Table 1S. Atomic positional and thermal parameters for title compound.

	x	y	z	U(eq)
Ni(1)	15000	5000	5000	28(1)
Ni(2)	9703(1)	6887(1)	3383(1)	31(1)
Ni(3)	9439(1)	2438(1)	3818(1)	38(1)
Fe(1)	10000	5000	5000	21(1)
Fe(2)	9272(1)	270(1)	2372(1)	30(1)
N(1)	14714(6)	4413(3)	5706(2)	41(1)
N(2)	15409(6)	3824(3)	4683(2)	51(2)
N(3)	9559(7)	7594(3)	2704(2)	53(2)
N(4)	10877(6)	5995(3)	3030(2)	41(1)
N(5)	8506(6)	7756(3)	3750(2)	44(2)
N(6)	11403(6)	7561(3)	3629(2)	48(2)
N(7)	7425(6)	2302(4)	3945(2)	54(2)
N(8)	9723(7)	1515(3)	4376(2)	56(2)
N(9)	9056(7)	3341(4)	3260(2)	63(2)
N(10)	11472(6)	2546(4)	3715(3)	70(2)
N(11)	12987(5)	4887(4)	4845(2)	44(2)
N(12)	9794(6)	6127(3)	4046(2)	39(1)
N(13)	9513(6)	3397(3)	4381(2)	46(2)
N(14)	9392(7)	1536(4)	3245(2)	54(2)
N(15)	11469(7)	-768(4)	2897(2)	59(2)
N(16)	11205(7)	1331(5)	1761(3)	68(2)
N(17)	7357(8)	-756(6)	3005(3)	104(3)
N(18)	6976(6)	1241(3)	1870(2)	42(1)
N(19)	9052(7)	-1010(4)	1497(2)	55(2)
C(1)	14101(8)	3578(4)	5716(3)	52(2)
C(2)	14810(10)	2976(5)	5415(3)	80(3)
C(3)	14707(11)	3114(5)	4844(3)	91(3)
C(4)	9693(10)	7185(5)	2208(3)	67(3)
C(5)	10847(10)	6616(6)	2184(3)	75(3)
C(6)	10815(8)	5836(5)	2482(3)	58(2)
C(7)	8967(10)	8150(6)	4220(3)	77(3)
C(8)	10284(9)	8533(5)	4195(3)	64(2)
C(9)	11372(9)	7958(5)	4139(3)	64(2)
C(10)	6851(9)	1461(5)	3978(3)	70(3)
C(11)	7476(10)	986(5)	4419(3)	78(3)
C(12)	8893(10)	774(5)	4366(3)	68(3)
C(13)	9948(10)	3984(6)	3166(4)	88(3)
C(14)	11317(12)	3699(6)	3104(4)	95(4)
C(15)	12061(10)	3329(7)	3547(4)	97(3)
C(16)	11873(6)	4908(4)	4890(2)	31(2)
C(17)	9857(6)	5694(4)	4386(2)	31(2)
C(18)	9693(6)	3988(4)	4606(2)	28(1)
C(19)	9364(7)	1069(4)	2919(2)	40(2)
C(20)	10683(7)	-370(4)	2694(2)	40(2)
C(21)	10499(7)	934(4)	1989(3)	40(2)
C(22)	8043(8)	-381(5)	2768(3)	51(2)
C(23)	7831(7)	887(4)	2054(2)	33(2)
C(24)	9156(7)	-544(4)	1826(2)	38(2)
O(5)	13316(20)	-356(14)	3691(6)	191(10)
O(6)	15455(17)	-1174(12)	3733(7)	184(10)
O(7)	15769(29)	-2212(13)	2932(10)	102(10)
Cl	6816(6)	-974(5)	5415(3)	113(2)
O(1)	5801(9)	-807(6)	5035(4)	109(6)
O(2)	7809(13)	-362(9)	5355(7)	270(17)
O(3)	7386(18)	-1761(7)	5292(8)	401(30)

Table 2S. Anistropic coefficients for title compound.

