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Investigación

Infrared and Raman Spectra (Solid State) of Diamminediiodidecadmium (II) Complex with ^{15}N and ^{2}H Isotopic Subtitution

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In Memory to Prof. Dr. Jacobo Gómez Lara

Abstract. The Raman and infrared spectra of the $Cd(NH_3)_2I_2$ complex with ^{15}N and ^{2}H substitution have been obtained in the solid state. Based on a normal coordinate treatment as an eleven-body problem, the vibrational spectra were assigned. With exclusion of the ammine torsional vibration, the vibrational modes of the ligand, framework-coupling and skeletal frequencies have been determined. Valence force constants values f_{CdN} and f_{CdI} were compared with the analogous force constants of $Cd(NH_3)_2Cl_2$ and $Cd(NH_3)_2Br_2$. The results of the calculations are discussed in terms of the present assignment for $Cd(NH_3)_2I_2$ and previously reported potential constants for the $Cd(NH_3)_2X_2$ and $Zn(NH_3)_2X_2$ (X = Cl, Br, I).
Key Words: Infrared, Raman spectra. Diamminediiodidecadmium (II) isotopic complex. Force constants.

Resumen. Se obtuvieron en el estado sólido los espectros Raman e infrarrojo del complejo $Cd(NH_3)_2I_2$, con substitución isotópica ^{15}N y ^{2}H. El espectro vibracional se asignó con la ayuda del análisis de coordenadas normales considerando un problema de once núcleos. Con la exclusión de las vibraciones torsionales de los grupos $-NH_3$, se determinaron los modos vibracionales y los números de onda correspondientes a los ligantes, acoplamiento ligantes-esqueleto, y esqueleto estructural. Las constantes de fuerza de valencia f_{CdN} y f_{CdI} se compararon con constantes de fuerza análogas de los complejos $Cd(NH_3)_2Cl_2$ y $Cd(NH_3)_2Br_2$. Los resultados de los cálculos se discuten en términos de la presente asignación vibracional para $Cd(NH_3)_2I_2$, y en términos de las constantes de potencial reportadas previamente para los complejos $Cd(NH_3)_2X_2$ y $Zn(NH_3)_2X_2$ (X = Cl, Br, I).
Palabras clave: Infrarrojo, espectros Raman, complejo diamino diyoduro de cadmio (II), constantes de potencial.

Introduction

There are many scientific works concerning the infrared and Raman active vibration of coordinated amine groups [1,2], but there is not enough information about the low-frequencies framework or skeletal metal-ligand modes, specifically on the diammine complexes. As a continuation of our studies on the infrared and Raman spectra and structure of diamminedichloridezinc (II), diamminedibromidezinc (II), diamminediiodidezinc (II), diamminedichloridecadmium (II) and diamminedibromidecadmium (II) complexes with ^{15}N and ^{2}H isotopic substitution [3], we have investigated the infrared and Raman spectra (solid state) of normal diamminediiodidecadmium (II) and with ^{15}N and ^{2}H - labeled isotopomers from 70 to 4000 cm^{-1}.

Assignment of the ammine vibrational modes is straightforward and follows the conventional pattern [1,3]. The experimental vibrational attribution of skeletal metal-ligand modes, have been made using the ^{15}N and ^{2}H isotopic labeled complexes, assuming that the di-ammine cadmium complexes have a C_{2v} planar symmetry, and by comparison with the analogous infrared and Raman spectra of the $Cd(NH_3)_2Cl_2$ and $Cd(NH_3)_2Br_2$. The assignment of the vibrational spectra was confirmed by means of the normal coordinate analysis.

The obtained valence force constants were compared with the values of the $Zn(NH_3)_2X_2$ (X = Cl, Br, I) complexes. Bond orders were also obtained.

