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ANOMALOUS SCATTERING BY COBALT AND CHLORINE AND CRYSTAL STRUCTURE OF (+)-TRIS (ETHYLENEDIAMINE) COBALT (III) CHLORIDE (+)-TARTRATE PENTAHYDRATE

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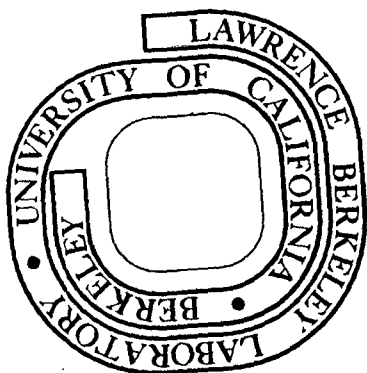
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ANOMALOUS SCATTERING BY COBALT AND  
CHLORINE AND CRYSTAL STRUCTURE OF  
(+)-TRIS(ETHYLENEDIAMINE)COBALT(III)  
CHLORIDE (+)-TARTRATE PENTAHYDRATE

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ABSTRACT

Crystals of  $\text{Co}(\text{C}_2\text{H}_8\text{N}_2)_3\text{Cl}(\text{C}_4\text{H}_4\text{O}_6) \cdot 5\text{H}_2\text{O}$  are triclinic, space group  $P1$ ;  $a = 8.261(3) \text{ \AA}$ ,  $b = 8.507(3) \text{ \AA}$ ,  $c = 8.149(3) \text{ \AA}$ ,  $\alpha = 101.20(1)$ ,  $\beta = 95.27(1)$ ,  $\gamma = 102.31(1)^\circ$ ,  $Z = 1$ . The structure and absolute configuration,  $\Lambda$  for (+)- $\text{Co}(\text{en})_3$ , were determined with 7688 observed reflections ( $\text{MoK}\alpha$  radiation) refined to  $R = 0.022$ . All hydrogen atom positions were refined. These data and 3198 reflections measured with  $\text{CuK}\alpha$  radiation ( $R = 0.029$ ) were used to determine anomalous scattering terms. At  $\text{MoK}\alpha$ ,  $f''(\text{Co}) = 0.962(10)$ ;  $f''(\text{Cl}) = 0.155(10)$ . At  $\text{CuK}\alpha$ ,  $f'$ ,  $f''(\text{Co}) = -2.36(2)$ ,  $3.92(2)$ ;  $f'$ ,  $f''(\text{Cl}) = 0.23(2)$ ,  $0.72(2)$  electrons.

equipped with a graphite monochromator and Mo radiation ( $\lambda = 0.70926 \text{ \AA}$  for  $K\alpha_1$ ). Cell dimensions were derived by least-squares from the setting angles of 12 reflections ( $50^\circ < 2\theta < 55^\circ$ ). Diffraction intensities were measured by the  $\theta$ - $2\theta$  scan technique at  $1^\circ \text{ min}^{-1}$  for  $2\theta$ , for all reflections in the full sphere up to  $2\theta = 65^\circ$  or  $d = 0.66 \text{ \AA}$ . The scan width was  $1.2^\circ$  in  $2\theta$  plus the  $\alpha_1$ - $\alpha_2$  splitting. Background was counted for 4 s at  $0.5^\circ$  past each end of the scan. Three reflections (600, 060, and 006) checked at intervals of 200 measurements indicated a uniform decrease in intensity of about 10% during 2.5 weeks of data collection, and each measurement was adjusted accordingly. An absorption correction ( $\mu = 10.1 \text{ cm}^{-1}$ ) was made using the program HORSE (Hamilton, 1969) that approximates the crystal as an array of points (480 in this case). The extreme correction factors were 1.15 and 1.22. Before the final refinement each structure factor was multiplied by  $1.0 + 1.8 \times 10^{-7} I$ , an empirical correction for extinction which was 1.18 for the strongest reflection,  $\bar{1}11$ ;  $I$  is the uncorrected observed intensity.

For 188 reflections the intensity was less than  $\sigma$  estimated from counting statistics, and these were given zero weight in the structure refinement. The remaining 7688 reflections, including both members of each Bijvoet pair, were assigned weights  $w = [\sigma(F)]^{-2}$ ;  $\sigma(F)$  was derived from

$$\sigma(F^2) = [S^2 + (pF^2)^2]^{1/2}$$

where  $S^2$  is the variance due to counting statistics and  $p = 0.03$ .

Another crystal,  $0.102 \times 0.084 \times 0.110 \text{ mm}$  in size, was used to measure diffraction intensities with  $\text{CuK}\alpha$  radiation. The technique

Werner (1912) demonstrated the optical activity and octahedral nature of complexes of cobalt and ethylenediamine by using the crystallization of (+)-tartrate salts to separate the enantiomers. One of the salts he isolated was (+)-tris(ethylenediamine)cobalt(III) chloride (+)-tartrate pentahydrate. We first became interested in this material when it was the subject of an experiment devised by McClain (1972) for the elementary chemistry laboratory course at Berkeley. We determined the crystal structure because lack of knowledge of it was an embarrassment in explanations to students. Later we realized that this salt is suitable for measuring anomalous scattering effects of cobalt and chlorine by a method described by Templeton and Templeton (1978).

In this paper we report the crystal structure and some measurements of scattering of  $\text{MoK}\alpha$  and  $\text{CuK}\alpha$  radiation. This study provides a foundation for some similar experiments with synchrotron radiation near the Co K absorption edge which will be described elsewhere.

## EXPERIMENTAL

Crystals provided by Professor McClain had been prepared by air oxidation of an aqueous solution of ethylenediamine, HCl, and  $\text{CoSO}_4$  in the presence of activated charcoal, followed by reaction with solid barium tartrate on a steam bath, concentration by boiling, and then cooling. Recrystallization from water yielded excellent orange-brown crystals for diffraction study. A crystal with dimensions  $0.16 \times 0.28 \times 0.20$  mm was used for measurements with a Picker FACS-I diffractometer

chlorine and the carbon and nitrogen atoms of ethylenediamine from a three-dimensional Patterson function. An electron density difference function phased with that partial structure revealed the rest of the non-hydrogen atoms. The absolute configuration was adjusted to correspond to the known configuration of the (+)-tartrate ion. After least-squares refinement with anisotropic thermal parameters an electron density difference function revealed the positions of all of the hydrogen atoms. The final full matrix refinement with isotropic thermal parameters for hydrogen and anisotropic ones for all other atoms (411 independent parameters) reduced  $R_w = [\sum w(\Delta F)^2 / \sum w|F_o|^2]^{1/2}$  to 0.024; the conventional  $R = \sum |\Delta F| / \sum |F_o|$  was 0.022 for the 7688 reflections given weight, and 0.024 for all 7876 reflections. The resulting atomic coordinates are listed in Table 1.\* The largest shift of any parameter in the last cycle was 7% of its standard deviation. The standard deviation of an observation of unit weight was 1.039.

The atomic scattering factors of Stewart, Davidson and Simpson (1965) were used for hydrogen and those of Doyle and Turner (1968) for the other atoms. The anomalous scattering factors reported by Cromer and Liberman (1970) for  $MoK\alpha_1$  were used for Co, Cl, O, N, and C.

A refinement of the reverse configuration of the structure, which gave  $R_w = 0.063$  and  $R = 0.049$  for the 7688 reflections, confirms

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\*Lists of structure factors and thermal parameters have been deposited with the British Lending Division as Supplementary Publication

the absolute configuration and indicates how much effect  $f'' = 0.973$  for Co has on the structure factors.

A less exhaustive refinement of the  $\text{CuK}\alpha$  data gave  $R = 0.029$  and  $R_w = 0.032$  for 3198 independent reflections ( $I > 3\sigma$ ). The atomic coordinates are generally in good agreement with those in Table 1, but have standard deviations two or three times larger because of the lower resolution of the less extensive data set.

#### DESCRIPTION OF THE STRUCTURE

Bond distances and bond angles are listed in Tables 2 and 3. The corresponding bromide salt is isomorphous and has a similar atomic arrangement according to Kushi, Kuramoto and Yoneda (1976), but numerical coordinates were not published. Pepinsky and Okaya (1956) also studied the bromide, but gave no details. The cation consists of a cobalt atom complexed to three ethylenediamine ligands in the form of a left-handed propeller as shown in Fig. 1. The absolute configuration, described as  $\Lambda(+)_589[\text{Co}(\text{en})_3\delta\delta\delta]^{3+}$  (IUPAC, 1970), is already well established by several other studies by Saito, Nakatsu, Shiro and Kuroya (1955), Nakatsu (1962), Iwata, Nakatsu and Saito (1969), and Witiak, Clardy and Martin (1972). The dimensions of this complex have also been measured by Duesler and Raymond (1971), Veal and Hodgson (1972), Whuler, Brouty, Spinat and Herpin (1975), Brouty, Spinat, Whuler and Herpin (1976), and Haupt, Huber and Preut (1976). Our bond distances fell



within the ranges listed in most of the earlier reports. Our confidence in their accuracy is enhanced by the high degree of consistency of values for bonds which are chemically equivalent.

Chemically equivalent bonds in the tartrate ion also have closely equal lengths, and are in good agreement generally with other studies of tartrate and bitartrate salts (Bommel and Bijvoet, 1958; Ambady and Kartha, 1968; Hinazumi and Mitsui, 1972; Yadava and Padmanabhan, 1973; Perez, 1976, 1977; Templeton and Templeton, 1978). The molecular conformation and atomic numbering scheme are shown in Fig. 2. The absolute configuration is the same as that first demonstrated for (+)-tartrate by Bijvoet, Peerdeman and Bommel (1951).\*

The chloride ion is near one cobalt complex on the pseudo three-fold axis of the octahedron, Fig. 3. Its six nearest neighbors are hydrogen atoms (attached to nitrogen or oxygen) at distances from 2.42 to 2.75 Å. The corresponding Cl-O and Cl-N distances range from 3.18 to 3.32 Å and 3.24 to 3.45 Å, respectively (Table 4) and have geometry appropriate for weak hydrogen bonds. All the other hydrogen atoms on nitrogen or oxygen are located near lines to oxygen neighbors at N-O distances 2.89 to 3.22 Å or O-O distances 2.65 to 2.86 Å (Table 4). In each case the bond angles are appropriate for hydrogen bonding, but the bonding must be rather weak in the case of the longer N-O distances.

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\* While (+)-tartrate is commonly designated as D-tartrate in the older literature, it may be noted that the current practice in carbohydrate chemistry (IUPAC, 1972) is to use L to describe this absolute configuration.

## ANOMALOUS SCATTERING

Anomalous scattering effects are not especially large for this crystal and  $\text{MoK}\alpha$  radiation, but they are significant. We used the molybdenum radiation data set to determine  $f''$  for both Co and Cl by the method of least squares (Templeton and Templeton, 1978). Both can be determined because they contribute differently to different reflections. Not all the  $f''$  values can be determined, because it is necessary to have a definition of zero phase angle. In the present example, the considerable number of oxygen, nitrogen, carbon and hydrogen atoms give that definition. We assume for them that the rather small values of  $f''$  calculated by Cromer and Liberman (1970) are correct. In principle one could also determine  $f''$  for some of the light atoms, using just one element as a standard, but there are other substances which seem more suitable for that objective.

A refinement with only a scale factor and  $f''$  for Co and Cl as variables, using the values determined above for all the other parameters, yielded values listed in Table 5, which are in excellent agreement with those calculated by Cromer and Liberman (1970) for  $\text{MoK}\alpha_1$ . Another calculation, refining  $f''$  of Co, a scale factor, and all positional and thermal parameters of Co, Cl and six N atoms (except xyz of Co) yielded  $f'' = 0.964 \pm 0.009$  and trivial changes of other parameters; this calculation confirms that  $f''$  is not much correlated with other parameters. As a test of the variation of  $f''$  with scattering angle, a calculation with  $f''$  defined as a linear function of  $s^2 = (\sin^2\theta)\lambda^{-2}$  yielded:

$$f''(\text{Co}) = (0.97 \pm 0.02) - (0.02 \pm 0.08)s^2, \text{ MoK}\alpha$$

$$f''(\text{Cl}) = (0.15 \pm 0.02) + (0.01 \pm 0.08)s^2.$$

In this case the thermal parameters of Co and Cl were allowed to vary, but they hardly changed. These results show no change with angle at the accuracy of the experiment; we report them to set an upper limit on the effect.

It is evident in advance that  $f'$  will be more sensitive than  $f''$  to changes in scale factor or thermal parameters or to any errors in the experiment or thermal model which are correlated with diffraction angle. However, as an experiment we made a calculation with scale factor and  $f'$ ,  $f''$ , and thermal parameters for Co and Cl as variables. The results were  $f'(\text{Co}) = 0.20(2)$  and  $f'(\text{Cl}) = 0.06(2)$ , surprisingly close to the values 0.299 and 0.132 calculated by Cromer and Liberman (1970); the estimated standard deviations, however, appear to be unrealistic, and we expect that systematic errors are present. The values obtained for  $f''$ , 0.957(10) for Co and 0.156(10) for Cl, are nearly the same as before. Correlation coefficients between each  $f'$  and the diagonal anisotropic thermal parameters of the same atom ranged from 0.66 to 0.74.

In all of the above calculations the R values were almost identical, as is to be expected in view of the small changes in the scattering factors which resulted.

The copper data set was refined with a scale factor and anomalous scattering terms for Co and Cl as variables. All coordinates and thermal parameters were held at the values determined with the MoK $\alpha$  data set.

Anomalous scattering terms for C, O, and N were taken from Cromer and Liberman (1970). The results in Table 5 were obtained with  $R = 0.029$  and  $R_w = 0.035$ . This value of  $R_w$  is not quite as good as that obtained in the earlier refinement, but one must note that it is achieved with only 5 adjustable parameters rather than 411 of them. There is a significant discrepancy with the value calculated by Cromer and Liberman (1970) for  $f''$  of Co; pending further investigation we ascribe it to the effect called extended x-ray absorption fine structure ("EXAFS") which is expected to occur at this photon energy which is only about 300 eV from the cobalt K edge. The theoretical value is calculated for an isolated atom which is free of this effect.

A calculation to test the variation of  $f''$  with angle for Co and Cl yielded the values

$$f''(\text{Co}) = (4.01 \pm 0.04) - (0.6 \pm 0.2)s^2, \text{ CuK}\alpha$$

$$f''(\text{Cl}) = (0.69 \pm 0.04) + (0.2 \pm 0.3)s^2,$$

where  $s = \lambda^{-1} \sin\theta$  as before. In this refinement also  $R = 0.029$  and  $R_w = 0.035$ . The variation of  $f''(\text{Cl})$  with angle is not significant. The equation for  $f''(\text{Co})$  gives  $f'' = 3.8$  at  $\theta = 63^\circ$ , the upper limit of the experiment. This 5% reduction (relative to zero angle) is similar to the 3.3% reduction at this angle estimated by Hazell (1975) from orbital Fourier transforms, an approximate method which may be expected to give the order of magnitude of the change. Thus our result is plausible, but it must be regarded as tentative because of the marginal statistical significance and because some calculations with the data partitioned into shells for intervals of  $s$  indicate some small

systematic errors of unidentified origin which are correlated with diffraction angle. However, our result serves to define an upper limit for this effect which still lacks any definitive measurement. Hall and Maslen (1966) report a somewhat similar result for  $f''$  of iodine at  $\text{CuK}\alpha$ .

We thank Professor W. M. McClain for providing this compound and suggesting that we study it. This research was supported by the Division of Nuclear Sciences, Office of Basic Energy Sciences, U.S. Department of Energy.

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Table I. Coordinates for  $\underline{d}$ -[Co(C<sub>2</sub>H<sub>8</sub>N<sub>2</sub>)<sub>3</sub>] Cl(C<sub>4</sub>H<sub>4</sub>O<sub>6</sub>)·5H<sub>2</sub>O<sup>α</sup>

	x	y	z
Co	0	0	0
Cl	.23162(5)	-.28567(5)	-.30803(5)
N(1)	.0324(2)	.2390(2)	.0206(2)
N(2)	.2409(1)	.0133(2)	.0093(2)
N(3)	.0396(2)	.0274(2)	.2461(2)
N(4)	-.0446(2)	-.2411(1)	-.0402(2)
N(5)	-.2418(2)	-.0299(2)	.0077(2)
N(6)	-.0244(2)	-.0143(2)	-.2452(2)
C(1)	-.2260(2)	-.3121(2)	-.0987(2)
C(2)	-.0101(2)	.2744(2)	-.1468(2)
C(3)	-.3202(2)	-.2048(2)	.0045(2)
C(4)	.3032(2)	-.0208(2)	.1719(2)
C(5)	.2221(2)	.0696(2)	.3060(2)
C(6)	.0422(2)	.1513(2)	-.2778(2)
C(7)	.6874(1)	.2328(1)	.4322(1)
C(8)	.7332(1)	.3736(1)	.3396(1)
C(9)	.9057(1)	.4796(1)	.4205(1)
C(10)	.9584(2)	.6181(2)	.3272(2)
O(1)	.6415(2)	.2720(1)	.5735(1)
O(2)	.7027(1)	.0930(1)	.3641(1)
O(3)	.7350(1)	.3148(1)	.1644(1)
O(4)	1.0197(1)	.3760(1)	.4169(1)
O(5)	.8840(2)	.7328(1)	.3520(2)
O(6)	1.0654(1)	.6090(1)	.2299(1)
O(7)	.4310(1)	.3632(1)	.0387(2)
O(8)	.6460(2)	.8262(2)	.5158(2)
O(9)	.4078(2)	.4210(2)	.7204(2)
O(10)	.5205(2)	.0624(2)	.7741(2)
O(11)	.3816(2)	.5711(3)	.3086(2)
H(1)	-.022(2)	.284(3)	.091(3)
H(2)	.136(3)	.283(2)	.051(2)
H(3)	.263(2)	.943(2)	.930(3)
H(4)	.298(2)	.110(2)	.999(2)
H(5)	-.001(3)	.111(3)	.296(3)
H(6)	-.009(2)	.934(2)	.274(2)
H(7)	-.016(2)	.726(2)	.054(2)
H(8)	.019(2)	.726(2)	.886(3)
H(9)	.708(2)	.003(2)	.927(2)
H(10)	.742(2)	.026(3)	.104(3)
H(11)	.874(2)	.952(2)	.710(2)
H(12)	.031(2)	.917(2)	.708(2)
H(13)	.755(3)	.691(3)	.788(3)
H(14)	.748(3)	.574(3)	.922(3)



Table 1 (continued)

H(15)	.872(3)	.257(2)	-.173(2)
H(16)	.041(3)	.377(3)	-.149(3)
H(17)	.563(2)	.771(2)	.952(2)
H(18)	.690(2)	.780(2)	.126(3)
H(19)	.424(3)	.011(3)	.192(3)
H(20)	.269(3)	-.138(3)	.161(3)
H(21)	.267(2)	.186(2)	.321(2)
H(22)	.242(3)	.035(3)	.417(3)
H(23)	.165(3)	.164(3)	.728(3)
H(24)	.001(3)	.158(3)	.614(3)
H(25)	.661(2)	.442(2)	.357(2)
H(26)	.896(2)	.527(2)	.531(2)
H(27)	.650(3)	.322(3)	.118(3)
H(28)	.097(3)	.421(3)	.463(3)
H(29)	.443(4)	.398(4)	-.046(4)
H(30)	.415(3)	.439(3)	.099(3)
H(31)	.639(3)	.901(3)	.465(3)
H(32)	.696(3)	.790(3)	.473(3)
H(33)	.473(4)	.402(3)	.666(4)
H(34)	.381(3)	.492(4)	.698(4)
H(35)	.539(4)	.111(4)	.705(4)
H(36)	.475(4)	-.032(4)	.713(4)
H(37)	.293(4)	.574(3)	.296(3)
H(38)	.443(4)	.663(4)	.365(5)

<sup>a</sup> Estimated standard deviations of the least significant digit(s) are given in parentheses.

Table 2. Distances Å

<u>tris(ethylenediamine)Co(III)</u>					
Co -N(1)	1.965(1)	C(2)-C(6)	1.505(2)	N(6)-H(12)	0.87(2)
Co -N(2)	1.962(1)	C(4)-C(5)	1.504(2)	C(1)-H(13)	0.93(2)
Co -N(3)	1.962(1)	N(1)-H(1)	0.85(2)	C(1)-H(14)	1.00(2)
Co -N(4)	1.961(1)	N(1)-H(2)	0.85(2)	C(2)-H(15)	0.95(2)
Co -N(5)	1.968(1)	N(2)-H(3)	0.85(2)	C(2)-H(16)	0.89(2)
Co -N(6)	1.967(1)	N(2)-H(4)	0.88(2)	C(3)-H(17)	0.98(2)
N(1)-C(2)	1.481(2)	N(3)-H(5)	0.90(2)	C(3)-H(18)	1.03(2)
N(2)-C(4)	1.480(2)	N(3)-H(6)	0.89(2)	C(4)-H(19)	0.96(2)
N(3)-C(5)	1.485(2)	N(4)-H(7)	0.90(2)	C(4)-H(20)	0.96(2)
N(4)-C(1)	1.486(2)	N(4)-H(8)	0.88(2)	C(5)-H(21)	0.96(2)
N(5)-C(3)	1.484(2)	N(5)-H(9)	0.87(2)	C(5)-H(22)	1.02(2)
N(6)-C(6)	1.484(2)	N(5)-H(10)	0.87(2)	C(6)-H(23)	1.00(2)
C(1)-C(3)	1.507(2)	N(6)-H(11)	0.85(2)	C(6)-H(24)	0.93(2)
<u>tartrate</u>					
C(7)-O(1)	1.251(2)	C(7)-C(8)	1.536(2)	C(8)-H(25)	0.92(2)
C(7)-O(2)	1.249(2)	C(8)-C(9)	1.525(2)	C(9)-H(26)	0.93(2)
C(10)-O(5)	1.254(2)	C(9)-C(10)	1.531(2)	O(3)-H(27)	0.78(2)
C(10)-O(6)	1.246(2)	C(8)-O(3)	1.421(1)	O(4)-H(28)	0.70(3)
		C(9)-O(4)	1.419(1)		
<u>water</u>					
O(7)-H(29)	0.81(3)	O(8)-H(32)	0.65(3)	O(10)-H(36)	0.85(3)
O(7)-H(30)	0.77(3)	O(9)-H(33)	0.75(3)	O(11)-H(37)	0.74(3)
O(8)-H(31)	0.83(3)	O(9)-H(34)	0.74(3)	O(12)-H(38)	0.85(3)
		O(10)-H(35)	0.77(3)		

Table 3. Angles, Deg.