	U11	U22	U33	U23	U13	U12
Ni(1)	19(1)	38(1)	27(1)	-1(1)	3(1)	2(1)
Ni(2)	33(1)	31(1)	29(1)	4(1)	-3(1)	0(1)
Ni(3)	53(1)	30(1)	30(1)	-6(1)	-2(1)	1(1)
Fe(1)	20(1)	22(1)	21(1)	0(1)	-1(1)	-1(1)
Fe(2)	32(1)	34(1)	25(1)	-3(1)	1(1)	2(1)
N(1)	42(4)	50(4)	31(3)	2(3)	6(3)	-5(3)
N(2)	64(4)	43(4)	45(4)	1(3)	11(3)	8(3)
N(3)	77(5)	36(3)	46(4)	10(3)	-8(3)	7(3)
N(4)	46(4)	38(3)	40(3)	2(3)	1(3)	1(3)
N(5)	44(4)	41(3)	47(4)	-3(3)	1(3)	7(3)
N(6)	40(4)	49(4)	55(4)	-4(3)	-6(3)	-3(3)
N(7)	55(4)	47(4)	59(4)	-5(3)	-5(3)	4(3)
N(8)	79(5)	41(4)	47(4)	4(3)	-3(4)	6(3)
N(9)	80(5)	52(4)	55(4)	14(3)	7(4)	7(4)
N(10)	54(5)	67(5)	89(5)	-2(4)	8(4)	-1(4)
N(11)	24(3)	65(4)	43(3)	5(3)	-1(3)	1(3)
N(12)	50(4)	33(3)	34(3)	10(3)	-2(3)	0(3)
N(13)	66(4)	34(3)	39(3)	-4(3)	-7(3)	-1(3)
N(14)	76(5)	51(4)	35(4)	-15(3)	-8(3)	13(3)
N(15)	54(4)	57(4)	66(5)	10(4)	-6(4)	8(4)
N(16)	46(4)	97(6)	62(5)	24(4)	-2(4)	-22(4)
N(17)	58(5)	124(7)	133(8)	69(6)	28(5)	2(5)
N(18)	35(4)	47(4)	45(4)	-1(3)	-3(3)	2(3)
N(19)	74(5)	49(4)	41(4)	-10(3)	2(3)	-2(3)
C(1)	58(5)	54(5)	45(5)	18(4)	3(4)	-12(4)
C(2)	117(8)	46(5)	80(7)	11(5)	38(6)	4(5)
C(3)	135(10)	55(6)	84(7)	-18(5)	31(7)	-22(6)
C(4)	107(8)	62(5)	30(4)	15(4)	-9(5)	3(5)
C(5)	93(8)	85(7)	48(5)	0(5)	21(5)	-2(6)
C(6)	69(6)	56(5)	49(5)	-3(4)	11(4)	18(4)
C(7)	102(8)	70(6)	60(6)	-18(5)	24(6)	19(6)
C(8)	96(7)	45(5)	52(5)	-19(4)	6(5)	-10(5)
C(9)	76(6)	54(5)	61(6)	-2(4)	-26(5)	-12(5)
C(10)	73(6)	64(6)	71(6)	1(5)	7(5)	-22(5)
C(11)	98(8)	60(6)	76(7)	13(5)	12(6)	-23(6)
C(12)	107(8)	38(5)	60(6)	5(4)	-2(5)	-3(5)
C(13)	90(8)	69(6)	106(8)	29(6)	-5(7)	-14(6)
C(14)	118(10)	81(7)	87(8)	28(6)	47(7)	-5(7)
C(15)	71(7)	111(9)	110(9)	4(7)	30(7)	-20(7)
C(16)	32(4)	30(4)	32(4)	7(3)	-6(3)	0(3)
C(17)	29(4)	26(3)	38(4)	1(3)	-1(3)	-2(3)
C(18)	31(4)	28(3)	25(3)	-3(3)	-4(3)	4(3)
C(19)	46(4)	50(4)	24(4)	-3(3)	0(3)	6(4)
C(20)	46(4)	38(4)	36(4)	-7(3)	2(3)	-3(4)
C(21)	29(4)	51(4)	40(4)	-4(4)	-7(3)	2(4)
C(22)	44(5)	60(5)	49(5)	14(4)	4(4)	5(4)
C(23)	35(4)	36(4)	28(4)	-4(3)	5(3)	-2(3)
C(24)	41(4)	42(4)	31(4)	-1(3)	0(3)	-1(3)
O(5)	184(19)	289(25)	96(12)	64(15)	-75(12)	-112(18)
O(6)	149(16)	224(20)	184(17)	143(16)	116(14)	21(14)
O(7)	154(27)	45(13)	104(20)	32(14)	-53(19)	-40(16)
Cl	60(4)	171(7)	110(5)	53(5)	6(4)	-1(4)
O(1)	59(8)	40(7)	229(18)	31(9)	24(10)	17(6)
O(2)	113(18)	488(51)	205(24)	-89(29)	-75(18)	88(26)
O(3)	103(18)	452(52)	642(68)	378(52)	-130(30)	37(26)
O(4)	403(45)	285(32)	146(20)	127(22)	-80(24)	-78(32)

