

# Powder diffraction study of some mixed ligand complexes of Mn(II), Ni(II), Cu(II), Zn(II), and Cd(II)

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The mixed ligand complexes of manganese(II), nickel(II), copper(II), zinc(II), and cadmium(II) involving aspartic acid and benzoic acid have been synthesized. The complexes were studied by various spectroscopic techniques such as infrared, electronic, X-ray diffraction, and magnetic measurements. The complexes were found to have octahedral geometry. The X-ray powder diffraction results show that the crystal systems of Mn(II)-Asp-Ben complex are hexagonal, and Ni(II)-Asp-Ben, Cu(II)-Asp-Ben, Zn(II)-Asp-Ben, and Cd(II)-Asp-Ben complexes are found to be triclinic. The value of unit-cell parameters and XRD data for the five mixed ligand complexes are reported. © 2011 International Centre for Diffraction Data. [DOI: 10.1154/1.3543995]

Key words: aspartic acid, benzoic acid, mixed ligand complexes

## I. INTRODUCTION

Benzoic acid has its biological importance (Buhler *et al.*, 2009). Benzoic acid or its sodium, potassium, or calcium salt is intentionally added to certain food as food preservative or may naturally be present in specific foods. Sodium benzoate is used as one of the main antimicrobial preservatives in foods and beverages.

Benzoic acid is used as an antiseptic, antimycotic, and antipyretic. Estimation of intake of benzoic acid in Belgium adult population was investigated by Vandevijvere *et al.* (2009). The effects of toxic and nontoxic metals on the aromatic system of benzoic acid have been studied by Raman, infrared spectra, and ultraviolet spectroscopic techniques (Lewandowski, 1988). Hofmann-type complexes  $M(\text{Ben})_2\text{Ni}(\text{CN})_4$  were studied using benzoic acid, where  $M$  is Ni, Cd, Co, and Mn (Kartal and Senturk, 2005). The amino acid aspartic acid is well known for its biological values. The complexes of some amino acids with vanadium(III) were reported (Bukietyńska *et al.*, 2003). Metal complexes of aspartic acid were studied by various methods (Yasui and Ama, 1975; Ishizuka *et al.*, 1973; Battaglia *et al.*, 1982; Wojciechowska *et al.*, 1987).

In biological systems there is a possibility of the formation of mixed ligand complexes by the interaction of protein and food intake with the metal ions present. The present paper deals with the synthesis, spectroscopic, and powder X-ray diffraction studies of mixed ligand complexes of Mn(II), Ni(II), Cu(II), Zn(II), and Cd(II) with benzoic acid (Ben) and aspartic acid (Asp).

## II. EXPERIMENTAL

All the chemicals and reagents used were of analytical grade. Asp was obtained from E. Merck, while Ben and metal sulphates were from Fluka.

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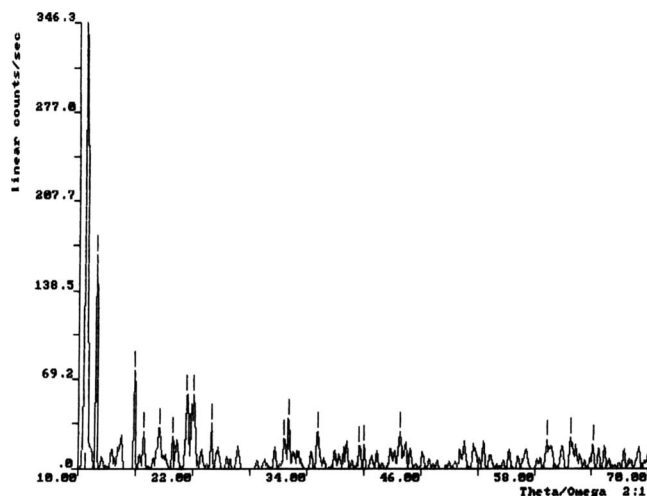


Figure 1. X-ray diffraction pattern of Mn(II)-Asp-Ben complex.