<u>tris(ethylenediamine)Co(III)</u>					
N(1) -Co -N(2)	92.4(1)	N(3) -Co -N(6)	175.7(1)	H(3) -N(2)-H(4)	105(2)
N(1) -Co -N(3)	91.6(1)	N(4) -Co -N(5)	85.6(1)	H(5) -N(3)-H(6)	110(3)
N(1) -Co -N(4)	174.9(1)	N(4) -Co -N(6)	89.9(1)	H(7) -N(4)-H(8)	107(2)
N(1) -Co -N(5)	92.2(1)	N(5) -Co -N(6)	93.2(1)	H(9) -N(5)-H(10)	108(2)
N(1) -Co -N(6)	85.5(1)	Co -N(1)-C(2)	110.0(1)	H(11)-N(6)-H(12)	108(2)
N(2) -Co -N(3)	85.4(1)	Co -N(2)-C(4)	108.7(1)	H(13)-C(1)-H(14)	114(3)
N(2) -Co -N(4)	90.2(1)	Co -N(3)-C(5)	110.1(1)	H(15)-C(2)-H(16)	111(3)
N(2) -Co -N(5)	173.7(1)	Co -N(4)-C(1)	109.1(1)	H(17)-C(3)-H(18)	112(2)
N(2) -Co -N(6)	91.5(1)	Co -N(5)-C(3)	110.4(1)	H(19)-C(4)-H(20)	108(3)
N(3) -Co -N(4)	93.0(1)	Co -N(6)-C(6)	109.2(1)	H(21)-C(5)-H(22)	110(2)
N(3) -Co -N(5)	90.1(1)	H(1) -N(1)-H(2)	109(3)	H(23)-C(6)-H(24)	108(3)
<u>tartrate</u>					
O(1) -C(7)-O(2)	126.1(1)	C(8) -C(9)-O(4)	108.3(1)	C(9) -C(8)-H(25)	106(1)
O(1) -C(7)-C(8)	115.5(1)	O(4) -C(9)-C(10)	112.1(1)	C(8) -O(3)-H(27)	107(2)
O(2) -C(7)-C(8)	118.4(1)	C(9) -C(10)-O(5)	115.9(1)	C(8) -C(9)-H(26)	107(1)
C(7) -C(8)-O(3)	112.4(1)	C(9) -C(10)-C(6)	119.6(1)	O(4) -C(9)-H(26)	111(1)
C(7) -C(8)-C(9)	108.4(1)	O(5) -C(10)-O(6)	124.3(1)	C(10)-C(9)-H(26)	108(1)
O(3) -C(8)-C(9)	109.5(1)	C(7) -C(8)-H(25)	110(1)	C(9) -O(4)-H(28)	109(2)
		O(3) -C(8)-H(25)	111(1)		
<u>water</u>					
H(29)-O(7)-H(30)	101(4)	H(33)-O(9) -H(34)	107(4)	H(37)-O(11)-H(38)	112(4)
H(31)-O(8)-H(32)	101(4)	H(35)-O(10)-H(36)	100(4)		

Table 4. Hydrogen Bond Distances and Angles

Atom	Dist. Å		Angle, deg.
O(3)-N(1) -O(7)	2.956	3.216	144.2
C1 -N(2) -O(7)	3.239	3.007	123.8
O(4)-N(3) -O(5)	3.066	2.889	123.9
C1 -N(4) -O(6)	3.328	2.918	103.2
O(2)-N(5) -O(10)	3.001	2.941	109.2
C1 -N(6) -O(8)	3.448	3.078	107.1
O(9)-O(7) -O(11)	2.729	2.663	123.6
O(2)-O(8) -O(5)	2.765	2.649	85.5
C1 -O(9) -O(1)	3.180	2.765	139.8
C1 -O(10)-O(1)	3.292	2.743	132.0
O(6)-O(11)-O(8)	2.733	2.865	123.6
O(7)-O(3)	2.768		
C1 -O(4)	3.316		

Table 5. Anomalous Scattering Terms

	$\lambda, \text{\AA}$	Experiment	Theory <sup>a</sup>
$f''(\text{Co})$	0.711 <sup>b</sup>	0.962(10)	0.973
	1.542 <sup>c</sup>	3.92(2)	3.608
$f'(\text{Co})$	1.542	-2.36(2)	-2.464
$f''(\text{Cl})$	0.711	0.155(10)	0.159
	1.542	0.72(2)	0.702
$f'(\text{Cl})$	1.542	0.23(2)	0.348

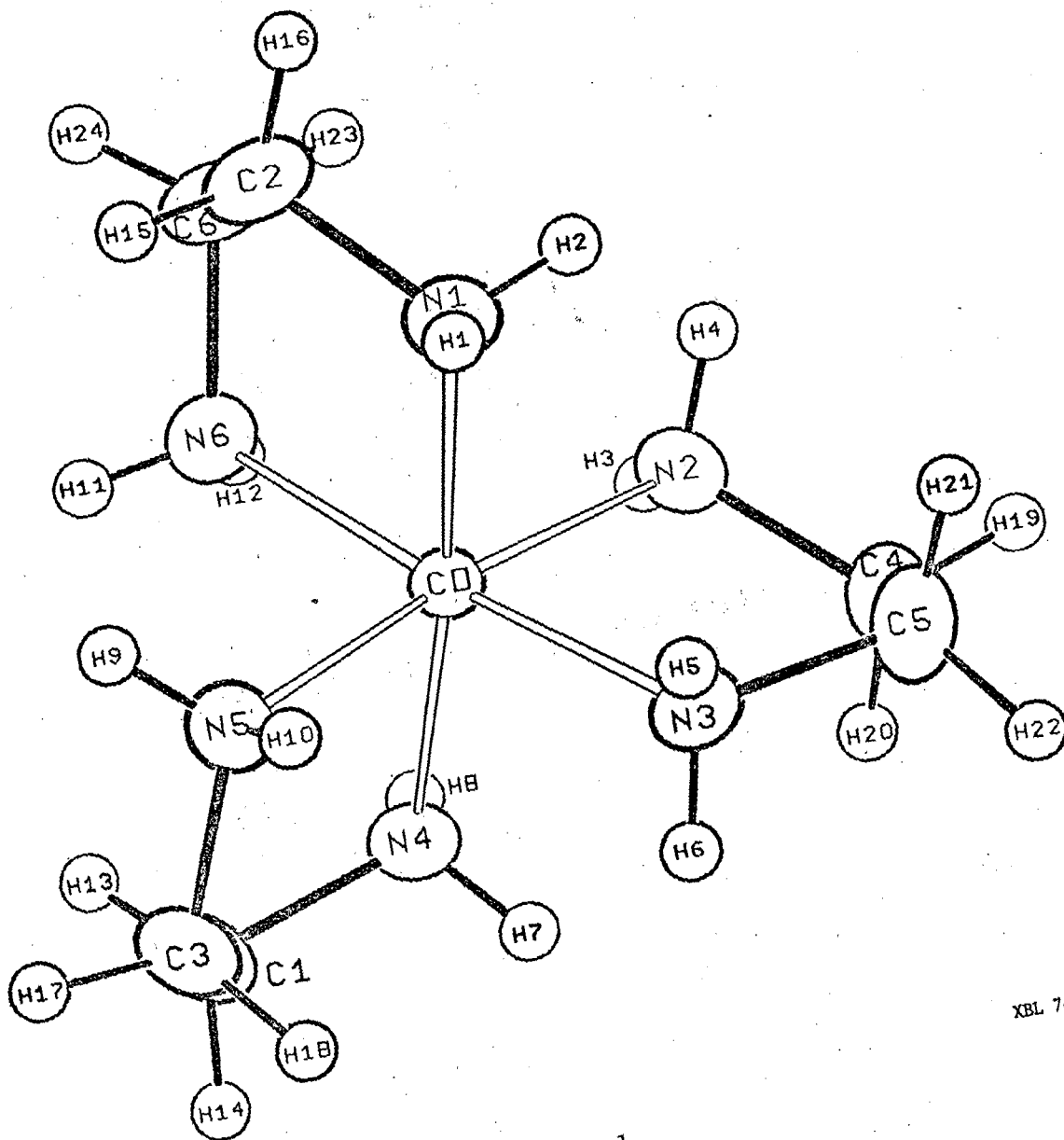
<sup>a</sup>Cromer and Liberman (1970) at  $K\alpha_1$ .

<sup>b</sup> $\text{MoK}\bar{\alpha}$ .

<sup>c</sup> $\text{CuK}\bar{\alpha}$ .

FIGURE CAPTIONS

- Fig. 1. The  $\text{Co(en)}_3^{3+}$  ion.
- Fig. 2. The (+)-tartrate ion,  $(\text{C}_4\text{H}_4\text{O}_4)^{2-}$ .
- Fig. 3. Packing diagram as viewed down the pseudo three-fold axis of the cation.



XBL 745-895

Fig. 1

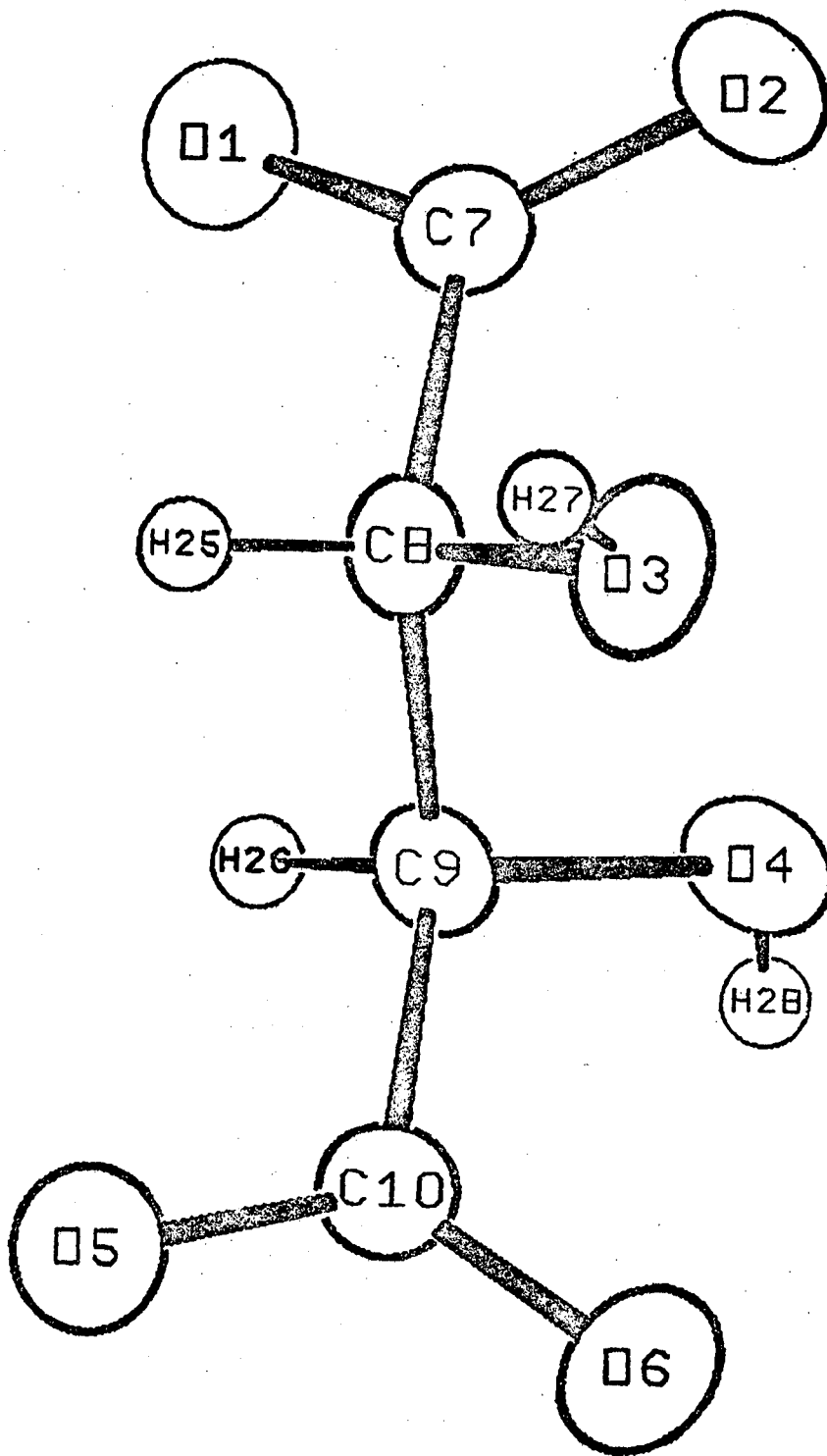
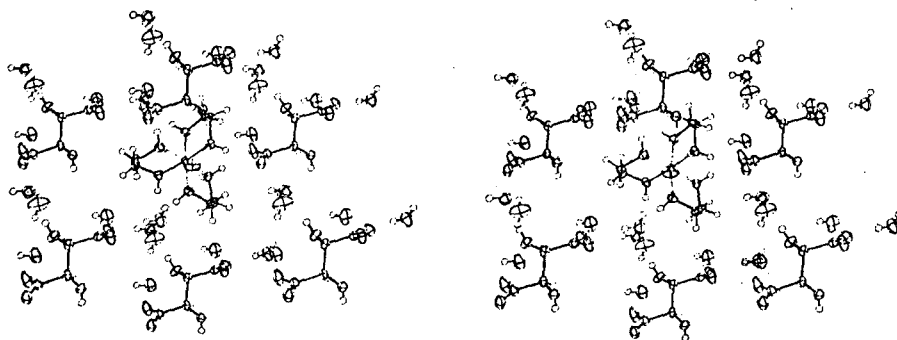


Fig. 2

XBL 745-897





XPL 731-82

Fig. 3

SUPPLEMENTARY MATERIALS FOR THE PAPER:

"Anomalous Scattering by Cobalt and Chlorine and  
Crystal Structure of (+)-tris(ethylenediamine)  
cobalt(III) Chloride (+)-tartrate Pentahydrate"

by David H. Templeton, Allan Zalkin, Helena W. Ruben and Lieselotte  
K. Templeton

Isotropic Thermal Parameters of  $d\text{-}[\text{Co}(\text{C}_2\text{H}_8\text{N}_2)_3] \text{Cl}(\text{C}_4\text{H}_4\text{O}_6) \cdot 5\text{H}_2\text{O}$

ATOM	B ( $\text{\AA}$ )
H(1)	2.6(4)
H(2)	2.4(3)
H(3)	2.5(3)
H(4)	2.7(3)
H(5)	3.2(4)
H(6)	2.2(3)
H(7)	2.3(3)
H(8)	2.5(4)
H(9)	2.0(3)
H(10)	3.1(4)
H(11)	1.7(3)
H(12)	2.7(4)
H(13)	4.8(5)
H(14)	4.1(4)
H(15)	2.9(3)
H(16)	4.3(5)
H(17)	2.9(3)
H(18)	3.0(4)
H(19)	3.5(4)
H(20)	4.5(5)
H(21)	2.5(3)
H(22)	3.5(4)
H(23)	4.9(5)
H(24)	3.7(4)
H(25)	1.9(3)
H(26)	2.2(3)
H(27)	3.4(4)
H(28)	4.2(5)
H(29)	6.3(7)
H(30)	4.4(5)
H(31)	4.8(5)
H(32)	4.4(6)
H(33)	5.6(7)
H(34)	5.2(6)
H(35)	6.6(7)
H(36)	6.5(7)
H(37)	4.9(6)
H(38)	7.3(8)

Anisotropic Thermal Parameters of  $d\text{-}[\text{Co}(\text{C}_2\text{H}_8\text{N}_2)_3] \text{Cl}(\text{C}_4\text{H}_4\text{O}_6) \cdot 5\text{H}_2\text{O}^a$

ATOM	B11	B22	B33	B12	B13	B23
CO	1.491(4)	1.418(4)	1.401(4)	.315(3)	.268(3)	.313(3)
CL	2.88(1)	3.76(2)	3.66(2)	.77(1)	.58(1)	-.89(1)
N(1)	2.44(4)	1.77(4)	2.20(4)	.48(3)	.45(3)	.40(3)
N(2)	1.88(4)	2.11(4)	2.33(4)	.33(3)	.51(3)	.33(3)
N(3)	2.39(4)	2.14(4)	1.67(4)	.59(3)	.44(3)	.57(3)
N(4)	2.25(4)	1.70(4)	2.18(4)	.47(3)	.50(3)	.47(3)
N(5)	1.95(4)	2.17(4)	2.40(4)	.55(3)	.32(3)	.44(3)
N(6)	2.72(5)	2.34(5)	1.77(4)	.50(4)	.30(4)	.34(3)
C(1)	2.57(5)	1.86(4)	3.25(5)	-.05(3)	.19(4)	.14(4)
C(2)	3.66(6)	2.33(5)	2.81(5)	.94(4)	.44(4)	1.22(4)
C(3)	1.96(4)	2.56(5)	3.49(6)	.06(4)	.64(4)	.77(4)
C(4)	2.00(4)	3.28(5)	3.06(5)	.77(4)	-.06(4)	.78(4)
C(5)	2.67(5)	4.02(7)	2.13(5)	.69(5)	-.23(4)	.30(4)
C(6)	3.92(6)	2.74(5)	2.07(4)	.55(4)	.75(4)	1.04(4)
C(7)	1.81(4)	2.06(4)	2.42(4)	.47(3)	.34(3)	.67(3)
C(8)	2.21(4)	1.96(4)	1.86(4)	.87(3)	.47(3)	.48(3)
C(9)	2.46(4)	1.55(3)	1.86(4)	.59(3)	.42(3)	.55(3)
C(10)	2.46(4)	2.05(4)	3.02(5)	.78(3)	.76(4)	1.17(4)
O(1)	4.60(5)	3.21(4)	3.31(4)	1.34(4)	2.08(4)	1.40(3)
O(2)	3.34(4)	2.00(3)	3.43(4)	.65(3)	.58(3)	.62(3)
O(3)	2.56(3)	3.41(4)	1.81(3)	1.24(3)	.19(3)	.41(3)
O(4)	2.17(3)	1.84(3)	3.25(4)	.52(3)	-.34(3)	.72(3)
O(5)	4.47(5)	2.88(4)	6.60(7)	2.10(4)	2.75(5)	2.82(5)
O(6)	3.26(4)	3.63(4)	3.23(4)	1.27(3)	1.37(3)	1.77(3)
O(7)	3.20(4)	2.83(4)	3.19(4)	.59(3)	.14(3)	.31(4)
O(8)	4.44(6)	3.98(5)	4.46(6)	1.63(5)	2.14(5)	1.64(5)
O(9)	4.98(7)	4.49(6)	5.04(7)	2.08(5)	1.98(5)	1.90(5)
O(10)	5.10(6)	3.43(5)	2.91(4)	.62(4)	1.03(4)	1.16(4)
O(11)	3.73(6)	6.73(9)	5.79(8)	2.62(6)	.30(5)	-1.59(6)

<sup>a</sup> The form of the temperature factor ( $B_{ij}$  in units of  $\text{Å}^2$ ) is  $T = \exp$   
 $[-0.25(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^* + 2B_{13}hla^*c^* +$   
 $2B_{23}k\ell b^*c^*)]$ .

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X13.0) FOR D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O F(0,0,0) = 3543

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS. SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/. \* INDICATES ZERO WEIGHTED DATA.

Table with 16 columns: L, FOB, SG, DEL, L, FOB, SG, DEL, L, FOB, SG, DEL, L, FOB, SG, DEL, L, FOB, SG, DEL. Rows contain numerical data with various annotations like H,K=-12, H,K=-11, H,K=-10, and asterisks indicating zero weighted data.

