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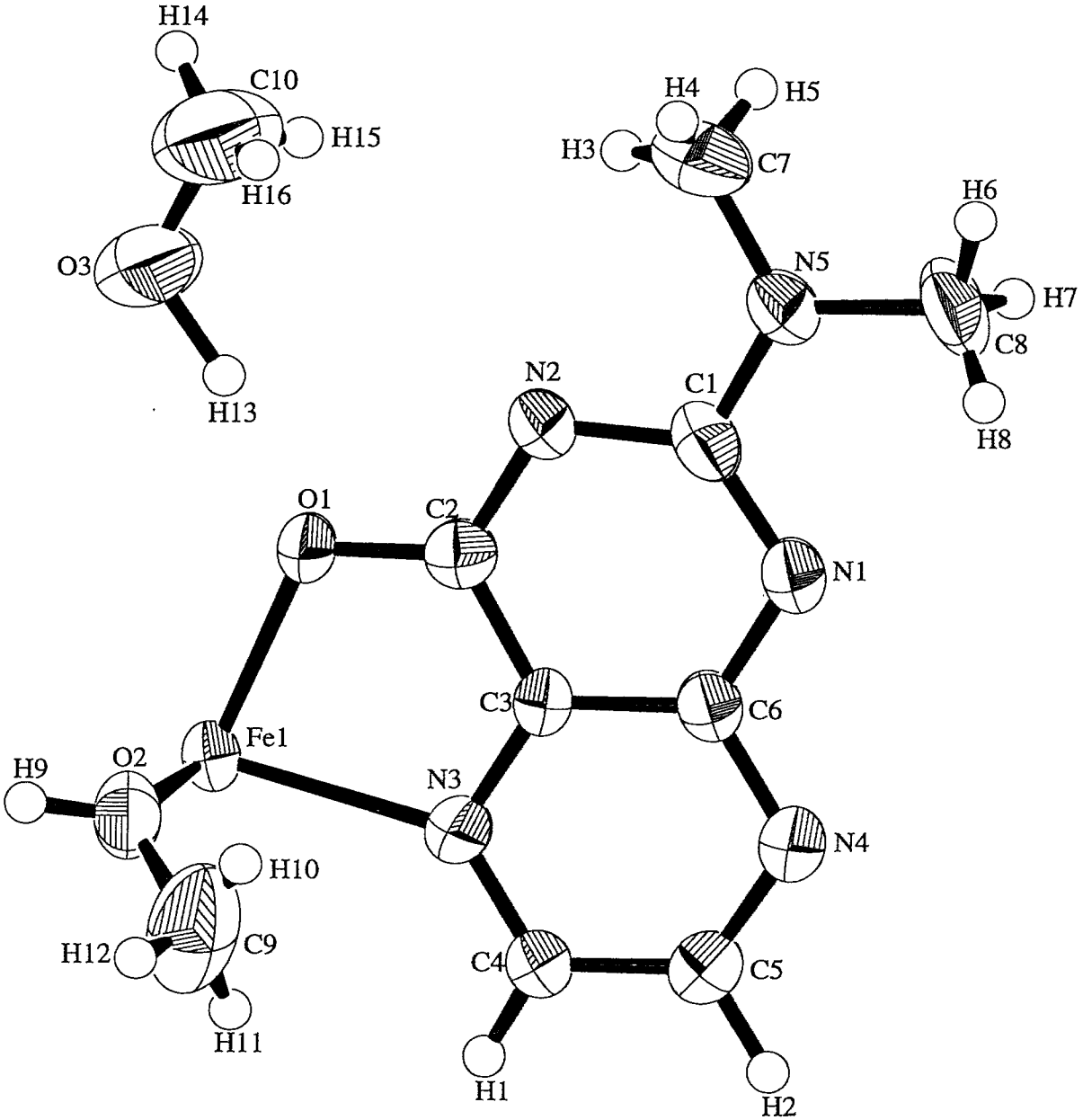
$[Fe(NDMP)_2(MeOH)_2]\cdot 2MeOH$ (**1**)



Positional parameters and B(eq) for position

atom	x	y	z	B(eq)
Fe(1)	0	0	0	3.34(3)
O(1)	0.1005(3)	0.1549(3)	0.1548(3)	3.87(7)
O(2)	-0.1606(3)	0.1672(3)	-0.1268(3)	4.18(8)
O(3)	0.3724(5)	0.2514(6)	0.1139(5)	10.8(2)
N(1)	-0.0873(4)	0.2338(3)	0.5805(3)	3.44(9)
N(2)	0.1062(4)	0.2676(3)	0.4082(4)	3.47(9)
N(3)	-0.1510(4)	0.0271(3)	0.1930(3)	3.16(8)
N(4)	-0.2808(4)	0.0895(4)	0.4851(4)	4.0(1)
N(5)	0.1063(4)	0.3775(4)	0.6641(4)	4.1(1)
C(1)	0.0387(5)	0.2884(4)	0.5488(5)	3.5(1)
C(2)	0.0436(5)	0.1804(4)	0.2907(5)	3.2(1)
C(3)	-0.0915(4)	0.1167(4)	0.3125(4)	2.8(1)
C(4)	-0.2757(5)	-0.0294(5)	0.2183(5)	3.6(1)
C(5)	-0.3365(6)	0.0019(5)	0.3655(5)	4.4(1)
C(6)	-0.1524(5)	0.1469(4)	0.4601(4)	3.0(1)
C(7)	0.2499(9)	0.432(1)	0.645(1)	5.9(2)
C(8)	0.038(1)	0.4229(8)	0.8151(7)	5.5(2)
C(9)	-0.326(1)	0.208(1)	-0.120(1)	7.7(2)
C(10)	0.430(1)	0.352(1)	0.219(2)	9.1(3)
H(1)	-0.322(4)	-0.089(4)	0.137(4)	4(1)
H(2)	-0.437(4)	-0.036(4)	0.384(4)	5(1)
H(3)	0.324(7)	0.360(6)	0.585(7)	12(2)
H(4)	0.232(8)	0.525(7)	0.625(8)	13(3)
H(5)	0.316(7)	0.429(7)	0.725(6)	10(2)
H(6)	0.069(5)	0.510(5)	0.859(5)	7(1)
H(7)	0.082(6)	0.355(5)	0.883(6)	8(2)
H(8)	-0.086(8)	0.445(6)	0.799(7)	13(2)
H(9)	-0.1379	0.1862	-0.2181	8.7
H(10)	-0.32(1)	0.282(8)	-0.059(8)	15(4)
H(11)	-0.36(1)	0.123(8)	-0.108(9)	17(4)
H(12)	-0.381(8)	0.260(8)	-0.193(7)	13(3)
H(13)	0.269(7)	0.204(6)	0.144(6)	12(2)
H(14)	0.54(1)	0.342(8)	0.22(1)	17(3)
H(15)	0.43(1)	0.33(1)	0.30(1)	18(5)
H(16)	0.349(8)	0.422(7)	0.236(9)	11(3)

