

The Infra-red Spectra of Some Inorganic Azide Compounds

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The infra-red spectra of crystals of $\text{Cu}(\text{N}_3)_2$, $[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]$, $[\text{Cu}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$, $[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]$, $[\text{Zn}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$, and $[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$ have been registered. The azide, pyridine, and ammine vibration modes are discussed and the spectra are interpreted in terms of general symmetry properties of the compounds. Attempts have been made to correlate the frequencies of the azide stretching modes with the degree of asymmetry within the azide group, and the ammine vibration frequencies with the effects of hydrogen bonding and of coordination.

The crystal and molecular structures of six inorganic azide compounds, namely $\text{Cu}(\text{N}_3)_2$,^{1,2} $[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]$,³ $[\text{Cu}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$,⁴ $[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]$,⁵ $[\text{Zn}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$,⁶ and $[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$ ⁷ have been determined by X-ray methods and published previously. In connection with these investigations, the infra-red spectra of the compounds were also registered. The spectra have now been analysed in order to see whether or not a confirmation of the conclusions drawn from the crystallographical investigations is possible and whether or not additional information concerning these compounds can be obtained.

EXPERIMENTAL

The methods of preparation of the compounds have been described elsewhere.¹⁻⁷ Samples of all compounds except $\text{Cu}(\text{N}_3)_2$ were pulverised and mixed with KBr, $\text{Cu}(\text{N}_3)_2$ being pulverised in nujol. The spectra were registered in the region 3600–600 cm^{-1} . For $\text{Cu}(\text{N}_3)_2$ a Perkin-Elmer-225 spectrophotometer was used and for $[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]$ a Perkin-Elmer-337, whereas the spectra of the remaining compounds were registered on a Beckman IR 9 spectrophotometer. The spectra recorded are shown in Figs. 1–6. Owing to differences in experimental technique, it is not possible to make a comparison of peak heights between the spectra of the different compounds.

RESULTS AND DISCUSSION

Symmetry properties. A general rule for infra-red activity is that, if the number of atoms in two molecules are equal, the more symmetric the molecule the fewer the expected infra-red active bands. Symmetry selection rules for

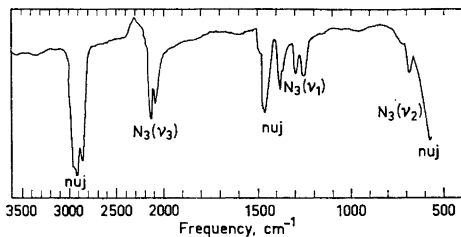


Fig. 1. Infra-red spectrum of $\text{Cu}(\text{N}_3)_2$. Notation, see Table 1; the peaks denoted by *nuj* are due to *nujol*.

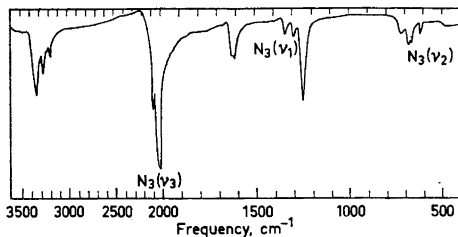


Fig. 2. Infra-red spectrum of $[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]$. Notation, see Table 1.

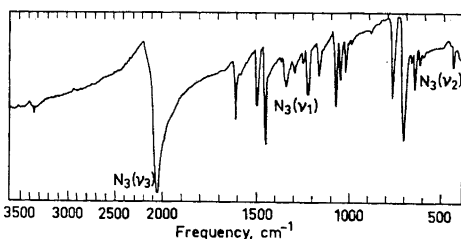


Fig. 3. Infra-red spectrum of $[\text{Cu}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$. Notation, see Table 1.

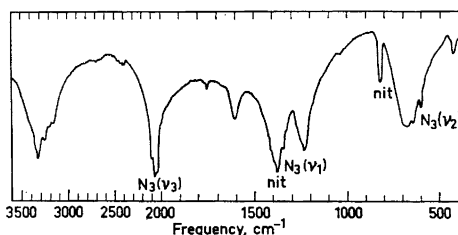


Fig. 4. Infra-red spectrum of $[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]$. The sample also contained nitrate, the peaks due to the latter being denoted by *nit*. Notation, see Table 1.