Results and Discussion

Vibrational irreducible representations: Information: the $Cd(NH_3)_2Cl_2$ complex, has a rhombic unit cell. The space group is $C_{2v}{}^{11}$ - C_{mm} with two formula weights per unit cell [5]. Assuming a C_{2v} symmetry for a geometrical structure of trans planar configuration of $Cd(NH_3)_2I_2$, the $3n - 6 = 27$ normal vibrations after discarding two torsional NH_3-Cd frequencies (a_2 and b_1) and two out of plane skeletal bending modes (a_1) can be distributed among the symmetry species:

$$\Gamma_{vib} = 7\ a_1(IR,R) + 4a_2(R) + 5b_1(IR,R) + 7b_2(IR,R)$$

The observed infrared absorption's bands and the Raman shifts with the approximate assignments are given in Table 1.

Ligand vibrations: The ν(NH) stretching, δ(HNH) bending and ρ(NH_3) rocking modes are considered as characteristic frequencies in amine complexes [1,2] and their assignments are straightforward.

Metal-nitrogen and metal-halogen stretching vibrations: According to the assumed C_{2v} symmetry for the trans geometry of the $Cd(NH_3)_2I_2$ complex, the metal-nitrogen and metal-halogen stretching vibrations should be infrared and Raman active. The $\nu_{as}(CdN)(b_2)$ modes were observed in the spectra at 367, 355 and 349 cm^{-1} for the normal $Cd(NH_3)_2I_2$ and for the ^{15}N and ^{2}H isotopomers, respectively. In the Raman spectra the $\nu_s(CdN)(a_1)$ vibrational modes were found at 320, 311 and 304 cm^{-1} for the normal and for the ^{15}N and ^{2}H isotopic complexes. The infrared bands found at 136, 130 and 122 cm^{-1} for the three isotopic complexes, were assigned to the $\nu_{as}(CdI)(b_1)$ vibrational modes. The Raman shifts at 133, 130 and 126 cm^{-1} in the normal compound and in the two isotopomers, were assigned to the $\nu_s(CdI)(a_1)$ stretching modes. Table 2 are listed the Cd-N and Cd-I stretching frequencies together with literature values.

X-Cd-X deformations: The Raman shifts at 115, 112 and at 110 cm^{-1} for $Cd(NH_3)_2I_2$, $Cd(^{15}NH_3)_2I_2$ and $Cd(ND_3)_2I_2$ isotopic complexes were assigned to the δ(NCdI)(a_2) vibrational mode. For the b_1 and b_2 δ(NCdI) vibrational modes, we assig

Table 1. Infrared and Raman spectra and assignments for $Cd(NH_3)_2I_2$ and ^{15}N, ^{2}H isotopic labeled isotopomers. (Observed wavenumbers in cm^{-1}).

Infrared spectrum			
$Cd(NH_3)_2I_2$	$Cd(15NH_3)_2I_2$	$Cd(ND_3)_2I_2$	Assignments
3329	3323	2434	ν_{as} (NH/ND)
		2356	ν_s (ND)
3239	3236	2384	ν_s (NH/ND)
3136			1602,0 × 2 = 3204
	3134		1595 × 2 = 3190
1602	1595	1124	δ_{as} (HNH/DND)
	1425		1595 – 130 = 1465
1431			1602 – 136 = 1466
	1425		1595 – 130 = 1465
1202	1195	925	δ_s (HNH/DND)
573	565	462	ρ (NH_3/ND_3)
367	355	349	ν_{as} (Cd-N)
147	144	141	ν_{as} (Cd-I)
136	130	122	ν_s (Cd-I)
90	82	81	δ (N-Cd-I)
74	74	71	δ (N-Cd-I)
Raman spectrum			
$Cd(NH_3)_2I_2$	$Cd(15NH_3)_2I_2$	$Cd(ND_3)_2I_2$	Assignments
3331	3319	2435	ν_{as} (NH/ND)
3239	3235	2357	ν_s (NH/ND)
		2384	ν_s (NH/ND)
3137			1596 × 2 = 3192
	3130		1529 × 2 = 3178
		2307	2393 – 74 = 2319
		1210	1124 + 95 = 1219
1596	1588	1117	δ_{as} (HNH/DND)
		1021	936 + 95 = 1031
		1021	936 + 82 = 1018
1198	1204	928	δ_s (HNH/DND)
566	563	433	ρ (NH_3/ND_3)
320	311	304	ν_s (Cd-N)
133	130	126	ν_s (Cd-I)
115	112	110	δ (NCdI)