U values for position

atom	U11	U22	U33	U12	U13	U23
Fe(1)	0.0472(7)	0.0559(7)	0.0275(6)	-0.0189(5)	0.0120(5)	-0.0057(5)
O(1)	0.058(2)	0.066(2)	0.032(2)	-0.032(2)	0.020(2)	-0.010(1)
O(2)	0.052(2)	0.073(2)	0.036(2)	-0.010(2)	0.011(2)	0.006(1)
O(3)	0.113(4)	0.220(5)	0.106(3)	-0.113(4)	0.055(3)	-0.065(3)
N(1)	0.053(2)	0.050(2)	0.031(2)	-0.016(2)	0.011(2)	-0.003(2)
N(2)	0.053(2)	0.051(2)	0.032(2)	-0.022(2)	0.008(2)	-0.006(2)
N(3)	0.038(2)	0.049(2)	0.037(2)	-0.014(2)	0.011(2)	-0.002(2)
N(4)	0.054(2)	0.066(3)	0.037(2)	-0.024(2)	0.015(2)	-0.003(2)
N(5)	0.067(3)	0.057(2)	0.036(2)	-0.028(2)	0.010(2)	-0.010(2)
C(1)	0.054(3)	0.045(3)	0.031(3)	-0.009(2)	0.004(2)	-0.003(2)
C(2)	0.043(3)	0.041(3)	0.039(3)	-0.012(2)	0.007(2)	0.001(2)
C(3)	0.039(2)	0.042(3)	0.027(2)	-0.012(2)	0.008(2)	0.003(2)
C(4)	0.050(3)	0.058(3)	0.033(3)	-0.024(2)	0.010(2)	-0.007(2)
C(5)	0.058(3)	0.072(3)	0.046(3)	-0.032(3)	0.016(3)	-0.004(2)
C(6)	0.044(3)	0.042(3)	0.030(2)	-0.009(2)	0.006(2)	0.001(2)
C(7)	0.074(5)	0.085(6)	0.066(5)	-0.038(4)	0.004(4)	-0.018(4)
C(8)	0.109(6)	0.074(5)	0.030(3)	-0.032(4)	0.015(4)	-0.015(3)
C(9)	0.056(4)	0.15(1)	0.079(5)	0.021(5)	0.021(4)	0.042(6)
C(10)	0.085(7)	0.130(8)	0.14(1)	-0.048(6)	0.041(6)	-0.042(6)
H(1)	0.05(1)					
H(2)	0.07(1)					
H(3)	0.16(3)					
H(4)	0.17(4)					
H(5)	0.13(3)					
H(6)	0.09(2)					
H(7)	0.11(2)					
H(8)	0.16(3)					
H(9)	0.1107					
H(10)	0.19(5)					
H(11)	0.21(5)					
H(12)	0.16(4)					
H(13)	0.16(2)					
H(14)	0.21(4)					
H(15)	0.23(7)					
H(16)	0.14(3)					

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
Fe(1)	O(1)	2.064(4)	N(2)	C(2)	1.328(5)
Fe(1)	O(2)	2.151(4)	N(3)	C(3)	1.341(5)
Fe(1)	N(3)	2.187(3)	N(3)	C(4)	1.329(5)
O(1)	C(2)	1.291(4)	N(4)	C(5)	1.318(5)
O(2)	C(9)	1.398(7)	N(4)	C(6)	1.361(5)
O(3)	C(10)	1.330(9)	N(5)	C(1)	1.346(5)
N(1)	C(1)	1.347(5)	N(5)	C(7)	1.449(7)
N(1)	C(6)	1.351(5)	N(5)	C(8)	1.466(6)
N(2)	C(1)	1.374(4)	C(2)	C(3)	1.438(5)
			C(3)	C(6)	1.400(5)
			C(4)	C(5)	1.397(5)

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle
O(1)	Fe(1)	O(1)	180.00
O(1)	Fe(1)	O(2)	91.3(2)
O(1)	Fe(1)	O(2)	88.7(2)
O(1)	Fe(1)	N(3)	79.5(2)
O(1)	Fe(1)	N(3)	100.5(2)
O(2)	Fe(1)	O(2)	180.00
O(2)	Fe(1)	N(3)	92.0(1)
O(2)	Fe(1)	N(3)	88.0(1)
N(3)	Fe(1)	N(3)	180.00
Fe(1)	O(1)	C(2)	113.5(3)
Fe(1)	O(2)	C(9)	126.5(5)
C(1)	N(1)	C(6)	115.6(3)
C(1)	N(2)	C(2)	116.7(3)
Fe(1)	N(3)	C(3)	108.1(2)