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
-2	22	6	-1	-3	56	3	0	H,K=-9,	-3	3	161	3	0	6	99	2	2			
-1	28	4	-4	-2	28	4	0	-4	70	3	1	4	38	5	-2	7	45	4	-4	
0	104	2	1	-1	99	2	2	-3	87	3	2	5	141	3	-1	8	49	3	5	
1	35	3	-2	0	47	7	-4	-2	76	2	1	6	109	2	-1	H,K=-9,		4		
2	43	3	-3	1	81	5	-1	-1	117	4	2	7	79	3	-1	-7	62	3	4	
3	64	2	-2	2	95	4	4	0	64	2	-3	8	71	6	-2	-6	68	2	-1	
4	37	7	1	3	23	6	-5	1	97	3	-2	9	76	8	-3	-5	48	3	2	
5	47	2	2	4	15	16	9*	2	111	3	-2	H,K=-9,		1	-4	98	2	-1		
6	48	4	-4	5	54	2	4	3	80	4	-2	-7	61	6	4	-3	130	2	2	
7	36	4	4	H,K=-10,				4	72	4	-4	-6	26	27	-4*	-2	71	2	0	
H,K=-10,				4	-4	57	4	-2	5	87	2	-3	-5	91	4	-1	-1	65	2	2
-6	41	4	-3	-3	21	8	3	6	80	3	-1	-4	95	2	3	0	155	3	-2	
-5	43	5	-7	-2	73	5	-0	7	46	3	1	-3	110	2	-3	1	116	2	-3	
-4	48	3	-2	-1	4	17	-3*	8	60	3	1	-2	111	2	1	2	50	3	-6	
-3	59	2	2	0	43	4	-4	H,K=-9,		-2	-1	111	2	-4	3	164	3	1		
-2	54	2	6	1	73	2	0	-5	96	3	4	0	122	2	-0	4	42	5	0	
-1	59	2	1	2	44	4	3	-4	67	4	3	1	98	2	-5	5	116	2	-2	
0	74	2	-1	3	13	17	2*	-3	89	2	-1	2	145	3	-4	6	125	3	4	
1	87	2	-3	4	54	8	2	-2	119	3	-0	3	125	2	-4	7	65	2	6	
2	116	2	-0	H,K=-10,				9	-1	77	4	-2	4	111	2	-3	8	77	3	-5
3	50	3	4	-3	102	2	6	0	31	6	-12	5	92	2	-0	H,K=-9,		5		
4	10	15	-2*	-2	41	5	2	1	108	2	-5	6	168	3	3	-7	78	3	-1	
5	86	3	-3	-1	14	20	-6*	2	107	2	-1	7	60	3	0	-6	73	3	1	
6	54	3	1	0	87	3	-2	3	21	5	-1	8	57	3	-1	-5	90	2	-1	
7	42	5	4	1	51	4	3	4	106	2	-3	9	129	3	4	-4	90	3	-2	
H,K=-10,				5	2	63	2	3	5	103	3	2	H,K=-9,		2	-3	65	3	-4	
-6	43	5	-5	H,K=-9,				-6	6	61	3	0	-7	83	3	4	-2	149	3	1
-5	34	6	-8	0	38	4	5	7	48	3	-2	-6	91	2	1	-1	155	3	-1	
-4	53	3	-1	1	58	4	-1	8	58	6	-1	-5	64	3	-1	0	69	2	-1	
-3	87	4	2	2	82	3	2	9	59	4	-4	-4	61	3	-1	1	164	3	0	
-2	75	4	-6	3	55	3	1	H,K=-9,		-1	-3	121	2	2	2	195	4	-2		
-1	57	2	2	4	36	8	-7	-6	106	3	5	-2	156	3	2	3	67	2	-4	
0	74	2	0	5	55	5	0	-5	32	8	4	-1	72	3	-1	4	111	2	2	
1	119	2	0	H,K=-9,				-5	-4	40	4	0	0	90	2	-5	5	200	3	0
2	46	2	2	-2	80	5	1	-3	125	3	2	1	187	3	-5	6	82	2	2	
3	42	3	1	-1	35	5	-3	-2	83	2	-3	2	97	3	-2	7	60	3	-1	
4	134	2	2	0	0	26	-19*	-1	48	2	-5	3	48	7	-3	H,K=-9,		6		
5	71	2	4	1	63	2	3	0	93	4	-1	4	164	3	1	-7	87	3	2	
6	51	3	-1	2	59	3	0	1	158	3	-3	5	131	3	1	-6	67	3	3	
7	86	3	0	3	38	5	-1	2	32	4	-4	6	89	3	-1	-5	79	2	2	
H,K=-10,				6	4	63	5	0	3	64	2	2	7	76	3	6	-4	62	3	-5
-6	46	5	4	5	75	3	0	4	132	2	-4	8	57	6	-1	-3	114	2	-1	
-5	46	6	-3	6	38	4	3	5	96	2	-2	9	18	14	-5	-2	117	2	-1	
-4	92	3	0	7	64	4	3	6	103	3	2	H,K=-9,		3	-1	101	2	-3		
-3	97	3	-4	H,K=-9,				-4	7	86	2	2	-7	115	3	1	0	170	3	1
-2	57	3	-5	-3	67	6	-0	8	29	5	7	-6	65	3	-3	1	90	2	-2	
-1	56	2	-1	-2	40	9	-2	9	69	3	2	-5	42	4	-0	2	67	4	-2	
0	110	2	4	-1	0	18	-21*	H,K=-9,		0	-4	75	2	1	3	63	2	2		
1	111	3	-1	0	106	2	4	-6	40	5	-6	-3	135	3	3	4	151	3	-0	
2	62	4	-2	1	53	3	-4	-5	28	7	-6	-2	97	2	2	5	85	5	1	
3	106	4	-1	2	45	4	-6	-4	98	4	0	-1	138	2	-4	6	52	3	2	
4	69	3	2	3	80	2	-0	-3	90	4	-1	0	177	3	-3	7	69	3	4	
5	80	2	2	4	88	2	-1	-2	135	3	-1	1	59	3	-2	H,K=-9,		7		
6	65	2	2	5	84	3	-2	-1	119	2	-3	2	62	2	-7	-7	48	4	1	
H,K=-10,				7	6	78	2	3	0	125	2	-5	3	118	3	-1	-6	77	3	1
-5	46	4	-0	7	70	4	-3	1	91	2	-5	4	79	2	1	-5	52	3	-1	
-4	97	4	1	8	38	11	-3	2	105	3	-5	5	78	2	-2	-4	77	3	1	

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-3	111	2	0	2	70	3	-1	-3	139	3	1	-4	170	3	-4	-5	65	5	-0
-2	36	6	-6	3	82	2	4	-2	128	2	-2	-3	168	3	-0	-4	113	2	4
-1	87	2	3	4	51	5	-2	-1	128	2	-3	-2	90	2	1	-3	170	3	-2
0	96	2	1	5	63	7	1	0	125	2	-5	-1	195	4	1	-2	114	3	-3
1	102	2	-1	6	83	2	1	1	56	5	-6	0	155	3	-3	-1	82	2	-1
2	87	2	-1	7	57	5	2	2	221	4	-3	1	141	2	-3	0	144	2	1
3	44	5	-3		H,K=-8,	-5		3	185	3	-1	2	200	3	-3	1	181	3	0
4	65	5	-1	-4	60	3	3	4	94	2	-2	3	208	3	-3	2	70	2	-3
5	53	5	-2	-3	63	3	-2	5	165	3	1	4	191	4	1	3	138	2	0
6	74	3	1	-2	61	4	7	6	76	2	0	5	177	3	0	4	188	3	-1
	H,K=-9,	8		-1	71	3	1	7	70	4	-4	6	98	2	1	5	85	3	-1
-6	59	6	2	0	21	13	2	8	102	2	4	7	96	2	-1	6	130	2	0
-5	60	4	0	1	43	6	-2	9	79	3	3	8	61	3	-1	7	67	2	2
-4	121	4	1	2	136	3	2	10	61	4	-3	9	117	3	0	8	64	4	1
-3	17	9	6	3	87	2	1		H,K=-8,	-1		10	69	4	-6	9	113	3	6
-2	65	6	-3	4	48	4	-2	-7	45	8	-2		H,K=-8,	2		H,K=-8,	5		
-1	103	3	-2	5	82	2	2	-6	73	4	-2	-8	95	3	2	-8	70	3	3
0	69	3	-0	6	102	2	2	-5	99	2	-1	-7	102	2	3	-7	59	3	1
1	88	2	1	7	37	4	-3	-4	90	3	2	-6	68	3	1	-6	39	4	-2
2	84	2	5	8	76	3	1	-3	135	2	2	-5	108	2	1	-5	78	2	7
3	79	3	1		H,K=-8,	-4		-2	112	2	1	-4	208	4	-3	-4	151	3	4
4	35	4	2	-5	59	2	4	-1	130	2	-2	-3	109	3	-4	-3	94	2	-1
5	105	2	5	-4	32	4	5	0	59	2	-3	-2	183	3	-2	-2	137	3	-4
	H,K=-9,	9		-3	110	2	4	1	186	3	-5	-1	169	3	-2	-1	100	3	-1
-5	77	3	4	-2	95	3	3	2	185	3	-5	0	79	2	-1	0	109	2	-0
-4	39	4	1	-1	47	3	-3	3	32	3	4	1	240	4	-3	1	142	3	1
-3	88	3	0	0	112	3	-2	4	150	3	-1	2	186	3	-4	2	162	3	-3
-2	77	3	-2	1	189	4	2	5	102	3	1	3	126	3	-2	3	147	3	-2
-1	49	6	-2	2	75	2	2	6	95	2	-1	4	81	2	-0	4	73	2	0
0	95	3	0	3	104	2	-2	7	61	3	-2	5	164	3	5	5	112	3	-4
1	122	3	1	4	132	2	4	8	96	3	1	6	93	2	3	6	107	2	3
2	50	3	4	5	75	2	0	9	93	2	2	7	40	4	-7	7	35	13	3
3	43	4	8	6	88	2	-3	10	55	5	-4	8	84	3	1	8	81	3	-3
4	141	4	0	7	116	2	2		H,K=-8,	0		9	82	3	4		H,K=-8,	6	
	H,K=-9,	10		8	83	3	-1	-7	74	5	0		H,K=-8,	3		-8	69	6	1
-4	77	3	2	9	62	3	0	-6	87	3	2	-8	73	4	-2	-7	69	2	4
-3	76	3	3		H,K=-8,	-3		-5	34	3	4	-7	100	2	0	-6	58	3	-3
-2	76	3	2	-6	92	3	2	-4	76	4	-3	-6	59	3	0	-5	80	2	1
-1	95	3	4	-5	41	3	7	-3	114	2	-1	-5	96	2	-1	-4	92	2	0
0	84	2	6	-4	104	2	-1	-2	104	2	-2	-4	61	3	1	-3	97	2	-2
1	102	5	2	-3	158	3	5	-1	87	2	-0	-3	143	2	-2	-2	134	3	0
2	50	6	-4	-2	111	2	1	0	154	3	-3	-2	122	3	-3	-1	129	2	1
	H,K=-8,	-7		-1	97	3	-1	1	117	2	2	-1	110	2	1	0	114	2	-2
-1	68	5	5	0	161	3	0	2	104	2	-3	0	172	3	-3	1	144	3	2
0	109	3	6	1	136	3	-5	3	150	3	-7	1	176	3	-2	2	145	3	-0
1	117	5	3	2	117	2	1	4	98	2	3	2	137	2	2	3	44	7	-6
2	105	4	2	3	170	3	-1	5	119	2	0	3	91	2	-4	4	94	3	1
3	80	3	-1	4	77	2	-3	6	171	3	-2	4	163	3	3	5	153	3	3
4	84	3	-1	5	126	3	-2	7	109	2	2	5	141	2	2	6	32	5	1
5	47	5	-3	6	133	3	-0	8	98	2	-1	6	53	3	-5	7	26	6	1
6	89	4	4	7	112	3	-3	9	81	3	1	7	107	2	3	8	93	4	-3
	H,K=-8,	-6		8	63	2	5	10	95	3	1	8	99	3	2		H,K=-8,	7	
-3	80	4	-5	9	88	3	-2		H,K=-8,	1		9	71	3	-3	-8	103	3	3
-2	84	5	-2		H,K=-8,	-2		-8	60	3	-3		H,K=-8,	4		-7	73	4	1
-1	55	4	1	-6	60	3	3	-7	90	3	2	-8	89	2	4	-6	58	3	2
0	83	3	2	-5	69	4	-4	-6	24	11	-14	-7	62	3	-2	-5	86	2	0
1	72	2	-1	-4	152	3	7	-5	69	4	-4	-6	70	2	-1	-4	46	4	-1

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
-3	181	3	2	-1	84	3	3	-2	99	2	0	-3	43	3	-2	-8	107	2	6	
-2	99	2	-2	0	76	3	-1	-1	115	2	3	-2	103	2	1	-7	75	3	-1	
-1	50	2	2	1	87	4	3	0	84	3	-4	-1	85	5	-2	-6	45	5	1	
0	127	2	1	2	94	4	-5	1	169	3	-2	0	110	3	5	-5	33	3	1	
1	91	4	-2	3	83	4	2	2	114	2	-1	1	79	2	-3	-4	229	4	-0	
2	23	5	2	4	56	3	2	3	68	3	2	2	126	2	-3	-3	99	2	-2	
3	53	3	-3	5	101	4	-0	4	155	3	-0	3	63	2	-1	-2	111	3	-0	
4	118	3	1	6	102	3	5	5	131	3	3	4	30	2	4	-1	182	3	-2	
5	58	2	5	H,K=-7,				6	143	3	2	5	198	3	-1	0	158	3	-0	
6	54	4	-1	-3	87	3	0	7	75	5	-6	6	105	2	1	1	232	4	4	
7	67	3	0	-2	67	4	2	8	120	2	1	7	12	27	-3*	2	231	4	-0	
H,K=-8,				-1	94	2	3	9	110	2	4	8	67	3	0	3	122	2	4	
-7	64	3	3	0	59	4	-4	10	65	3	1	9	109	2	2	4	95	2	-1	
-6	38	5	-6	1	106	3	6	H,K=-7,		-3	10	63	6	-3	5	137	3	-4		
-5	30	6	-2	2	93	3	4	-7	57	3	4	H,K=-7,		0	6	94	3	4		
-4	92	3	1	3	40	4	1	-6	85	3	-3	-8	46	4	2	7	83	3	2	
-3	88	2	-4	4	87	4	-1	-5	100	2	3	-7	53	3	0	8	77	2	2	
-2	12	27	2*	5	48	10	2	-4	88	2	2	-6	62	2	1	9	53	3	1	
-1	62	2	2	6	82	3	-0	-3	128	2	4	-5	116	2	-2	10	75	2	4	
0	83	2	5	7	65	4	-4	-2	161	3	-0	-4	76	2	5	H,K=-7,			3	
1	46	8	-4	8	60	3	4	-1	48	3	-3	-3	91	3	-3	-9	63	3	1	
2	64	2	0	H,K=-7,				-6	0	144	2	-2	-2	130	2	-4	-8	33	12	3
3	133	3	8	-4	73	7	-5	1	290	5	-1	-1	96	2	5	-7	79	2	2	
4	32	5	-5	-3	60	2	7	2	128	2	-4	0	116	2	4	-6	70	2	-2	
5	62	2	2	-2	88	3	2	3	76	3	-1	1	283	5	-1	-5	95	2	1	
6	61	7	-2	-1	56	3	-1	4	189	4	-3	2	169	3	-2	-4	84	2	-1	
H,K=-8,				9	0	74	2	5	5	140	3	-1	3	175	3	-2	-3	80	2	-2
-6	15	17	-6*	1	115	3	-3	6	158	4	-2	4	84	2	-1	-2	155	3	-1	
-5	44	4	2	2	60	2	1	7	100	2	1	5	193	3	-1	-1	170	3	1	
-4	69	2	0	3	69	2	3	8	63	4	-3	6	153	3	-1	0	126	2	1	
-3	64	5	2	4	74	2	-3	9	71	2	3	7	114	2	2	1	115	2	4	
-2	56	4	2	5	82	2	2	10	60	11	-1	8	115	2	0	2	181	3	1	
-1	103	2	2	6	51	4	-2	H,K=-7,		-2	9	64	2	1	3	83	2	1		
0	74	2	-0	7	71	3	1	-7	106	4	3	10	40	9	-4	4	87	2	0	
1	88	4	-5	8	48	4	1	-6	91	3	-0	H,K=-7,		1	5	126	2	-1		
2	88	4	0	9	36	5	0	-5	38	5	-2	-9	32	5	-0	6	81	3	4	
3	60	3	1	H,K=-7,		-5	-4	107	4	-4	-8	75	2	6	7	59	2	1		
4	77	3	0	-5	36	5	-3	-3	144	3	2	-7	79	7	-2	8	105	2	6	
5	102	3	5	-4	68	3	0	-2	82	2	-2	-6	127	2	4	9	56	3	0	
H,K=-8,				10	-3	85	3	2	-1	87	2	0	-5	103	3	-4	10	31	5	0
-5	0	23	-11*	-2	62	2	1	0	198	3	-1	-4	83	2	4	H,K=-7,			4	
-4	76	11	-0	-1	84	2	-0	1	51	2	-4	-3	229	4	-1	-9	34	5	-1	
-3	85	3	2	0	136	3	1	2	113	3	-3	-2	32	3	-3	-8	54	5	5	
-2	93	4	4	1	12	16	-11*	3	134	3	-0	-1	130	2	2	-7	48	8	-1	
-1	76	3	-2	2	99	2	-3	4	17	7	-5	0	289	5	0	-6	88	4	2	
0	55	5	-2	3	113	2	-2	5	123	2	1	1	179	3	1	-5	69	5	1	
1	77	4	-4	4	31	4	4	6	99	2	3	2	175	3	-3	-4	27	4	-1	
2	0	22	-18*	5	103	2	-0	7	21	5	6	3	117	2	1	-3	88	2	-1	
3	41	3	6	6	90	2	2	8	28	4	-1	4	221	4	3	-2	45	2	2	
H,K=-8,				11	7	82	3	3	9	73	2	7	5	92	3	-1	-1	50	2	0
-4	48	4	2	8	14	16	2*	10	53	4	-3	6	109	2	-2	0	64	2	-1	
-3	60	4	-1	9	85	3	-0	H,K=-7,		-1	7	124	2	4	1	232	4	-1		
-2	0	20	-26*	H,K=-7,		-4	-8	74	3	1	8	23	10	-2	2	72	2	-4		
-1	21	15	5	-6	31	6	-4	-7	56	2	6	9	86	3	2	3	62	3	3	
0	91	3	-0	-5	63	3	1	-6	22	7	1	10	47	4	-4	4	240	4	-1	
1	27	9	13	-4	82	2	6	-5	80	3	6	H,K=-7,		2	5	44	3	-2		
H,K=-7,				-8	-3	69	3	-4	-4	86	4	0	-9	37	5	-8	6	39	9	-3



OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	90	3	4	5	89	2	2	-1	9	20	-9*	-3	97	2	1	-6	101	2	-0
8	89	2	1	6	17	9	15	0	40	5	3	-2	72	3	1	-5	75	3	-1
9	27	6	-1	7	50	4	-3	1	62	3	3	-1	26	11	1	-4	67	2	-2
				H,K=-7,	5			2	52	4	-4	0	117	3	0	-3	126	3	-2
-9	34	6	-6	-8	20	15	-11	3	53	3	4	1	63	2	-1	-2	98	2	-4
-8	36	4	4	-7	28	7	-6	4	58	4	6	2	85	2	-2	-1	82	2	1
-7	87	2	2	-6	27	7	3	5	48	4	-2	3	74	2	1	0	59	3	5
-6	31	3	1	-5	45	2	2	6	57	5	3	4	85	3	-2	1	170	3	-3
-5	49	3	1	-4	43	4	0		H,K=-6,	-8	5	101	3	0	2	24	4	6	
-4	115	2	-0	-3	69	4	1	-3	43	4	0	6	124	2	-1	3	66	2	1
-3	156	3	2	-2	57	2	2	-2	59	3	2	7	89	3	-2	4	122	2	-1
-2	93	3	-1	-1	48	4	-4	-1	40	5	-2	8	35	5	1	5	72	2	2
-1	157	3	2	0	119	2	2	0	75	3	-1	9	84	2	1	6	75	3	-5
0	120	2	-0	1	73	3	3	1	38	12	-1	10	84	5	3	7	68	2	-1
1	170	3	3	2	20	6	-2	2	60	3	-1		H,K=-6,	-4	8	38	5	-2	
2	148	2	-2	3	108	2	5	3	58	8	-4	-7	65	3	1	9	60	3	-2
3	140	2	2	4	111	3	5	4	0	32	-9*	-6	37	3	4	10	38	10	-0
4	141	3	-1	5	25	5	4	5	105	5	4	-5	19	10	-5	11	38	6	-1
5	68	2	-1	6	57	4	-1	6	80	3	-1	-4	97	3	2		H,K=-6,	-1	
6	72	2	-4	7	61	6	4	7	54	3	-2	-3	80	2	-2	-9	33	5	-1
7	85	4	7		H,K=-7,	9		8	29	7	3	-2	97	2	2	-8	66	2	2
8	27	7	-6	-7	37	5	-2		H,K=-6,	-7	-1	162	3	2	-7	86	2	-2	
9	83	4	0	-6	20	8	5	-4	48	5	3	0	101	3	-3	-6	57	3	1
				H,K=-7,	6			-3	88	4	1	1	54	2	-2	-5	20	6	-10
-9	67	3	-5	-4	116	2	6	-2	83	2	4	2	116	2	-3	-4	118	2	-0
-8	70	2	2	-3	112	2	1	-1	95	2	2	3	143	3	-0	-3	135	2	-6
-7	58	3	5	-2	51	3	1	0	69	2	4	4	128	3	-1	-2	89	2	6
-6	86	2	3	-1	66	3	1	1	38	3	5	5	139	2	0	-1	184	3	-2
-5	136	3	3	0	126	5	-4	2	128	3	2	6	122	2	-0	0	195	3	2
-4	160	3	2	1	15	11	6	3	78	2	3	7	80	2	1	1	44	2	5
-3	139	3	-2	2	101	4	4	4	57	3	-1	8	90	2	-1	2	145	2	-2
-2	138	2	4	3	73	2	4	5	84	2	1	9	91	3	0	3	135	2	-2
-1	172	3	1	4	59	5	2	6	93	2	1	10	56	4	-2	4	141	3	-2
0	131	2	-1	5	49	6	-2	7	58	3	-1		H,K=-6,	-3	5	147	3	2	
1	106	3	4		H,K=-7,	10		8	12	25	-2*	-8	51	7	-0	6	151	3	-3
2	121	2	1	-7	47	4	-2	9	67	3	3	-7	86	4	4	7	41	6	-5
3	117	2	0	-6	57	4	-4		H,K=-6,	-6	-6	-6	49	4	-8	8	30	4	-7
4	84	2	3	-5	53	4	-4	-5	32	10	-6	-5	102	2	-1	9	125	2	1
5	97	2	3	-4	85	4	-0	-4	79	2	5	-4	83	2	-3	10	55	2	2
6	65	3	1	-3	90	3	3	-3	82	2	1	-3	67	7	-3	11	36	6	-4
7	13	16	2*	-2	42	5	-7	-2	75	2	-1	-2	154	3	4		H,K=-6,	0	
8	63	3	-0	-1	77	3	-1	-1	68	2	-2	-1	73	2	-2	-9	25	25	-11*
				H,K=-7,	7			0	73	2	3	0	74	2	-1	-8	80	3	1
-9	38	5	-3	1	93	2	2	1	121	2	3	1	221	4	-2	-7	85	2	-3
-8	81	3	1	2	43	4	3	2	79	2	0	2	179	3	4	-6	40	3	1
-7	71	2	3	3	32	5	4	3	48	7	-4	3	42	4	-4	-5	102	2	-0
-6	60	3	2	4	66	3	2	4	60	2	2	4	128	2	-2	-4	142	3	0
-5	77	4	-2		H,K=-7,	11		5	74	2	1	5	163	3	-1	-3	95	3	2
-4	86	2	2	-5	61	3	4	6	72	2	3	6	75	2	-1	-2	277	4	0
-3	16	8	4	-4	37	4	1	7	39	4	8	7	56	4	-2	-1	118	2	-2
-2	67	3	-1	-3	57	6	-1	8	81	2	5	8	93	2	3	0	167	3	-1
-1	27	4	4	-2	56	3	-1	9	0	22	-16*	9	78	2	3	1	186	3	-4
0	55	4	-0	-1	22	7	2	10	68	3	0	10	34	4	-2	2	197	3	-2
1	138	3	2	0	93	3	-2		H,K=-6,	-5	11	22	13	-11	3	169	3	-4	
2	0	23	-16*	1	50	4	-5	-6	44	8	2		H,K=-6,	-2	4	98	2	-2	
3	14	18	-5*	2	62	3	5	-5	5	16	-5*	-8	50	7	0	5	229	4	4
4	72	2	5		H,K=-6,	-9		-4	44	11	-1	-7	52	3	3	6	125	2	-0

OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	60	3	-2	-3	147	2	2	H,K=-6,	6	H,K=-6,	9	0	17	18	9*				
8	113	2	2	-2	130	2	-2	-9	61	3	1	-8	49	4	0	1	74	3	1
9	120	2	-1	-1	116	2	2	-8	101	3	-1	-7	59	5	0	2	40	3	5
10	76	5	1	0	170	3	-1	-7	78	2	0	-6	45	4	-5	3	43	10	-1
11	37	11	2	1	83	3	-3	-6	85	2	2	-5	80	2	5	4	68	6	-3
	H,K=-6,		1	2	59	2	4	-5	108	2	1	-4	105	2	-1	5	46	5	-2
-9	43	6	1	3	141	2	0	-4	116	4	2	-3	145	3	0	6	68	4	4
-8	65	5	-0	4	47	2	1	-3	222	4	1	-2	69	2	1	7	32	21	-8
-7	38	8	5	5	138	3	-2	-2	20	13	-3	-1	76	2	2		H,K=-5,		-8
-6	81	3	0	6	87	4	6	-1	121	3	-2	0	146	3	-0	-4	74	3	4
-5	155	3	2	7	42	2	1	0	221	4	-3	1	98	2	1	-3	59	3	-1
-4	22	6	-14	8	45	4	-4	1	60	2	-1	2	46	2	4	-2	90	2	4
-3	127	2	-3	9	96	2	-3	2	82	2	2	3	129	3	0	-1	57	2	2
-2	112	2	-1	10	44	5	0	3	133	3	3	4	144	3	3	0	76	2	2
-1	122	2	-0		H,K=-6,		4	4	125	3	1	5	64	3	2	1	117	3	1
0	338	5	1	-10	25	10	3	5	26	5	5	6	60	4	-1	2	66	4	-4
1	229	4	-2	-9	49	5	4	6	117	2	1		H,K=-6,	10	3	107	3	-1	
2	170	3	7	-8	59	3	-3	7	47	4	-0	-7	86	3	3	4	66	7	-2
3	89	2	-2	-7	59	3	4	8	4	16	-1*	-6	50	7	-0	5	111	2	-0
4	295	5	-3	-6	111	2	-1	9	83	2	2	-5	89	3	3	6	121	2	-1
5	116	2	2	-5	80	2	1		H,K=-6,		7	-4	118	3	3	7	55	2	4
6	68	3	1	-4	113	2	-1	-9	52	6	3	-3	89	2	-1	8	75	2	8
7	131	2	-1	-3	113	2	-7	-8	84	2	1	-2	48	3	-4	9	67	4	2
8	100	4	-4	-2	42	2	-4	-7	84	3	4	-1	140	3	5		H,K=-5,		-7
9	60	4	-2	-1	168	3	-2	-6	42	3	-2	0	95	2	2	-5	77	5	0
10	59	4	1	0	213	3	-1	-5	73	2	2	1	79	5	-1	-4	70	3	-3
11	63	5	4	1	382	6	1	-4	148	3	1	2	116	3	-1	-3	103	2	4
	H,K=-6,		2	2	90	2	1	-3	71	2	0	3	64	5	3	-2	79	4	0
-10	46	3	5	3	97	2	-1	-2	53	2	4	4	35	8	-8	-1	98	4	-2
-9	56	2	7	4	190	3	-2	-1	98	2	2	5	56	4	-2	0	139	3	2
-8	76	2	-3	5	210	3	-1	0	106	3	-1		H,K=-6,	11	1	62	2	1	
-7	99	3	-3	6	82	2	2	1	147	3	2	-6	55	7	3	2	143	3	4
-6	124	3	-2	7	114	2	2	2	126	2	3	-5	94	3	3	3	80	4	-1
-5	77	3	-2	8	138	3	-2	3	78	2	5	-4	44	4	-2	4	88	2	1
-4	123	2	-5	9	79	3	-2	4	50	2	-1	-3	0	17	-21*	5	46	3	0
-3	282	4	-3	10	40	4	8	5	108	2	2	-2	91	2	6	6	91	4	2
-2	98	2	-1		H,K=-6,		5	6	52	2	5	-1	26	6	-7	7	85	4	-1
-1	152	2	3	-10	27	9	0	7	0	18	-14*	0	69	4	-6	8	23	8	-5
0	224	4	-1	-9	54	9	-2	8	82	4	3	1	67	3	-3	9	76	4	-2
1	156	3	-1	-8	84	4	4		H,K=-6,		8	2	25	6	-1	10	47	10	4
2	121	2	-3	-7	125	3	-0	-9	21	10	1	3	44	3	4		H,K=-5,		-6
3	69	2	-1	-6	156	3	1	-8	55	3	-1		H,K=-6,	12	-6	13	30	-5*	
4	211	4	2	-5	80	2	-1	-7	95	2	1	-4	52	3	1	-5	64	5	4
5	70	2	-1	-4	193	3	0	-6	63	3	1	-3	33	7	-2	-4	88	2	1
6	137	3	-3	-3	151	3	1	-5	50	3	-3	-2	34	7	-1	-3	42	3	-1
7	27	4	-5	-2	184	3	-3	-4	128	2	0	-1	49	6	1	-2	90	2	2
8	47	3	-2	-1	149	2	-2	-3	41	3	5	0	34	10	-0	-1	64	2	1
9	40	4	2	0	213	4	1	-2	111	2	-1		H,K=-5,-10		0	58	2	6	
10	64	3	0	1	221	4	1	-1	112	3	-1	0	0	20	-16*	1	96	2	-3
	H,K=-6,		3	2	131	2	4	0	90	2	-3	1	38	4	7	2	126	2	-2
-10	48	6	0	3	118	2	2	1	141	3	-3	2	55	3	-2	3	78	2	3
-9	58	3	2	4	182	3	-1	2	33	5	1	3	29	12	1	4	47	2	3
-8	89	2	-1	5	189	3	2	3	60	3	5	4	11	20	-7*	5	133	2	-2
-7	120	4	3	6	77	2	0	4	93	4	-4	5	40	12	4	6	47	8	-1
-6	25	4	1	7	96	3	1	5	73	3	0		H,K=-5,		-9	7	22	7	-5
-5	121	2	2	8	64	2	4	6	43	4	1	-2	45	4	-2	8	124	2	1
-4	69	2	-4	9	39	3	4	7	87	4	-1	-1	22	25	-6*	9	95	4	-2

OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
10	62	4	-4	6	86	2	-3	-4	248	4	-0	7	128	3	1	-3	157	3	-3
	H,K=-5,	-5		7	71	2	1	-3	225	4	1	8	132	2	-1	-2	230	4	-3
-7	33	5	3	8	117	2	2	-2	54	2	-2	9	75	2	-1	-1	171	3	6
-6	33	4	4	9	134	3	-3	-1	358	5	-6	10	75	2	2	0	279	4	4
-5	69	2	1	10	66	8	-1	0	326	5	-1	11	63	4	-3	1	217	4	2
-4	39	4	1	11	56	2	6	1	234	4	5		H,K=-5,	3	2	236	4	3	
-3	144	3	-2		H,K=-5,	-2		2	291	4	-3	-10	79	3	-5	3	211	3	3
-2	78	2	-1	-9	77	3	1	3	305	5	-0	-9	54	6	-1	4	142	2	5
-1	49	4	1	-8	87	3	1	4	238	4	-1	-8	104	2	-2	5	305	5	5
0	90	2	2	-7	59	2	2	5	175	4	-2	-7	210	4	1	6	78	2	1
1	160	3	-0	-6	108	2	-1	6	259	4	-2	-6	103	3	2	7	79	2	-0
2	106	2	0	-5	148	3	2	7	120	2	0	-5	120	2	-4	8	164	3	3
3	197	3	-2	-4	152	3	-1	8	81	3	-1	-4	85	2	1	9	49	4	0
4	88	2	1	-3	270	4	-3	9	124	4	-3	-3	375	6	-0		H,K=-5,	6	
5	136	3	1	-2	263	4	-5	10	118	3	-2	-2	244	4	-5	-10	53	5	2
6	101	3	-3	-1	141	2	0	11	67	2	5	-1	98	2	-2	-9	91	3	2
7	76	2	-2	0	184	3	-2		H,K=-5,	1	0	0	376	6	0	-8	148	3	0
8	103	3	3	1	260	4	-0	-10	55	5	0	1	219	3	2	-7	113	2	2
9	72	3	3	2	259	4	-3	-9	67	2	1	2	89	2	2	-6	132	2	-0
10	76	3	-1	3	100	2	2	-8	104	3	0	3	284	4	-2	-5	174	3	-1
11	54	4	-2	4	203	3	-7	-7	111	2	1	4	272	4	-1	-4	61	3	0
	H,K=-5,	-4		5	154	3	-4	-6	59	4	-5	5	108	2	2	-3	243	4	2
-8	68	3	-2	6	83	2	1	-5	223	4	-2	6	168	3	-0	-2	208	4	-1
-7	47	6	-3	7	116	2	2	-4	239	4	0	7	137	3	0	-1	193	3	-3
-6	127	3	2	8	115	2	-4	-3	264	4	1	8	63	2	1	0	264	4	-4
-5	52	3	1	9	76	2	-1	-2	392	6	-1	9	111	3	-1	1	115	2	1
-4	67	2	-1	10	74	3	-1	-1	199	3	-6	10	83	3	-1	2	90	2	-1
-3	179	3	-1	11	34	6	-10	0	131	2	3		H,K=-5,	4	3	194	3	-4	
-2	41	3	-4		H,K=-5,	-1		1	370	6	-1	-10	58	7	-1	4	220	4	3
-1	165	3	-3	-9	75	2	3	2	320	5	2	-9	63	4	-2	5	94	2	4
0	148	3	2	-8	78	2	-2	3	178	3	-0	-8	155	3	1	6	66	2	-1
1	250	4	-1	-7	71	2	2	4	227	4	-2	-7	56	2	3	7	76	4	1
2	47	2	-3	-6	138	2	1	5	250	4	-1	-6	100	2	4	8	41	6	-2
3	124	2	-1	-5	62	2	0	6	110	2	-2	-5	172	3	0	9	42	5	-9
4	207	3	-1	-4	79	2	-1	7	155	3	-0	-4	235	4	-3		H,K=-5,	7	
5	101	2	-2	-3	171	3	-4	8	119	3	-0	-3	138	2	-1	-10	39	8	2
6	142	2	2	-2	143	2	-1	9	105	2	-1	-2	173	3	-3	-9	93	2	2
7	102	2	1	-1	19	6	1	10	70	2	1	-1	341	5	-3	-8	146	3	2
8	81	3	0	0	114	2	-2	11	29	5	1	0	158	3	-1	-7	97	2	-2
9	87	2	1	1	236	4	-4		H,K=-5,	2	1	1	164	3	2	-6	38	3	-0
10	57	2	1	2	55	2	-2	-10	52	4	-4	2	322	5	-1	-5	111	2	0
11	48	8	-1	3	39	2	-1	-9	93	2	3	3	291	5	2	-4	166	3	0
	H,K=-5,	-3		4	296	5	1	-8	108	2	0	4	235	4	3	-3	145	2	1
-8	81	2	5	5	113	2	-5	-7	148	3	-2	5	138	3	2	-2	83	2	5
-7	113	2	-1	6	207	4	-3	-6	167	3	-2	6	176	3	3	-1	220	4	-2
-6	50	3	3	7	129	3	3	-5	116	2	0	7	55	3	0	0	206	3	-2
-5	56	2	2	8	100	2	-3	-4	248	4	3	8	146	4	1	1	53	4	-0
-4	208	4	4	9	99	2	-0	-3	268	4	-0	9	179	3	6	2	46	2	-0
-3	118	2	-2	10	107	2	1	-2	142	2	-2	10	28	12	-10	3	166	3	0
-2	170	3	-1	11	60	2	2	-1	220	3	-2		H,K=-5,	5	4	4	87	4	0
-1	190	3	0		H,K=-5,	0		0	197	3	1	-10	27	5	4	5	77	4	3
0	188	3	0	-10	51	3	2	1	316	5	5	-9	79	2	3	6	106	2	4
1	160	3	1	-9	34	3	6	2	45	2	2	-8	66	2	-1	7	51	3	-2
2	367	6	2	-8	70	3	-0	3	248	4	4	-7	118	3	4	8	63	3	-5
3	120	2	-1	-7	171	3	4	4	180	3	-0	-6	145	3	-3		H,K=-5,	8	
4	46	2	-1	-6	13	15	-6*	5	204	3	-1	-5	117	2	1	-9	27	18	-4
5	353	5	-2	-5	76	2	1	6	123	3	-0	-4	270	4	-2	-8	56	2	2

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-7	86	4	-2	2	75	2	1	-2	98	2	4	-6	162	3	4	6	183	3	-3
-6	61	2	1	3	26	30	-8*	-1	118	2	-0	-5	112	3	-2	7	43	3	1
-5	106	2	3		H,K=	-5,	12	0	117	2	-0	-4	77	2	-2	8	124	2	-0
-4	156	3	0	-5	88	3	1	1	225	4	-1	-3	188	3	2	9	158	3	-0
-3	93	2	-2	-4	53	10	-3	2	160	3	1	-2	216	3	-4	10	64	2	-0
-2	75	2	3	-3	45	4	-1	3	82	4	-0	-1	176	3	-3	11	74	2	-0
-1	184	3	-1	-2	53	3	6	4	131	3	2	0	253	4	1	12	74	3	2
0	104	2	-2	-1	72	3	-1	5	86	2	4	1	507	8	-0		H,K=	-4,	-1
1	138	3	3	0	50	5	-5	6	105	2	-3	2	256	4	-8	-10	38	10	-2
2	196	3	-2	1	77	4	-0	7	128	2	4	3	209	4	-0	-9	95	3	-0
3	76	3	2		H,K=	-4,-	-11	8	75	3	2	4	373	6	-2	-8	86	3	-3
4	125	2	2	2	42	8	-8	9	43	3	2	5	102	2	0	-7	86	3	4
5	181	3	2	3	46	5	-8	10	80	5	1	6	209	4	1	-6	72	2	-5
6	64	2	2		H,K=	-4,-	-10		H,K=	-4,	-6	7	222	4	-2	-5	207	3	3
7	78	3	-3	-1	35	5	-2	-7	87	4	-2	8	172	3	0	-4	151	2	-0
	H,K=	-5,	9	0	70	3	0	-6	63	3	3	9	81	4	-1	-3	125	2	-5
-9	88	2	4	1	53	6	2	-5	70	4	-3	10	77	2	-3	-2	180	3	-2
-8	92	3	-1	2	78	2	-1	-4	148	3	-2	11	75	4	-3	-1	123	2	-7
-7	45	3	2	3	30	6	-8	-3	110	2	7		H,K=	-4,	-3	0	423	7	-1
-6	110	3	6	4	26	28	8*	-2	98	2	-1	-9	65	4	-3	1	493	8	-0
-5	100	3	-2	5	66	3	1	-1	161	3	-2	-8	63	4	1	2	63	1	-4
-4	135	2	0	6	61	4	-5	0	151	3	2	-7	148	3	1	3	321	5	-1
-3	105	2	2	7	39	5	1	1	138	3	-2	-6	184	3	4	4	339	5	0
-2	141	2	-4		H,K=	-4,	-9	2	118	2	1	-5	108	2	1	5	228	4	-2
-1	144	3	-1	-3	51	10	-3	3	147	2	1	-4	236	4	-4	6	86	2	1
0	176	3	2	-2	93	4	-2	4	62	2	-2	-3	308	5	-2	7	219	4	-3
1	149	3	2	-1	88	2	2	5	93	2	-0	-2	198	3	-8	8	163	3	-1
2	66	4	1	0	44	7	-5	6	140	3	-1	-1	231	4	-4	9	103	2	1
3	122	2	-1	1	79	2	-1	7	67	2	-2	0	556	9	-9	10	103	2	1
4	173	3	3	2	136	3	1	8	51	3	-6	1	346	5	1	11	44	5	1
5	111	3	-2	3	44	2	4	9	95	3	4	2	146	3	0		H,K=	-4,	0
6	25	27	-0*	4	108	2	-0	10	50	4	-3	3	260	4	-6	-10	51	4	-7
	H,K=	-5,	10	5	132	3	3	11	57	3	-1	4	219	3	-1	-9	68	3	-0
-8	89	3	2	6	103	3	-0		H,K=	-4,	-5	5	187	3	-3	-8	94	2	1
-7	68	3	-1	7	85	4	2	-8	60	3	2	6	258	4	-3	-7	144	3	-5
-6	77	3	3	8	64	5	4	-7	89	3	1	7	54	2	3	-6	176	3	3
-5	45	2	7		H,K=	-4,	-8	-6	46	4	1	8	159	3	-5	-5	103	3	1
-4	112	3	-3	-5	64	3	0	-5	117	2	2	9	105	2	0	-4	233	4	-3
-3	116	2	1	-4	71	7	-1	-4	70	2	4	10	62	3	-5	-3	409	6	-3
-2	79	2	-2	-3	103	3	3	-3	115	2	-2	11	28	6	-5	-2	143	2	3
-1	95	3	0	-2	112	3	-0	-2	223	4	-1		H,K=	-4,	-2	-1	410	6	-0
0	129	3	1	-1	85	3	0	-1	60	2	1	-10	74	3	5	0	664	10	-17
1	82	3	-2	0	86	2	2	0	114	2	-1	-9	60	3	-3	1	533	8	-6
2	36	3	-1	1	170	3	1	1	170	3	3	-8	113	2	-0	2	208	3	5
3	72	2	-2	2	137	3	-1	2	183	3	0	-7	113	2	1	3	368	6	7
4	84	3	-4	3	96	2	5	3	132	2	-0	-6	96	2	-1	4	264	4	2
5	36	5	-1	4	117	2	0	4	162	3	4	-5	189	3	2	5	289	5	2
	H,K=	-5,	11	5	148	3	0	5	245	4	-6	-4	239	4	-2	6	235	4	-1
-7	73	3	4	6	138	3	2	6	94	3	-2	-3	206	3	-2	7	174	3	-2
-6	41	3	8	7	59	2	-0	7	157	3	3	-2	180	3	-5	8	134	2	1
-5	96	3	-2	8	89	2	1	8	87	3	3	-1	211	3	4	9	139	3	-1
-4	72	3	-1	9	71	3	7	9	135	3	-0	0	206	3	-3	10	78	3	-4
-3	31	4	-2		H,K=	-4,	-7	10	86	4	2	1	140	2	-2	11	63	2	0
-2	71	2	-1	-6	85	3	-1	11	83	3	2	2	399	6	-3		H,K=	-4,	1
-1	82	3	1	-5	60	4	1		H,K=	-4,	-4	3	197	3	0	-11	67	3	-1
0	71	4	-2	-4	78	2	1	-8	72	3	-1	4	109	2	1	-10	87	3	-1
1	35	5	-3	-3	116	3	2	-7	54	2	1	5	258	4	-0	-9	50	2	-1