Table 2. Vibrational spectra of the metal-ligand region for $Cd(NH_3)_2X_2$ (X = Cl, Br, I) complexes and for the ^{15}N and ^{2}H isotopic labeled isotopomer. (Observed wavenumbers in cm^{-1}).

Infrared	ν_{as} (CdN)	ν_{as} (CdX)	δ_s (NCdX)	δ_{as} (NCdX)	Liter
$Cd(NH_3)_2Cl_2$	380	192	123	117	15
	375	215	-	-	16
	374	-	-	-	17
	370	-	-	-	18
$Cd(^{15}NH_3)_2Cl_2$	365	188	124	117	19
$Cd(ND_3)_2Cl_2$	353	185	120	117	19
	350	-	-	-	18
$Cd(NH_3)_2Br_2$	371	150	97	90	3
	368	<200	-	-	16
	370	-	-	-	18
$Cd(^{15}NH_3)_2Br_2$	365	152	97	92	3
$Cd(ND_3)_2Br_2$	350	142	97	90	3
$Cd(NH_3)_2I_2$	367	<200	-	-	16
	370	-	-	-	18
	367	136	90	74	present work
$Cd(^{15}NH_3)_2I_2$	355	130	82	74	present work
$Cd(ND_3)_2I_2$	355	-	-	-	18
	349	122	81	71	present work
Raman	ν_s(CdN)	ν_s(CdX)	δ(NCdX)		
$Cd(NH_3)_2Cl_2$	351	162	112	15	
$Cd(15NH_3)_2Cl_2$	345	159	107	19	
$Cd(ND_3)_2Cl_2$	325	154	99	15	
$Cd(NH_3)_2Br_2$	334	152	99	3	
$Cd(15NH_3)_2Br_2$	331	153	112	19	
$Cd(ND_3)_2Br_2$	311	140	97	3	
$Cd(NH_3)_2I_2$	320	133	115	present work	
$Cd(15NH_3)_2I_2$	311	130	112	present work	
$Cd(ND_3)_2I_2$	304	126	110	present work	

ned tentatively the values of 90, 82 and 81 cm^{-1} for Cd $(NH_3)_2I_2$, and his isotopomers. The values of 74, 74 and 71 cm^{-1} were assigned tentatively for the b_2 δ(NCdI) vibrational modes. Table 2 shows also our approximate assignments together with another values of wavenumbers found for the $Cd(NH_3)_2X_2$ (X = Cl, Br) with ^{15}N and ^{2}H isotopic substitution. Fig. 1 illustrates the low region of the Raman spectra.

Normal coordinate analysis (NCA)

A normal coordinate analysis for the whole structure of diamminediiodidecadmium (II) was carried out to aid principally the assignment of the framework or skeletal frequencies. The molecular structure and the internal coordinates for Cd $(NH_3)_2I_2$ are shown in Fig. 2. Some of the geometrical parameters which describes the skeletal structure CdA_2I_2 (A = NH_3), were taken from the literature [5], other geometrical parameters were assumed: d_{Cd-N} = 2.10 Å; d_{Cd-I} = 2.90 Å; d_{N-H} = 1 Å; N-Cd-I angle = 90° and M-N-H angle = 109.47°.