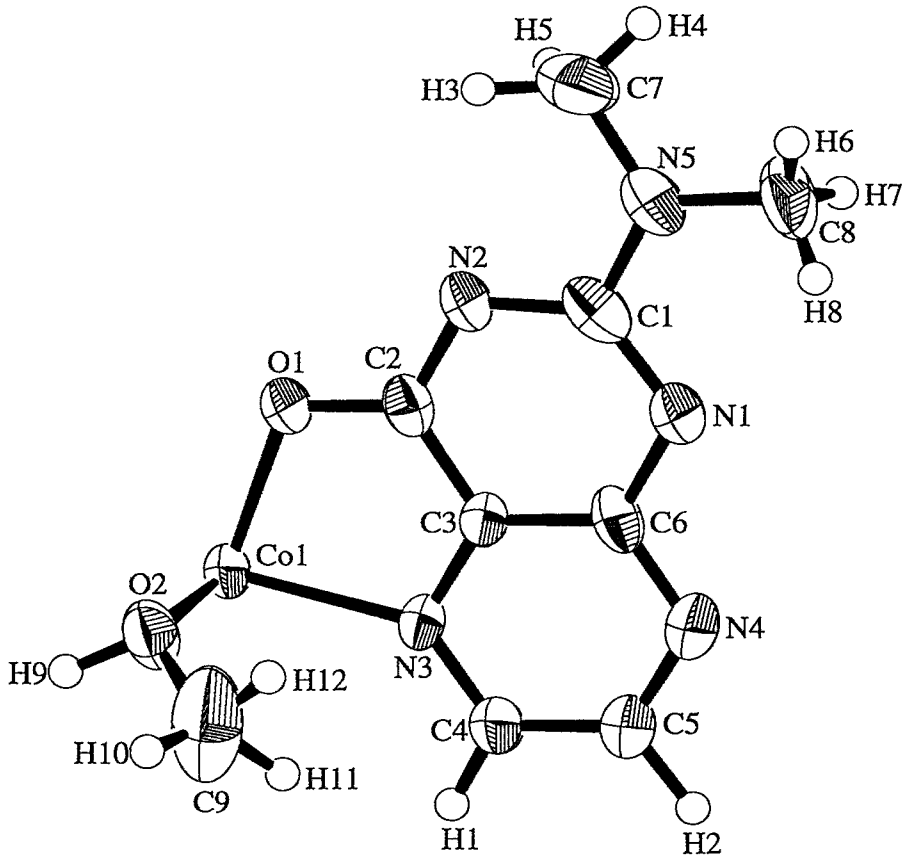
atom	atom	atom	angle
Fe(1)	N(3)	C(4)	134.9(3)
C(3)	N(3)	C(4)	116.9(3)
C(5)	N(4)	C(6)	115.7(4)
C(1)	N(5)	C(7)	121.5(4)
C(1)	N(5)	C(8)	121.3(4)
C(7)	N(5)	C(8)	117.2(5)
N(1)	C(1)	N(2)	127.5(4)
N(1)	C(1)	N(5)	118.0(4)
N(2)	C(1)	N(5)	114.5(4)
O(1)	C(2)	N(2)	120.6(4)
O(1)	C(2)	C(3)	119.4(4)
N(2)	C(2)	C(3)	120.0(4)
N(3)	C(3)	C(2)	118.9(3)
N(3)	C(3)	C(6)	122.6(3)
C(2)	C(3)	C(6)	118.5(4)
N(3)	C(4)	C(5)	120.2(4)
N(4)	C(5)	C(4)	124.3(4)
N(1)	C(6)	N(4)	118.2(4)
N(1)	C(6)	C(3)	121.6(4)
N(4)	C(6)	C(3)	120.3(4)

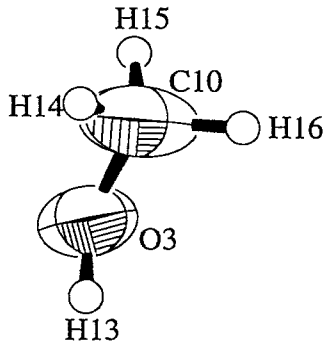
Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
Fe(1)	O(1)	C(2)	N(2)	174.0(3)	N(1)	C(1)	N(5)	C(7)	175.1(6)
Fe(1)	O(1)	C(2)	C(3)	-7.8(5)	N(1)	C(1)	N(5)	C(8)	-4.5(7)
Fe(1)	O(1)	C(2)	N(2)	-174.0(3)	N(1)	C(6)	N(4)	C(5)	-178.0(4)
Fe(1)	O(1)	C(2)	C(3)	7.8(5)	N(1)	C(6)	C(3)	N(3)	177.9(4)
Fe(1)	N(3)	C(3)	C(2)	3.3(4)	N(1)	C(6)	C(3)	C(2)	0.1(6)
Fe(1)	N(3)	C(3)	C(6)	-174.4(3)	N(2)	C(1)	N(1)	C(6)	1.1(6)
Fe(1)	N(3)	C(4)	C(5)	173.7(3)	N(2)	C(1)	N(5)	C(7)	-6.8(7)
Fe(1)	N(3)	C(3)	C(2)	-3.3(4)	N(2)	C(1)	N(5)	C(8)	173.7(5)
Fe(1)	N(3)	C(3)	C(6)	174.4(3)	N(2)	C(2)	C(3)	N(3)	-179.0(4)
Fe(1)	N(3)	C(4)	C(5)	-173.7(3)	N(2)	C(2)	C(3)	C(6)	-1.1(6)
O(1)	Fe(1)	O(2)	C(9)	-106.7(7)	N(3)	Fe(1)	O(1)	C(2)	7.1(3)
O(1)	Fe(1)	O(2)	C(9)	-73.3(7)	N(3)	Fe(1)	O(1)	C(2)	172.9(3)
O(1)	Fe(1)	N(3)	C(3)	-5.4(2)	N(3)	Fe(1)	O(2)	C(9)	-27.2(7)
O(1)	Fe(1)	N(3)	C(4)	178.9(4)	N(3)	Fe(1)	O(2)	C(9)	-152.8(7)
O(1)	Fe(1)	N(3)	C(3)	-174.6(2)	N(3)	C(3)	C(6)	N(4)	-2.6(6)
O(1)	Fe(1)	N(3)	C(4)	1.1(4)	N(3)	C(4)	C(5)	N(4)	1.8(7)
O(1)	C(2)	N(2)	C(1)	-179.8(3)	N(4)	C(6)	N(1)	C(1)	-179.6(3)
O(1)	C(2)	C(3)	N(3)	2.8(6)	N(4)	C(6)	C(3)	C(2)	179.6(4)
O(1)	C(2)	C(3)	C(6)	-179.3(4)	N(5)	C(1)	N(1)	C(6)	179.0(4)
O(2)	Fe(1)	O(1)	C(2)	98.9(3)	N(5)	C(1)	N(2)	C(2)	180.0(4)
O(2)	Fe(1)	O(1)	C(2)	81.1(3)	C(1)	N(1)	C(6)	C(3)	-0.1(6)
O(2)	Fe(1)	N(3)	C(3)	-96.4(3)	C(1)	N(2)	C(2)	C(3)	1.9(6)
O(2)	Fe(1)	N(3)	C(4)	87.9(4)	C(2)	C(3)	N(3)	C(4)	179.9(4)
O(2)	Fe(1)	N(3)	C(3)	-83.6(3)	C(3)	N(3)	C(4)	C(5)	-1.7(6)
O(2)	Fe(1)	N(3)	C(4)	92.1(4)	C(3)	C(6)	N(4)	C(5)	2.4(6)
N(1)	C(1)	N(2)	C(2)	-2.1(6)	C(4)	N(3)	C(3)	C(6)	2.1(6)
					C(4)	C(5)	N(4)	C(6)	-2.1(7)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

