Supporting Information

Hydrazide based novel selective and sensitive optical chemosensor for the detection of Ni^{2+}: Applications in living cell imaging, molecular logic gate and smart phone

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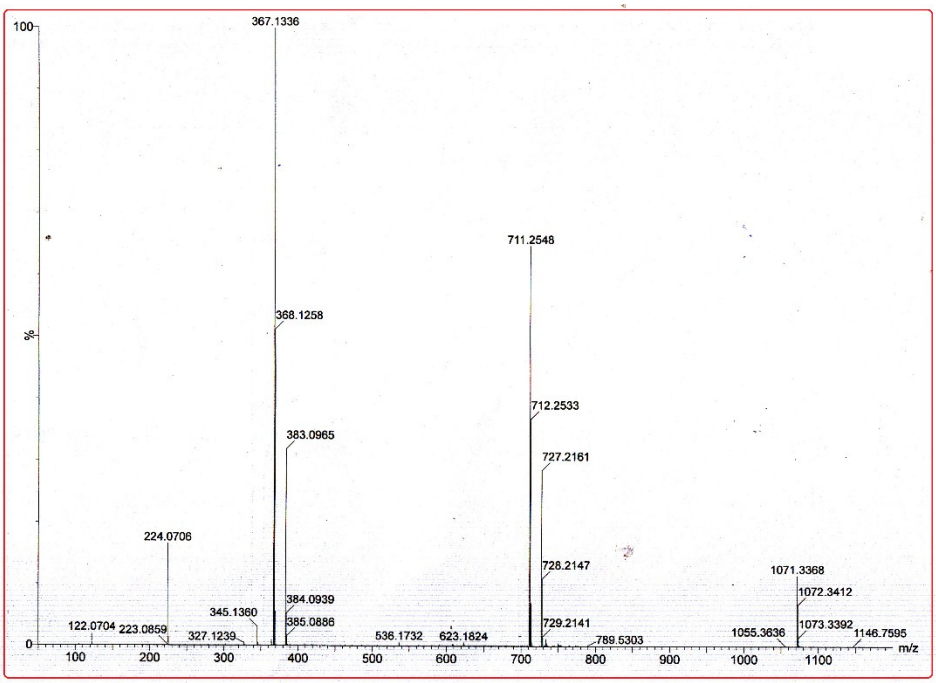

Fig. S1 ESI-mass spectra of **L**.