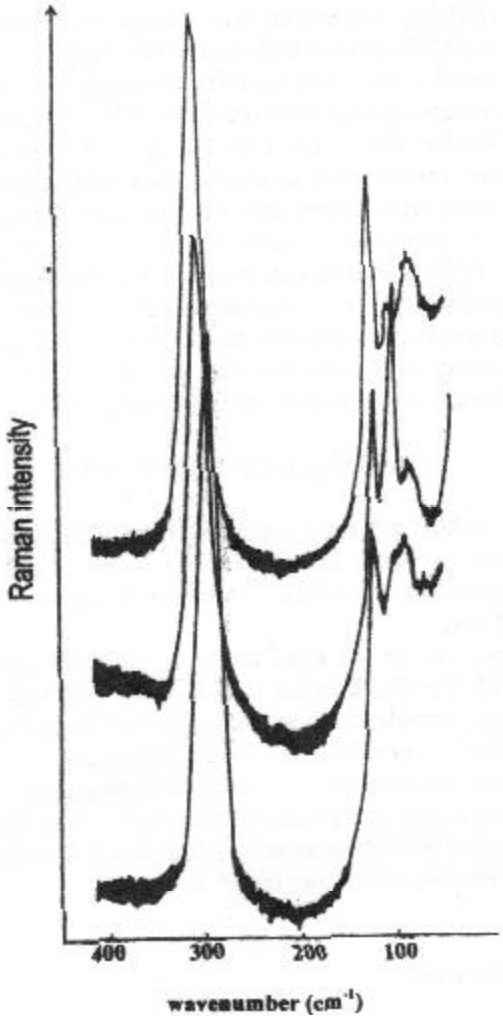

Fig.1. Raman spectra in the low-energy region for $Cd(NH_3)_2I_2$, $Cd(^{15}NH_3)_2I_2$ and $Cd(ND_3)_2I_2$.

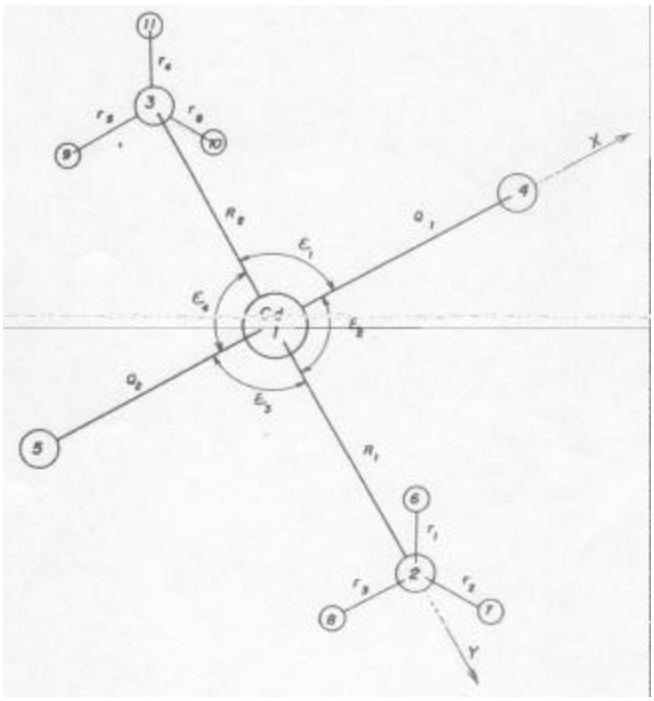

Fig. 2. Molecular structure and internal coordinates for $Cd(NH_3)_2I_2$.