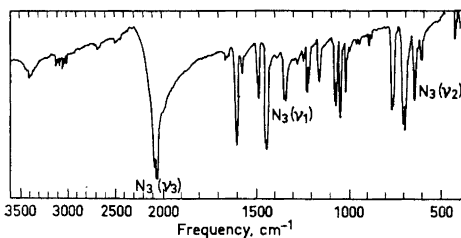


Fig. 5. Infra-red spectrum of $[\text{Zn}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$. Notation, see Table 1.

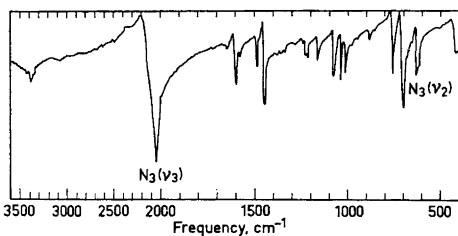


Fig. 6. Infra-red spectrum of $[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$. Notation, see Table 1.

infra-red transitions can be determined using the character table for the point group to which the molecule belongs.⁸ Formally allowed transitions in the infra-red are, however, sometimes of low intensity, or accidentally degenerate with other allowed modes, thus making the interpretation somewhat ambiguous.

The symmetry properties of the three copper azide compounds $\text{Cu}(\text{N}_3)_2$, $[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]$, and $[\text{Cu}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$ (Figs. 7–9) are similar. The two

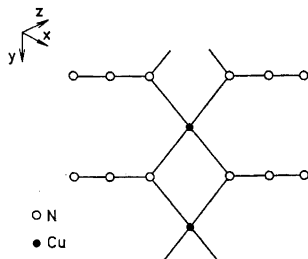


Fig. 7. Structure of $\text{Cu}(\text{N}_3)_2$. The atoms lie close to the plane of the paper.

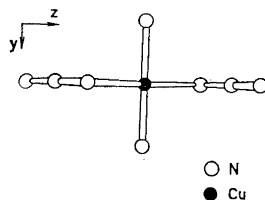


Fig. 8. Structure of $[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]$. The hydrogen atoms are not indicated.

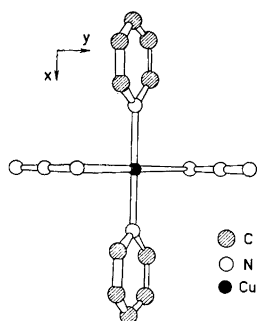


Fig. 9. Structure of $[\text{Cu}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$. The hydrogen atoms are not indicated.

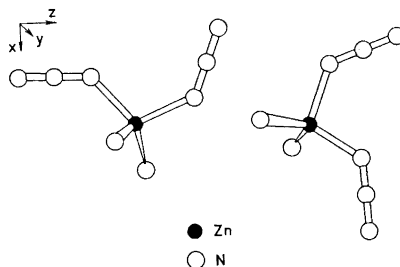


Fig. 10. Structure of $[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]$. The hydrogen atoms are not indicated.

azide groups in each compound are crystallographically independent and are situated in a mirror plane. There are no further symmetry operations, apart from the identity operation, and, consequently, the point group is C_s . Using the character table for point group C_s ,⁹ it can be shown for the azide groups, that the number of times the infra-red active species A' contributes to the total irreducible representation is equal to 2 ($n_{A'} = 2$), while $n_{A''} = 0$ (for notation, method of calculation and further references see Ref. 8). Thus, two peaks are expected to appear in the infra-red spectra due to the antisymmetric stretching mode (ν_3) of the azide groups, and, similarly, two further peaks are expected to occur corresponding to the symmetric stretching mode (ν_1). An inspection of the spectra (Figs. 1–3, Table 1) supports this prediction for all three copper compounds, although in $[\text{Cu}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$ the antisymmetric stretching peak is not resolved. It appears, however, to be split into two components, one of which has a slightly higher frequency than the value given in the table. Each of the peaks due to antisymmetric stretching and to symmetric stretching can thus be assigned to a particular azide group.

In the crystal structure of $[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]$ (Fig. 10) there are two independent molecules. The two azide groups belonging to each molecule are also independent and all four azide groups are situated in a mirror plane.