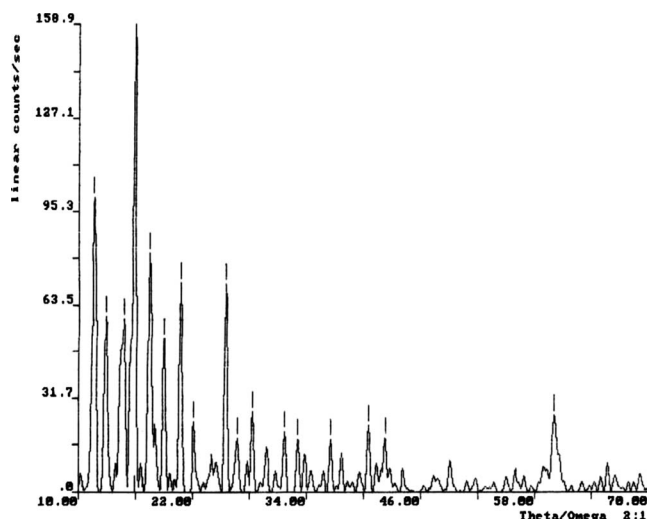


Figure 2. X-ray diffraction pattern of Ni(II)-Asp-Ben complex.

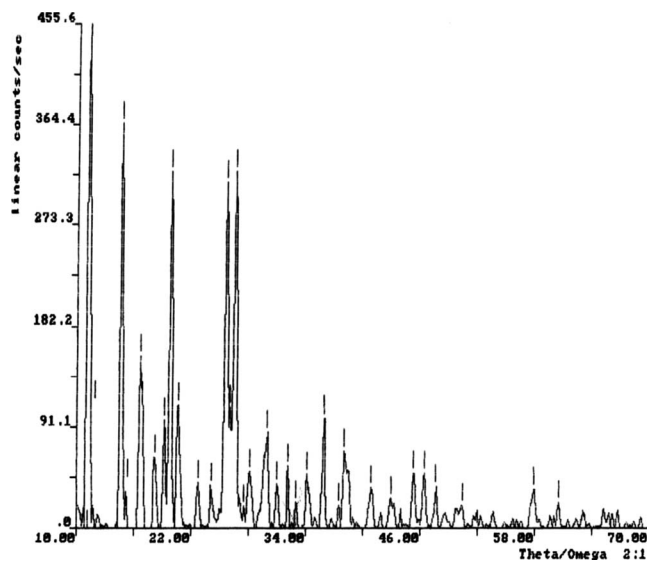


Figure 3. X-ray diffraction pattern of Cu(II)-Asp-Ben complex.

To synthesize the various mixed ligand complexes, aqueous solution of metal(II) sulphate was added to an aqueous solution of Asp in 1:1 molar ratio in hot condition. Further an equimolar amount of methanolic solution of Ben was added to it. The *pH* values of the resultant mixtures were raised to between 6.0 and 7.5 by adding sodium hydroxide solution depending on the metal ion. The *pH* for Mn(II) was 7.2, for Ni(II) 7.5, for Cu(II) 6.05, for Zn(II) 7.2, and Cd(II) 6.8. Each of the resultant solution was heated until it boils and concentrated to half of its initial volume; precipitates of the complexes appeared which were filtered off and washed with hot water several times and with acetone. The precipitates were dried in an oven  $\sim 50^\circ\text{C}$ .