For the $Cd(NH_3)_2I_2$ complexes, initial symmetry force constants values for the NH_3-ligands were transferred from the values given by Cyvin *et al*. [6], while the rocking force constants value was calculated from $F_{ii} = \lambda_{ii} / G_{ii}$, in which, G_{ii} means the ith element of the kinematics coefficient matrix (it is not the kinetic energy matrix), and $\lambda_{ii} = 0.589141\ (\omega_i / 1000)^2$. Using the point mass model (PMM) in conjunction with the isotopic shifts, the starting set of skeletal force constants was obtained. The initial set of force constants F_0 so obtained was refined by two methods to reproduce the experimental frequencies. In the least square method [7,8] a Modified General Valence Force Field (MGVFF) was used in which the off diagonal force constants pertaining to different blocks between i) NH_3-ligand and rocking vibration, ii) NH_3-ligand and framework vibrations as well as iii) framework and rocking vibrations were all constrained to zero. In the iterative autoconsistency method [8], the off diagonal force constants between the different blocks were not constrained to zero. Results also show, that there are no significant differences between the force constants obtained by the two methods. Table 3 shows the more significative set of valence force constants. The symmetry coordinates used in the calculations are given below:

a_1: $S_1 = 1/\sqrt{6}\Delta(r_1 + r_2 + r_3 + r_4 + r_5 + r_6)$,
$S_2 = 1/\sqrt{12}\Delta[(-\alpha_1 - \alpha_2 - \alpha_3 - \alpha_4 - \alpha_5 - \alpha_6) + (\beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5 + \beta_6)]$,
$S_3 = 1/\sqrt{12}\Delta[(2r_1 - r_2 - r_3) + (2r_4 - r_5 - r_6)]$,
$S_4 = 1/\sqrt{12}\Delta[(2\alpha_1 - \alpha_2 - \alpha_3) + (2\alpha_4 - \alpha_5 - \alpha_6)]$,
$S_5 = 1/\sqrt{12}\ \Delta[(2\beta_1 - \beta_2 - \beta_3) + (2\beta_4 - \beta_5 - \beta_6)]$, $S_6 = 1/\sqrt{2}\Delta(R_1 + R_2)$,
$S_7 = 1\sqrt{(2\Delta(Q_1 + Q_2)}$

a_2: $S_8 = 1/2\,\Delta(-r_2 + r_3 - r_5 + r_6)$, $S_9 = 1/2\Delta(-\alpha_2 + \alpha_3 - \alpha_5 + \alpha_6)$,
$S_{10} = 1/2\Delta(-\beta_2 + \beta_3 - \beta_5 + \beta_6)$, $S_{11} = 1/2\Delta(-\in_1 + \in_2 - \in_3 + \in_4)$
b_1: $S_{12} = 1/2\Delta(-r_2 + r_3 + r_5 - r_6)$, $S_{13} = 1/2\Delta(-\alpha_2 + \alpha_3 + \alpha_5 - \alpha_6)$,
$S_{14} = 1/2\Delta(-\beta_2 + \beta_3 + \beta_5 - \beta_6)$
$S_{15} = 1/\sqrt{2}\Delta(Q_1 - Q_2)$, $S_{16} = 1/2\Delta(\in_1 + \in_2 - \in_3 - \in_4)$
b_2: $S_{17} = 1/\sqrt{12}\Delta(2r_1 - r_2 - r_3 - 2r_4 + r_5 + r_6)$,
$S_{18} = 1/\sqrt{12}\Delta[(-\alpha_1 - \alpha_2 - \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6) +$
$(\beta_1 + \beta_2 + \beta_3 - \beta_4 - \beta_5 - \beta_6)]$
$S_{19} = 1/\sqrt{6}\Delta(r_1 + r_2 + r_3 - r_4 - r_5 - r_1)$,
$S_{20} = 1/\sqrt{12}\Delta(2\alpha_1 - \alpha_2 - \alpha_3 - 2\alpha_4 + \alpha_5 + \alpha_6)$
$S_{21} = 1/\sqrt{12}\Delta(2\beta_1 - \beta_2 - \beta_3 - 2\beta_4 + \beta_5 + \beta_6)$, $S_{22} = 1/\sqrt{2}\Delta(R_1 - R_2)$,
$S_{23} = 1/2\Delta(-\in_1 + \in_2 + \in_3 - \in_4)$

