	N1—Fe1—Cl2	94.51(19)
C23—C22—C21	117.59(88)	N2—Fe1—Cl2	92.77(21)
C24—C23—C22	120.90(88)	N7—Fe1—Cl1	90.04(21)
C23—C24—C25	120.61(91)	N1—Fe1—Cl1	144.68(22)
C20—C25—C24	118.47(88)	N2—Fe1—Cl1	131.38(22)
C20—C25—C26	119.65(89)	Cl2—Fe1—Cl1	101.53(11)
C24—C25—C26	121.85(87)		

Table S2. Selected geometric parameters (Å,°) of complex **2‘**

C1—N1	1.486(8)	C29—H29	0.951(7)
C1—C2	1.492(9)	C30—N6	1.340(9)
C1—H1A	0.991(7)	C30—C31	1.515(9)
C1—H1B	0.989(7)	C31—N1	1.494(8)
C2—N2	1.332(9)	C31—H31A	0.992(7)
C2—C3	1.388(9)	C31—H31B	0.990(6)
C3—C4	1.38(1)	C32—N1	1.472(7)
C3—H3	0.951(9)	C32—C33	1.518(10)
C4—C5	1.342(12)	C32—H32A	0.991(5)
C4—H4	0.950(7)	C32—H32B	0.989(6)
C5—C6	1.400(8)	C33—N7	1.325(7)
C5—H5	0.950(7)	C33—C34	1.379(9)
C6—N2	1.363(8)	C34—C35	1.391(12)
C6—C7	1.475(10)	C34—H34	0.951(7)
C7—C12	1.397(8)	C35—C36	1.322(11)
C7—C8	1.402(8)	C35—H35	0.950(7)
C8—C9	1.359(11)	C36—C37	1.362(9)
C8—H8	0.951(7)	C36—H36	0.950(9)
C9—C10	1.379(10)	C37—N7	1.357(9)
C9—H9	0.950(7)	C37—H37	0.950(7)
C10—C11	1.386(8)	N1—Fe1	2.242(5)
C10—H10	0.950(8)	N2—Fe1	2.142(5)
C11—C12	1.398(9)	N3—H3N	0.867(29)
C11—N3	1.414(7)	N5—H5N	0.857(38)
C12—O3	1.355(6)	N7—Fe1	2.170(5)
C13—O1	1.230(8)	O3—Fe1	1.887(4)

C13—N3	1.338(10)	O4—Fe1	1.955(5)
C13—C14	1.518(10)	O4—Fe1^{i}	2.022(4)
C14—N4	1.351(8)	O4—H4W	0.832(37)
C14—C15	1.382(11)	O5—Fe3	1.754(6)
C15—C16	1.352(10)	O5—Fe2	1.790(7)
C15—H15	0.950(6)	Cl1—Fe2	2.232(7)
C16—C17	1.386(10)	Cl2—Fe2	2.233(3)
C16—H16	0.950(9)	Cl3—Fe3	2.225(9)
C17—C18	1.389(11)	Cl4—Fe3	2.204(3)
C17—H17	0.949(7)	Fe1—O4^{i}	2.022(4)
C18—N4	1.341(9)	Fe2—Cl2^{ii}	2.233(3)
C18—C19	1.509(10)	Fe3—Cl4^{ii}	2.204(3)
C19—O2	1.212(9)	C38—N8	1.137(16)
C19—N5	1.334(10)	C38—C39	1.467(18)
C20—C21	1.366(10)	C39—H39A	0.98(4)
C20—C25	1.395(9)	C39—H39B	0.982(43)
C20—H20	0.949(6)	C39—H39C	0.976(57)
C21—C22	1.407(9)	C40—N9	1.109(30)
C21—N5	1.409(8)	C40—C41	1.428(25)
C22—C23	1.367(10)	C40—C40^{iii}	1.582(28)
C22—H22	0.950(8)	C41—C40^{iii}	1.428(25)
C23—C24	1.367(11)	C41—H41A	0.981(40)
C23—H23	0.950(7)	C41—H41B	0.987(29)
C24—C25	1.390(9)	C41—H41C	0.979(79)
C24—H24	0.950(6)	C42—C43	1.038(26)
C25—C26	1.458(10)	C42—C42^{ii}	1.173(28)
C26—N6	1.358(7)	C42—N10	1.269(23)
C26—C27	1.414(9)	C42—C43^{ii}	1.941(28)
C27—C28	1.360(11)	C43—C42^{ii}	1.941(28)
C27—H27	0.951(7)	C43—H43A	0.993(53)
C28—C29	1.368(9)	C43—H43B	0.979(45)
C28—H28	0.949(7)	C43—H43C	0.972(35)
C29—C30	1.391(9)	N10—C42^{ii}	1.269(23)