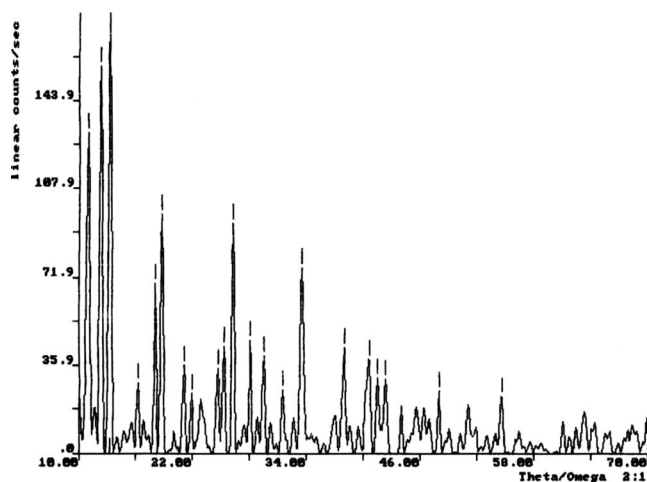


Figure 4. X-ray diffraction pattern of Zn(II)-Asp-Ben complex.

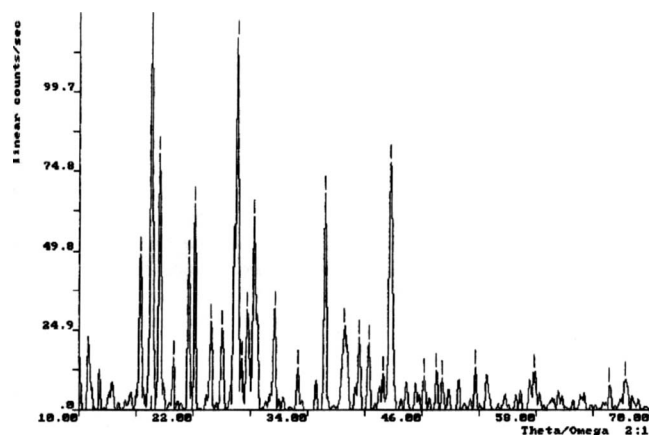


Figure 5. X-ray diffraction pattern of Cd(II)-Asp-Ben complex.

TABLE I. X-ray diffraction data of Mn(II)-Asp-Ben  $[\text{Mn}_2(\text{C}_4\text{H}_5\text{NO}_4) \times (\text{C}_7\text{H}_5\text{O}_2)(\text{OH})(\text{H}_2\text{O})_4]$  complex.

Line	$2\theta_{\text{obs}}$	$2\theta_{\text{calc}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	<i>I</i>	$\Delta 2\theta$	<i>h</i>	<i>k</i>	<i>l</i>
1	10.840	10.511	8.1551	8.409 42	100	-0.329	1	1	2
				8.409 03		-0.328	1	2	0
		10.512		8.409 03		-0.328	2	1	0
2	11.908	11.923	7.4260	7.416 67	48	0.015	0	0	3
		11.924		7.416 06		0.016	3	-3	0
3	15.916	15.920	5.5639	5.562 50	22	0.004	0	0	4
		15.920		5.562 30		0.004	1	2	3
4	16.896	16.893	5.2433	5.244 16	8	-0.003	3	-3	3
		16.893		5.244 16		-0.003	3	0	3
		16.893		5.244 16		-0.003	0	3	3
5	18.547	18.691	4.7801	4.743 49	9	0.144	1	-4	3
		18.691		4.743 49		0.144	3	1	3
		18.691		4.743 49		0.144	1	3	3
6	19.913	19.936	4.4552	4.450 00	7	0.023	0	0	5
		19.937		4.449 87		0.024	0	3	4
7	21.455	21.490	4.1383	4.131 67	17	0.035	0	2	5
		21.490		4.131 67		0.035	2	0	5
		21.490		4.131 57		0.035	1	3	4
8	22.206	22.229	4.0000	3.995 93	16	0.023	3	3	2
		22.229		3.995 93		0.023	1	5	0
9	24.004	23.978	3.7043	3.708 33	10	-0.026	0	0	6
		23.979		3.708 11		-0.025	3	3	3
10	31.640	31.639	2.8256	2.825 70	7	-0.001	1	-4	7
		31.639		2.825 70		-0.001	1	3	7
		31.639		2.825 70		-0.001	1	3	7
11	32.141	32.159	2.7827	2.781 15	11	0.018	2	4	6
		32.160		2.781 11		0.019	2	5	5
		32.160		2.781 11		0.019	2	5	5
12	35.163	35.136	2.5501	2.552 07	8	-0.027	2	7	3
		35.136		2.552 04		-0.027	6	4	0
13	39.553	39.443	2.2766	2.282 74	5	-0.110	1	5	8
		39.445		2.282 62		-0.108	1	9	2
14	40.094	40.087	2.2471	2.247 50	57	-0.007	0	7	7
		40.089		2.247 41		-0.005	8	3	1
		40.089		2.247 41		-0.005	8	3	1
15	43.799	43.786	2.0653	2.065 84	8	-0.013	0	4	10
		43.789		2.065 73		-0.010	1	9	5
16	59.300	59.430	1.5571	1.554 00	6	0.130	0	3	14
		59.430		1.554 00		0.130	3	0	14
		59.431		1.554 00		0.131	0	6	13
17	61.799	61.798	1.5000	1.500 02	7	-0.001	3	10	9
		61.800		1.499 98		0.001	1	14	3
18	64.241	62.262	1.4904	1.489 96	5	0.021	3	3	14
		64.266	1.4487	1.448 25	5	0.025	1	14	5