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
-8	146	3	1	1	285	4	-4	H,K=-4,	6	4	74	2	1	1	32	6	-4			
-7	168	3	-2	2	210	3	-1	-11	66	3	2	5	64	6	-4	2	93	4	-2	
-6	128	2	0	3	223	4	1	-10	78	3	-0	6	107	2	2	H,K=-3,-11	0	65	4	-6
-5	181	3	1	4	134	2	-4	-9	101	2	3	7	60	5	3	0	65	4	-6	
-4	460	7	7	5	202	4	-2	-8	167	3	4	H,K=-4,	9	1	73	3	-4			
-3	404	6	0	6	103	2	-3	-7	99	2	-2	-9	57	4	-1	2	69	3	-2	
-2	74	1	-1	7	158	3	1	-6	101	2	-2	-8	78	4	-3	3	44	4	-4	
-1	581	9	-3	8	122	2	4	-5	249	4	4	-7	35	3	9	4	63	6	4	
0	506	8	-5	9	74	3	-4	-4	122	2	0	-6	87	2	-3	5	75	3	-2	
1	185	3	1	10	87	2	0	-3	190	3	-0	-5	139	3	4	6	42	5	-2	
2	442	7	6	11	57	5	-4	-2	211	3	1	-4	76	3	4	H,K=-3,-10	3	103	3	-3
3	449	7	4	H,K=-4,	4	-1	119	2	-2	-3	134	2	-4	-3	103	3	-3			
4	305	5	-3	-11	42	4	1	0	219	4	-3	-2	86	3	2	-2	69	6	0	
5	209	3	-5	-10	49	3	-2	1	223	4	-1	-1	101	3	-0	-1	35	5	-4	
6	210	3	2	-9	32	5	-6	2	75	2	5	0	109	2	-1	0	79	3	-2	
7	150	3	1	-8	106	3	-6	3	80	2	-5	1	124	2	2	1	87	3	-4	
8	161	3	-2	-7	119	2	2	4	157	3	-0	2	124	3	-3	2	54	10	-1	
9	143	3	-2	-6	83	2	-1	5	100	4	0	3	57	4	0	3	91	2	1	
10	75	2	-5	-5	115	2	-1	6	34	4	-4	4	116	2	-2	4	63	2	-1	
11	50	4	-6	-4	228	4	-2	7	117	3	-2	5	78	7	-3	5	63	3	1	
H,K=-4,	2	-3	263	4	-7	8	75	3	-2	6	32	5	1	6	100	4	-2			
-11	87	3	-3	-2	194	3	5	9	45	4	-2	H,K=-4,	10	7	64	4	-2			
-10	74	2	1	-1	404	6	6	H,K=-4,	7	-8	89	3	-0	8	79	3	-1			
-9	96	3	-5	0	192	3	-9	-10	0	27	-12*	-7	66	5	1	H,K=-3,-9	4	69	11	-4
-8	172	3	-0	1	405	6	4	-9	77	4	-2	-6	67	3	-0	-4	69	11	-4	
-7	112	2	-2	2	163	3	-1	-8	126	2	5	-5	86	2	-1	-3	77	3	0	
-6	108	2	-1	3	148	2	-2	-7	74	2	0	-4	70	4	-1	-2	69	2	0	
-5	237	4	-6	4	434	7	5	-6	73	2	-1	-3	124	3	2	-1	82	4	-2	
-4	463	7	4	5	224	4	2	-5	125	2	0	-2	127	2	-6	0	77	3	-0	
-3	255	4	1	6	170	3	-5	-4	207	4	5	-1	79	2	-1	1	80	7	-3	
-2	278	4	-4	7	148	3	-0	-3	80	2	-0	0	103	2	-0	2	79	2	-4	
-1	140	2	-6	8	110	2	-2	-2	226	4	-4	1	90	3	-5	3	121	3	-0	
0	378	6	-6	9	131	3	0	-1	97	2	3	2	8	26	-12*	4	109	2	-2	
1	567	9	8	10	67	3	-5	0	155	3	2	3	70	4	-2	5	131	3	1	
2	340	5	3	H,K=-4,	5	1	245	4	-3	4	78	5	-3	6	95	2	-1			
3	75	2	-4	-11	56	5	-2	2	48	2	-0	5	36	10	-7	7	89	2	4	
4	390	6	-3	-10	37	7	-5	3	135	2	2	H,K=-4,	11	8	93	4	1			
5	317	5	-8	-9	99	4	-3	4	162	3	0	-7	64	6	3	9	74	3	2	
6	27	7	-4	-8	135	3	-1	5	94	3	4	-6	73	3	-9	H,K=-3,-8	6	37	14	2
7	56	4	-3	-7	116	2	-1	6	103	2	2	-5	48	3	2	-6	37	14	2	
8	185	3	2	-6	64	2	-1	7	117	2	5	-4	79	3	-4	-5	70	3	-2	
9	109	2	-0	-5	249	4	-3	8	80	3	-0	-3	62	2	-1	-4	67	7	-1	
10	51	10	-10	-4	365	6	0	H,K=-4,	8	-2	37	4	-3	-3	82	2	4			
11	59	3	6	-3	261	4	-4	-10	67	7	-2	-1	67	3	1	-2	124	3	-2	
H,K=-4,	3	-2	201	3	2	-9	47	7	2	0	60	2	-2	-1	139	3	-1			
-11	57	3	2	-1	261	4	-6	-8	63	3	1	1	12	16	-7*	0	136	2	-1	
-10	47	4	-3	0	195	3	2	-7	79	2	1	2	25	16	-2	1	125	2	1	
-9	123	2	3	1	372	6	6	-6	53	4	-1	3	97	3	-1	2	170	3	-1	
-8	113	2	-2	2	371	6	-5	-5	81	2	-2	4	24	8	-1	3	88	2	-6	
-7	165	3	-2	3	227	4	3	-4	154	3	-1	H,K=-4,	12	4	129	2	-2			
-6	109	2	-1	4	136	2	2	-3	186	3	0	-6	16	19	-5*	5	208	4	1	
-5	135	2	1	5	235	4	1	-2	110	2	5	-5	72	3	2	6	86	2	-0	
-4	216	3	-4	6	127	2	-1	-1	79	3	-1	-4	49	4	-1	7	59	3	1	
-3	144	2	-3	7	17	8	3	0	187	3	1	-3	25	6	2	8	49	5	5	
-2	242	4	-1	8	115	3	-2	1	33	8	-0	-2	0	17	-11*	9	115	4	2	
-1	26	2	0	9	118	3	2	2	191	3	1	-1	80	3	-3	10	47	9	-6	
0	427	7	1	10	20	8	3	3	174	3	-0	0	25	9	-11	H,K=-3,-7	3	174	3	-0

OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-7	56	3	1	9	173	3	1	-4	132	3	-3	4	259	4	-2	H,K=-3,	-3	3	
-6	104	4	1	10	138	3	-2	-3	464	7	-8	5	333	5	4	-11	77	2	2
-5	97	3	-0	11	45	4	-1	-2	89	2	2	6	223	4	-1	-10	34	5	3
-4	76	4	-3	H,K=-3,	-3,	-4	-1	190	3	-3	7	260	4	-3	-9	59	3	-11	
-3	187	3	0	-9	49	9	-6	0	257	4	-7	8	163	3	-2	-8	84	2	0
-2	153	3	-3	-8	105	2	5	1	270	4	1	9	117	2	-4	-7	53	4	-0
-1	107	2	-2	-7	103	3	2	2	215	3	-0	10	97	2	3	-6	58	2	1
0	197	3	2	-6	74	2	-2	3	300	5	-2	11	62	2	2	-5	146	3	-1
1	163	3	-1	-5	129	2	6	4	159	2	-3	12	64	3	3	-4	31	2	3
2	131	2	-3	-4	158	3	0	5	105	2	-0	H,K=-3,	-3,	1	-3	167	3	1	
3	94	3	-4	-3	215	4	-4	6	308	5	2	-11	70	3	-1	-2	157	2	4
4	85	2	-0	-2	274	4	-3	7	98	2	-2	-10	28	9	-7	-1	80	2	-5
5	110	2	-3	-1	279	4	-2	8	48	2	1	-9	51	5	-1	0	280	4	9
6	64	3	1	0	211	4	-1	9	146	3	-4	-8	99	2	-2	1	346	5	1
7	101	2	-0	1	433	7	-3	10	64	2	-1	-7	200	3	-2	2	134	2	-6
8	56	3	-0	2	344	5	-1	11	53	10	-6	-6	278	4	4	3	150	2	3
9	64	3	4	3	38	3	2	12	63	3	-1	-5	151	2	6	4	151	2	-0
10	75	2	5	4	355	5	-5	H,K=-3,	-3,	-1	-4	226	4	-7	5	266	4	-1	
H,K=-3,	-3,	-6	5	240	4	-2	-10	48	5	4	-3	447	7	0	6	27	5	-3	
-8	52	3	0	6	109	2	-2	-9	45	5	-4	-2	334	5	-5	7	144	3	-3
-7	89	3	1	7	160	3	3	-8	168	3	3	-1	249	4	-4	8	177	3	-1
-6	119	2	2	8	138	3	-2	-7	141	2	-4	0	791	12	-19	9	66	3	-2
-5	47	2	2	9	112	4	-2	-6	71	2	-2	1	257	4	-4	10	33	5	6
-4	167	3	-2	10	70	3	2	-5	125	2	-0	2	270	4	-1	11	56	4	-3
-3	129	2	-2	11	75	4	-0	-4	292	5	1	3	412	6	12	H,K=-3,	-3,	4	
-2	113	2	3	12	44	10	-2	-3	154	2	3	4	357	5	-6	-11	29	5	1
-1	117	2	-3	H,K=-3,	-3,	-3	-2	322	5	4	5	135	2	-0	-10	37	6	4	
0	137	3	-5	-10	53	4	-2	-1	399	6	3	6	218	4	2	-9	76	2	-7
1	174	3	-1	-9	71	2	1	0	76	2	-1	7	74	2	-2	-8	47	2	-3
2	99	2	1	-8	50	3	-3	1	369	6	2	8	99	2	-3	-7	77	2	-3
3	114	2	2	-7	156	3	3	2	253	4	-3	9	62	2	6	-6	251	4	1
4	179	3	-3	-6	137	2	2	3	284	4	8	10	44	3	3	-5	180	3	-1
5	116	2	2	-5	152	3	1	4	346	5	2	11	54	5	-4	-4	123	2	-2
6	129	2	1	-4	216	4	-2	5	295	5	-4	H,K=-3,	-3,	2	-3	229	4	4	
7	53	2	-1	-3	226	4	-3	6	126	2	-4	-11	78	3	-1	-2	170	3	-6
8	145	3	4	-2	207	3	-8	7	92	3	-4	-10	78	3	-6	-1	425	7	8
9	73	2	-1	-1	143	2	4	8	163	3	-0	-9	54	3	-2	0	572	9	15
10	91	2	3	0	304	5	2	9	144	3	-3	-8	185	3	-3	1	267	4	-8
11	57	4	2	1	435	7	-7	10	75	2	-5	-7	140	2	-1	2	226	4	7
H,K=-3,	-3,	-5	2	170	3	6	11	78	2	0	-6	31	2	2	3	180	3	-2	
-8	60	4	-3	3	139	2	-3	12	73	3	-3	-5	158	3	-3	4	234	4	-0
-7	150	3	4	4	116	2	-1	H,K=-3,	-3,	0	-4	227	4	-1	5	207	3	2	
-6	40	4	2	5	279	4	0	-11	65	3	-0	-3	188	3	2	6	61	2	-3
-5	36	4	-5	6	127	2	0	-10	23	20	4	-2	158	2	-1	7	176	3	1
-4	164	3	5	7	93	2	-1	-9	46	4	1	-1	357	5	4	8	100	2	2
-3	180	3	1	8	108	2	3	-8	106	3	-3	0	239	4	-2	9	34	4	-3
-2	110	2	-2	9	111	3	1	-7	97	4	-3	1	336	5	7	10	40	4	2
-1	147	2	2	10	73	3	-7	-6	80	2	0	2	28	2	3	H,K=-3,	-3,	5	
0	314	5	-4	11	14	25	5*	-5	191	3	9	3	214	3	-10	-11	68	4	3
1	210	4	-2	12	47	5	-5	-4	186	3	6	4	128	2	6	-10	48	2	6
2	223	4	-0	H,K=-3,	-3,	-2	-3	221	3	-0	5	137	2	5	-9	113	3	-1	
3	168	3	-2	-10	60	4	-4	-2	333	5	-2	6	84	2	-0	-8	119	2	1
4	239	4	-5	-9	4	27	-19*	-1	401	6	3	7	83	2	-4	-7	112	2	-1
5	275	4	-2	-8	124	3	-3	0	808	12	-35	8	100	2	-6	-6	127	3	-4
6	235	4	0	-7	155	3	-2	1	425	7	2	9	97	3	-1	-5	91	2	-1
7	84	3	1	-6	129	2	-1	2	376	6	3	10	30	6	0	-4	329	5	-2
8	80	2	-1	-5	129	3	-1	3	188	3	-1	11	68	2	2	-3	157	3	-2



OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	277	4	-1	4	479	7	7	11	34	5	-2	-4	124	2	1	7	66	2	5
-3	157	3	-0	5	274	4	0		H,K=-2,	2	-3	111	2	-0	8	28	6	2	
-2	268	4	-5	6	239	4	-1	-11	49	3	-4	-2	72	3	-3	9	49	4	-8
-1	140	2	1	7	123	2	-2	-10	67	4	-3	-1	165	3	-1		H,K=-2,	7	
0	242	4	-2	8	200	3	-3	-9	89	2	-4	0	314	5	7	-11	43	4	-1
1	147	2	-4	9	102	2	-8	-8	90	2	1	1	302	5	-0	-10	43	3	0
2	314	5	5	10	105	2	-5	-7	197	3	2	2	386	6	2	-9	75	4	-5
3	216	3	1	11	55	4	-2	-6	15	6	8	3	113	3	-5	-8	117	2	-3
4	171	3	1	12	70	3	-1	-5	40	2	1	4	274	4	-3	-7	103	3	3
5	293	5	-1		H,K=-2,	0	-4	481	7	1	5	5	201	3	3	-6	74	3	2
6	246	4	-5	-11	22	10	-8	-3	362	5	5	6	73	2	-1	-5	31	3	2
7	64	3	0	-10	30	4	1	-2	277	4	3	7	97	2	-2	-4	142	2	-2
8	159	3	-4	-9	45	3	-4	-1	266	4	6	8	172	3	5	-3	129	3	-1
9	81	3	-6	-8	160	3	-2	0	536	8	11	9	63	4	-1	-2	121	2	1
10	37	7	1	-7	123	3	2	1	346	5	6	10	23	7	0	-1	268	4	-2
11	17	25	-19*	-6	92	2	-1	2	595	9	28		H,K=-2,	5	0	113	2	0	
12	42	5	2	-5	239	4	-4	3	229	4	-3	-11	40	4	2	1	106	2	3
	H,K=-2,	-2	-2	-4	396	6	-5	4	274	4	4	-10	0	16	-12*	2	145	2	2
-10	84	2	2	-3	222	3	-3	5	214	3	4	-9	125	2	4	3	82	2	-1
-9	80	2	0	-2	35	1	1	6	109	2	-1	-8	73	2	-3	4	109	2	-5
-8	113	2	1	-1	469	7	3	7	59	2	0	-7	114	2	-4	5	113	4	0
-7	142	3	3	0	278	4	-9	8	70	2	-1	-6	137	3	1	6	68	2	0
-6	126	2	-3	1	294	4	2	9	111	2	-2	-5	88	2	-2	7	42	4	2
-5	105	3	-3	2	391	6	11	10	41	8	0	-4	260	4	2	8	113	4	-4
-4	81	2	-5	3	232	4	-4	11	49	8	-5	-3	283	4	-2		H,K=-2,	8	
-3	234	4	1	4	405	6	10		H,K=-2,	3	-2	293	5	-8	-10	42	4	-1	
-2	149	2	4	5	321	5	-1	-11	22	17	-4	-1	42	2	-2	-9	48	3	2
-1	284	4	3	6	18	8	-0	-10	33	5	-6	0	557	8	4	-8	52	5	2
0	407	6	-1	7	34	5	-1	-9	69	2	-2	1	218	3	3	-7	105	2	2
1	249	4	7	8	167	3	-3	-8	198	3	-1	2	143	3	1	-6	104	3	-2
2	267	4	7	9	131	2	-6	-7	95	3	5	3	228	4	-4	-5	103	2	2
3	133	2	-2	10	35	6	2	-6	56	2	5	4	138	2	1	-4	68	2	-5
4	288	4	-5	11	34	14	2	-5	91	3	-2	5	126	2	4	-3	175	3	-3
5	100	2	4	12	39	18	-4	-4	188	3	-4	6	133	2	-4	-2	128	2	1
6	122	2	-1		H,K=-2,	1	-3	302	5	6	7	65	4	-0	-1	140	2	-5	
7	180	3	-1	-11	76	4	-4	-2	473	7	2	8	58	2	4	0	267	4	-3
8	31	6	-0	-10	70	2	1	-1	48	2	6	9	47	5	3	1	169	3	1
9	150	3	-1	-9	119	2	-1	0	89	2	-1	10	65	3	-2	2	125	2	-3
10	78	2	-1	-8	125	3	-2	1	306	5	12		H,K=-2,	6	3	100	2	0	
11	42	7	-1	-7	70	2	2	2	76	1	-4	-11	62	5	-0	4	144	3	-1
12	70	3	-2	-6	161	3	-1	3	148	2	-3	-10	38	5	-2	5	97	2	-0
	H,K=-2,	-1	-1	-5	318	5	-1	4	332	5	2	-9	104	2	-2	6	49	3	-0
-11	45	4	0	-4	28	3	5	5	233	4	-0	-8	162	3	3	7	124	4	1
-10	17	23	-4*	-3	259	4	-2	6	187	3	-2	-7	148	3	-1		H,K=-2,	9	
-9	43	5	1	-2	180	3	4	7	23	15	-4	-6	31	4	-1	-10	57	4	5
-8	93	3	-1	-1	547	8	3	8	111	2	-0	-5	231	4	1	-9	76	3	-1
-7	84	2	-1	0	276	4	4	9	137	3	1	-4	144	2	4	-8	96	2	-1
-6	5	12	-4*	1	595	9	11	10	51	2	3	-3	277	4	-2	-7	63	3	-4
-5	113	2	2	2	357	5	4	11	53	4	0	-2	239	4	-2	-6	137	2	2
-4	321	5	-2	3	168	3	5		H,K=-2,	4	-1	150	2	1	-5	112	3	-2	
-3	239	4	8	4	282	4	-2	-11	35	5	1	0	83	2	-0	-4	152	3	-1
-2	222	3	8	5	182	3	13	-10	31	7	-2	1	105	2	-4	-3	131	2	-2
-1	821	13	3	6	82	2	-3	-9	77	2	-1	2	108	2	2	-2	153	3	-8
0	491	8	-8	7	158	3	-1	-8	152	3	-1	3	131	2	-0	-1	139	3	-2
1	437	7	9	8	83	2	1	-7	49	2	-1	4	78	2	0	0	111	2	-1
2	254	4	3	9	52	5	-3	-6	139	2	-2	5	185	3	-1	1	66	3	-9
3	332	5	9	10	42	2	6	-5	236	4	-3	6	77	2	4	2	58	3	-0



OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	142	3	-1	3	74	2	2	H,K=-1,-7	5	306	5	-2	-11	66	5	1			
4	108	2	2	4	40	3	4	-8	82	5	2	6	73	2	1	-10	31	4	-1
5	22	6	2	5	82	4	-3	-7	100	4	4	7	146	2	1	-9	86	2	0
6	62	3	-3	6	50	3	5	-6	49	3	-1	8	125	2	-2	-8	133	3	-4
H,K=-2,10				7	42	5	5	-5	85	2	1	9	149	3	-2	-7	14	7	6
-9	99	5	-2	H,K=-1,-10				-4	164	3	0	10	70	2	0	-6	24	5	0
-8	42	5	-3	-4	43	4	1	-3	122	2	-1	11	44	4	-1	-5	275	4	0
-7	95	2	-3	-3	32	5	-3	-2	47	3	3	12	52	4	-6	-4	100	2	1
-6	58	3	-1	-2	25	16	0	-1	172	3	2	H,K=-1,-4				-3	304	5	7
-5	102	2	-1	-1	45	9	0	0	171	3	-1	-10	54	3	0	-2	227	4	12
-4	144	4	-2	0	31	5	-3	1	234	4	-0	-9	22	10	-2	-1	203	3	2
-3	40	2	4	1	65	3	-5	2	107	2	2	-8	115	2	2	0	456	7	-5
-2	89	2	-2	2	97	2	-2	3	110	3	3	-7	141	3	0	1	463	7	15
-1	105	2	-4	3	32	3	7	4	45	2	-2	-6	181	3	3	2	582	9	37
0	49	2	-1	4	96	3	-2	5	102	3	5	-5	143	3	-1	3	204	3	7
1	38	3	1	5	64	4	-0	6	148	3	-7	-4	267	4	-4	4	302	5	-2
2	82	2	-3	6	76	3	2	7	50	2	4	-3	286	5	1	5	203	3	-3
3	60	3	-5	7	65	3	1	8	39	3	2	-2	144	3	-4	6	41	2	-4
4	32	4	4	8	36	5	-1	9	61	4	3	-1	284	4	-6	7	202	3	3
5	70	6	-1	9	104	3	-3	10	60	3	-0	0	503	8	-1	8	119	2	-1
H,K=-2,11				H,K=-1,-9				11	0	18	-8*	1	427	7	2	9	125	2	-3
-8	65	3	3	-6	38	6	-5	H,K=-1,-6				2	417	6	8	10	96	2	-5
-7	49	3	1	-5	43	4	-1	-8	85	4	0	3	210	3	-5	11	61	3	0
-6	55	2	5	-4	48	4	1	-7	65	3	1	4	174	3	2	12	43	4	-2
-5	89	4	0	-3	58	5	-8	-6	54	6	0	5	197	3	5	H,K=-1,-1			
-4	6	18	-6*	-2	102	2	-5	-5	86	2	-1	6	288	4	-3	-11	55	3	-1
-3	21	9	-3	-1	77	2	-4	-4	92	2	4	7	78	2	-5	-10	0	25	-22*
-2	57	6	-3	0	40	3	-6	-3	36	2	4	8	100	2	-1	-9	91	3	-3
-1	98	2	-2	1	126	2	0	-2	62	2	0	9	80	3	-1	-8	47	3	-1
0	44	4	-7	2	117	2	-2	-1	77	2	1	10	35	4	-1	-7	142	2	-1
1	58	5	-3	3	50	2	1	0	48	2	-5	11	37	4	-4	-6	193	3	-6
2	59	9	-0	4	136	3	0	1	151	2	5	12	62	4	-4	-5	35	2	0
3	0	18	-9*	5	92	2	-2	2	135	2	-2	H,K=-1,-3				-4	249	4	-1
4	60	6	-7	6	74	2	-0	3	63	2	3	-10	31	6	-4	-3	443	7	-10
H,K=-2,12				7	60	3	-2	4	128	2	-3	-9	103	2	2	-2	380	6	5
-6	50	5	4	8	64	3	2	5	154	3	-0	-8	176	3	0	-1	103	2	6
-5	93	2	3	9	77	4	0	6	19	6	-4	-7	120	2	3	0	471	7	10
-4	41	4	0	10	81	3	-0	7	47	2	1	-6	131	2	-1	1	377	6	10
-3	47	4	-5	H,K=-1,-8				8	91	2	1	-5	138	2	-2	2	371	6	16
-2	55	5	-4	-7	65	5	-1	9	136	3	-1	-4	269	4	-3	3	470	7	8
-1	76	3	1	-6	54	8	1	10	26	13	-3	-3	188	3	4	4	198	3	4
0	69	3	-2	-5	40	6	6	11	83	3	-3	-2	232	4	5	5	181	3	1
1	41	13	0	-4	113	2	-1	H,K=-1,-5				-1	116	2	-2	6	136	2	2
2	34	4	4	-3	146	3	-0	-9	48	4	-1	0	311	5	1	7	278	4	-1
H,K=-1,-12				-2	49	3	2	-8	32	4	-1	1	712	11	17	8	129	2	-2
0	38	11	-7	-1	108	2	-3	-7	33	5	-5	2	563	9	14	9	95	3	3
1	93	3	-3	0	198	3	-5	-6	27	5	7	3	228	4	2	10	81	2	-1
2	48	4	0	1	163	3	-1	-5	93	2	1	4	111	2	-1	11	71	3	-2
3	33	4	4	2	98	2	0	-4	115	2	1	5	272	4	-2	12	60	4	-6
4	59	3	-2	3	120	3	4	-3	201	3	-3	6	152	2	-2	H,K=-1,-0			
5	46	5	-5	4	121	2	-4	-2	142	2	-1	7	135	2	-3	-11	40	3	2
H,K=-1,-11				5	148	3	-0	-1	172	3	1	8	226	4	-5	-10	82	4	-0
-2	16	18	-4*	6	109	2	2	0	243	4	-7	9	111	3	2	-9	95	2	-0
-1	15	18	-11*	7	73	2	-3	1	372	6	5	10	34	8	-7	-8	165	3	-2
0	66	3	-1	8	103	2	2	2	125	2	-6	11	41	9	-4	-7	200	3	-4
1	30	4	5	9	94	2	6	3	66	2	1	12	63	4	-8	-6	76	2	2
2	44	3	2	10	39	5	-4	4	274	4	0	H,K=-1,-2				-5	95	2	1

OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	319	5	-4	2	88	2	2	9	119	4	-1	-2	151	2	-2	-1	143	3	-4
-3	339	5	4	3	151	2	1	10	29	6	-2	-1	284	4	-3	0	116	3	-1
-2	696	11	8	4	414	6	-4		H,K=-1,	5	0	243	4	1	1	31	9	2	
-1	612	9	8	5	134	2	5	-11	60	6	-4	1	100	2	-1	2	40	5	-15
0	639	10	-64	6	25	8	4	-10	88	2	-2	2	146	2	-2	3	123	3	-3
1	213	3	4	7	223	4	-4	-9	137	2	-4	3	249	4	-1	4	21	8	-2
2	535	8	21	8	144	3	0	-8	159	3	-3	4	107	2	1	5	54	5	-2
3	448	7	0	9	53	7	-2	-7	67	5	3	5	104	2	-2		H,K=-1,	11	
4	343	5	7	10	61	3	0	-6	197	3	2	6	105	2	-1	-8	57	3	2
5	489	7	8	11	48	4	-7	-5	445	7	2	7	52	3	1	-7	41	4	-3
6	150	2	1		H,K=-1,	3	-4	326	5	4	8	95	3	-3	-6	62	2	-0	
7	160	3	-2	-12	44	4	-6	-3	254	4	3		H,K=-1,	8	-5	55	4	-5	
8	134	3	-2	-11	19	26	-9*	-2	210	3	-2	-10	79	2	4	-4	74	2	-2
9	109	3	-5	-10	64	3	-1	-1	312	5	-2	-9	78	2	2	-3	65	8	1
10	59	2	-0	-9	106	2	-1	0	250	4	11	-8	73	2	-0	-2	60	3	2
11	60	4	-5	-8	87	2	1	1	344	5	6	-7	52	2	0	-1	99	3	-7
12	67	3	-2	-7	238	4	3	2	73	2	-2	-6	69	5	-0	0	47	3	-7
	H,K=-1,	1	-6	62	2	2	2	3	222	4	-1	-5	167	3	-2	1	57	3	1
-12	57	8	3	-5	105	2	2	4	198	3	1	-4	167	3	-1	2	92	5	-3
-11	101	7	-4	-4	334	5	-2	5	136	2	1	-3	167	3	-3	3	44	10	-1
-10	82	2	-4	-3	43	2	-5	6	85	2	1	-2	140	2	1		H,K=-1,	12	
-9	64	5	-4	-2	61	2	0	7	95	2	2	-1	144	2	0	-6	44	12	-6
-8	221	4	-3	-1	337	5	6	8	139	3	1	0	242	4	-5	-5	97	3	-3
-7	80	3	1	0	504	8	-5	9	62	3	1	1	91	4	1	-4	74	2	4
-6	187	3	-1	1	290	4	12	10	27	6	1	2	220	4	-4	-3	65	2	1
-5	230	4	6	2	317	5	2		H,K=-1,	6	3	132	3	-2	-2	88	3	-1	
-4	508	8	3	3	340	5	-4	-11	52	4	-7	4	94	3	-0	-1	82	3	-3
-3	612	9	-3	4	382	6	-2	-10	103	3	0	5	142	3	0	0	51	4	-6
-2	449	7	17	5	204	3	2	-9	100	3	1	6	63	2	2	1	77	3	-7
-1	523	8	8	6	219	4	3	-8	150	4	-2	7	74	3	-2		H,K=0,-12		
0	243	4	-8	7	173	3	4	-7	174	3	-4		H,K=-1,	9	-1	49	4	-7	
1	990	15	43	8	85	2	-3	-6	82	3	4	-10	82	5	-1	0	48	3	5
2	484	7	20	9	115	2	-1	-5	177	3	1	-9	68	3	-0	1	67	3	-3
3	313	5	6	10	91	3	2	-4	188	3	4	-8	125	3	4	2	64	5	4
4	543	8	21	11	51	3	-2	-3	237	4	3	-7	55	3	0	3	0	17	-9*
5	26	4	0		H,K=-1,	4	-2	171	3	-2	-6	122	2	0	4	81	3	-3	
6	78	2	3	-12	29	16	-6	-1	152	2	1	-5	191	3	2	5	63	9	-2
7	186	3	-2	-11	62	2	3	0	323	5	4	-4	67	2	-3	6	57	3	0
8	209	3	-4	-10	68	3	-9	1	164	3	2	-3	164	3	-3		H,K=0,-11		
9	62	4	-1	-9	84	2	-3	2	95	2	-1	-2	175	3	-3	-3	81	5	-0
10	70	2	-0	-8	124	2	-3	3	268	4	-4	-1	140	2	-2	-2	71	3	-0
11	86	5	1	-7	69	2	-3	4	223	4	-1	0	89	3	-9	-1	22	8	1
	H,K=-1,	2	-6	112	2	-1	5	86	2	2	1	159	3	-4	0	88	7	-3	
-12	88	3	-0	-5	308	5	2	6	91	2	3	2	95	3	-1	1	76	2	2
-11	56	2	2	-4	275	4	-1	7	155	3	2	3	80	2	1	2	43	4	-8
-10	108	2	-1	-3	276	4	2	8	32	5	-2	4	186	4	-0	3	85	3	1
-9	177	3	-3	-2	464	7	4	9	41	5	-11	5	48	7	-7	4	83	5	-3
-8	52	2	2	-1	557	8	0		H,K=-1,	7	6	46	5	-2	5	72	3	-6	
-7	158	3	7	0	270	4	2	-11	61	7	2		H,K=-1,	10	6	87	3	-1	
-6	294	5	0	1	423	6	2	-10	55	3	-3	-9	143	3	-1	7	0	22	-14*
-5	315	5	1	2	362	6	-0	-9	115	2	-5	-8	72	3	-2	8	59	4	2
-4	397	6	8	3	394	6	7	-8	129	4	1	-7	100	4	2		H,K=0,-10		
-3	459	7	9	4	286	5	-3	-7	72	3	0	-6	64	2	3	-5	31	6	-6
-2	648	10	11	5	170	3	2	-6	123	3	-4	-5	72	2	-0	-4	54	4	-4
-1	306	5	-4	6	173	3	0	-5	97	2	2	-4	157	4	1	-3	67	6	-5
0	422	7	11	7	117	3	-2	-4	263	4	-4	-3	80	2	2	-2	25	7	-5
1	379	6	15	8	152	3	2	-3	52	3	-2	-2	75	6	-8	-1	57	3	-4

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
0	101	2	1	1	246	4	1	-10	80	3	-1	-3	403	6	5	5	262	4	8
1	87	2	-1	2	220	4	-4	-9	102	3	0	-2	525	8	4	6	286	4	-0
2	106	3	-1	3	80	2	2	-8	85	5	3	-1	288	4	7	7	270	4	2
3	62	2	-4	4	111	2	-6	-7	162	3	0	0	160	2	-6	8	98	2	0
4	64	2	-2	5	48	3	-1	-6	183	3	-5	1	518	8	17	9	128	3	-5
5	101	3	4	6	128	2	5	-5	237	4	-4	2	449	7	12	10	81	2	-2
6	89	2	-3	7	104	3	-1	-4	99	2	4	3	138	2	-2	11	36	4	-7
7	53	8	-3	8	78	4	2	-3	334	5	-7	4	460	7	-5	H,K= 0,			1
8	52	8	-6	9	55	5	-0	-2	359	5	1	5	284	4	3	-12	59	5	-3
9	99	3	3	10	62	3	-0	-1	194	3	4	6	69	2	-3	-11	98	4	0
H,K= 0,			-9	11	64	5	-2	0	449	7	2	7	134	2	1	-10	93	2	-5
-6	46	4	1	H,K= 0,			-6	1	700	11	6	8	151	3	-1	-9	92	3	-2
-5	50	3	3	-9	20	32	2*	2	352	5	12	9	152	3	-3	-8	234	4	-5
-4	89	4	-4	-8	81	2	2	3	152	2	-3	10	77	2	-5	-7	244	4	2
-3	52	4	-3	-7	103	2	2	4	479	7	4	11	82	2	2	-6	208	3	4
-2	137	3	-3	-6	45	5	-2	5	246	4	3	12	61	5	-4	-5	432	7	-5
-1	153	3	-2	-5	91	2	0	6	118	2	1	H,K= 0,			-1	-4	634	10	6
0	51	2	-3	-4	177	3	-1	7	226	4	-1	-11	77	3	-2	-3	515	8	7
1	163	3	-6	-3	82	2	1	8	142	2	-2	-10	83	2	1	-2	351	5	9
2	151	3	-1	-2	201	3	-7	9	98	2	-2	-9	106	2	-5	-1	659	10	-16
3	99	4	0	-1	255	4	4	10	50	3	1	-8	166	3	-2	0	443	7	-16
4	114	2	-3	0	96	2	-1	11	77	3	-5	-7	78	2	0	1	490	7	-3
5	213	4	0	1	215	3	-4	12	79	4	2	-6	201	3	-1	2	308	5	7
6	116	2	0	2	226	4	2	H,K= 0,			-3	-5	265	4	1	3	122	2	2
7	73	3	-2	3	147	2	-1	-11	66	4	-2	-4	292	4	8	4	287	4	5
8	112	3	-1	4	199	3	3	-10	67	2	0	-3	145	2	3	5	273	4	3
9	63	9	1	5	212	4	-3	-9	81	2	-2	-2	295	5	5	6	193	3	-1
10	94	5	-4	6	141	2	1	-8	101	2	3	-1	506	8	4	7	95	2	1
H,K= 0,			-8	7	137	2	2	-7	186	3	3	0	432	7	-20	8	167	3	-1
-7	68	4	2	8	188	3	1	-6	140	2	-1	1	655	10	-15	9	107	2	-2
-6	81	3	-2	9	95	2	1	-5	245	4	-3	2	355	5	8	10	72	2	-2
-5	122	3	-2	10	88	3	-2	-4	303	5	0	3	522	8	10	11	83	3	-1
-4	66	3	2	11	65	6	1	-3	230	4	-1	4	635	10	2	H,K= 0,			2
-3	197	4	-1	H,K= 0,			-5	-2	196	3	7	5	419	6	-6	-12	59	11	-4
-2	144	3	-3	-9	79	3	-2	-1	610	9	-15	6	210	3	4	-11	76	5	-2
-1	158	3	-2	-8	104	3	-1	0	810	12	-27	7	237	4	1	-10	80	2	-3
0	214	3	-3	-7	81	2	-1	1	431	7	12	8	240	4	-2	-9	158	3	-3
1	76	2	2	-6	137	2	1	2	193	3	9	9	96	2	-3	-8	149	3	0
2	207	4	1	-5	153	3	-2	3	649	10	5	10	94	3	-5	-7	122	3	1
3	145	2	-4	-4	220	4	-0	4	98	2	-1	11	100	2	-0	-6	75	2	-6
4	137	2	5	-3	258	4	2	5	177	3	-3	12	54	11	-7	-5	276	4	2
5	193	3	-1	-2	277	4	-3	6	217	4	-1	H,K= 0,			0	-4	461	7	-5
6	98	2	1	-1	285	5	-3	7	149	3	-5	-11	48	4	-1	-3	151	2	-3
7	88	2	1	0	289	4	5	8	110	2	-3	-10	70	4	-6	-2	424	7	10
8	51	4	1	1	359	5	9	9	153	3	-3	-9	124	2	-8	-1	502	8	15
9	101	3	4	2	259	4	-2	10	55	2	4	-8	96	2	1	0	165	3	-4
10	51	3	0	3	233	4	2	11	24	7	-5	-7	264	4	2	1	298	5	7
H,K= 0,			-7	4	495	8	1	12	91	2	1	-6	276	4	-0	2	502	8	3
-8	73	3	2	5	315	5	6	H,K= 0,			-2	-5	270	4	8	3	412	6	3
-7	125	3	4	6	131	2	-2	-11	56	3	-4	-4	461	7	-5	4	315	5	0
-6	127	3	3	7	110	2	-3	-10	69	3	-1	-3	766	12	-18	5	274	4	-2
-5	34	8	1	8	186	3	2	-9	84	3	-1	-2	255	4	-2	6	117	2	0
-4	142	3	-1	9	128	3	-3	-8	199	3	-0	-1	389	6	-10	7	104	2	-0
-3	157	3	1	10	93	2	-1	-7	102	2	-1	1	407	6	-6	8	201	3	-1
-2	7	16	-7*	11	71	3	-5	-6	132	2	3	2	234	4	-3	9	79	3	-5
-1	132	3	-1	12	78	3	-1	-5	283	4	-0	3	775	12	-17	10	77	2	1
0	203	3	3	H,K= 0,			-4	-4	310	5	-0	4	460	7	-5	11	62	3	-1

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
	H,K=	0,	3	-5	313	5	5	8	68	3	0	-6	79	3	-4	H,K=	1,	-9	
-12	87	3	-0	-4	496	8	-1	H,K=	0,	8	-5	81	2	-1	-6	51	5	2	
-11	17	23	-9*	-3	220	3	1	-10	33	5	-7	-4	75	2	2	-5	64	2	4
-10	60	2	-1	-2	258	4	-1	-9	101	2	6	-3	77	3	-4	-4	188	3	2
-9	146	3	-5	-1	346	5	8	-8	60	3	-2	-2	60	2	-1	-3	78	2	-1
-8	111	3	1	0	288	4	5	-7	93	2	0	-1	66	3	-3	-2	91	2	-4
-7	133	2	-6	1	287	5	-2	-6	85	2	-2	0	88	3	-0	-1	166	3	-2
-6	214	3	1	2	276	4	-4	-5	188	3	-1	1	19	15	10	0	86	2	-5
-5	169	3	-3	3	250	4	1	-4	138	2	3	2	77	2	4	1	138	3	-1
-4	98	2	-1	4	222	4	-1	-3	136	2	-4	3	82	3	0	2	188	3	-1
-3	661	10	7	5	159	3	-0	-2	210	3	-0	H,K=	0,	12	3	168	3	-2	
-2	173	3	10	6	128	2	0	-1	72	5	4	-6	53	4	-3	4	75	2	-2
-1	420	6	11	7	86	3	-1	0	208	4	-3	-5	67	4	0	5	191	3	5
0	820	13	-24	8	104	3	-2	1	168	3	-1	-4	81	3	-2	6	128	3	1
1	613	9	-16	9	86	2	3	2	141	3	-2	-3	22	7	15	7	47	3	4
2	192	3	5	H,K=	0,	6	3	196	3	-2	-2	62	6	3	8	129	2	6	
3	249	4	-2	-11	68	3	2	4	67	3	0	-1	70	3	-5	9	76	2	1
4	303	5	1	-10	87	2	-1	5	124	3	-2	0	42	5	1	10	77	3	-1
5	244	4	-1	-9	98	2	-1	6	79	3	-2	1	59	3	2	H,K=	1,	-8	
6	142	2	-4	-8	181	3	-0	7	67	5	2	H,K=	1,-	-12	-7	72	3	-4	
7	185	3	1	-7	129	2	2	H,K=	0,	9	-1	82	3	-2	-6	64	3	-2	
8	101	2	1	-6	131	2	-3	-10	100	3	0	0	54	7	-4	-5	145	3	-2
9	89	4	2	-5	208	3	-1	-9	66	3	2	1	84	3	-1	-4	98	2	3
10	67	2	1	-4	203	3	4	-8	108	3	-1	2	92	3	-1	-3	127	2	1
11	63	6	-2	-3	158	3	0	-7	80	2	1	3	70	7	-4	-2	230	4	-4
H,K=	0,	4	-2	212	3	1	-6	114	2	0	4	75	4	5	-1	88	2	-1	
-12	74	2	1	-1	214	3	-3	-5	209	4	-4	5	103	3	1	0	244	4	-3
-11	72	3	-3	0	102	2	-3	-4	118	2	-6	6	51	3	0	1	155	3	-0
-10	56	4	5	1	249	4	3	-3	97	2	-2	H,K=	1,-	-11	2	125	2	-0	
-9	101	2	-1	2	207	4	-5	-2	153	3	-1	-3	41	5	-4	3	175	3	-1
-8	139	2	-4	3	98	2	-1	-1	162	3	-6	-2	96	3	-1	4	169	3	-1
-7	225	4	-1	4	173	3	0	0	64	2	-1	-1	63	3	-2	5	168	3	-2
-6	129	2	2	5	79	3	-2	1	152	3	-3	0	54	4	1	6	73	2	1
-5	248	4	-0	6	52	3	2	2	143	3	-2	1	107	3	-2	7	56	2	4
-4	483	7	4	7	104	2	1	3	57	5	-0	2	51	3	1	8	75	2	-2
-3	134	2	-4	8	83	3	3	4	92	4	-1	3	65	4	-1	9	80	2	5
-2	347	5	8	9	29	8	4	5	37	7	-6	4	79	3	-3	10	86	2	2
-1	703	11	5	H,K=	0,	7	6	27	8	-9	5	58	3	-2	H,K=	1,	-7		
0	455	7	2	-11	59	5	0	H,K=	0,	10	6	62	2	-2	-8	99	3	-1	
1	178	3	1	-10	66	5	4	-9	97	3	0	7	40	5	-10	-7	52	3	-3
2	361	6	-0	-9	54	2	5	-8	63	3	4	8	57	4	2	-6	103	2	-2
3	327	5	-8	-8	85	2	3	-7	47	7	-3	H,K=	1,-	-10	-5	103	2	0	
4	88	2	3	-7	99	3	-2	-6	93	3	0	-5	58	2	3	-4	104	2	3
5	242	4	-3	-6	115	2	5	-5	91	4	-1	-4	25	5	2	-3	249	4	-2
6	189	3	-2	-5	61	2	3	-4	75	2	-0	-3	121	3	-2	-2	151	3	1
7	158	3	0	-4	120	2	-4	-3	68	2	-2	-2	56	5	-3	-1	112	2	-1
8	90	4	2	-3	89	2	0	-2	99	3	-5	-1	21	9	-11	0	244	4	3
9	103	3	1	-2	200	3	-6	-1	82	3	-2	0	118	3	2	1	282	4	-2
10	77	2	0	-1	252	4	-2	0	95	2	-1	1	141	3	-0	2	147	2	1
H,K=	0,	5	0	198	3	2	1	62	2	2	2	77	2	-8	3	62	2	-4	
-12	79	3	-2	1	119	2	-2	2	20	20	1*	3	72	2	1	4	270	4	-2
-11	74	4	1	2	24	13	-2	3	68	6	-6	4	158	3	-0	5	105	2	2
-10	88	2	1	3	148	3	-3	4	45	5	-15	5	74	2	-3	6	137	2	-1
-9	134	3	-3	4	139	2	-2	5	23	9	-8	6	58	3	-0	7	82	2	-2
-8	186	3	-0	5	25	5	-2	H,K=	0,	11	7	106	2	2	8	128	4	1	
-7	109	2	-1	6	128	2	2	-8	59	3	-0	8	67	3	-5	9	118	3	-5
-6	124	2	-2	7	120	3	0	-7	0	25	-3*	9	145	3	1	10	64	3	1