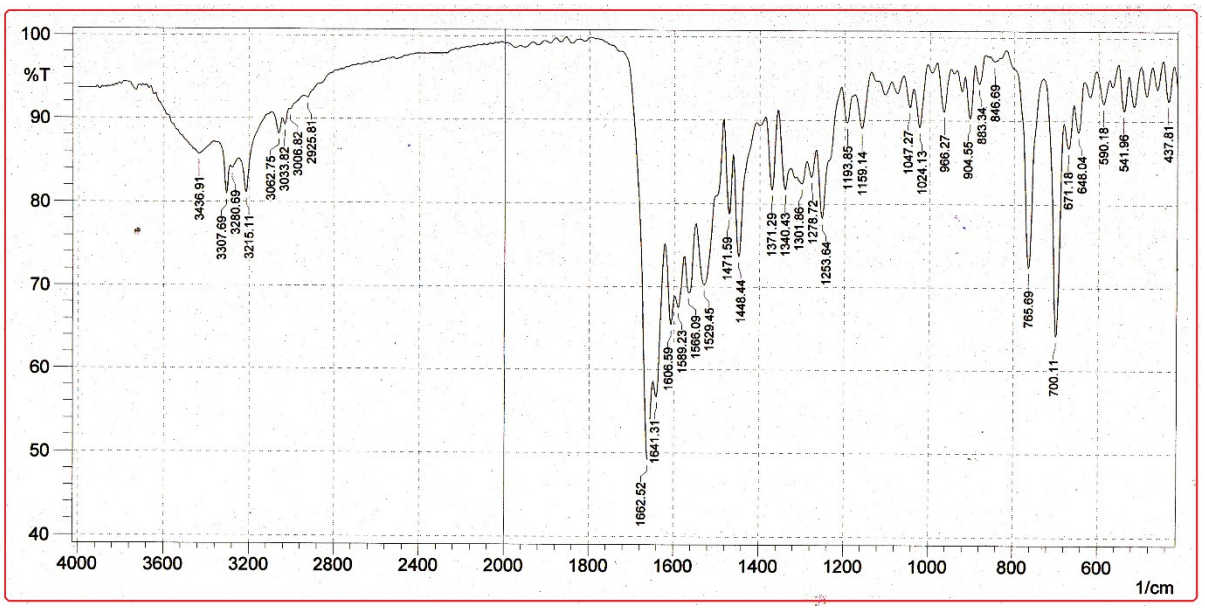

Fig. S2 FTIR spectra of **L.**

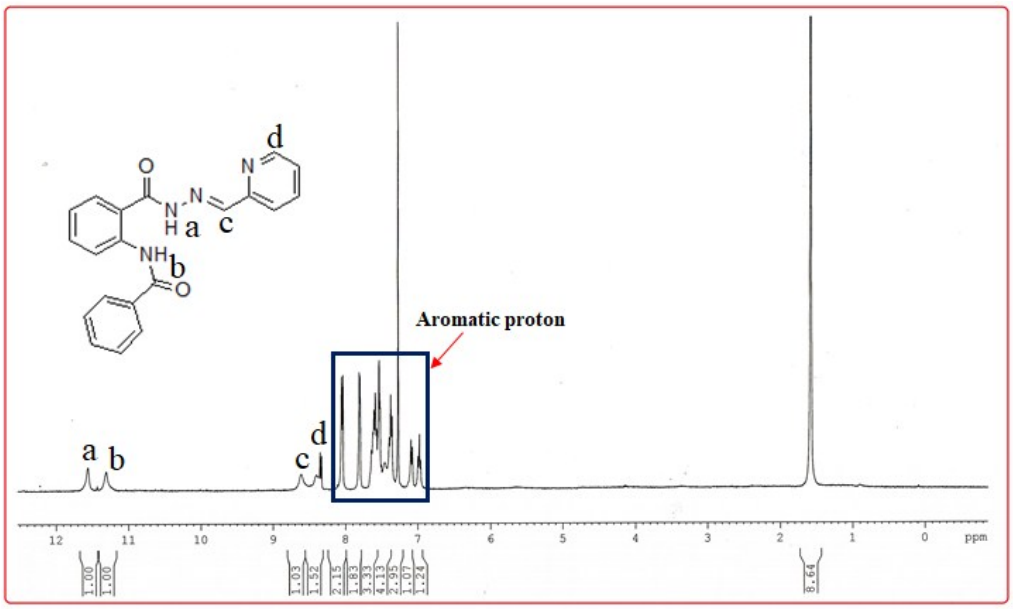

Fig. S3 ^{1}H NMR spectra of **L.**

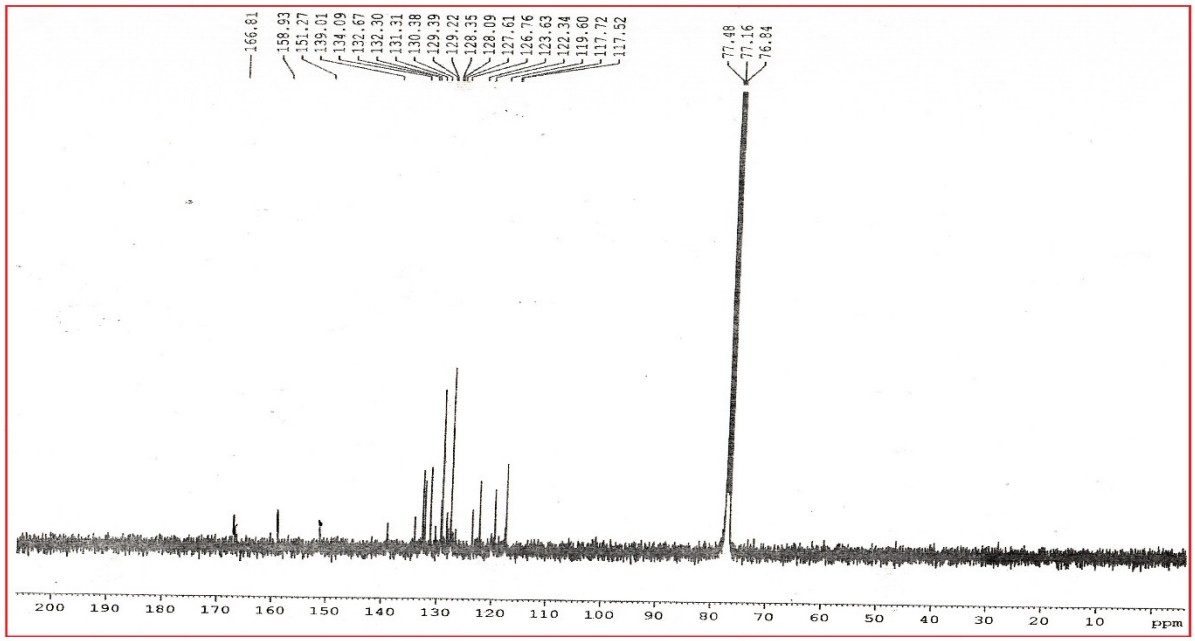