TABLE II. X-ray diffraction data of Ni(II)-Asp-Ben  $[\text{Ni}_2(\text{C}_4\text{H}_5\text{NO}_4) \times (\text{C}_7\text{H}_5\text{O}_2)(\text{OH})(\text{H}_2\text{O})_4]$  complex.

Line	$2\theta_{\text{obs}}$	$2\theta_{\text{calc}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I$	$\Delta 2\theta$	$h$	$k$	$l$
1	11.657	11.665	7.5853	7.580 18	58	0.008	2	0	0
2	12.930	12.928	6.8413	6.842 35	35	-0.002	0	2	0
		12.938		12.938		0.008	1	0	-2
3	14.813	14.747	5.9755	6.002 29	35	-0.066	0	2	1
		14.747		6.002 17		-0.066	0	-2	1
4	15.930	15.928	5.5590	5.559 86	93	-0.002	2	0	1
		15.933		5.558 05		0.003	3	-1	0
5	17.517	17.513	5.0588	5.060 04	48	-0.004	-2	3	1
		17.523		5.056 97		0.006	-3	0	2
6	19.050	19.142	4.6550	4.632 81	30	0.092	-2	1	3
7	20.797	20.802	4.2677	4.266 63	42	0.005	2	2	0
8	22.183	22.185	4.0041	4.003 82	14	0.002	-1	2	3
9	25.526	25.507	3.4868	3.489 39	42	-0.019	4	-2	1
		25.530		3.486 21		0.004	4	-1	1
10	26.782	26.779	3.3261	3.326 43	11	-0.003	4	-4	0
		26.782		3.326 05		0.000	3	0	2
11	28.385	28.470	3.1418	3.132 58	16	0.085	-3	3	4
12	31.706	31.712	2.8198	2.819 37	12	0.006	-6	4	1
		31.692		2.821 08		-0.014	5	0	-4
13	33.143	33.142	2.7008	2.700 85	11	-0.001	1	-2	4
14	36.610	36.603	2.4526	2.453 06	100	-0.007	4	3	0
15	40.596	40.597	2.2205	2.220 47	13	0.001	1	5	-3
		40.597		2.220 47		0.001	-1	-5	3
16	48.334	42.324	2.1333	2.133 74	11	-0.010	3	3	3
		42.333		2.133 31		-0.001	4	4	0
17	60.090	60.095	1.5385	1.538 38	15	0.005	0	6	6
		60.075		1.538 86		-0.015	5	6	0

All the complexes were analyzed for metal, sulphate, carbon, hydrogen, and nitrogen by standard methods.