N1—C1—C2	111.25(44)	N7—C33—C34	121.74(51)
N1—C1—H1A	109.38(50)	N7—C33—C32	114.17(46)
C2—C1—H1A	109.33(57)	C34—C33—C32	124.08(50)
N1—C1—H1B	109.41(47)	C33—C34—C35	118.09(57)
C2—C1—H1B	109.33(59)	C33—C34—H34	120.93(64)
H1A—C1—H1B	108.07(67)	C35—C34—H34	120.98(69)
N2—C2—C3	122.44(53)	C36—C35—C34	119.99(72)
N2—C2—C1	116.57(57)	C36—C35—H35	120.05(70)
C3—C2—C1	120.91(50)	C34—C35—H35	119.96(64)
C4—C3—C2	117.84(59)	C35—C36—C37	119.95(65)
C4—C3—H3	121.04(79)	C35—C36—H36	120.01(78)
C2—C3—H3	121.12(66)	C37—C36—H36	120.04(63)
C5—C4—C3	119.63(75)	N7—C37—C36	121.63(51)
C5—C4—H4	120.16(67)	N7—C37—H37	119.22(62)
C3—C4—H4	120.21(66)	C36—C37—H37	119.15(62)
C4—C5—C6	121.60(57)	C32—N1—C1	111.20(46)
C4—C5—H5	119.20(78)	C32—N1—C31	110.16(46)
C6—C5—H5	119.20(54)	C1—N1—C31	106.53(44)
N2—C6—C5	118.19(48)	C32—N1—Fe1	107.17(34)
N2—C6—C7	120.02(56)	C1—N1—Fe1	101.44(37)
C5—C6—C7	121.77(50)	C31—N1—Fe1	119.97(37)
C12—C7—C8	117.61(49)	C2—N2—C6	120.00(56)
C12—C7—C6	124.16(47)	C2—N2—Fe1	113.08(33)