Fig. S4 ^{13}C NMR spectra of **L.**

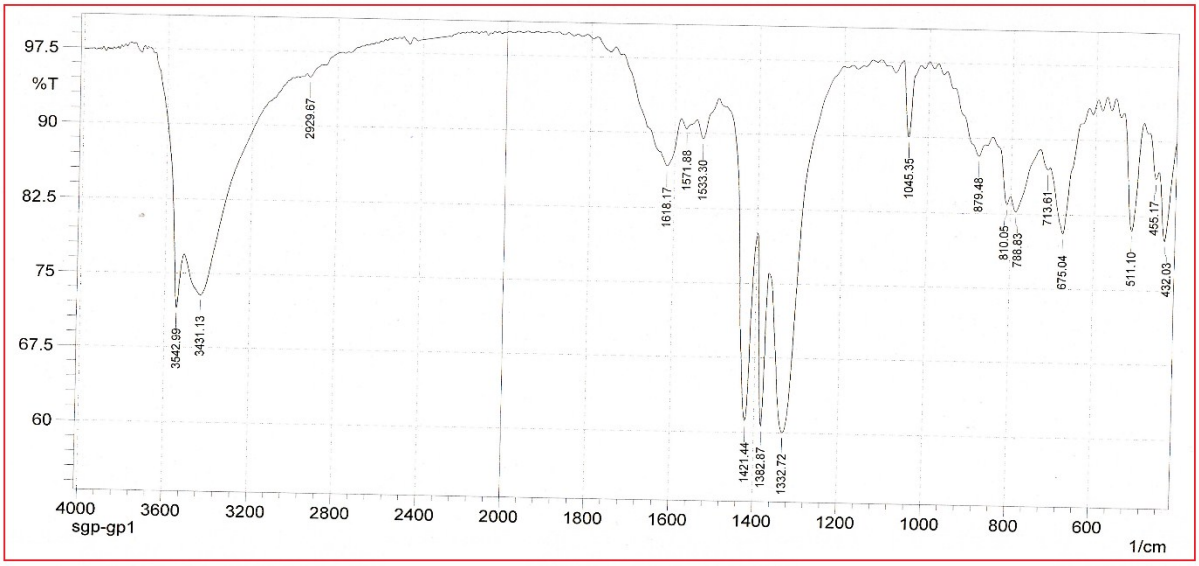

Fig. S5 IR spectra of **L.**

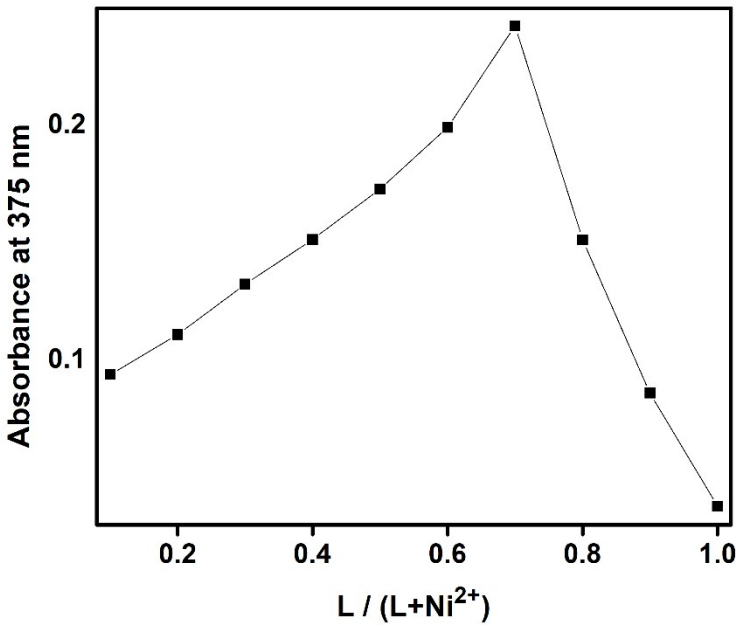

Fig. S6 Job's plot.