Table 3S. H-atoms coordinates and isotropic displacement coefficients for title compound.

	x	y	z	U(eq)
H(1A)	15504(6)	4374(3)	5865(2)	49
H(1B)	14218(6)	4755(3)	5894(2)	49
H(2A)	15286(6)	3868(3)	4344(2)	61
H(2B)	16270(6)	3722(3)	4740(2)	61
H(3A)	8773(7)	7851(3)	2701(2)	64
H(3B)	10175(7)	7996(3)	2725(2)	64
H(4A)	11717(6)	6127(3)	3108(2)	50
H(4B)	10715(6)	5506(3)	3183(2)	50
H(5A)	8322(6)	8165(3)	3525(2)	53
H(5B)	7742(6)	7500(3)	3815(2)	53
H(6A)	12094(6)	7210(3)	3627(2)	58
H(6B)	11555(6)	7962(3)	3399(2)	58
H(7A)	7251(6)	2568(4)	4237(2)	64
H(7B)	6989(6)	2575(4)	3695(2)	64
H(8A)	10564(7)	1343(3)	4360(2)	67
H(8B)	9632(7)	1759(3)	4681(2)	67
H(9A)	8922(7)	3069(4)	2965(2)	75
H(9B)	8288(7)	3583(4)	3337(2)	75
H(10A)	11869(6)	2410(4)	4013(3)	84
H(10B)	11697(6)	2151(4)	3490(3)	84
H(1C)	14075(8)	3384(4)	6065(3)	63
H(1D)	13202(8)	3617(4)	5587(3)	63
H(2C)	14481(10)	2424(5)	5490(3)	97
H(2D)	15731(10)	2992(5)	5519(3)	97
H(3C)	15043(11)	2626(5)	4672(3)	109
H(3D)	13788(11)	3176(5)	4745(3)	109
H(4C)	9771(10)	7609(5)	1948(3)	80
H(4D)	8900(10)	6869(5)	2132(3)	80
H(5C)	10965(10)	6468(6)	1830(3)	90
H(5D)	11620(10)	6927(6)	2294(3)	90
H(6C)	10012(8)	5535(5)	2398(3)	69
H(6D)	11551(8)	5488(5)	2390(3)	69
H(7C)	8982(10)	7735(6)	4488(3)	92
H(7D)	8341(10)	8577(6)	4312(3)	92
H(8C)	10283(9)	8918(5)	3911(3)	77
H(8D)	10439(9)	8856(5)	4502(3)	77
H(9C)	11312(9)	7526(5)	4395(3)	77
H(9D)	12190(9)	8255(5)	4199(3)	77
H(10C)	6994(9)	1162(5)	3663(3)	84
H(10D)	5910(9)	1504(5)	4025(3)	84
H(11A)	7382(10)	1315(5)	4725(3)	93
H(11B)	6989(10)	473(5)	4465(3)	93
H(12A)	9164(10)	406(5)	4642(3)	82
H(12B)	9010(10)	480(5)	4049(3)	82
H(13A)	9928(10)	4379(6)	3445(4)	106
H(13B)	9664(10)	4276(6)	2859(4)	106
H(14A)	11820(12)	4171(6)	2985(4)	114
H(14B)	11308(12)	3288(6)	2833(4)	114
H(15A)	12962(10)	3228(7)	3451(4)	116
H(15B)	12075(10)	3723(7)	3826(4)	116

Table S4. Molar magnetic susceptibility vs temperature data for title compound.