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
11	63	3	-1	0	278	4	4	7	157	3	3	-12	70	2	1	-5	280	4	0
	H,K=	1,	-6	1	557	8	2	8	55	2	3	-11	70	3	-7	-4	90	2	-2
-9	54	3	4	2	451	7	5	9	175	3	-4	-10	87	4	-3	-3	241	4	2
-8	34	4	3	3	281	4	3	10	108	4	-4	-9	81	2	3	-2	589	9	14
-7	153	3	1	4	289	4	1	11	53	2	2	-8	134	2	-2	-1	693	11	15
-6	83	2	-1	5	315	5	4	12	89	3	1	-7	285	4	0	0	312	5	4
-5	88	3	-3	6	122	2	-1		H,K=	1,	-1	-6	139	2	3	1	124	2	1
-4	227	4	2	7	62	2	-5	-11	80	2	3	-5	185	3	1	2	223	4	6
-3	265	4	-3	8	133	2	0	-10	56	5	-6	-4	194	3	3	3	187	3	6
-2	77	2	-3	9	83	2	-2	-9	62	3	-7	-3	460	7	10	4	275	4	-2
-1	178	3	0	10	82	3	0	-8	203	3	-5	-2	348	5	11	5	127	2	-5
0	327	5	7	11	64	3	-3	-7	178	3	-2	-1	387	6	12	6	130	2	3
1	140	2	0	12	39	8	-2	-6	79	2	7	0	456	7	2	7	126	2	5
2	178	3	0		H,K=	1,	-3	-5	47	2	-2	1	98	2	8	8	169	3	-1
3	251	4	3	-11	46	4	-5	-4	531	8	18	2	403	6	6	9	97	5	-2
4	184	3	3	-10	88	2	-3	-3	319	5	6	3	431	7	-12	10	33	6	-7
5	179	3	-1	-9	119	2	1	-2	474	7	17	4	243	4	0		H,K=	1,	4
6	84	2	5	-8	91	2	-1	-1	988	15	33	5	30	3	2	-12	64	4	3
7	175	3	-1	-7	174	3	3	0	253	4	-6	6	202	3	-5	-11	41	5	-2
8	155	3	1	-6	226	4	6	1	508	8	0	7	153	3	2	-10	46	3	1
9	102	2	1	-5	197	3	-1	2	440	7	14	8	40	2	2	-9	71	2	-2
10	98	4	0	-4	394	6	-2	3	609	9	-6	9	96	3	-3	-8	101	2	1
11	55	9	-4	-3	346	5	0	4	509	8	2	10	17	8	2	-7	79	2	-3
	H,K=	1,	-5	-2	308	5	0	5	234	4	5	11	52	3	-4	-6	291	5	-1
-10	0	19	-19*	-1	312	5	13	6	187	3	-2		H,K=	1,	2	-5	200	3	6
-9	56	3	0	0	515	8	-1	7	87	2	4	-12	46	10	-4	-4	167	3	1
-8	140	3	-1	1	336	5	6	8	214	4	-4	-11	65	2	1	-3	198	3	-5
-7	88	3	1	2	83	2	2	9	60	3	-10	-10	95	3	-4	-2	405	6	9
-6	77	3	-1	3	48	2	-5	10	85	2	-1	-9	122	2	-4	-1	439	7	6
-5	148	3	-1	4	347	5	-1	11	102	3	-6	-8	114	2	-2	0	495	8	-0
-4	192	3	3	5	124	2	2	12	52	3	-1	-7	206	3	3	1	278	4	-5
-3	220	4	2	6	78	2	0		H,K=	1,	0	-6	57	2	-3	2	147	2	-4
-2	73	2	-1	7	234	4	3	-12	64	3	-1	-5	195	3	-1	3	293	5	1
-1	332	5	7	8	95	2	1	-11	67	2	4	-4	317	5	-0	4	260	4	-5
0	263	4	12	9	107	2	-0	-10	54	3	-4	-3	194	3	6	5	136	3	2
1	314	5	0	10	63	3	-6	-9	111	2	-3	-2	579	9	34	6	191	3	2
2	200	3	-1	11	13	17	-9*	-8	134	2	-2	-1	470	7	15	7	135	2	1
3	246	4	4	12	48	3	-0	-7	171	3	0	0	478	7	-4	8	114	2	1
4	328	5	8		H,K=	1,	-2	-6	145	3	-1	1	222	3	5	9	36	4	1
5	447	7	3	-11	59	3	-2	-5	479	7	8	2	231	4	12	10	48	4	2
6	180	3	-3	-10	53	4	-2	-4	364	6	10	3	304	5	7		H,K=	1,	5
7	68	2	3	-9	52	3	-5	-3	460	7	1	4	112	2	2	-12	66	3	2
8	156	3	-4	-8	142	2	1	-2	528	8	19	5	279	4	1	-11	46	3	-1
9	134	2	-5	-7	226	4	-4	-1	210	3	3	6	38	5	1	-10	63	3	-4
10	88	2	-1	-6	8	22	2*	0	608	9	-85	7	13	9	5	-9	152	3	2
11	62	5	-7	-5	144	2	3	1	621	9	3	8	140	2	0	-8	128	2	0
	H,K=	1,	-4	-4	407	6	-4	2	671	10	6	9	83	4	-2	-7	145	3	-3
-10	24	25	-4*	-3	137	2	1	3	347	5	5	10	25	28	-2*	-6	82	2	5
-9	123	2	-0	-2	70	2	1	4	323	5	-3	11	62	5	-5	-5	310	5	-2
-8	149	3	2	-1	353	5	12	5	85	2	-1		H,K=	1,	3	-4	272	4	6
-7	111	2	-1	0	430	7	11	6	82	2	1	-12	68	3	-2	-3	46	2	1
-6	186	3	1	1	318	5	-5	7	199	3	-5	-11	39	6	-5	-2	124	2	-5
-5	152	3	-1	2	656	10	8	8	157	3	-4	-10	45	3	-1	-1	380	6	4
-4	281	4	-2	3	435	7	7	9	83	4	-5	-9	106	2	0	0	246	4	-6
-3	398	6	7	4	391	6	9	10	90	4	-3	-8	226	4	-4	1	179	3	-1
-2	375	6	2	5	324	5	1	11	26	12	-3	-7	149	3	2	2	147	2	1
-1	422	6	5	6	289	5	-2		H,K=	1,	1	-6	150	2	-0	3	198	3	-2

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
4	104	2	3	-2	99	2	-1	-3	36	8	2	6	137	3	-0	2	222	4	-2	
5	101	2	-1	-1	171	3	-4	-2	41	6	-4	7	60	4	0	3	290	4	-0	
6	34	3	5	0	198	3	-5	-1	96	6	-6	8	87	3	-6	4	137	2	4	
7	30	4	3	1	115	3	-1	0	43	4	-2	9	84	3	-0	5	220	4	3	
8	46	3	3	2	58	2	-0	H,K=	2,-12	10	54	3	4	6	35	3	-6	3	-6	
9	48	6	-1	3	142	4	1	-2	28	7	-3	H,K=	2,-8	7	141	3	-2	3	-2	
H,K=	1,	6	4	111	2	-1	-1	26	10	-15	-7	121	3	0	8	162	3	4	4	
-11	94	3	1	5	33	9	-0	0	70	3	-0	-6	44	3	4	9	98	3	-2	
-10	23	6	-2	6	54	3	1	1	73	3	-1	-5	102	2	2	10	43	3	-1	
-9	138	3	-0	7	64	3	0	2	61	4	-3	-4	146	3	-1	11	56	11	-3	
-8	97	2	2	H,K=	1,	9	3	52	7	-1	-3	100	2	3	H,K=	2,-5	5	-5	-5	
-7	35	3	-1	-10	83	4	-2	4	40	4	-0	-2	133	2	0	-10	67	3	-3	
-6	41	2	1	-9	80	4	1	5	84	4	-2	-1	162	3	-3	-9	23	30	-10*	
-5	170	3	-0	-8	59	3	1	6	53	3	6	0	262	5	-2	-8	54	3	1	
-4	122	2	-1	-7	60	3	-3	H,K=	2,-11	1	149	3	-2	-7	70	2	3	3	3	
-3	65	2	4	-6	82	4	2	-4	60	4	-6	2	128	3	0	-6	119	2	-4	
-2	160	3	1	-5	99	2	-2	-3	0	25	-15*	3	175	3	-1	-5	132	2	4	
-1	145	3	2	-4	138	3	3	-2	61	3	2	4	73	2	-3	-4	143	2	2	
0	41	3	-1	-3	42	5	-10	-1	57	3	-2	5	108	4	3	-3	229	4	-4	
1	56	2	1	-2	116	3	1	0	46	3	-2	6	97	2	-3	-2	162	3	1	
2	61	2	-0	-1	127	2	-1	1	96	2	-1	7	107	2	1	-1	200	3	0	
3	45	2	2	0	48	4	2	2	52	10	-5	8	58	5	2	0	556	8	4	
4	87	4	1	1	66	4	-7	3	13	18	-6*	9	54	4	3	1	57	2	0	
5	89	2	-2	2	104	2	-4	4	22	7	-1	10	41	5	-8	2	306	5	-7	
6	44	3	4	3	61	2	5	5	88	3	-1	H,K=	2,-7	3	275	4	-3	4	-3	
7	73	2	3	4	51	3	1	6	48	4	-3	-8	115	3	-4	4	260	4	1	
8	86	3	0	5	46	5	-1	7	45	4	-4	-7	42	3	2	5	83	2	1	
H,K=	1,	7	6	39	4	3	8	71	3	5	-6	75	2	5	6	130	3	0	0	
-11	20	9	16	H,K=	1,	10	H,K=	2,-10	-5	118	2	3	7	118	2	-1	7	118	2	-1
-10	63	3	1	-9	118	3	5	-5	62	4	-7	-4	106	2	-2	8	76	2	-2	
-9	66	2	1	-8	29	6	0	-4	31	5	1	-3	82	2	-1	9	125	2	1	
-8	35	4	1	-7	55	7	-1	-3	64	3	-0	-2	149	2	-1	10	11	18	1*	
-7	42	3	7	-6	81	4	-1	-2	86	2	-2	-1	106	2	3	11	36	4	-1	
-6	153	3	-5	-5	62	4	-1	-1	26	5	-1	0	97	3	1	H,K=	2,-4	4	-4	
-5	102	2	3	-4	99	2	-1	0	53	5	-3	1	269	4	-1	-10	29	4	4	
-4	60	2	0	-3	39	3	2	1	108	3	-4	2	130	3	0	-9	67	2	2	
-3	115	2	3	-2	91	6	-4	2	93	2	-2	3	111	3	-3	-8	170	3	2	
-2	91	2	3	-1	64	2	-2	3	23	7	-3	4	146	2	2	-7	105	3	-2	
-1	237	4	2	0	36	6	3	4	139	3	-3	5	44	2	2	-6	80	2	0	
0	187	3	1	1	56	4	1	5	115	2	0	6	70	2	-1	-5	214	4	4	
1	163	3	1	2	0	18	-13*	6	53	3	2	7	114	3	5	-4	273	4	-1	
2	49	2	4	3	41	4	-3	7	96	2	-2	8	106	2	-4	-3	129	2	-4	
3	137	2	-0	4	53	4	2	8	46	4	-3	9	74	2	1	-2	398	6	4	
4	168	4	2	H,K=	1,	11	9	95	3	-0	10	36	14	-9	-1	306	5	2	2	
5	80	3	-1	-7	47	13	1	H,K=	2,-9	11	39	5	-4	0	312	5	8	8	8	
6	52	3	-3	-6	37	4	1	-6	62	3	-2	H,K=	2,-6	1	169	3	3	3	3	
7	100	3	2	-5	90	2	-2	-5	17	13	-3	-9	56	5	-5	2	89	2	-2	
8	79	4	-0	-4	39	13	-4	-4	106	2	1	-8	20	7	6	3	107	2	0	
H,K=	1,	8	-3	63	3	-1	-3	142	3	-5	-7	69	2	2	4	141	2	2	2	
-10	44	8	0	-2	55	6	-0	-2	44	4	-2	-6	89	2	3	5	226	4	-1	
-9	83	3	-2	-1	37	4	2	-1	80	3	-4	-5	170	3	0	6	143	2	-2	
-8	102	3	-5	0	67	9	-4	0	106	2	-2	-4	82	2	-4	7	65	5	-1	
-7	78	2	-1	1	39	3	7	1	135	2	-2	-3	131	2	0	8	150	3	1	
-6	111	4	-1	2	26	14	-1	2	161	3	-6	-2	90	2	3	9	70	2	-3	
-5	152	3	2	H,K=	1,	12	3	137	3	1	-1	99	2	-4	10	24	5	-0	-0	
-4	125	2	-7	-5	51	4	-5	4	149	3	-0	0	92	2	-1	11	40	7	-1	
-3	108	2	2	-4	60	3	-2	5	102	2	-2	1	138	2	-1	H,K=	2,-3	3	-3	

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-11	50	3	4	-2	365	6	5	5	97	2	2	-11	59	5	-1	2	119	2	3
-10	49	5	-5	-1	590	9	10	6	12	15	-3*	-10	37	14	-1	3	152	3	-0
-9	145	3	1	0	288	4	6	7	92	2	-0	-9	139	3	-3	4	99	3	-1
-8	108	2	-1	1	530	8	-0	8	94	2	-0	-8	144	3	1	5	92	2	0
-7	42	2	0	2	163	3	2	9	45	7	-4	-7	54	4	-9	6	77	2	1
-6	199	3	-1	3	266	4	-1	10	31	4	0	-6	151	3	1	7	49	3	-1
-5	222	4	-1	4	17	5	-6	11	39	8	-1	-5	261	4	-0	8	44	5	-4
-4	318	5	1	5	305	5	-3		H,K=	2,	2	-4	153	3	0		H,K=	2,	7
-3	168	3	-1	6	151	3	-4	-12	72	3	0	-3	151	2	-5	-11	33	6	-2
-2	80	2	-4	7	62	2	-1	-11	51	5	-3	-2	286	4	-4	-10	52	5	-1
-1	293	4	13	8	119	2	-2	-10	74	2	-2	-1	143	2	2	-9	96	5	-4
0	88	2	-1	9	115	3	-6	-9	147	3	-5	0	40	2	3	-8	69	2	2
1	54	2	2	10	53	4	-3	-8	43	2	1	1	409	6	-7	-7	69	2	2
2	447	7	-3	11	70	3	-6	-7	166	3	-0	2	109	2	-2	-6	116	2	-4
3	312	5	5		H,K=	2,	0	-6	142	3	0	3	168	3	-2	-5	101	2	-2
4	196	3	-3	-12	50	3	3	-5	117	2	1	4	172	3	4	-4	73	3	0
5	90	2	-0	-11	22	16	-3	-4	291	4	-6	5	60	2	-3	-3	57	2	-5
6	50	5	4	-10	27	4	3	-3	121	2	-1	6	73	2	2	-2	199	3	1
7	92	2	5	-9	141	3	-5	-2	246	4	6	7	68	2	2	-1	70	2	-2
8	197	3	-2	-8	173	3	-4	-1	273	4	8	8	93	2	0	0	120	2	-1
9	67	2	-5	-7	42	3	-3	0	390	6	-3	9	11	18	-9*	1	62	4	-3
10	42	3	1	-6	31	2	-1	1	288	4	3		H,K=	2,	5	2	157	3	3
11	27	5	2	-5	316	5	-3	2	128	2	4	-11	38	7	5	3	129	2	-1
	H,K=	2,	-2	-4	410	6	13	3	228	4	1	-10	100	5	-3	4	98	4	2
-11	58	3	-1	-3	211	3	-5	4	77	3	-2	-9	104	3	0	5	97	2	3
-10	44	8	-3	-2	408	6	10	5	105	2	0	-8	122	2	-1	6	56	6	3
-9	103	3	-3	-1	296	5	2	6	124	2	-5	-7	98	2	2	7	73	3	5
-8	66	2	-5	0	283	4	-8	7	127	2	-1	-6	97	2	-4		H,K=	2,	8
-7	59	2	4	1	451	7	5	8	121	3	3	-5	158	3	3	-10	55	4	-1
-6	90	2	0	2	18	2	5	9	78	3	-3	-4	243	4	0	-9	67	7	3
-5	209	3	6	3	218	3	-3	10	75	3	-0	-3	185	3	2	-8	46	6	4
-4	278	4	3	4	403	6	-5		H,K=	2,	3	-2	51	2	1	-7	75	2	0
-3	225	4	-2	5	250	4	-4	-12	43	4	1	-1	211	3	-1	-6	126	2	2
-2	585	9	27	6	82	2	0	-11	26	15	4	0	211	3	4	-5	100	2	1
-1	368	6	7	7	120	2	3	-10	29	4	7	1	77	2	-1	-4	60	3	-4
0	521	8	9	8	160	3	-1	-9	84	2	-4	2	22	4	2	-3	100	2	1
1	247	4	5	9	41	3	1	-8	161	3	-1	3	177	3	0	-2	117	2	-3
2	298	5	4	10	38	4	-2	-7	84	2	4	4	120	2	0	-1	98	3	0
3	386	6	7	11	45	3	7	-6	234	4	-4	5	33	5	0	0	169	4	1
4	463	7	-1		H,K=	2,	1	-5	295	5	-2	6	83	2	-0	1	135	2	-2
5	25	6	-10	-12	64	6	-5	-4	163	3	1	7	96	2	2	2	103	3	-1
6	23	4	-3	-11	57	6	-4	-3	200	3	0	8	43	3	2	3	96	3	-2
7	187	3	-1	-10	118	3	-1	-2	319	5	7	9	46	13	-0	4	112	3	-3
8	89	2	-2	-9	108	2	-1	-1	145	2	-2		H,K=	2,	6	5	39	3	-1
9	92	2	-2	-8	202	3	-2	0	234	4	-2	-11	63	6	-1	6	43	4	3
10	62	4	-7	-7	140	2	-2	1	138	2	1	-10	46	6	-1		H,K=	2,	9
11	40	4	-2	-6	238	4	-2	2	267	4	-6	-9	97	2	-2	-9	62	5	2
	H,K=	2,	-1	-5	263	4	2	3	146	2	1	-8	164	3	0	-8	73	4	5
-11	40	4	-2	-4	486	7	7	4	281	4	1	-7	65	2	1	-7	66	4	-2
-10	36	3	1	-3	347	5	9	5	264	4	0	-6	55	2	1	-6	103	2	1
-9	46	3	-3	-2	230	4	3	6	141	3	-1	-5	103	2	4	-5	106	2	5
-8	81	2	-3	-1	459	7	12	7	91	2	-1	-4	140	2	-4	-4	76	4	-8
-7	151	3	-1	0	515	8	-10	8	89	3	2	-3	195	3	6	-3	141	3	-1
-6	98	2	0	1	798	12	-10	9	92	2	-5	-2	164	3	5	-2	73	2	0
-5	201	3	12	2	241	4	7	10	0	20	-21*	-1	117	2	-0	-1	152	3	-3
-4	275	4	0	3	258	4	8		H,K=	2,	4	0	109	3	0	0	33	4	-4
-3	183	3	4	4	327	5	-1	-12	45	5	-8	1	68	2	-5	1	20	6	7