[Co(NDMP)$_2$(MeOH)$_2$]·2MeOH (**2**)





Positional parameters and B(eq) for position

atom	x	y	z	B(eq)
Co(1)	1.0000	0	1.0000	3.18(5)
O(1)	1.1032(6)	0.1543(5)	1.1514(5)	3.7(1)
O(2)	0.8451(7)	0.1627(5)	0.8722(5)	3.9(2)
O(3)	0.378(1)	0.251(1)	0.1146(8)	11.3(3)
N(1)	0.9111(8)	0.2311(7)	1.5800(7)	3.3(2)
N(2)	1.1069(8)	0.2650(7)	1.4045(7)	3.7(2)
N(3)	0.8504(8)	0.0257(6)	1.1875(6)	2.9(2)
N(4)	0.7160(9)	0.0842(8)	1.4830(7)	4.3(2)
N(5)	1.105(1)	0.3752(7)	1.6631(8)	4.3(2)
C(1)	1.039(1)	0.2856(9)	1.545(1)	3.8(3)
C(2)	1.045(1)	0.1805(8)	1.2867(8)	2.9(2)
C(3)	0.909(1)	0.1146(8)	1.3097(8)	2.7(2)
C(4)	0.725(1)	-0.031(1)	1.216(1)	3.6(3)
C(5)	0.660(1)	-0.001(1)	1.360(1)	4.3(3)
C(6)	0.845(1)	0.1444(8)	1.4577(9)	3.2(2)
C(7)	1.249(1)	0.435(1)	1.643(1)	6.3(4)
C(8)	1.036(2)	0.420(2)	1.814(1)	5.5(4)
C(9)	0.681(2)	0.211(2)	0.883(1)	8.3(4)
C(10)	0.425(1)	0.356(1)	0.222(1)	9.2(4)
H(1)	0.674(9)	-0.087(7)	1.125(7)	5(2)
H(2)	0.56(1)	-0.040(8)	1.389(8)	7(2)
H(3)	1.26(2)	0.46(1)	1.53(2)	24(7)
H(4)	1.30(1)	0.45(1)	1.75(1)	13(5)
H(5)	1.3348	0.3531	1.6272	13.4
H(6)	1.05(1)	0.510(9)	1.84(1)	6(3)
H(7)	1.07(1)	0.34(1)	1.88(1)	7(4)
H(8)	0.92(2)	0.42(2)	1.80(2)	25(8)
H(9)	0.8486	0.1270	0.7584	4.6
H(10)	0.64(1)	0.26(1)	0.80(1)	8(3)
H(11)	0.63(2)	0.15(1)	0.94(1)	16(6)
H(12)	0.6778	0.2811	0.9734	10.7
H(13)	0.2622	0.2844	0.0703	13.3
H(14)	0.4169	0.4395	0.1629	17.2
H(15)	0.5355	0.3212	0.2565	4.8
H(16)	0.3752	0.3644	0.3344	32.8