Table 1. Infra-red azide vibration frequencies. The frequencies (cm^{-1}) due to azide are given in the region 2200–600 cm^{-1} together with interatomic distances (\AA) for some azide compounds. In the regions marked with an asterisk there is some ambiguity in the interpretation, owing to absorption by other groups.

	Azide antisymm. stretch. ν_3	Azide symm. stretch. ν_1	Azide bend ν_2	N–N distances ^a	
KN_3^{10}	2041	(1344) (Raman-active)	645	1.15(2)	1.15(2)
$\text{HN}_3^{10,11}$	2140	1269	658	1.24(1)	1.13(1)
$\text{Cu}(\text{N}_3)_2^2$	2125 2080	1253 1295	680*	1.21(1) 1.21(1)	1.09(2) 1.13(1)
$[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]^3$	2080 2030	1290* 1340	611*	1.19(1) 1.17(1)	1.14(1) 1.14(1)
$[\text{Cu}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]^4$	2040	1295 1333	611*	1.14(4) 1.23(3)	1.08(4) 1.19(4)
$[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]^5$	2110 2080 2070	1350*	611*	1.20(2) 1.19(2) 1.18(3) 1.17(2)	1.14(3) 1.16(3) 1.15(3) 1.18(3)
$[\text{Zn}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]^6$	2095 2070	1340 1348	609*	1.17(2) 1.15(3)	1.13(2) 1.13(3)
$[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]^7$	2055	—	625*	1.17(2)	1.14(2)

^a For asymm. azides the N–N distance closest to the Me–N (H–N) bond is given in the first column.

The appropriate point group is thus C_s and, accordingly, four peaks are expected in the infra-red spectrum resulting from the antisymmetric stretching of the azide groups and four from the symmetric stretching. From an inspection of the relevant antisymmetric stretching frequencies (Table 1, Fig. 4), the split band might appear to support this prediction whereas the interpretation of the symmetric stretching region is difficult, owing to absorption by other groups.

Since there are no symmetry relations between the ligands in the compound $[\text{Zn}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$ (Fig. 11), two peaks, one due to each azide group, would be expected to appear for both stretching modes in the infra-red spectrum. This is also the case, as is indicated by Table 1 and Fig. 5.

Finally, in $[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$ (Fig. 12), the cadmium atom is situated in a centre of symmetry. The appropriate point group is C_i , and it can be shown that, for the azide groups, $n_{A_g} = 1$ (infra-red non-active) and $n_{A_u} = 1$ (infra-red active). Thus only one azide peak is expected to occur in the infra-red spectrum. An examination of the spectrum registered (Table 1, Fig. 6) shows

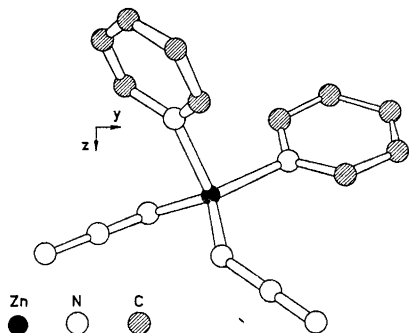


Fig. 11. Structure of $[\text{Zn}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$. The hydrogen atoms are not indicated.

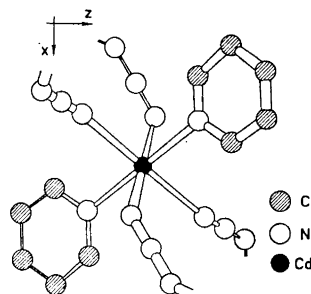


Fig. 12. Structure of $[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$. The hydrogen atoms are not indicated.

that the antisymmetric azide stretching band is single (the symmetric azide stretching band vanishes for this compound, as is discussed later).

There are three compounds in this series which contain pyridine ligands, namely $[\text{Cu}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$, $[\text{Zn}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$, and $[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$. In the spectra registered only the zinc complex shows a distinct splitting of several pyridine peaks (Table 2, Figs. 3, 5, 6). The zinc complex is also the only one which contains two crystallographically different pyridine groups. For the copper complex, no splitting due to coupling of the two crystallographically identical pyridine rings is apparent from the spectrum, and in the cadmium complex the pyridine peaks are expected to be single, owing to the inversion centre.