Infrared spectra in nujol mulls were recorded on a Hitachi 270-50 IR spectrophotometer in the range from 4000 to 250  $\text{cm}^{-1}$ , and electronic spectra in the solid state were recorded with a Hitachi 330 spectrophotometer in the range from 200 to 2500 nm. The magnetic moment measurements were carried out by the Gouy method using  $\text{Hg}[\text{Co}(\text{SCN})_4]$  as a calibrant. X-ray diffraction patterns were taken with a Seifert-Rich ID 3000 X-ray diffractometer operated at 40 kV and 30 mA. Cu  $K\alpha$  X-rays ( $\lambda = 1.540\ 598\ \text{\AA}$ ) with a Ni filter were used. Ito's method was used for automatic indexing of the observed diffraction patterns (Azaroff and Buerger, 1958).

### III. RESULTS AND DISCUSSION

The analytical data of the complexes show that the mixed ligand complexes are of the composition  $M_2(\text{C}_4\text{H}_5\text{NO}_4)(\text{C}_7\text{H}_5\text{O}_2)(\text{OH})(\text{H}_2\text{O})_4$ . All the synthesized

TABLE III. X-ray diffraction data of Cu(II)-Asp-Ben  $[\text{Cu}_2(\text{C}_4\text{H}_5\text{NO}_4) \times (\text{C}_7\text{H}_5\text{O}_2)(\text{OH})(\text{H}_2\text{O})_4]$  complex.

Line	$2\theta_{\text{obs}}$	$2\theta_{\text{calc}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I$	$\Delta 2\theta$	$h$	$k$	$l$
1	11.184	11.250	7.9051	7.859 08	100	0.066	1	0	0
2	11.974	11.992	7.3852	7.373 96	25	0.018	0	1	0
3	14.691	14.757	6.0249	5.998 10	80	0.066	0	0	1
4	15.407	15.640	5.7465	5.661 59	9	0.233	4	-3	0
5	16.714	16.643	5.3000	5.322 36	34	-0.071	0	1	-1
		16.643		5.322 36		-0.071	0	-1	1
6	18.245	18.104	4.8585	4.895 92	14	-0.141	-2	2	1
7	19.226	19.144	4.6128	4.632 40	21	-0.082	3	-4	0
8	19.815	19.747	4.4770	4.492 35	71	-0.068	2	-1	1
		19.753		4.490 79		-0.062	-3	2	1
9	20.654	20.639	4.2970	4.300 03	24	-0.015	-3	3	1
10	22.778	22.786	3.9009	3.899 51	9	0.008	3	-1	0
11	24.112	24.119	3.6880	3.686 98	8	0.007	0	2	0
12	25.606	25.701	3.4761	3.463 43	68	0.095	1	-3	0
		25.709		3.462 43		0.103	5	-6	0
13	26.054	26.116	3.4173	3.409 35	24	0.062	1	-3	1
14	26.612	26.664	3.3469	3.340 50	70	0.052	-5	5	1
15	27.522	27.522	3.2383	3.238 28	4	0.000	-3	4	1
16	28.163	28.397	3.1660	3.140 42	11	0.234	-5	3	1
17	29.977	29.985	2.9784	2.977 69	19	0.008	-6	6	1
18	31.035	31.011	2.8793	2.881 42	9	-0.024	-2	1	2
19	32.177	32.025	2.7796	2.792 49	12	-0.152	9	-8	0
20	33.032	33.043	2.7096	2.708 74	5	0.011	-1	3	1
21	34.195	34.200	2.6201	2.619 69	11	0.005	3	0	0
		34.216		2.618 51		0.021	2	0	-2
22	35.450	35.462	2.5301	2.529 33	22	0.012	6	-7	2
23	37.508	37.515	2.3959	2.395 51	4	0.007	10	-10	1
24	38.097	38.076	2.3602	2.361 49	15	-0.021	1	-4	0
25	40.931	40.932	2.2031	2.203 05	8	0.001	2	0	2
26	42.954	42.959	2.1039	2.103 67	6	0.005	0	3	1
27	45.341	45.321	1.9985	1.999 37	11	-0.020	0	0	3
28	46.474	46.484	1.9524	1.952 01	11	0.010	3	1	0
29	47.623	47.637	1.9080	1.907 44	8	0.014	11	-8	1
30	50.430	50.449	1.8082	1.807 52	4	0.019	10	-12	1
31	57.953	57.965	1.5900	1.589 75	8	0.012	15	-14	2
32	60.567	60.590	1.5275	1.527 00	5	0.023	-13	11	2