U values for position

atom	U11	U22	U33	U12	U13	U23
Co(1)	0.038(1)	0.060(2)	0.026(1)	-0.014(1)	0.010(1)	-0.004(1)
O(1)	0.051(4)	0.066(4)	0.028(3)	-0.027(3)	0.012(3)	-0.012(3)
O(2)	0.047(4)	0.066(4)	0.033(3)	0.000(4)	0.008(3)	-0.000(3)
O(3)	0.096(7)	0.24(1)	0.113(6)	-0.094(7)	0.041(5)	-0.068(6)
N(1)	0.048(5)	0.047(5)	0.032(4)	-0.010(4)	0.008(4)	-0.003(3)
N(2)	0.053(5)	0.063(5)	0.027(4)	-0.021(4)	0.009(4)	-0.010(4)
N(3)	0.034(5)	0.049(5)	0.029(4)	-0.009(4)	0.011(4)	0.003(3)
N(4)	0.054(6)	0.075(6)	0.041(4)	-0.021(5)	0.020(4)	-0.002(4)
N(5)	0.066(6)	0.061(6)	0.036(4)	-0.014(5)	0.005(4)	-0.010(4)
C(1)	0.057(7)	0.041(7)	0.037(5)	-0.002(6)	-0.004(5)	-0.005(5)
C(2)	0.042(6)	0.041(6)	0.026(5)	-0.002(5)	0.003(5)	0.006(4)
C(3)	0.034(6)	0.043(6)	0.028(5)	-0.008(5)	0.008(4)	0.004(4)
C(4)	0.039(6)	0.066(8)	0.033(5)	-0.015(6)	0.010(5)	-0.006(5)
C(5)	0.052(7)	0.078(8)	0.038(5)	-0.023(6)	0.015(5)	-0.004(5)
C(6)	0.056(7)	0.037(6)	0.026(4)	-0.002(5)	0.010(5)	-0.005(4)
C(7)	0.063(9)	0.11(1)	0.063(8)	-0.035(8)	0.003(7)	-0.023(8)
C(8)	0.12(1)	0.07(1)	0.035(6)	-0.04(1)	0.024(7)	-0.016(7)
C(9)	0.07(1)	0.16(1)	0.074(9)	0.04(1)	0.023(8)	0.056(9)
C(10)	0.07(1)	0.13(1)	0.14(1)	-0.032(9)	-0.006(9)	-0.032(8)
H(1)	0.06(3)					
H(2)	0.08(3)					
H(3)	0.30(9)					
H(4)	0.16(6)					
H(5)	0.1701					
H(6)	0.08(4)					
H(7)	0.09(5)					
H(8)	0.3(1)					
H(9)	0.0581					
H(10)	0.11(4)					
H(11)	0.20(7)					
H(12)	0.1352					
H(13)	0.1684					
H(14)	0.2183					
H(15)	0.0610					
H(16)	0.4157					

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
Co(1)	O(1)	2.062(4)	N(2)	C(2)	1.312(8)
Co(1)	O(2)	2.099(5)	N(3)	C(3)	1.351(8)
Co(1)	N(3)	2.126(5)	N(3)	C(4)	1.330(9)
O(1)	C(2)	1.283(7)	N(4)	C(5)	1.321(9)
O(2)	C(9)	1.39(1)	N(4)	C(6)	1.374(9)
O(3)	C(10)	1.341(9)	N(5)	C(1)	1.362(9)
N(1)	C(1)	1.36(1)	N(5)	C(7)	1.47(1)
N(1)	C(6)	1.362(8)	N(5)	C(8)	1.46(1)
N(2)	C(1)	1.363(8)	C(2)	C(3)	1.45(1)
			C(3)	C(6)	1.404(8)
			C(4)	C(5)	1.382(9)

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

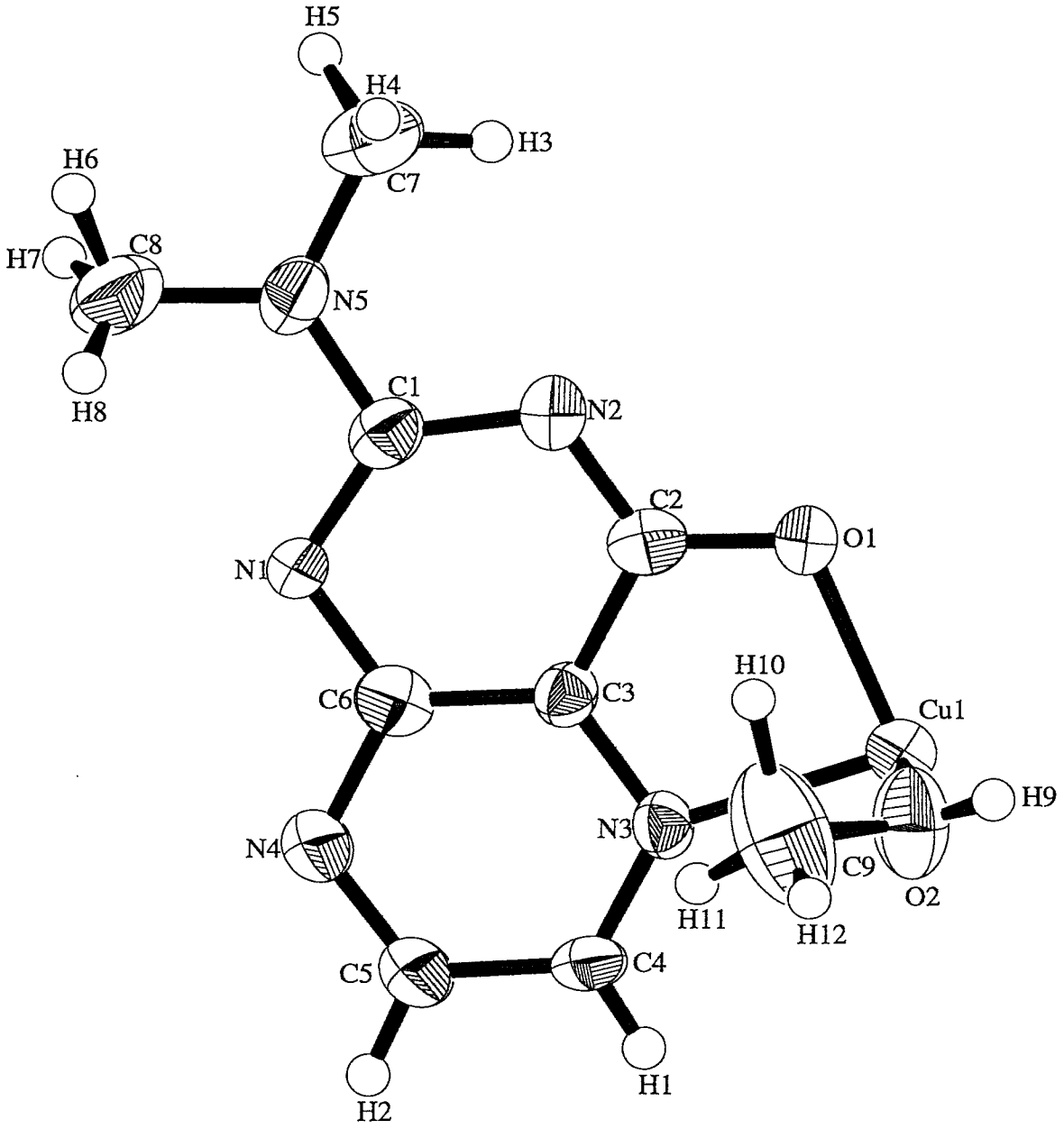
atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Co(1)	O(1)	180.00	Co(1)	N(3)	C(4)	135.9(6)
O(1)	Co(1)	O(2)	90.5(2)	C(3)	N(3)	C(4)	115.1(7)
O(1)	Co(1)	O(2)	89.5(2)	C(5)	N(4)	C(6)	115.1(7)
O(1)	Co(1)	N(3)	80.8(2)	C(1)	N(5)	C(7)	121.0(8)
O(1)	Co(1)	N(3)	99.2(2)	C(1)	N(5)	C(8)	122.3(9)
O(2)	Co(1)	O(2)	180.00	C(7)	N(5)	C(8)	116.7(9)
O(2)	Co(1)	N(3)	92.2(2)	N(1)	C(1)	N(2)	128.6(8)
O(2)	Co(1)	N(3)	87.8(2)	N(1)	C(1)	N(5)	116.0(8)
N(3)	Co(1)	N(3)	180.0000(1	N(2)	C(1)	N(5)	115.4(8)
Co(1)	O(1)	C(2)	112.7(5)	O(1)	C(2)	N(2)	121.4(8)
Co(1)	O(2)	C(9)	127.0(7)	O(1)	C(2)	C(3)	119.1(7)
C(1)	N(1)	C(6)	114.5(7)	N(2)	C(2)	C(3)	119.5(7)
C(1)	N(2)	C(2)	117.3(7)	N(3)	C(3)	C(2)	118.1(7)
Co(1)	N(3)	C(3)	108.7(5)	N(3)	C(3)	C(6)	123.0(7)
				C(2)	C(3)	C(6)	119.0(7)
				N(3)	C(4)	C(5)	122.4(9)
				N(4)	C(5)	C(4)	124.0(9)
				N(1)	C(6)	N(4)	118.5(7)
				N(1)	C(6)	C(3)	121.2(8)
				N(4)	C(6)	C(3)	120.4(7)

Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
Co(1)	O(1)	C(2)	N(2)	173.3(6)	N(1)	C(1)	N(5)	C(7)	176.7(9)
Co(1)	O(1)	C(2)	C(3)	-6.5(8)	N(1)	C(1)	N(5)	C(8)	-5(1)
Co(1)	O(1)	C(2)	N(2)	-173.3(6)	N(1)	C(6)	N(4)	C(5)	-178.9(8)
Co(1)	O(1)	C(2)	C(3)	6.5(8)	N(1)	C(6)	C(3)	N(3)	177.9(7)
Co(1)	N(3)	C(3)	C(2)	4.6(8)	N(1)	C(6)	C(3)	C(2)	-1(1)
Co(1)	N(3)	C(3)	C(6)	-174.7(6)	N(2)	C(1)	N(1)	C(6)	0(1)
Co(1)	N(3)	C(4)	C(5)	174.0(6)	N(2)	C(1)	N(5)	C(7)	-5(1)
Co(1)	N(3)	C(3)	C(2)	-4.6(8)	N(2)	C(1)	N(5)	C(8)	174(1)
Co(1)	N(3)	C(3)	C(6)	174.7(6)	N(2)	C(2)	C(3)	N(3)	-178.6(7)
Co(1)	N(3)	C(4)	C(5)	-174.0(6)	N(2)	C(2)	C(3)	C(6)	1(1)
O(1)	Co(1)	O(2)	C(9)	-104.0(9)	N(3)	Co(1)	O(1)	C(2)	6.8(5)
O(1)	Co(1)	O(2)	C(9)	-76.0(9)	N(3)	Co(1)	O(1)	C(2)	173.2(5)
O(1)	Co(1)	N(3)	C(3)	-5.9(5)	N(3)	Co(1)	O(2)	C(9)	-23.2(9)
O(1)	Co(1)	N(3)	C(4)	179.8(8)	N(3)	Co(1)	O(2)	C(9)	-156.8(9)
O(1)	Co(1)	N(3)	C(3)	-174.1(5)	N(3)	C(3)	C(6)	N(4)	-1(1)
O(1)	Co(1)	N(3)	C(4)	0.2(8)	N(3)	C(4)	C(5)	N(4)	-1(1)
O(1)	C(2)	N(2)	C(1)	-179.3(7)	N(4)	C(6)	N(1)	C(1)	179.8(7)
O(1)	C(2)	C(3)	N(3)	1(1)	N(4)	C(6)	C(3)	C(2)	179.7(7)
O(1)	C(2)	C(3)	C(6)	-179.6(7)	N(5)	C(1)	N(1)	C(6)	178.7(7)
O(2)	Co(1)	O(1)	C(2)	99.0(5)	N(5)	C(1)	N(2)	C(2)	-179.4(7)
O(2)	Co(1)	O(1)	C(2)	81.0(5)	C(1)	N(1)	C(6)	C(3)	1(1)
O(2)	Co(1)	N(3)	C(3)	-96.0(5)	C(1)	N(2)	C(2)	C(3)	0(1)
O(2)	Co(1)	N(3)	C(4)	89.6(8)	C(2)	C(3)	N(3)	C(4)	-179.8(7)
O(2)	Co(1)	N(3)	C(3)	-84.0(5)	C(3)	N(3)	C(4)	C(5)	0(1)
O(2)	Co(1)	N(3)	C(4)	90.4(8)	C(3)	C(6)	N(4)	C(5)	0(1)
N(1)	C(1)	N(2)	C(2)	-1(1)	C(4)	N(3)	C(3)	C(6)	1(1)
					C(4)	C(5)	N(4)	C(6)	1(1)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