T	χ_M	$\chi_M T$	T	χ_M	$\chi_M T$
5.001	20.5755	102.898	104.99	0.0341792	3.58847
6.0122	19.7423	118.694	109.99	0.0325645	3.58117
8.0084	17.8129	142.653	114.99	0.0311168	3.57812
10.024	6.1242	61.3889	119.95	0.0298035	3.57493
12.029	1.32523	15.9412	125	0.0285939	3.57424
14.018	0.71514	10.0248	130.03	0.027436	3.56753
16.02	0.466022	7.46567	135.04	0.0263725	3.56135
18.035	0.349613	6.30528	140.06	0.0254145	3.55955
20.055	0.282625	5.66805	145.07	0.024514	3.55624
22.064	0.238427	5.26066	150.1	0.0236884	3.55563
24.075	0.206747	4.97744	155.12	0.0229223	3.55571
26.08	0.182552	4.76095	160.1	0.0221908	3.55275
28.07	0.163784	4.59741	165.12	0.0215361	3.55604
30.069	0.148549	4.46671	170.13	0.0209159	3.55843
32.114	0.135462	4.35023	175.15	0.020338	3.5622
34.034	0.125277	4.26367	180.14	0.019792	3.56533
36.036	0.116199	4.18735	185.17	0.0192753	3.565921
38.027	0.108379	4.12132	190.15	0.0187671	3.56856
39.989	0.102204	4.08704	195.18	0.0182946	3.57074
42.007	0.0960526	4.03488	200.17	0.017834	3.56983
43.993	0.0906267	3.98694	205.18	0.0174214	3.57452
46.006	0.0857711	3.94598	210.18	0.0170047	3.57405
48.003	0.0813417	3.90464	215.2	0.016625	3.57769
50.001	0.0775862	3.87939	220.21	0.0162736	3.58361
51.999	0.0741782	3.85719	225.22	0.015933	3.58843
54.992	0.069887	3.84323	230.24	0.0155893	3.58928
56.994	0.0673431	3.83815	235.25	0.0152739	3.59318
59.969	0.0634186	3.80315	240.25	0.0149546	3.59284
64.985	0.0577988	3.75606	245.26	0.0146474	3.59241
69.982	0.0531409	3.71891	250.26	0.0144139	3.60722
74.987	0.04918	3.68786	260.25	0.0138965	3.61656
79.988	0.0457855	3.66229	270.24	0.01339	3.61851
84.966	0.0428229	3.63849	280.24	0.0130357	3.65314
89.999	0.0402828	3.62541	290.26	0.0126084	3.6597
94.999	0.0380038	3.61032	300.2	0.0121775	3.65569
99.997	0.0359801	3.5979			

Table S5. The field-cooled magnetization (FCM) vs temperature data (100 to 5 K) under a weak magnetic field of 10 G for title compound.

T	M(per mol)	T	M(per mol)
4.9995	573.077	39.996	1.101
6.0012	481.724	42.005	1.03741
8.0072	197.394	43.994	0.980766
10.018	23.8212	46.002	0.930309
12.013	8.79046	48	0.884153
14.008	5.64859	50.003	0.844447
16.01	4.21629	51.998	0.808237
18.027	3.3698	53.993	0.777939
20.041	2.81884	55.975	0.749255
22.056	2.42371	58	0.721837
24.081	2.128	59.988	0.694266
26.069	1.90144	61.946	0.668884
28.057	1.71938	64.921	0.633556
30.07	1.56794	69.986	0.584712
32.042	1.44256	74.987	0.543356
34.039	1.33566	79.99	0.506914
36.116	1.23927	89.977	0.447817
38.034	1.16374	99.989	0.400931

Table S6. The magnetization (H) vs magnetic field data at 5K (including hysteresis data).