complexes are coloured except those of Zn(II) and Cd (II) which are white. The complexes were insoluble in water and common organic solvents. The complexes did not melt up to 300 °C.

In the mixed ligand complexes Asp behaves as a bidentate ligand. Asp forms bonds with the  $\alpha$ -carboxylate and  $\beta$ -carboxylate O atoms. The presence of multiple bands in the mixed ligand complexes in the region of asymmetric and symmetric modes of the carboxylate groups (Battaglia *et al.*, 1980) shows that both the carboxylate groups of Asp are coordinated to the metal ions. The benzoate ion behaves as a bidentate ligand in the mixed ligand complexes.

TABLE IV. X-ray diffraction data of Zn(II)-Asp-Ben  $[\text{Zn}_2(\text{C}_4\text{H}_5\text{NO}_4)(\text{C}_7\text{H}_5\text{O}_2)(\text{OH})(\text{H}_2\text{O})_4]$  complex.

Line	$2\theta_{\text{obs}}$	$2\theta_{\text{calc}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I$	$\Delta 2\theta$	$h$	$k$	$l$
1	10.981	10.978	8.0507	8.052 98	73	-0.003	0	1	0
2	12.369	12.367	7.1503	7.151 50	88	-0.002	1	0	-1
		12.367		7.151 50		-0.002	-1	0	1
3	13.282	13.178	6.6607	6.713 20	100	-0.104	1	1	0
4	16.292	16.193	5.4363	5.469 23	16	-0.099	2	0	-1
		16.193		5.469 23		-0.099	-2	0	1
5	18.081	18.273	4.9022	4.851 17	39	0.192	2	1	0
6	18.783	18.848	4.7206	4.704 53	54	0.065	1	1	-2
		18.848		4.704 53		0.065	-1	-1	2
7	21.099	21.105	4.2073	4.206 17	20	0.006	0	2	-2
		21.105		4.206 17		0.006	0	-2	2
8	21.902	21.906	4.0549	4.054 11	13	0.004	3	0	-1
		21.906		4.054 11		0.004	-3	0	1
		21.917		4.052 14		0.015	3	0	0
9	24.684	24.657	3.6038	3.607 66	19	-0.027	0	0	2
10	25.300	25.414	3.5174	3.501 96	24	0.114	3	2	-1
		25.414		3.501 96		0.114	-3	-2	1
11	26.292	26.197	3.3869	3.398 98	52	-0.095	1	3	-2
		26.197		3.398 98		-0.095	-1	-3	2
12	28.098	28.107	3.1732	3.172 16	26	0.009	3	0	1
13	29.474	29.504	3.0281	3.025 14	22	0.030	2	-2	2
		29.560		3.019 52		0.086	1	-3	1
14	31.502	31.438	2.8377	2.843 26	14	-0.064	4	1	0
15	33.494	33.352	2.6733	2.684 33	42	-0.142	0	3	0
16	38.002	38.052	2.3659	2.362 92	24	0.050	4	3	-1
		38.052		2.362 92		0.050	-4	-3	1
		38.060		2.362 43		0.058	1	-4	2
17	40.639	40.728	2.2183	2.213 63	22	0.089	4	0	-3
		40.728		2.213 63		0.089	-4	0	3
18	41.500	41.434	2.1742	2.177 52	17	-0.066	4	-1	2
19	42.405	42.411	2.1299	2.129 57	17	0.006	0	2	2
20	48.013	47.979	1.8934	1.894 64	14	-0.034	2	-3	4
21	54.635	54.642	1.6785	1.678 30	13	0.007	4	4	0