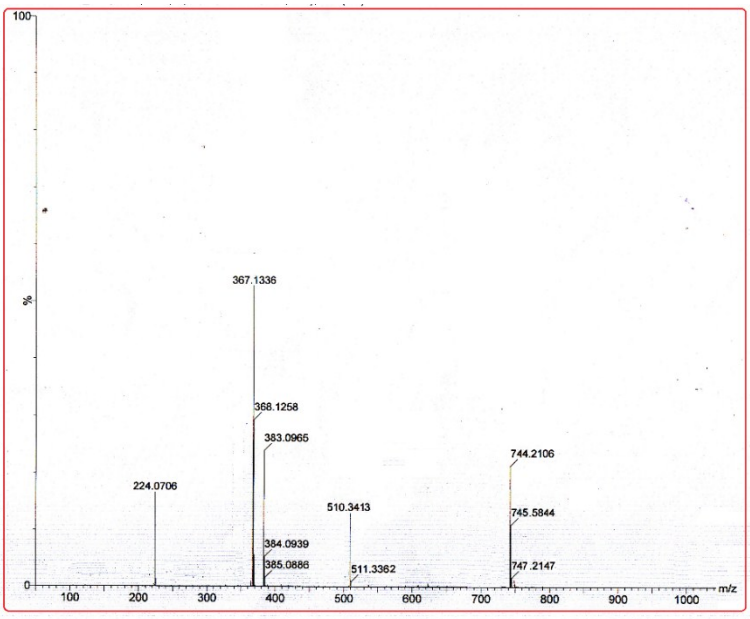

Fig. S7 ESI-mass spectra of **L**-Ni^{2+}.

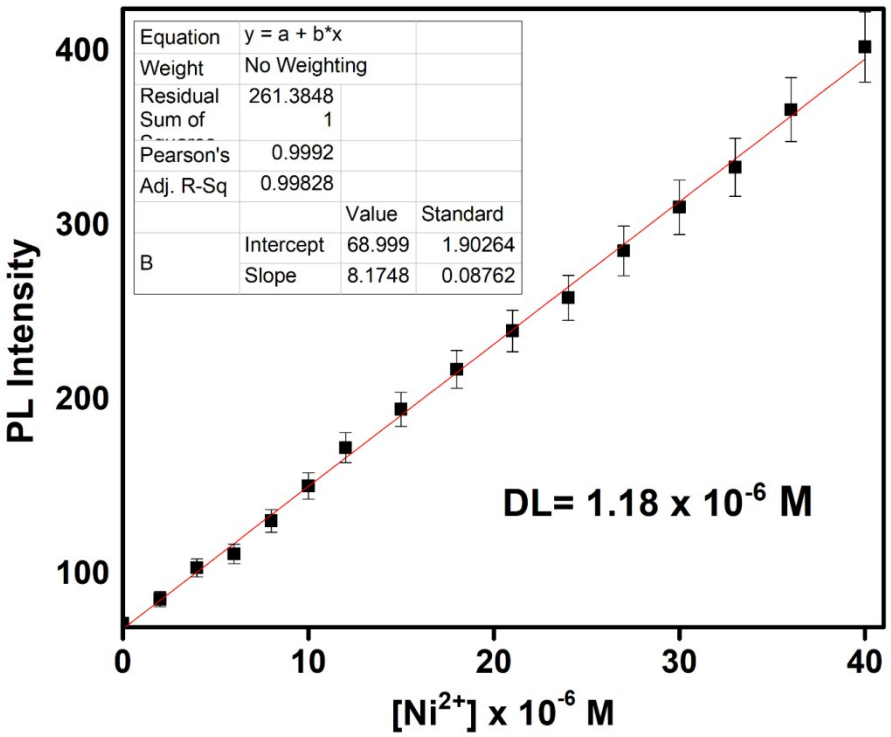

Fig. S8 Fluorometric Detection limit of **L** in presence of Ni^{2+}.