Azide group frequencies. The vibration frequencies due to the azide group are given in Table 1, together with the nitrogen-nitrogen distances found in the six azide compounds investigated. For the purpose of comparison, the vibration frequencies and nitrogen-nitrogen distances for potassium azide and hydrogen azide, *i.e.* for a typically symmetrical and a typically asymmetrical azide, have also been included.

The antisymmetric azide stretching frequency (ν_3), which is to be found just above 2000 cm^{-1} ,¹⁰ is expected to be higher for those azides in which one nitrogen-nitrogen bond is stronger and consequently shorter, while the other is weaker and thus longer, than for those azides in which the nitrogen-nitrogen bonds are of equal strength.⁹ In Fig. 13a ν_3 has been plotted against the difference in the two nitrogen-nitrogen distances for the compounds listed in Table 1. It would appear from the figure that there is a relationship between the antisymmetric stretching frequency and the degree of asymmetry of an azide group, although the nature of this relationship is not quite explicit and, moreover, experimental errors cannot be neglected. From the figure it would seem that the frequency is throughout higher for the zinc compounds than for the copper compounds.

The symmetric stretching frequency (ν_1), which is observed in the region around 1300 cm^{-1} , is infra-red active only for asymmetric azide groups.¹⁰ The crystal structure determinations of the six compounds have revealed azide

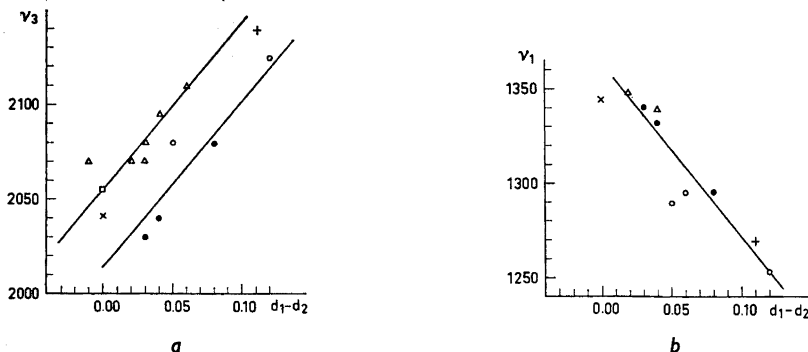


Fig. 13. The frequency of the two azide stretching modes (ν_3 and ν_1 , respectively) versus the degree of asymmetry, as measured by the difference between the two N—N distances ($d_1 - d_2$) within the azide group, where d_1 is the N—N distance closest to the Me—N bond. (Since in the Cd complex d_1 and d_2 are equally close to a Me—N bond $d_1 - d_2$ has been put equal to zero.) The standard deviations of the distances are given in Table 1. The errors in the frequencies are of the magnitude of 15 cm^{-1} .

Notations. Δ , azide group coordinated through one end to Zn. \circ , azide group coordinated through one end to Cu. \bullet , azide group coordinated through both ends to Cu. \square , azide group coordinated through both ends to Cd. \times , azide group of KN_3 . $+$, azide group of HN_3 .

groups which deviate more or less from symmetry, but only in some of the compounds the asymmetry has been statistically ascertained. In the infra-red spectra registered, symmetric stretching bands have been found for all compounds except $[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$, although in some cases absorption due to other ligands has made the interpretation of this region somewhat ambiguous. This suggests that the azide groups are symmetrical in $[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$, which seems reasonable from a consideration of the structural environment of these groups⁷ (Fig. 12).