A sharp band about  $3600\text{ cm}^{-1}$  in the complexes suggests  $\nu\text{OH}$  stretching band, and the band appearing at  $950\text{ cm}^{-1}$  indicates a bridging OH bonding in the complexes. This suggests the polymeric structure of the complexes, which is also reflected from the insolubility of various complexes.

In all the synthesized complexes a broad band appears in the region between  $3500$  to  $3200\text{ cm}^{-1}$ , showing the presence of aquo group in the complexes.  $\nu\text{M-O}$  aquo bands at about  $440\text{ cm}^{-1}$  in the complexes confirm the coordination of water molecule. The assignments (Nakamoto, 1970) of  $\nu\text{M-O}$  around  $280\text{ cm}^{-1}$  (Goodgame and Johns, 1978) favours the coordination number six for the metal ions.

The magnetic moment value for Mn(II) complex is in the range of 5.2 to 6.0 B. M., indicating that the Mn(II) complex is typically high spin complex and having octahedral structure. The Ni(II) complex exhibits the magnetic moment value in the range of 2.8 to 3.2 B. M., indicating octa-

hedral coordination of the ligands around Ni(II) ion. The Cu(II) complex shows magnetic moment in the range of 1.61 to 1.85 B. M., suggesting distorted octahedral nature for the complex. The UV-visible spectra also show octahedral geometry for the complexes.

X-ray powder diffraction patterns for the mixed ligand complexes of Mn(II), Ni(II), Cu(II), Zn(II), and Cd(II) involving Asp and Ben are plotted in Figures 1–5. The observed and calculated values of  $2\theta$ ,  $d$ ,  $I$ , and  $\Delta 2\theta$  of the diffraction peaks and their ( $hkl$ ) Miller indices determined by Ito's method are listed in Tables I–V. The unit-cell parameters were also obtained from the automatic indexing results for the mixed ligand complexes. The crystal systems of Mn(II)-Asp-Ben complex is hexagonal, while Ni(II)-Asp-Ben, Cu(II)-Asp-Ben, Zn(II)-Asp-Ben, and Cd(II)-Asp-Ben complexes are triclinic. The values of unit-cell parameters for the five mixed ligand complexes are listed in Table VI.

TABLE V. X-ray diffraction data of Cd(II)-Asp-Ben  $[\text{Cd}_2(\text{C}_4\text{H}_5\text{NO}_4)(\text{C}_7\text{H}_5\text{O}_2)(\text{OH})(\text{H}_2\text{O})_4]$  complex.