C8—C7—C6	118.22(52)	C6—N2—Fe1	125.53(34)
C9—C8—C7	121.75(62)	C13—N3—C11	126.55(52)
C9—C8—H8	119.11(66)	C13—N3—H3N	120.68(221)
C7—C8—H8	119.15(64)	C11—N3—H3N	111.81(301)
C8—C9—C10	120.72(63)	C18—N4—C14	116.74(55)
C8—C9—H9	119.59(68)	C19—N5—C21	130.11(60)
C10—C9—H9	119.69(67)	C19—N5—H5N	117.01(238)
C9—C10—C11	119.35(61)	C21—N5—H5N	112.39(239)
C9—C10—H10	120.32(66)	C30—N6—C26	119.01(46)
C11—C10—H10	120.32(65)	C33—N7—C37	118.41(52)
C10—C11—C12	120.23(53)	C33—N7—Fe1	116.89(34)
C10—C11—N3	122.28(50)	C37—N7—Fe1	123.46(34)
C12—C11—N3	117.46(47)	C12—O3—Fe1	130.46(35)
O3—C12—C7	123.56(45)	Fe1—O4—Fe1^{i}	101.60(18)
O3—C12—C11	116.08(47)	Fe1—O4—H4W	102.59(339)
C7—C12—C11	120.29(48)	Fe1^{i}—O4—H4W	120.82(344)
O1—C13—N3	124.65(62)	Fe3—O5—Fe2	140.38(34)
O1—C13—C14	118.93(58)	O3—Fe1—O4	100.61(17)
N3—C13—C14	116.42(57)	O3—Fe1—O4^{i}	99.38(17)
N4—C14—C15	122.53(62)	O4—Fe1—O4^{i}	78.40(16)
N4—C14—C13	118.99(57)	O3—Fe1—N2	88.13(18)
C15—C14—C13	118.49(60)	O4—Fe1—N2	166.37(17)
C16—C15—C14	120.37(66)	O4^{i}—Fe1—N2	89.93(16)
C16—C15—H15	119.86(68)	O3—Fe1—N7	89.75(18)
C14—C15—H15	119.77(67)	O4—Fe1—N7	93.30(17)
C15—C16—C17	118.34(68)	O4^{i}—Fe1—N7	168.61(16)
C15—C16—H16	120.82(74)	N2—Fe1—N7	97.22(15)
C17—C16—H16	120.84(80)	O3—Fe1—N1	157.34(19)
C16—C17—C18	118.86(72)	O4—Fe1—N1	98.22(18)
C16—C17—H17	120.61(69)	O4^{i}—Fe1—N1	96.65(17)
C18—C17—H17	120.53(69)	N2—Fe1—N1	75.94(19)
N4—C18—C17	123.13(62)	N7—Fe1—N1	76.65(19)
N4—C18—C19	118.39(57)	O5—Fe2—Cl1	108.60(19)
C17—C18—C19	118.47(64)	O5—Fe2—Cl2	110.60(4)
O2—C19—N5	125.45(66)	Cl1—Fe2—Cl2	109.21(4)
O2—C19—C18	119.89(63)	O5—Fe2—Cl2^{ii}	110.60(4)
N5—C19—C18	114.66(65)	Cl1—Fe2—Cl2^{ii}	109.21(4)
C21—C20—C25	122.06(62)	Cl2—Fe2—Cl2^{ii}	108.60(6)
C21—C20—H20	118.93(58)	O5—Fe3—Cl4	112.29(6)
C25—C20—H20	119.02(57)	O5—Fe3—Cl4^{ii}	112.29(6)
C20—C21—C22	118.73(56)	Cl4—Fe3—Cl4^{ii}	104.18(8)
C20—C21—N5	118.35(60)	O5—Fe3—Cl3	107.79(19)
C22—C21—N5	122.92(54)	Cl4—Fe3—Cl3	110.14(5)
C23—C22—C21	119.32(61)	Cl4^{ii}—Fe3—Cl3	110.14(5)
C23—C22—H22	120.37(70)	N8—C38—C39	179.49(115)
C21—C22—H22	120.31(64)	C38—C39—H39A	107.84(395)
C24—C23—C22	121.69(71)	C38—C39—H39B	107.49(259)
C24—C23—H23	119.12(67)	H39A—C39—H39B	110.19(462)
C22—C23—H23	119.19(70)	C38—C39—H39C	109.03(338)
C23—C24—C25	120.13(60)	H39A—C39—H39C	112.02(473)
C23—C24—H24	120.03(70)	H39B—C39—H39C	110.12(453)
C25—C24—H24	119.84(64)	N9—C40—C41	178.42(205)
C24—C25—C20	118.07(54)	N9—C40—C40^{iii}	122.98(211)
C24—C25—C26	121.48(50)	C41—C40—C40^{iii}	56.34(99)
C20—C25—C26	120.44(58)	C40—C41—C40^{iii}	67.31(108)
N6—C26—C27	119.51(49)	C40—C41—H41A	108.37(266)
N6—C26—C25	117.79(46)	C40^{iii}—C41—H41A	43.59(262)