It would appear that the symmetric stretching frequency (ν_1) of an azide group is also dependent on the nitrogen—nitrogen distances within the azide group. This is illustrated in Fig. 13b in which ν_1 has been plotted against the difference between the two nitrogen—nitrogen distances. One weaker and one stronger nitrogen—nitrogen bond in the azide group appears to have an effect on the symmetric stretching frequency which is opposite to that on the antisymmetric stretching frequency, the symmetric stretching frequency thus apparently decreasing with increasing asymmetry of the azide group. This is what could be expected from calculations based on classical mechanics.²⁴ From such calculations the following secular determinant is obtained:

$$\begin{vmatrix} \mu F - \lambda & -\mu F & 0 \\ -\mu F & \mu(F + F') - \lambda & -\mu F' \\ 0 & -\mu F' & \mu F' - \lambda \end{vmatrix} = 0$$

Here μ is the reciprocal of the mass of nitrogen, F and F' are the force constants for the two N-N bonds and $\nu = \sqrt{\lambda}/2\pi$, where ν is the frequency of vibration. If the equation is solved, the following expression for ν is obtained (except for one root, $\nu=0$):

$$\nu = k \sqrt{\frac{F + F' \pm F'}{F + F' + sF'}} \sqrt{1 - \frac{F}{F'} + \left(\frac{F'}{F'}\right)^2}; \quad k = \sqrt{\mu}/2\pi$$

If F' is the force constant of the short N-N bond and F is the force constant of the long N-N bond, then $F' \geq F$ and $1 \leq s \leq \sqrt{0.75}$.

Thus

$$\nu_a = k \sqrt{F + F' + sF'}; \quad \nu_b = k \sqrt{F + F' - sF'}$$

Consequently, for normal variations of F and F' , ν_a (the antisymmetric stretching frequency *i.e.* ν_3) will increase with increasing F' and ν_b (the symmetric stretching frequency *i.e.* ν_1) will decrease with decreasing F (F' vanishing as $s \approx 1$).

The bending frequency, ν_2 , is to be found in a region (700–600 cm^{-1})¹⁰ in which other groups present absorb, and it is likely that at least one more peak for each compound than that given in Table 1 is due to the bending of the azide group. It is, consequently, difficult to draw any conclusions from the bending mode.

Pyridine group frequencies. The absorption frequencies in the infra-red spectra due to the pyridine ligands in the complexes $[\text{Cu}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$, $[\text{Zn}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$, and $[\text{Cd}(\text{N}_3)_2(\text{C}_5\text{H}_5\text{N})_2]$ are listed in Table 2. For the purpose of comparison the frequencies of the infra-red peaks of the corresponding thiocyanato complexes and of pure pyridine have been included.¹² As seen from the table, there is a very great similarity between the spectra of the different complexes, including that of pure pyridine. According to the structural investigations of pyridine^{13,14} and of the three azide compounds,^{4,6,7} bond distances and angles are also practically invariant. This may be interpreted as indicating a similar electron density over the ring system in all these compounds.

Ammine group frequencies. The vibrational frequencies due to the ammine groups observed for $[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]$ and $[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]$ are listed in Table 3. For the purpose of comparison, the frequencies of two other ammine compounds with the same central atoms have also been included.

The stretching frequency of an unperturbed N-H bond is to be found somewhat above 3400 cm^{-1} (*cf.* Refs. 15 and 16). As seen from Table 3, the NH_3 stretching bands in the above complexes are shifted to lower frequencies. These changes are caused by several factors, *e.g.* hydrogen bonding, which is probably the most important factor, and the effect of coordination.^{9,23} Attempts have been made to quantitatively correlate the shift of the infra-red N-H stretching frequency with the N-H...N bond length.^{15,17} Since there are many other factors which may be of importance it is not, however, possible to make more than a very rough estimate. Of the two relationships cited it

Table 2. Infra-red pyridine vibration frequencies. The frequencies (cm^{-1}) due to pyridine (py) are given in the region 2200–600 cm^{-1} . Assignments are based on the work of Wilmshurst and Bernstein,²¹ using the notation of Kline and Turkevich.²² In the regions marked with an asterisk there is some ambiguity in the interpretation, owing to absorption by other groups.