Line	$2\theta_{\text{obs}}$	$2\theta_{\text{calc}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I$	$\Delta 2\theta$	$h$	$k$	$l$
1	16.465	16.443	5.3795	5.386 79	39	-0.022	0	2	0
2	17.598	17.588	5.0357	5.038 43	100	-0.010	2	0	-2
		17.588		5.038 43		-0.010	-2	0	2
3	18.519	18.535	4.7873	4.783 19	64	0.016	2	0	1
4	19.895	19.905	4.4592	4.457 01	13	0.010	3	0	0
5	21.489	21.697	4.1318	4.092 71	38	0.208	3	1	-1
		21.697		4.092 71		0.208	-3	-1	1
6	22.177	22.101	4.0052	4.018 84	52	-0.076	-3	2	1
		22.299		3.983 64		0.122	-3	1	2
7	23.828	23.781	3.7313	3.738 49	22	-0.047	2	-3	0
8	25.035	25.040	3.5541	3.553 34	21	0.005	4	-1	0
		25.046		3.552 54		0.011	0	1	-3
9	26.633	26.646	3.3443	3.342 75	94	0.013	4	0	0
		26.652		3.342 01		0.019	0	0	3
10	27.068	27.041	3.2916	3.294 77	13	-0.027	-1	3	1
		27.101		3.287 69		0.033	3	1	-3
11	27.638	27.658	3.2250	3.222 62	26	0.020	2	-3	2
12	28.404	28.481	3.1397	3.131 44	49	0.077	-3	1	3
13	30.551	30.556	2.9238	2.923 31	26	0.005	4	1	0
		30.562		2.922 75		0.011	0	1	3
14	32.993	33.006	2.7127	2.711 67	10	0.013	2	0	-4
		33.006		2.711 67		0.013	-2	0	4
15	35.803	35.800	2.5060	2.506 19	54	-0.003	4	-4	1
		35.821		2.504 80		0.018	3	-2	3
16	37.880	37.836	2.3732	2.375 92	21	-0.044	6	0	-1
		37.903		2.371 83		0.023	2	4	-3
		37.903		2.371 83		0.023	-2	-4	3
17	39.421	39.455	2.2839	2.282 06	18	0.034	4	3	-1
		39.455		2.282 06		0.034	-4	-3	1
18	40.463	40.444	2.2275	2.228 50	17	-0.019	6	0	0
		40.509		2.225 06		0.046	-2	2	4
19	41.915	41.893	2.1536	2.154 71	9	-0.022	0	5	0
		41.974		2.150 75		0.059	4	3	-4
20	42.763	42.738	2.1129	2.114 02	62	-0.025	4	3	0
		42.751		2.113 42		-0.012	6	0	-4
		42.751		2.113 42		-0.012	-6	0	4
21	46.301	46.299	1.9593	1.959 41	9	-0.002	0	4	-5
		46.299		1.959 41		-0.002	0	-4	5
		46.318		1.958 65		0.017	1	3	3
22	47.540	47.532	1.9111	1.911 41	10	-0.008	3	-6	2
23	48.198	48.200	1.8865	1.886 46	8	0.002	-1	3	4
24	51.601	51.596	1.7698	1.770 00	10	-0.005	2	5	-5
		51.596		1.770 00		-0.005	-2	-5	5
25	57.894	57.884	1.5915	1.591 79	10	-0.010	1	-7	0
26	65.772	65.796	1.4187	1.418 23	6	0.024	6	0	4
27	67.460	67.451	1.3872	1.387 39	8	-0.009	6	-8	1

TABLE VI. The unit-cell parameters for M(II)-Asp-Ben complexes.

Complex formula	$a$ (Å)	$b$ (Å)	$c$ (Å)	$\alpha$ (deg)	$\beta$ (deg)	$\gamma$ (deg)	$V$ (Å <sup>3</sup> )	Crystal system
$\text{C}_{11}\text{H}_{19}\text{Mn}_2\text{O}_{11}$	25.69	25.69	22.25	90	90	120	12 718.70	Hexagonal
$\text{C}_{11}\text{H}_{19}\text{Ni}_2\text{O}_{11}$	18.66	15.40	13.97	78.19	116.50	117.30	3192.31	Triclinic
$\text{C}_{11}\text{H}_{19}\text{Cu}_2\text{O}_{11}$	25.50	24.26	6.27	103.58	80.27	161.75	1162.47	Triclinic
$\text{C}_{11}\text{H}_{19}\text{Zn}_2\text{O}_{11}$	12.98	10.27	9.59	128.36	110.52	77.44	939.49	Triclinic
$\text{C}_{11}\text{H}_{19}\text{Cd}_2\text{O}_{11}$	11.81	14.91	11.18	107.49	104.02	104.02	1713.65	Triclinic

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