The following trends were observed in the internal (valence) force constants. The force constants value for the Cd-N stretching, f_R, increases from 1.05 mdyn/Å for Cd $(NH_3)_2I_2$ to 1.21 mdyn/Å for $Cd(NH_3)_2Cl_2$. The opposite trend was observed for the Cd-X (X = Cl, Br, I) stretching force constants, f_{R-}. The values goes from 0.86 mdyn/Å to 0.48 mdyn/Å. For the $Zn(NH_3)_2X_2$ (X = Cl, Br, I) complexes. The $f_{R-} = f_{ZnX}$ force constants increases from 0.78 to 1.15 mdyn/Å from $Zn(NH_3)_2Cl_2$ to $Zn(NH_3)_2I_2$ [9,10]. Structural differences also exist between the Zn(II) and Cd(II)-diamminedihalogenide complexes. The Zn (II) diamminedihalogenide one's are tetrahedral and the Cd(II) diamminedihalogenide have square-planar structures. The observed trend in the Cd-X (X = Cl, Br, I) force constants related to the Zn-X force constants can be explained as: 1) When X = Cl, we observed that $f_{Cd\text{-}Cl} = 0.48$ mdyn/Å and $f_{Zn\text{-}Cl} = 1.15$ mdyn/Å. This trend can be explained by the effect of the reduced mass for the differents oscillators M-X: (Cd-Cl = 26.95 and (Zn-Cl = 22.97, resulting from the almost 72% higher atomic mass of Cd compared with the Zn atomic mass. It is well know that when the reduced mass in a particular bond such as C-C, C-Si, C-Ge, C-Sn and C-Pb, increases, the force constants decreased. 2) When X = I, we observed that $f_{Cd\text{-}I} = 0.86$ mdyn/Å and $f_{Zn\text{-}I} = 0.78$ mdyn/Å. This trend can be explained through the different Pearson classification of Lewis acids [12]; Zn^{+2} is in the border line between hard and soft acids; Cd^{+2} is a soft acid. F^- and Cl^- are hard Lewis bases, and I^- is a soft base. The general rule is: hard acids are those acids that react preferentially with hard bases, whereas soft acids are those that react preferentially with soft bases. In our case, Cd^{+2} react preferentially with I^- (soft acid + soft base). The reaction between Zn^{+2} with I^- being a reaction between an acid of the border line with a soft base. We do not have the $K_{ps}{}^0$ values for the $Cd(NH_3)_2I_2$ and $Zn(NH_3)_2I_2$ complexes, but, for the above reasons we think that $Zn(NH_3)_2I_2$ has higher solubility than $Cd(NH_3)_2I_2$.

It is well known that the force constants for a particular bond increases with the bond order (for C_2H_2, C_2H_4 and C_2H_6, the bond orders for CC are 3.00, 2.12 and 1.11, respectively), magnitude which can be considered as a relative measure of the electronic cloud effective in holding the two atoms together, and represents the effective number of covalent (electron pair) or electrovalent (ionic) bonds acting between the two atoms considered [11]. As the normal coordinate has revealed, there are not coupling between the skeletal ν(CdN) and ν(CdI) normal modes, then as an approach the Cd-N and Cd-X bond order were calculated by the Gordy's equation [11]

$$F = 1.67\, N_{CdN}\, (X_{cd} \bullet X_N / d^2)^{3/4} + 0.30$$

where F is the Cd-N force constant, N is the bond order, d is the Cd-N bond length, and X_{cd} and X_N are the Cd and N atom eletronegativities according to Allred and Rochow [13] and Mulliken [14].

Table 4 gives the bond order of the Cd-N and Cd-X bonds with X = Cl, Br in the $Cd(NH_3)_2Cl_2$, $Cd(NH_3)_2Br_2$ and $Cd(NH_3)_2I_2$ complexes, these values reflect the influence of the halogenide ligand on the square planar coordination of Cd^{+2} cation, and indicate rather little covalent degree.