C27—C26—C25	122.70(61)	C40—C41—H41B	108.54(72)
C28—C27—C26	120.47(65)	C40^{iii}—C41—H41B	108.54(72)
C28—C27—H27	119.81(64)	H41A—C41—H41B	108.70(393)
C26—C27—H27	119.72(61)	C40—C41—H41C	109.47(326)
C27—C28—C29	119.61(60)	C40^{iii}—C41—H41C	138.32(347)
C27—C28—H28	120.15(69)	H41A—C41—H41C	110.28(492)
C29—C28—H28	120.25(63)	H41B—C41—H41C	111.40(443)
C28—C29—C30	118.49(59)	C43—C42—C42^{ii}	122.64(240)
C28—C29—H29	120.71(61)	C43—C42—N10	173.88(243)
C30—C29—H29	120.80(59)	C42^{ii}—C42—N10	62.45(145)
N6—C30—C29	122.89(60)	C43—C42—C43^{ii}	95.87(186)
N6—C30—C31	117.73(52)	C42^{ii}—C42—C43^{ii}	26.77(126)
C29—C30—C31	119.36(55)	N10—C42—C43^{ii}	89.16(130)
N1—C31—C30	116.04(47)	C42—C43—C42^{ii}	30.60(147)
N1—C31—H31A	108.31(56)	C42—C43—H43A	106.83(347)
C30—C31—H31A	108.23(50)	C42^{ii}—C43—H43A	90.30(318)
N1—C31—H31B	108.28(48)	C42—C43—H43B	108.38(292)
C30—C31—H31B	108.28(48)	C42^{ii}—C43—H43B	90.96(376)
H31A—C31—H31B	107.40(61)	H43A—C43—H43B	109.68(436)
N1—C32—C33	111.07(45)	C42—C43—H43C	109.54(299)
N1—C32—H32A	109.43(47)	C42^{ii}—C43—H43C	140.14(250)
C33—C32—H32A	109.39(49)	H43A—C43—H43C	110.17(398)
N1—C32—H32B	109.43(44)	H43B—C43—H43C	112.07(448)
C33—C32—H32B	109.44(51)	C42—N10—C42^{ii}	55.10(139)
H32A—C32—H32B	108.02(55)		

Symmetry codes:

(i) 1-x, 1-y, 1-z; (ii) x, 0.5-y, z; (iii) x, 1.5-y, z.

Table S3. Selected geometric parameters (Å,°) of complex **3**

C1—N1	1.475(4)	C22—H22	0.951(3)
C1—C2	1.511(6)	C23—C24	1.390(4)
C1—H1A	0.989(3)	C23—H23	0.949(3)
C1—H1B	0.990(3)	C24—H24	0.950(4)
C2—N2	1.350(5)	C25—N1	1.471(4)
C2—C3	1.383(5)	C25—C26	1.511(4)
C3—C4	1.377(5)	C25—H25A	0.989(3)
C3—H3	0.950(4)	C25—H25B	0.990(4)
C4—C5	1.383(6)	C26—N6	1.347(5)
C4—H4	0.949(3)	C26—C27	1.384(6)
C5—C6	1.388(5)	C27—C28	1.380(5)
C5—H5	0.950(4)	C27—H27	0.950(4)
C6—N2	1.358(5)	C28—C29	1.385(6)
C6—C7	1.483(6)	C28—H28	0.950(4)
C7—C8	1.389(5)	C29—C30	1.378(6)
C7—C12	1.398(4)	C29—H29	0.951(3)
C8—C9	1.404(6)	C30—N6	1.345(4)
C8—H8	0.950(3)	C30—H30	0.950(4)
C9—N3	1.375(5)	C31—C32	1.459(5)
C9—C10	1.402(4)	C31—H31A	0.980(5)
C10—C11	1.385(5)	C31—H31B	0.980(5)
C10—H10	0.950(4)	C31—H31C	0.980(4)