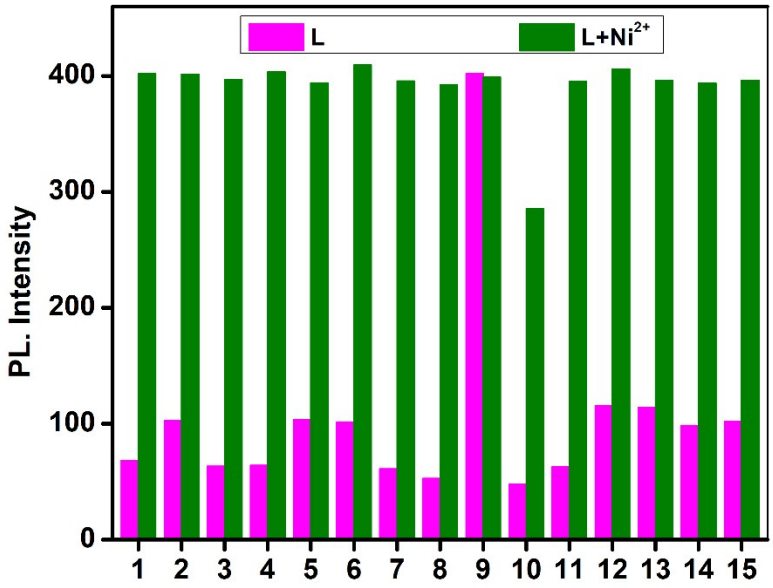

Fig. S9 Competitive experiment in presence of **L** and other metal ions (where 1 = **L**, 2 = Co^{2+}, 3 = Ag^{+}, 4 =Fe^{3+}, 5 = Cd^{2+}, 6 = Al^{3+}, 7 = Hg^{2+}, 8 = Fe^{2+}, 9 = Ni^{2+}, 10 = Cu^{2+}, 11 = Cr^{3+}, 12 = Mn^{2+} 13 = Zn^{2+} 14 = Pd^{2+} and 15 = Pt^{2+}

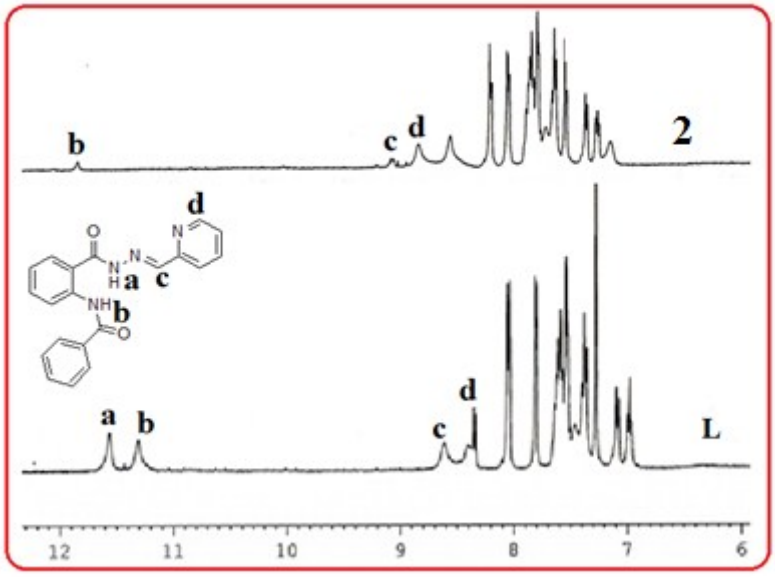

Fig. S10 Partial ^{1}H NMR Spectra of **L** and **2** in $CDCl_3$.

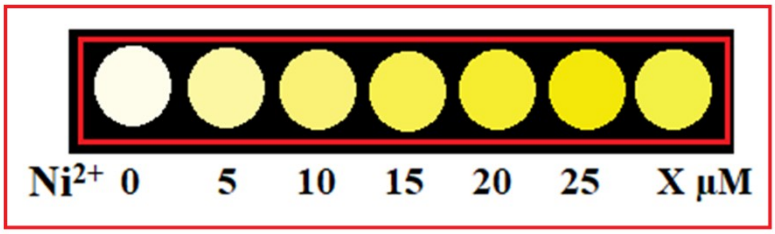

Fig. S11 Smartphone based image using RGB grabber.