[Cu(NDMP)$_2$(MeOH)$_2$] (**3**)



Positional parameters and B(eq) for position

atom	x	y	z	B(eq)
Cu(1)	1/2	0	1/2	3.16(4)
O(1)	0.5912(6)	0.0878(3)	0.3625(6)	3.2(1)
O(2)	0.3444(9)	-0.0792(4)	0.3036(7)	4.6(2)
N(1)	1.0218(7)	-0.0139(4)	0.2575(6)	3.0(2)
N(2)	0.8196(8)	0.1086(4)	0.2456(7)	3.3(2)
N(3)	0.6906(7)	-0.0789(4)	0.4692(6)	2.4(2)
N(4)	0.9767(7)	-0.1508(4)	0.3871(7)	3.7(2)
N(5)	1.0509(8)	0.1223(4)	0.1320(7)	3.5(2)
C(1)	0.960(1)	0.0700(5)	0.2165(8)	2.9(2)
C(2)	0.727(1)	0.0598(5)	0.3276(8)	2.8(2)
C(3)	0.784(1)	-0.0308(4)	0.3827(8)	2.4(2)
C(4)	0.741(1)	-0.1608(5)	0.516(1)	3.2(2)
C(5)	0.883(1)	-0.1963(5)	0.472(1)	4.0(3)
C(6)	0.926(1)	-0.0643(5)	0.3408(8)	2.9(2)
C(7)	1.007(2)	0.2176(9)	0.089(2)	5.9(4)
C(8)	1.198(2)	0.0897(7)	0.082(1)	5.1(4)
C(9)	0.392(2)	-0.126(1)	0.181(2)	7.7(4)
H(1)	0.689(7)	-0.193(4)	0.571(7)	2(2)
H(2)	0.913(7)	-0.256(4)	0.505(8)	6(2)
H(3)	0.92(1)	0.241(6)	0.14(1)	9(3)
H(4)	0.95(1)	0.211(6)	-0.006(9)	6(3)
H(5)	1.095(9)	0.262(5)	0.10(1)	7(3)
H(6)	1.21(1)	0.123(5)	-0.03(1)	10(3)
H(7)	1.28(1)	0.111(8)	0.11(1)	11(5)
H(8)	1.184(5)	0.035(3)	0.054(5)	-1(1)
H(9)	0.25(1)	-0.061(5)	0.27(1)	8(4)
H(10)	0.42(2)	-0.067(8)	0.10(2)	24(8)
H(11)	0.48(1)	-0.158(7)	0.22(1)	11(4)
H(12)	0.33(2)	-0.17(1)	0.16(2)	18(8)

U values for position

atom	U11	U22	U33	U12	U13	U23
Cu(1)	0.040(1)	0.0319(8)	0.050(1)	0.004(1)	0.0127(8)	0.004(1)
O(1)	0.035(4)	0.038(3)	0.050(4)	0.005(3)	0.016(3)	0.005(3)
O(2)	0.047(5)	0.074(4)	0.055(4)	0.006(4)	0.007(4)	-0.025(3)
N(1)	0.030(4)	0.032(4)	0.053(4)	0.003(3)	0.015(3)	0.010(4)
N(2)	0.035(5)	0.041(4)	0.052(5)	0.005(3)	0.013(4)	0.005(3)
N(3)	0.023(5)	0.031(3)	0.037(4)	0.002(3)	0.002(3)	-0.001(3)
N(4)	0.034(6)	0.039(4)	0.069(5)	0.007(3)	0.009(4)	0.010(4)
N(5)	0.037(5)	0.053(4)	0.047(4)	0.002(4)	0.016(4)	0.007(3)
C(1)	0.037(7)	0.037(5)	0.036(5)	-0.007(4)	0.007(5)	-0.003(4)
C(2)	0.041(8)	0.037(5)	0.028(5)	-0.004(5)	-0.000(5)	0.000(4)
C(3)	0.025(6)	0.034(5)	0.031(5)	-0.000(4)	0.002(4)	0.003(4)
C(4)	0.035(8)	0.028(5)	0.057(6)	-0.004(4)	0.008(5)	0.013(4)
C(5)	0.038(7)	0.037(5)	0.077(7)	0.008(5)	0.011(6)	0.014(5)
C(6)	0.035(7)	0.035(5)	0.039(5)	-0.001(4)	-0.006(5)	-0.000(4)
C(7)	0.07(1)	0.065(7)	0.10(1)	-0.003(7)	0.023(9)	0.034(7)
C(8)	0.07(1)	0.047(7)	0.08(1)	-0.018(7)	0.033(8)	-0.006(6)
C(9)	0.10(1)	0.12(1)	0.07(1)	0.04(1)	-0.01(1)	-0.038(8)
H(1)	0.03(2)					
H(2)	0.07(3)					
H(3)	0.11(4)					
H(4)	0.08(4)					
H(5)	0.08(3)					
H(6)	0.13(4)					
H(7)	0.14(6)					
H(8)	-0.01(2)					
H(9)	0.10(5)					
H(10)	0.3(1)					
H(11)	0.14(5)					
H(12)	0.2(1)					

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
Cu(1)	O(1)	1.969(5)	N(2)	C(2)	1.322(8)
Cu(1)	O(2)	2.386(6)	N(3)	C(3)	1.343(8)
Cu(1)	N(3)	2.006(5)	N(3)	C(4)	1.309(8)
O(1)	C(2)	1.278(8)	N(4)	C(5)	1.319(8)
O(2)	C(9)	1.38(1)	N(4)	C(6)	1.366(8)
N(1)	C(1)	1.352(8)	N(5)	C(1)	1.354(8)
N(1)	C(6)	1.355(8)	N(5)	C(7)	1.46(1)
N(2)	C(1)	1.353(8)	N(5)	C(8)	1.43(1)
			C(2)	C(3)	1.460(8)
			C(3)	C(6)	1.381(9)
			C(4)	C(5)	1.39(1)