C11—C12	1.393(6)	C32—N7	1.124(4)
C11—H11	0.949(3)	N1—Fe1	2.215(6)
C12—H12	0.949(3)	N2—Fe1	2.182(3)
C13—N1	1.473(4)	N3—H3A	0.880(4)
C13—C14	1.503(4)	N3—H3B	0.881(3)
C13—H13A	0.991(3)	N4—H4A	0.881(3)
C13—H13B	0.990(4)	N4—H4B	0.880(3)
C14—N5	1.358(3)	N5—Fe1	2.126(3)
C14—C15	1.383(4)	N6—Fe1	2.155(7)
C15—C16	1.383(5)	N7—Fe1	2.116(5)
C15—H15	0.950(3)	C33—F1	1.326(5)
C16—C17	1.384(4)	C33—F2	1.330(5)
C16—H16	0.951(3)	C33—F3	1.332(4)
C17—C18	1.387(4)	C33—S1	1.813(4)
C17—H17	0.950(3)	O1—S1	1.433(5)
C18—N5	1.356(4)	O2—S1	1.440(5)
C18—C19	1.482(4)	O3—S1	1.431(3)
C19—C20	1.384(6)	C34—F6	1.317(4)
C19—C24	1.402(5)	C34—F5	1.324(6)
C20—C21	1.404(4)	C34—F4	1.331(4)
C20—H20	0.950(3)	C34—S2	1.827(5)
C21—N4	1.365(6)	O4—S2	1.434(3)
C21—C22	1.397(5)	O5—S2	1.429(6)
C22—C23	1.383(7)	O6—S2	1.435(4)

N1—C1—C2	110.73(20)	N1—C25—H25B	109.6(2)
N1—C1—H1A	109.50(21)	C26—C25—H25B	109.61(19)
C2—C1—H1A	109.50(23)	H25A—C25—H25B	108.12(22)
N1—C1—H1B	109.5(2)	N6—C26—C27	122.22(22)
C2—C1—H1B	109.48(19)	N6—C26—C25	115.75(18)
H1A—C1—H1B	108.09(22)	C27—C26—C25	121.95(24)
N2—C2—C3	122.48(21)	C28—C27—C26	119.04(25)
N2—C2—C1	116.80(19)	C28—C27—H27	120.50(24)
C3—C2—C1	120.67(23)	C26—C27—H27	120.46(24)
C4—C3—C2	118.74(24)	C27—C28—C29	119.00(23)
C4—C3—H3	120.66(23)	C27—C28—H28	120.55(28)
C2—C3—H3	120.60(23)	C29—C28—H28	120.45(26)
C3—C4—C5	119.20(22)	C30—C29—C28	118.95(23)
C3—C4—H4	120.37(26)	C30—C29—H29	120.53(27)
C5—C4—H4	120.43(24)	C28—C29—H29	120.52(23)
C4—C5—C6	119.95(23)	N6—C30—C29	122.53(25)
C4—C5—H5	120.01(24)	N6—C30—H30	118.77(21)
C6—C5—H5	120.05(26)	C29—C30—H30	118.71(23)
N2—C6—C5	120.62(23)	C32—C31—H31A	109.49(28)
N2—C6—C7	117.46(19)	C32—C31—H31B	109.47(23)
C5—C6—C7	121.90(21)	H31A—C31—H31B	109.49(40)
C8—C7—C12	120.11(21)	C32—C31—H31C	109.50(26)
C8—C7—C6	119.05(19)	H31A—C31—H31C	109.46(39)
C12—C7—C6	120.84(21)	H31B—C31—H31C	109.41(41)
C7—C8—C9	120.88(20)	N7—C32—C31	178.04(27)
C7—C8—H8	119.58(23)	C25—N1—C13	112.07(20)
C9—C8—H8	119.54(23)	C25—N1—C1	110.85(19)
N3—C9—C10	121.61(22)	C13—N1—C1	111.92(19)
N3—C9—C8	119.85(20)	C25—N1—Fe1	108.14(12)
C10—C9—C8	118.51(22)	C13—N1—Fe1	106.14(12)
C11—C10—C9	120.37(22)	C1—N1—Fe1	107.42(12)
C11—C10—H10	119.75(23)	C2—N2—C6	118.81(18)