Assignment	py ¹²	[Cu(NCS) ₂ (py) ₂] ¹²	[Zn(NCS) ₂ (py) ₂] ¹²	[Cd(NCS) ₂ (py) ₂] ¹²	[Cu(N ₃) ₂ (py) ₂] ⁴	[Zn(N ₃) ₂ (py) ₂] ⁶	[Cd(N ₃) ₂ (py) ₂] ⁷
1+6b	1627	1632		1633			
or 6a+12	1539				1603	1606, 1597	1599
1+6a	1578	1604	1611	1598		1571	1571
8a	1570	1572		1570		1490, 1487	1485
8b	1478	1487		1483		1447, 1445	1444
19a	1436	1447	1487	1442	1489		
19b	1383	1383	1447	1442	1447		
14	1372	1383	1374	1363			
6a+10b	1350	1353					
	1235	1235	1243	1235	1242	1245	
9a	1217	1217	1218, 1214	1216		1222, 1215	1223, 1217
15	1145	1152	1154	1149	1158	1161	1160
18a	1067	1072	1069	1070	1071	1075, 1069	1074
12	1031	1042	1047, 1043	1036	1044	1048	1036
1	991	1016	1022, 1017	1008	1018	1018	1010
5	942	943					
4	747	755	755, 752	753	760	760, 757	755
11	700	692, 687	697, 687	692	700	701, 692	701
6b	650						
6a	601	637	641	625	640*	649, 640*	631*

Table 3. Infra-red ammine vibration frequencies. The frequencies (cm^{-1}) are given in the region 3600–600 cm^{-1} . In the regions marked with an asterisk there is some ambiguity in the interpretation, owing to absorption by other groups (sh = shoulder).

	Ammine stretch.	Ammine degen def.	Ammine symm. def.	Ammine rock
$[\text{Zn}(\text{NH}_3)_4]\text{I}_3^9$	3290	1600	1242	693
$[\text{Cu}(\text{NH}_3)_4]\text{Cl}_2^9$	3270	1596	1245	709
$[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]^5$	3330 3255 3200 sh 3170	1612	1238*	650–690*
$[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]^3$	3330 3255 3205 sh 3175	1610	1242*	660–730*

is easier to make at least an approximate correction for the effect of coordination, if the equation $\Delta\nu = 1.05 \times 10^3 (3.38 - R)$ (Ref. 17) is used, where $\Delta\nu$ is the frequency shift, in cm^{-1} , due to hydrogen bonding and R is the $\text{N}-\text{H}\cdots\text{N}$ distance in Å. The effect of coordination is assumed to cause a lowering of the $\text{N}-\text{H}$ stretching frequency to about 3400–3350 cm^{-1} for the copper and zinc complexes (cf. Ref. 9; 3380 cm^{-1} has been used in the calculations). Thus, according to the equation given above, and using the frequencies observed for the copper and zinc complexes (Table 3) it can be calculated that the $\text{N}-\text{H}\cdots\text{N}$ distances in the two complexes ought to lie within the range 3.18–3.33 Å. According to the results of the X-ray investigations, the distances between nitrogen atoms in positions such that development of attraction through interjacent hydrogen atoms is feasible are 3.18–3.31 Å for $[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]^3$ and 3.14–3.34 Å for $[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]^5$. In both structures the presumed hydrogen bonds are non-linear, and some are bi- or trifurcated and, consequently, very weak. It may therefore be concluded that the information concerning hydrogen bonding obtained from the $\text{N}-\text{H}$ stretching frequency in the infra-red supports the assumption that such attraction exists, while it is doubtful whether the quantitative calculations, although they show agreement with the results of the X-ray investigation, can be considered to be very reliable.

The frequencies of the three bending bands of the ammine group (Table 3) are also affected by coordination and hydrogen bonding and tend to be shifted towards higher values.⁹ The rocking and the symmetric deformation frequencies are regarded as being most sensitive to the central atom.^{9,18,19} The frequencies have been found, in general, to decrease as the stability of the ammine complexes, measured in terms of stability constants, decrease.²⁰ Although the differences are small, it might appear from Table 3 that the ammine group is a little more strongly coordinated to copper in $[\text{Cu}(\text{N}_3)_2(\text{NH}_3)_2]^3$ than to zinc in $[\text{Zn}(\text{N}_3)_2(\text{NH}_3)_2]^5$, which also seems to be quite reasonable, in view of

the fact that the same trend has been found for other comparable ammine complexes of zinc and copper.^{19,20}

The metal-nitrogen stretching bands, which are found below 500 cm^{-1} have not been registered for all the compounds and discussion based on these bands is also difficult because different ligands are bonded to the metal through nitrogen.

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