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Cu(1)	O(1)	180.00	Cu(1)	N(3)	C(4)	135.0(6)
O(1)	Cu(1)	O(2)	93.7(2)	C(3)	N(3)	C(4)	117.2(7)
O(1)	Cu(1)	O(2)	86.3(2)	C(5)	N(4)	C(6)	116.1(7)
O(1)	Cu(1)	N(3)	85.1(2)	C(1)	N(5)	C(7)	121.6(8)
O(1)	Cu(1)	N(3)	94.9(2)	C(1)	N(5)	C(8)	122.8(7)
O(2)	Cu(1)	O(2)	180.0000(1	C(7)	N(5)	C(8)	115.6(8)
O(2)	Cu(1)	N(3)	91.3(2)	N(1)	C(1)	N(2)	129.5(7)
O(2)	Cu(1)	N(3)	88.7(2)	N(1)	C(1)	N(5)	115.1(7)
N(3)	Cu(1)	N(3)	180.00	N(2)	C(1)	N(5)	115.4(7)
Cu(1)	O(1)	C(2)	111.1(5)	O(1)	C(2)	N(2)	123.8(7)
Cu(1)	O(2)	C(9)	130(1)	O(1)	C(2)	C(3)	118.1(8)
C(1)	N(1)	C(6)	113.2(6)	N(2)	C(2)	C(3)	118.0(8)
C(1)	N(2)	C(2)	117.5(6)	N(3)	C(3)	C(2)	117.7(8)
Cu(1)	N(3)	C(3)	107.8(5)	N(3)	C(3)	C(6)	123.2(7)
				C(2)	C(3)	C(6)	119.1(8)
				N(3)	C(4)	C(5)	120.2(8)
				N(4)	C(5)	C(4)	124.0(8)
				N(1)	C(6)	N(4)	118.2(8)
				N(1)	C(6)	C(3)	122.6(7)
				N(4)	C(6)	C(3)	119.3(8)

Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle
Cu(1)	O(1)	C(2)	N(2)	175.0(6)
Cu(1)	O(1)	C(2)	C(3)	-4.4(8)
Cu(1)	O(1)	C(2)	N(2)	-175.0(6)
Cu(1)	O(1)	C(2)	C(3)	4.4(8)
Cu(1)	N(3)	C(3)	C(2)	2.7(7)
Cu(1)	N(3)	C(3)	C(6)	-179.2(6)
Cu(1)	N(3)	C(4)	C(5)	179.7(6)
Cu(1)	N(3)	C(3)	C(2)	-2.7(7)
Cu(1)	N(3)	C(3)	C(6)	179.2(6)
Cu(1)	N(3)	C(4)	C(5)	-179.7(6)
O(1)	Cu(1)	O(2)	C(9)	120(1)
O(1)	Cu(1)	O(2)	C(9)	60(1)
O(1)	Cu(1)	N(3)	C(3)	3.9(5)
O(1)	Cu(1)	N(3)	C(4)	-178.1(8)
O(1)	Cu(1)	N(3)	C(3)	176.1(5)
O(1)	Cu(1)	N(3)	C(4)	-1.9(8)
O(1)	C(2)	N(2)	C(1)	-179.6(7)
O(1)	C(2)	C(3)	N(3)	-1.1(9)
O(1)	C(2)	C(3)	C(6)	177.1(7)
O(2)	Cu(1)	O(1)	C(2)	-95.6(5)
O(2)	Cu(1)	O(1)	C(2)	-84.4(5)
O(2)	Cu(1)	N(3)	C(3)	97.5(5)
O(2)	Cu(1)	N(3)	C(4)	-95.5(8)
O(2)	Cu(1)	N(3)	C(3)	82.5(5)
O(2)	Cu(1)	N(3)	C(4)	-84.5(8)
N(1)	C(1)	N(2)	C(2)	1(1)

(1)	(2)	(3)	(4)	angle
N(1)	C(1)	N(5)	C(7)	-175(1)
N(1)	C(1)	N(5)	C(8)	3(1)
N(1)	C(6)	N(4)	C(5)	178.1(7)
N(1)	C(6)	C(3)	N(3)	-177.8(7)
N(1)	C(6)	C(3)	C(2)	4(1)
N(2)	C(1)	N(1)	C(6)	-1(1)
N(2)	C(1)	N(5)	C(7)	6(1)
N(2)	C(1)	N(5)	C(8)	-175.6(9)
N(2)	C(2)	C(3)	N(3)	178.3(7)
N(2)	C(2)	C(3)	C(6)	-3(1)
N(3)	Cu(1)	O(1)	C(2)	-4.6(5)
N(3)	Cu(1)	O(1)	C(2)	-175.4(5)
N(3)	Cu(1)	O(2)	C(9)	-25(1)
N(3)	Cu(1)	O(2)	C(9)	-155(1)
N(3)	C(3)	C(6)	N(4)	1(1)
N(3)	C(4)	C(5)	N(4)	3(1)
N(4)	C(6)	N(1)	C(1)	179.4(6)
N(4)	C(6)	C(3)	C(2)	-177.3(6)
N(5)	C(1)	N(1)	C(6)	-179.4(6)
N(5)	C(1)	N(2)	C(2)	179.9(7)
C(1)	N(1)	C(6)	C(3)	-2(1)
C(1)	N(2)	C(2)	C(3)	1(1)
C(2)	C(3)	N(3)	C(4)	178.9(7)
C(3)	N(3)	C(4)	C(5)	-2(1)
C(3)	C(6)	N(4)	C(5)	-1(1)
C(4)	N(3)	C(3)	C(6)	1(1)
C(4)	C(5)	N(4)	C(6)	-1(1)