The potential energy distribution reveals that the vibrational modes pertaining to the ligands and framework coupling are nearly pure (values higher than 95%).

Table 3. Symmetry and valence force constants for $Cd(AB_3)_2I_2$ (A = ^{14}N / ^{15}N and B = H / D).

Force constants	Type	F_0	F (A)	F(B)
			Mdyn/Å	
Ligand				
$F_{(NH)as}$	a_1, a_2, b_1, b_2	6.45	5.93 ± 0.10	5.95 ± 0,04
$F_{(NH)s}$	a_1, b_2	6.48	6.20 ± 0.10	6.15 ± 04
$F_{(HNH)as}$	a_1, a_2, b_1, b_2	0.59	0.54 ± 03	0.55 ± 01
$F_{(HNH)s}$	a1, b2	0.24	0.37 ± 04	0.36 ± 01
Skeletal-ligand coupling				
$F_{(NH3)\,\rho}$	a_1	0.18	0.20 ± 02	0.19 ± 01
	a_2	0.19	0.20 ± 02	0.19 ± 01
	b_1	0.23	0.20 ± 03	0.19 ± 01
	b_2	0.18	0.20 ± 03	0.19 ± 01
Skeletal				
$F_{(Cd\text{-}N)s}$	a_1	1.00	1.07 ± 0.08	1.077 ± 0.07
$F_{(Cd\text{-}N)as}$	b_2	1.02	1.06 ± 0.07	1.04 ± 0.04
$F_{(Cd\text{-}I)s}$	a_1	0.80	1.27 ± 0.16	1.26 ± 0.19
$F_{(Cd\text{-}I)as}$	b_1	0.95	0.44 ± 07	0.46 ± 0.06
Valence force constants				
f_r = f(NH)		6.47	6.07 ± 0.04	6.05 ± 0.04
F_R = f(CdN)		0.98	1.07 ± 0.08	1.05 ± 0.06
f_Q = f(CdI)		0.91	0.86 ± 0.12	0.86 ± 0.13

F_0 - Initial force constant -
F(A) - refers to the mean value of the symmetry calculated force constants by the iterative autoconsistency method.
F(B) - refers to the mean value of the symmetry iterative least square force constants refinement.

Experimental

The complexes $Cd(NH_3)_2I_2$, $Cd(^{15}NH_3)_2I_2$ and $Cd(ND_3)_2I_2$ were prepared in mg quantities using the suggestion given by

Table 4. Bond orders calculated according the Gordy's equation.

	$Cd(NH_3)_2Cl_2$	$Cd(NH_3)_2Br_2$	$Cd(NH_3)_2I_2$
A			
NCd-N	0.54	0.49	0.44
NCd-X	0.17	0.42	0.69
B			
NCd-N	0.68	0.62	0.56
NCd-X	0.16	0.43	0.64

A - refers to the bond orders calculated using Allred's eletronegativities.
B - refers to the bond orders calculated using Mulliken's eletronegativities.

Perchard and Novak [4]. The samples as nujol mulls are on polyethylene supports. The infrared spectra from 4000 to 40 cm^{-1} were run with a Nicolet 60 SXB Fourier transform infrared (FT-IR) spectrometer equipped with a DTGS detector with polyethylene windows. For the IR measurements the resolution was 4 cm^{-1} in the 4000 - 1500 region, 2 cm^{-1} between 1500 and 700 cm^{-1} and 0.25 cm^{-1} in the range from 700 to 40 cm^{-1}. The Raman spectra were recorded on a Jarrel-Ash 25-300 double grating monochromator with an RCAC31034A photon counting system. The resolutions used in the measurement were: 5 cm^{-1} in the spectral range from 3500 to 2000 cm^{-1} and 2 cm^{-1} in the range from 2000 to 20 cm^{-1}. The measurement was carried out using 514.5 nm radiation from an Ar^{+} laser. The samples were sealed in capillary tubes.

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