C9—C10—H10	119.88(24)	C2—N2—Fe1	113.52(15)
C10—C11—C12	121.00(22)	C6—N2—Fe1	125.98(17)
C10—C11—H11	119.52(24)	C9—N3—H3A	119.93(21)
C12—C11—H11	119.48(24)	C9—N3—H3B	120.02(24)
C11—C12—C7	119.10(22)	H3A—N3—H3B	120.05(27)
C11—C12—H12	120.49(22)	C21—N4—H4A	119.95(24)
C7—C12—H12	120.42(23)	C21—N4—H4B	120.03(27)
N1—C13—C14	110.96(20)	H4A—N4—H4B	120.02(29)
N1—C13—H13A	109.44(24)	C18—N5—C14	118.99(19)
C14—C13—H13A	109.45(23)	C18—N5—Fe1	125.61(16)
N1—C13—H13B	109.50(19)	C14—N5—Fe1	115.05(15)
C14—C13—H13B	109.45(19)	C30—N6—C26	118.25(18)
H13A—C13—H13B	107.99(22)	C30—N6—Fe1	125.36(18)
N5—C14—C15	122.16(21)	C26—N6—Fe1	116.37(16)
N5—C14—C13	116.18(19)	C32—N7—Fe1	171.11(19)
C15—C14—C13	121.59(22)	N7—Fe1—N5	126.54(8)
C16—C15—C14	118.83(23)	N7—Fe1—N6	93.04(8)
C16—C15—H15	120.60(23)	N5—Fe1—N6	111.77(8)
C14—C15—H15	120.57(23)	N7—Fe1—N2	93.54(8)
C15—C16—C17	119.15(23)	N5—Fe1—N2	111.65(8)
C15—C16—H16	120.44(25)	N6—Fe1—N2	119.17(8)
C17—C16—H16	120.41(25)	N7—Fe1—N1	156.83(7)
C16—C17—C18	120.02(22)	N5—Fe1—N1	76.63(7)
C16—C17—H17	119.95(24)	N6—Fe1—N1	76.08(7)
C18—C17—H17	120.03(24)	N2—Fe1—N1	74.89(7)
N5—C18—C17	120.76(22)	F1—C33—F2	107.57(22)
N5—C18—C19	116.98(19)	F1—C33—F3	106.99(22)
C17—C18—C19	122.24(21)	F2—C33—F3	108.17(22)
C20—C19—C24	120.26(23)	F1—C33—S1	111.56(17)
C20—C19—C18	120.51(19)	F2—C33—S1	111.19(20)
C24—C19—C18	119.23(22)	F3—C33—S1	111.17(20)
C19—C20—C21	120.55(21)	O3—S1—O1	114.06(12)
C19—C20—H20	119.71(25)	O3—S1—O2	115.02(13)
C21—C20—H20	119.74(25)	O1—S1—O2	115.30(11)
N4—C21—C22	121.31(24)	O3—S1—C33	104.60(13)
N4—C21—C20	120.25(22)	O1—S1—C33	102.88(11)
C22—C21—C20	118.44(24)	O2—S1—C33	102.74(12)
C23—C22—C21	121.13(24)	F6—C34—F5	108.75(22)
C23—C22—H22	119.44(23)	F6—C34—F4	108.29(22)
C21—C22—H22	119.42(25)	F5—C34—F4	106.93(23)
C22—C23—C24	120.23(22)	F6—C34—S2	111.40(18)
C22—C23—H23	119.90(26)	F5—C34—S2	110.43(18)
C24—C23—H23	119.87(25)	F4—C34—S2	110.89(17)
C23—C24—C19	119.37(23)	O5—S2—O4	115.10(15)
C23—C24—H24	120.36(22)	O5—S2—O6	114.80(14)
C19—C24—H24	120.27(25)	O4—S2—O6	114.48(13)
N1—C25—C26	110.35(21)	O5—S2—C34	103.02(13)
N1—C25—H25A	109.57(22)	O4—S2—C34	104.47(12)
C26—C25—H25A	109.55(21)	O6—S2—C34	102.73(12)