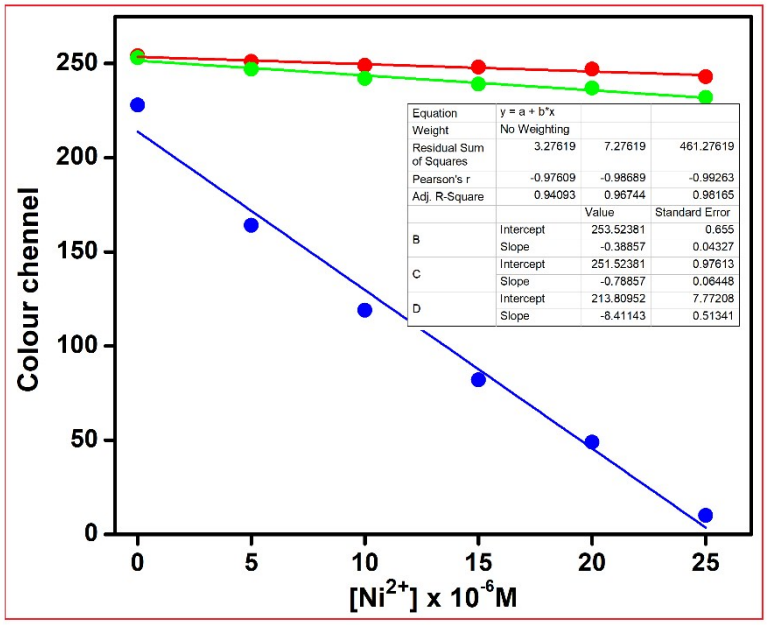

Fig. S12 Plot of red, green and blue colour channel level of signal images obtained from smartphone.

Table S1 Selected matric parameters for X-ray and geometry optimized structures of **L** and $NiL_2.H_2O$ (**2**.H_2O)

L	Experimental	Optimized	**$NiL_2.H_2O$ (2.H_2O)**	Experimental	Optimized
Bond length (Å)			Bond length (Å)		
N006-C00e	1.343(2)	1.3647	Ni1-O2	2.078(4)	2.0241
C00e-C009	1.462(3)	1.4705	Ni1-O5	2.086(3)	2.1008
C009-N004	1.273(2)	1.3023	Ni1-N3	1.958(4)	1.8987
N004-N003	1.373(2)	1.3806	Ni1-N9	1.965(3)	1.9448
N003-C007	1.353(2)	1.3837	Ni1-N4	2.084(4)	2.0212
C007-O002	1.219(2)	1.2442	Ni1-N10	2.106(3)	2.1641
C007-C00a	1.494(3)	1.4956	O2-C14	1.260(5)	1.2942
C00a-C00c	1.407(3)	1.4368	O5-C27	1.261(5)	1.2823
C00c-N005	1.401(2)	1.4074	N2-C14	1.335(6)	1.3625
N005-C00b	1.350(2)	1.3884	N5-C27	1.331(6)	1.3674
C00b-O001	1.232(2)	1.2619	N2-N3	1.371(6)	1.3697
C00b-C008	1.490(2)	1.5071	N5-N9	1.374(5)	1.3842
C008-C00g	1.386(3)	1.4157	N3-C15	1.276(6)	1.314
			N9-C26	1.255(5)	1.2947
			C15-C16	1.459(6)	1.4545
			C25-C26	1.452(6)	1.4618
			N4 -C16	1.351(6)	1.3681
			N5-C27	1.331(6)	1.3701
Bond angle (°)			Bond angle (°)		
N006-C00e-C009	114.50(16)	114.939	O2-Ni1-N3	75.77(13)	77.383
C00e-C009-N004	120.85(16)	120.809	O5-Ni1-N9	76.84(11)	75.557
C009-N004-N003	114.90(15)	117.583	N3-Ni1-N4	79.35(15)	82.657
N004-N003-C007	119.81(14)	120.273	N9-Ni1-N10	78.15(14)	74.573
N003-C007-O002	122.52(17)	121.108	N4-C16-C15	114.9(4)	113.903
N003-C007-C00a	114.58(15)	115.712	N10-C25-C26	114.3(3)	118.728
C007-C00a-C00c	120.40(15)	120.568	C16-C15-N3	115.7(4)	113.572
C00a-C00c-N005	118.70(15)	118.685	C25-C26-N9	116.4(4)	120.375
C00c-N005-C00b	128.49(15)	128.601	C15-N3-N2	121.0(4)	123.952
N005-C00b-O001	122.89(16)	123.346	C26-N9-N5	122.5(3)	118.989
O001-C00b -C008	121.31(14)	120.985	N3-N2-C14	108.3(4)	108.398
			N9-N5-C27	109.1(4)	114.392
			N2-C14-O2	123.9(4)	120.563
			N5-C27-O5	125.1(4)	123.428