H	M	H	M	H	M	H	M
0	60.5102	2000	10091.4	-340	170.51	-190	-4986.58
20	152.858	1800	9650.22	-370	-113.705	-160	-4852.57
40	276.846	1600	9179.83	-400	-390.64	-130	-4712.79
60	401.161	1400	8678.71	-500	-1156.75	-100	-4567.64
80	517.052	1200	8147.64	-600	-1927.09	-80	-4450.91
100	626.068	1000	7621.95	-800	-3216.13	-60	-4336.86
150	891.564	800	7093.96	-1000	-4325.72	-40	-4220.51
200	1138.28	600	6509.9	-1200	-5363.28	-20	-4096.09
400	2222.54	500	6193.48	-1400	-6324.04	0	-3961.7
600	3067.52	400	5842.9	-1600	-7147.72	20	-3795.89
800	3872.99	370	5713.49	-1800	-7830.46	40	-3613.53
1000	4626.78	340	5593.3	-2000	-8438.33	60	-3408.59
1200	5528.79	310	5466.58	-3000	-11028	80	-3190.78
1400	6424.65	280	5358.68	-4000	-12180	100	-2960.54
1600	7204.93	250	5233.11	-5000	-12862	130	-2598.43
1800	7863.49	220	5106.77	-10000	-14767.7	160	-2238.2
2000	8466.36	190	4977.37	-50000	-22055.2	190	-1861.85
3000	10968.5	160	4847.58	-10000	-14793.5	220	-1491.98
4000	12112.4	130	4708.57	-5000	-13016	250	-1135.67
5000	12795.9	100	4559.19	-4000	-12460.3	280	-779.475
6000	13296.3	80	4443.61	-3000	-11639.7	310	-474.735
7000	13706.4	60	4330.33	-2000	-10113.3	340	-154.82
8000	14063.1	40	4214.37	-1800	-9674.42	370	117.876
9000	14379.9	20	4091.49	-1600	-9200.56	400	419.555
10000	14671.4	0	3957.47	-1400	-8699.06	500	1171.04
15000	15913.6	-20	3798.65	-1200	-8167.61	600	1946.75
20000	16913.1	-40	3617.44	-1000	-7640	800	3233.91
25000	17754.1	-60	3418.26	-800	-7112.77	1000	4344.92
30000	19120.7	-80	3197.54	-600	-6527.18	1200	5380.95
35000	19975.9	-100	2970.45	-500	-6208.46	1400	6349.77
40000	20737	-130	2603.34	-400	-5856.72	1600	7169.22
45000	21426.3	-160	2250.03	-370	-5726.54	1800	7846.98
50000	22057.5	-190	1874.71	-340	-5605.97	2000	8456.38
10000	14784.6	-220	1507.88	-310	-5477.71	3000	11040.3
5000	13006.7	-250	1150.03	-280	-5366.36	4000	12184.6
4000	12447.6	-280	796.333	-250	-5243.09	5000	12863.1
3000	11624.4	-310	486.486	-220	-5116.76		

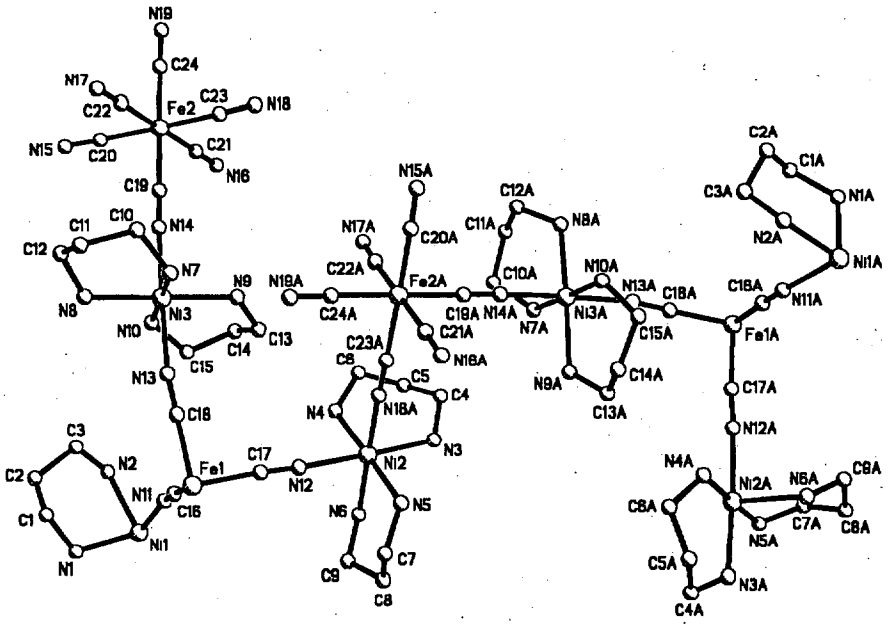

Figure 1S. The coordination environment surrounding of Fe2, Ni2 with the atom-numbering scheme.