2. UV-Vis spectroscopic data

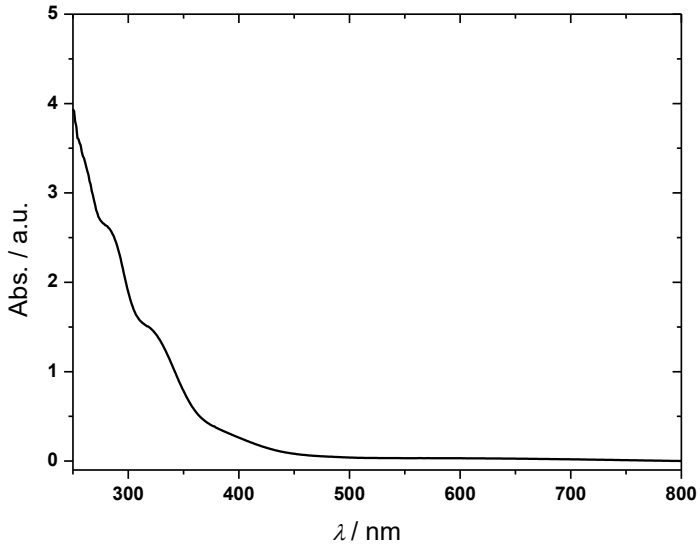

Figure S1. UV-Vis spectrum of complex **1** (1.4 mM) in CH_3CN.

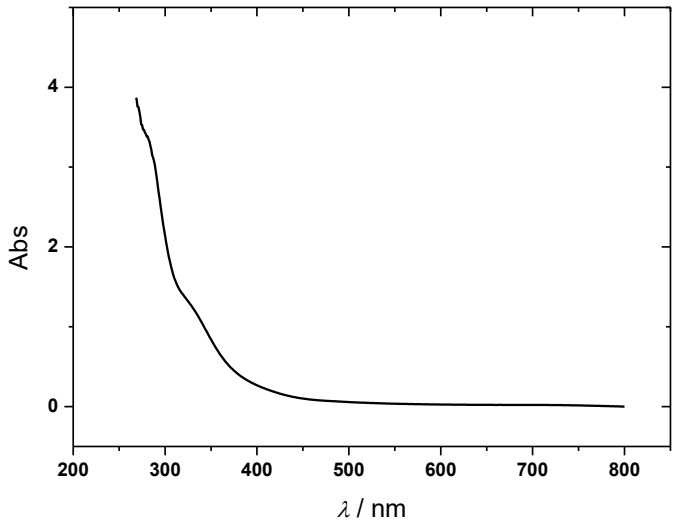

Figure S2. UV-Vis spectrum of complex **3** (2.5 mM) in CH_3CN.

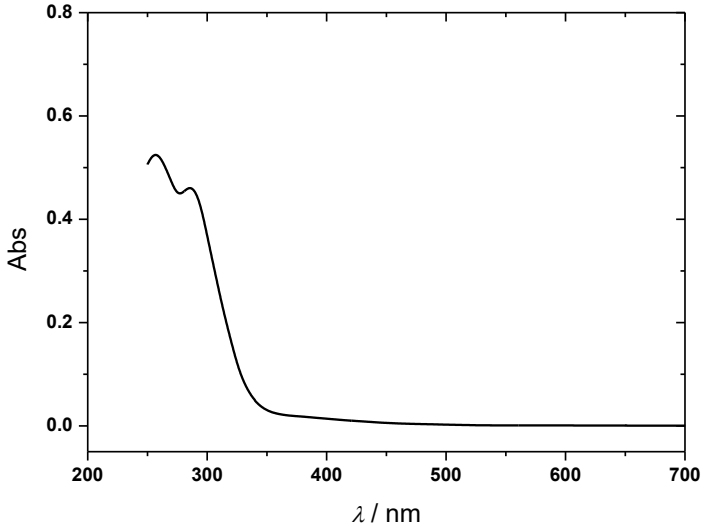

Figure S3. UV-Vis spectrum of complex **4** (0.5 mM) in CH_3CN.