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	80	3	-1	-1	74	2	-2	-1	152	3	-1	11	60	3	1	-3	237	4	-5
3	64	3	-3	0	59	3	-8	0	70	2	1	H,K= 3, -4		-2	54	2	3		
4	38	5	-7	1	71	2	-4	1	168	3	-4	-10	40	5	-7	-1	315	5	5
5	40	4	2	2	76	2	-2	2	190	3	2	-9	29	11	-4	0	264	4	0
H,K= 2, 10				3	46	2	0	3	187	3	-2	-8	97	3	-2	1	354	5	0
-8	58	3	0	4	120	2	-3	4	175	3	-7	-7	172	3	-3	2	138	2	-2
-7	65	4	-0	5	157	3	6	5	115	2	2	-6	45	3	-6	3	175	3	3
-6	101	2	6	6	28	20	-2	6	75	2	-2	-5	202	3	-0	4	222	4	-0
-5	44	4	-1	7	83	3	-2	7	71	5	-4	-4	240	4	-1	5	150	2	-3
-4	82	3	-3	8	91	3	3	8	72	2	2	-3	167	3	-7	6	45	2	3
-3	65	2	3	9	59	4	2	9	64	3	1	-2	215	3	8	7	134	2	0
-2	31	10	-11	H,K= 3, -9			10	25	20	-5	-1	268	4	-8	8	182	3	-4	
-1	81	3	-3	-6	70	3	-2	11	37	5	-5	0	548	8	9	9	58	3	-3
0	0	17	-5*	-5	48	7	6	H,K= 3, -6			1	430	7	7	10	78	7	-4	
1	46	3	4	-4	80	2	3	-9	62	4	-6	2	188	3	-3	11	72	3	-5
2	50	3	2	-3	129	2	-1	-8	74	3	1	3	207	3	0	H,K= 3, -1			
3	76	3	0	-2	71	3	-6	-7	48	4	-2	4	123	2	-2	-11	62	3	-2
4	39	10	4	-1	106	2	-2	-6	102	2	2	5	181	3	-3	-10	44	3	-1
H,K= 2, 11				0	137	3	-3	-5	45	4	1	6	247	4	0	-9	42	3	-1
-7	31	8	-13	1	164	3	-3	-4	142	3	-1	7	74	4	-4	-8	104	2	-4
-6	33	24	5	2	95	2	2	-3	37	2	3	8	54	5	-1	-7	66	2	-1
-5	88	2	3	3	135	3	-1	-2	189	3	-1	9	81	2	-5	-6	208	3	1
-4	19	22	2*	4	127	2	-5	-1	75	2	3	10	15	25	-9*	-5	146	3	2
-3	17	19	-2*	5	148	3	-2	0	178	3	0	11	26	7	-4	-4	373	6	-5
-2	88	4	-2	6	77	3	2	1	237	4	0	H,K= 3, -3			-3	397	6	9	
-1	64	3	2	7	23	7	2	2	146	2	1	-11	60	4	5	-2	271	4	-0
0	67	3	-1	8	57	3	-3	3	150	2	1	-10	0	21	-23*	-1	263	4	-0
1	61	5	-3	9	77	2	4	4	96	2	2	-9	71	3	-3	0	746	11	-50
H,K= 3, -12				10	57	3	2	5	222	4	0	-8	180	3	3	1	258	4	2
-2	55	3	0	H,K= 3, -8			6	83	2	1	-7	141	2	-3	2	350	5	-2	
-1	20	20	-2*	-8	38	3	8	7	36	4	-3	-6	19	5	-0	3	453	7	-1
0	68	7	-4	-7	94	2	4	8	112	3	-1	-5	271	4	-1	4	219	3	-7
1	64	7	-2	-6	42	4	-4	9	74	2	2	-4	139	2	-4	5	142	3	7
2	0	18	-11*	-5	51	2	2	10	76	3	-2	-3	132	2	2	6	282	4	2
3	20	29	-5*	-4	142	3	0	11	43	5	5	-2	134	2	-9	7	196	3	-2
4	80	3	-2	-3	158	3	-2	H,K= 3, -5			-1	347	5	0	8	103	2	-1	
5	46	3	3	-2	28	4	5	-10	62	9	-2	0	301	5	11	9	64	3	2
6	24	10	-6	-1	101	2	0	-9	66	6	-0	1	103	2	-3	10	26	7	-9
H,K= 3, -11				0	231	4	4	-8	63	4	-0	2	151	2	0	11	58	4	-10
-4	41	5	-7	1	79	2	-2	-7	88	2	-0	3	154	3	1	H,K= 3, 0			
-3	63	3	2	2	21	5	-0	-6	77	2	4	4	49	3	1	-12	59	3	-2
-2	33	4	5	3	103	2	-2	-5	104	2	0	5	146	2	-3	-11	66	3	-2
-1	43	3	1	4	87	4	1	-4	231	4	-6	6	57	2	1	-10	87	2	1
0	75	2	0	5	35	3	-1	-3	276	5	-4	7	67	2	3	-9	121	3	-2
1	17	23	4*	6	38	10	-1	-2	138	2	-5	8	75	2	0	-8	173	3	-2
2	25	5	0	7	101	2	4	-1	110	2	-1	9	68	2	-6	-7	261	4	-1
3	27	6	3	8	15	12	-1	0	366	6	1	10	0	18	-19*	-6	217	3	-2
4	42	3	3	9	59	3	-3	1	220	3	3	11	72	2	2	-5	340	5	7
5	44	4	3	10	34	4	0	2	190	3	2	H,K= 3, -2			-4	265	4	-1	
6	64	3	-5	H,K= 3, -7			3	168	3	-2	-11	61	3	-2	-3	193	3	1	
7	16	17	-4*	-8	90	2	2	4	326	5	-1	-10	28	12	-9	-2	373	6	1
8	49	4	-1	-7	86	3	0	5	88	2	-1	-9	96	2	-1	-1	426	7	4
H,K= 3, -10				-6	0	15	-12*	6	116	3	-3	-8	103	3	-4	0	784	12	-65
-5	58	6	2	-5	68	2	0	7	108	2	-2	-7	94	2	-2	1	418	6	0
-4	63	3	-4	-4	163	3	-1	8	116	3	2	-6	85	2	-2	2	322	5	-5
-3	10	21	-5*	-3	33	3	1	9	113	3	-2	-5	121	2	5	3	221	3	3
-2	17	11	-5	-2	114	2	-3	10	49	3	1	-4	141	2	5	4	188	3	7



OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	191	3	7	-11	11	28	-4*	0	321	5	-1	-3	99	3	1	-4	14	31	-12*
6	77	2	-2	-10	75	2	-5	1	143	3	2	-2	171	3	-2	-3	92	3	-2
7	97	2	-1	-9	109	3	0	2	107	3	0	-1	121	3	-1	-2	18	19	-13*
8	111	3	-2	-8	108	3	-1	3	191	3	3	0	135	3	-2	-1	19	9	-1
9	28	11	-10	-7	84	4	-3	4	167	3	2	1	142	3	2	0	57	4	-3
10	0	18	-11*	-6	131	2	0	5	26	10	-3	2	115	3	-5	1	63	3	1
11	71	4	2	-5	279	4	0	6	42	5	4	3	82	3	1	2	31	5	-1
	H,K=	3,	1	-4	126	2	-1	7	153	3	1	4	77	2	3	3	67	2	2
-12	81	2	1	-3	139	2	-1	8	63	4	-1	5	68	3	-0	4	85	2	0
-11	76	3	1	-2	190	3	6		H,K=	3,	6	6	34	6	0	5	49	3	-3
-10	78	2	-2	-1	433	7	-6	-11	45	9	-9		H,K=	3,	9	6	81	2	1
-9	147	3	-1	0	300	5	2	-10	87	3	-2	-9	77	5	2	7	64	3	0
-8	163	3	2	1	164	3	7	-9	64	6	-6	-8	89	3	2		H,K=	4,-10	
-7	111	2	-0	2	225	4	-4	-8	142	3	4	-7	91	3	2	-5	36	11	-8
-6	123	2	0	3	222	4	-0	-7	55	5	0	-6	100	3	1	-4	77	2	-0
-5	297	5	-2	4	212	4	0	-6	123	2	0	-5	130	3	-1	-3	70	2	1
-4	332	5	3	5	160	3	2	-5	121	2	3	-4	116	3	1	-2	31	4	1
-3	302	5	6	6	129	2	2	-4	180	3	-1	-3	115	2	-1	-1	91	2	-2
-2	255	4	-5	7	152	3	3	-3	105	2	1	-2	74	3	-5	0	109	3	4
-1	357	5	2	8	63	7	1	-2	81	2	0	-1	78	4	-2	1	79	3	-3
0	61	3	-2	9	63	3	-1	-1	180	3	-1	0	85	2	1	2	129	3	-3
1	387	6	5	10	46	8	-4	0	128	2	-5	1	72	3	-6	3	120	3	3
2	327	5	4		H,K=	3,	4	1	108	2	-2	2	71	5	-1	4	74	3	2
3	135	2	2	-12	47	6	-1	2	125	2	0	3	84	3	0	5	85	4	-1
4	283	4	0	-11	68	3	-2	3	131	3	-1	4	73	2	3	6	71	3	1
5	134	2	-1	-10	70	3	-2	4	164	3	-1		H,K=	3,	10	7	57	4	-2
6	57	2	-1	-9	116	3	-2	5	36	3	1	-8	82	3	1	8	86	3	-2
7	149	3	-1	-8	139	2	-4	6	117	3	1	-7	50	4	-4		H,K=	4,-9	
8	168	3	2	-7	152	3	0	7	87	2	1	-6	97	3	-1	-6	44	6	4
9	41	7	-7	-6	124	2	-3	8	47	6	-3	-5	58	4	-6	-5	85	2	-0
10	41	5	-2	-5	237	4	-0		H,K=	3,	7	-4	58	3	2	-4	116	5	-1
	H,K=	3,	2	-4	352	5	-5	-10	74	3	2	-3	86	2	1	-3	61	4	-2
-12	57	4	-2	-3	35	2	-1	-9	57	3	-2	-2	55	3	-3	-2	126	3	-2
-11	59	3	-2	-2	349	5	2	-8	54	3	2	-1	89	3	-2	-1	120	3	1
-10	61	3	-2	-1	446	7	-0	-7	93	3	-1	0	71	4	-8	0	104	2	-4
-9	148	3	2	0	203	3	2	-6	53	6	2	1	46	3	5	1	104	2	1
-8	44	2	2	1	273	4	2	-5	109	2	1	2	67	4	-1	2	89	2	2
-7	82	2	1	2	284	4	1	-4	80	4	1	3	107	3	2	3	131	2	-1
-6	309	5	4	3	211	3	-2	-3	85	2	-2		H,K=	3,	11	4	71	2	2
-5	96	2	-1	4	162	3	1	-2	131	2	-1	-6	36	7	1	5	131	3	2
-4	163	3	0	5	124	2	2	-1	173	3	1	-5	77	2	0	6	95	3	-4
-3	308	5	-2	6	72	3	-1	0	188	3	-0	-4	58	4	1	7	25	25	1*
-2	194	3	2	7	108	3	4	1	110	2	1	-3	43	4	-2	8	77	3	1
-1	262	4	1	8	104	2	-1	2	146	3	-1	-2	67	3	-7	9	58	3	-3
0	256	4	-5	9	46	4	-7	3	189	3	3	-1	74	5	-2		H,K=	4,-8	
1	192	3	-2		H,K=	3,	5	4	82	2	-2	0	68	3	-0	-7	62	3	0
2	70	1	2	-11	41	4	-3	5	97	2	6		H,K=	4,-12	-6	110	4	2	
3	477	7	-7	-10	132	3	-2	6	102	4	3	-2	92	3	-1	-5	62	4	-2
4	136	2	-0	-9	181	3	3	7	61	3	5	-1	40	4	1	-4	75	2	-1
5	115	3	-1	-8	71	3	2		H,K=	3,	8	0	28	6	-5	-3	173	3	2
6	133	2	-1	-7	81	2	2	-10	52	7	-1	1	89	3	3	-2	191	3	-3
7	158	3	2	-6	238	4	3	-9	115	3	2	2	0	20	-9*	-1	20	6	0
8	129	2	1	-5	278	4	1	-8	46	3	3	3	19	10	-1	0	184	3	-1
9	31	4	2	-4	243	4	-2	-7	54	3	-1	4	53	4	1	1	82	2	-3
10	60	3	1	-3	169	3	-1	-6	86	2	0	5	68	7	-4	2	95	2	6
	H,K=	3,	3	-2	229	4	1	-5	210	3	3	6	21	10	0	3	196	3	3
-12	56	3	3	-1	201	3	1	-4	133	3	1		H,K=	4,-11	4	163	3	3	

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	
5	90	2	2	-2	371	6	-5	8	127	3	-0	-7	170	3	2	3	209	3	2	
6	61	3	-2	-1	363	6	6	9	117	3	0	-6	230	4	0	4	253	4	-0	
7	84	4	3	0	205	3	5	10	44	4	-6	-5	294	5	5	5	182	3	2	
8	66	2	5	1	257	4	-6	11	51	4	-2	-4	277	4	2	6	89	3	-2	
9	45	4	2	2	197	3	1	H,K= 4,			-2	-3	351	5	9	7	116	2	3	
10	78	3	-1	3	258	4	-3	-11	50	3	3	-2	203	3	10	8	112	2	-1	
	H,K= 4,			-7	4	366	6	0	-10	54	4	4	-1	537	8	-7	9	60	4	-1
-8	81	3	-1	5	255	4	-2	-9	105	2	-2	0	647	10	-25	10	70	4	1	
-7	118	2	2	6	53	2	-0	-8	181	3	0	1	413	6	1	H,K= 4,			3	
-6	92	2	0	7	119	2	-1	-7	50	4	-1	2	123	2	3	-11	24	8	-4	
-5	86	2	1	8	133	2	-1	-6	50	4	2	3	405	6	-3	-10	60	10	-7	
-4	163	3	-0	9	100	4	-2	-5	325	5	-7	4	235	4	1	-9	108	4	-1	
-3	139	3	0	10	44	4	-1	-4	384	6	-1	5	106	2	1	-8	158	3	-2	
-2	44	2	2	11	52	6	-8	-3	72	2	-3	6	172	3	2	-7	52	2	2	
-1	249	4	-4	H,K= 4,			-4	-2	336	5	4	7	150	3	-1	-6	249	4	0	
0	162	3	3	-10	74	3	-1	-1	567	9	4	8	100	3	-0	-5	195	3	-1	
1	88	2	5	-9	128	3	-2	0	381	6	-6	9	67	3	-3	-4	226	4	-0	
2	236	4	-3	-8	114	2	2	1	149	2	-4	10	56	3	-3	-3	255	4	-2	
3	100	3	3	-7	150	3	0	2	289	4	-4	H,K= 4,			1	-2	147	2	2	
4	201	3	5	-6	179	3	-3	3	248	4	3	-11	34	5	-6	-1	344	5	8	
5	137	3	-2	-5	211	3	2	4	464	7	4	-10	92	3	-6	0	554	8	-14	
6	88	2	2	-4	438	7	6	5	245	4	-4	-9	99	2	1	1	229	4	-1	
7	71	2	1	-3	158	3	-2	6	116	2	-0	-8	165	3	1	2	200	3	-3	
8	121	3	2	-2	159	3	2	7	118	2	-3	-7	219	4	0	3	311	5	0	
9	85	2	0	-1	415	6	5	8	168	3	-2	-6	103	2	4	4	237	4	0	
10	27	5	10	0	190	3	-8	9	99	2	-4	-5	231	4	2	5	105	2	1	
	H,K= 4,			-6	1	395	6	5	10	67	3	-1	-4	337	5	3	6	185	3	5
-9	49	4	8	2	213	3	5	11	90	3	-2	-3	320	5	2	7	149	3	1	
-8	74	6	-4	3	273	4	-5	H,K= 4,			-1	-2	59	1	-1	8	57	3	-4	
-7	116	2	1	4	226	4	-1	-11	50	3	2	-1	488	7	-2	9	74	3	2	
-6	50	3	-0	5	119	2	-1	-10	79	4	-2	0	434	7	1	H,K= 4,			4	
-5	106	4	-1	6	97	2	-3	-9	144	3	-1	1	141	2	-4	-11	71	3	-2	
-4	149	3	-0	7	107	2	2	-8	152	3	-3	2	175	3	0	-10	72	5	-5	
-3	88	2	-2	8	113	3	-0	-7	155	3	0	3	124	2	-2	-9	82	2	3	
-2	73	2	0	9	45	3	1	-6	209	3	4	4	160	3	1	-8	173	3	3	
-1	223	4	-1	10	50	3	-3	-5	214	3	-0	5	210	3	1	-7	218	4	-0	
0	217	4	-4	11	50	6	2	-4	306	5	-1	6	80	4	-4	-6	215	3	1	
1	131	2	2	H,K= 4,			-3	-3	447	7	3	7	97	4	4	-5	105	2	4	
2	202	3	-0	-11	62	4	-6	-2	444	7	8	8	92	3	-3	-4	373	6	1	
3	193	3	1	-10	86	4	1	-1	204	3	1	9	91	2	-1	-3	217	4	4	
4	118	2	2	-9	81	4	-1	0	499	8	-9	10	34	5	-1	-2	250	4	-3	
5	242	4	4	-8	125	3	6	1	579	9	-5	H,K= 4,			2	-1	511	8	1	
6	106	5	-3	-7	151	3	-2	2	54	2	-2	-12	69	3	-0	0	252	4	3	
7	100	3	-5	-6	110	2	-0	3	408	6	0	-11	67	2	1	1	181	3	1	
8	168	3	4	-5	212	3	1	4	462	7	5	-10	69	3	-1	2	217	4	-3	
9	98	2	3	-4	140	3	-4	5	172	3	1	-9	158	3	-1	3	187	3	6	
10	75	3	1	-3	202	3	-1	6	119	2	-1	-8	119	2	-2	4	76	2	0	
11	64	3	-2	-2	226	4	1	7	169	3	-2	-7	36	3	4	5	118	2	1	
	H,K= 4,			-5	-1	296	5	-2	8	142	3	1	-6	191	3	-1	6	168	3	5
-10	16	28	6*	0	424	7	1	9	39	11	-9	-5	265	4	1	7	50	3	-1	
-9	112	2	-0	1	47	1	4	10	92	2	4	-4	101	2	2	8	76	2	-0	
-8	115	3	1	2	243	4	-2	11	72	4	1	-3	192	3	-2	H,K= 4,			5	
-7	26	5	1	3	130	2	-2	H,K= 4,			0	-2	407	6	-4	-11	74	3	-5	
-6	128	3	0	4	214	3	-4	-11	68	2	1	-1	124	2	1	-10	79	2	2	
-5	236	4	-0	5	146	3	0	-10	83	2	-0	0	225	4	0	-9	144	3	5	
-4	120	2	-1	6	104	2	-1	-9	138	3	-1	1	222	4	4	-8	92	3	1	
-3	225	4	3	7	171	3	-0	-8	136	3	1	2	173	3	-1	-7	153	3	6	

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	100	2	2	-6	140	3	5	7	74	3	4	-3	163	3	-3	-10	45	2	3
-5	251	4	-4	-5	149	3	1		H,K=	5,-10		-2	41	2	0	-9	177	3	4
-4	159	3	8	-4	115	2	-1	-5	38	4	2	-1	55	4	-1	-8	143	3	-5
-3	126	2	3	-3	92	2	3	-4	87	3	-4	0	214	4	-0	-7	59	3	-1
-2	179	3	-0	-2	138	3	3	-3	67	4	-6	1	211	4	-4	-6	177	3	3
-1	161	3	1	-1	166	3	-2	-2	49	3	3	2	63	2	1	-5	131	2	1
0	114	2	-0	0	79	2	1	-1	88	3	-3	3	148	3	0	-4	228	4	3
1	79	3	1	1	83	2	-2	0	126	2	-3	4	168	3	2	-3	307	5	3
2	214	3	-1	2	112	3	-1	1	91	4	0	5	116	2	2	-2	316	5	-2
3	119	2	-2	3	96	3	0	2	81	3	-1	6	48	3	1	-1	169	3	6
4	66	2	-0	4	74	4	-1	3	114	4	-0	7	96	2	-1	0	168	3	-0
5	114	2	-0	5	70	3	5	4	113	3	-1	8	142	3	1	1	338	5	-3
6	42	7	2		H,K=	4,	9	5	44	4	1	9	96	3	2	2	170	3	-2
7	89	3	0	-8	56	3	2	6	73	3	-1	10	41	4	0	3	134	4	2
8	59	3	2	-7	82	2	2	7	73	2	4		H,K=	5,	-6	4	243	4	-3
	H,K=	4,	6	-6	111	2	4	8	85	6	-2	-9	43	11	-2	5	175	3	1
-11	60	4	2	-5	127	2	3		H,K=	5,	-9	-8	51	3	4	6	108	2	1
-10	50	7	-4	-4	106	2	2	-6	27	6	3	-7	68	2	-2	7	47	5	0
-9	88	3	1	-3	44	7	-2	-5	120	3	5	-6	60	2	-1	8	157	3	4
-8	49	3	-4	-2	134	3	3	-4	171	3	1	-5	85	2	1	9	73	5	-2
-7	69	2	2	-1	74	7	-3	-3	121	2	-2	-4	221	4	-1	10	61	3	0
-6	131	2	1	0	51	6	2	-2	68	3	1	-3	186	3	-4		H,K=	5,	-3
-5	97	3	7	1	88	2	1	-1	148	3	-1	-2	101	2	2	-10	78	7	-2
-4	59	2	-5	2	98	3	0	0	174	3	5	-1	110	2	-1	-9	115	3	-0
-3	151	3	0	3	54	4	-4	1	147	3	-0	0	260	4	-2	-8	58	3	-2
-2	103	2	1		H,K=	4,	10	2	148	3	-2	1	195	3	-2	-7	137	2	1
-1	132	3	0	-7	40	8	6	3	112	2	4	2	203	3	-3	-6	165	3	1
0	162	3	2	-6	65	3	3	4	137	3	0	3	248	4	1	-5	106	2	3
1	154	3	-1	-5	69	5	-0	5	102	2	2	4	68	2	4	-4	271	4	-0
2	103	2	-1	-4	30	12	3	6	113	2	7	5	172	3	-1	-3	283	4	-2
3	113	2	4	-3	21	24	-8*	7	50	3	1	6	136	2	2	-2	102	2	3
4	147	3	1	-2	79	3	-3	8	93	3	-1	7	108	2	2	-1	219	3	2
5	62	3	-4	-1	48	4	-6	9	94	4	4	8	152	3	1	0	374	6	-2
6	67	3	6	0	65	3	0		H,K=	5,	-8	9	93	3	2	1	90	2	-3
7	92	5	-1	1	33	16	-1	-7	79	3	-2	10	55	3	7	2	239	4	-5
	H,K=	4,	7		H,K=	4,	11	-6	65	5	0		H,K=	5,	-5	3	387	6	0
-10	77	3	-1	-3	43	5	-5	-5	181	4	1	-9	55	3	3	4	77	4	0
-9	40	6	-1	-2	58	4	4	-4	126	3	3	-8	163	3	1	5	137	2	-3
-8	64	4	0		H,K=	5,-12		-3	78	2	4	-7	75	2	-2	6	108	2	2
-7	129	3	6	-1	76	6	-1	-2	197	3	-1	-6	75	2	3	7	206	3	-2
-6	109	2	-2	0	50	4	-0	-1	148	3	4	-5	311	5	4	8	112	2	-1
-5	80	2	4	1	67	6	-7	0	102	2	0	-4	139	2	2	9	52	7	-4
-4	140	3	1	2	56	5	1	1	191	3	1	-3	204	4	2	10	86	2	1
-3	78	2	-1	3	43	10	-6	2	85	3	2	-2	242	4	0		H,K=	5,	-2
-2	160	3	2	4	60	3	-1	3	93	2	-4	-1	211	4	3	-11	67	3	-0
-1	232	4	3	5	84	3	-2	4	163	3	1	0	287	4	8	-10	63	3	-1
0	120	3	1		H,K=	5,-11		5	109	2	4	1	186	3	5	-9	69	3	-1
1	116	4	3	-3	34	5	-3	6	57	3	1	2	233	4	-4	-8	141	2	-1
2	102	3	3	-2	73	3	-3	7	92	2	-0	3	153	3	2	-7	117	2	0
3	118	3	3	-1	38	13	-0	8	61	5	1	4	276	4	-1	-6	117	2	-0
4	73	3	3	0	77	3	-2	9	40	3	6	5	123	2	1	-5	211	3	-1
5	64	4	4	1	77	6	-3		H,K=	5,	-7	6	134	2	-2	-4	183	3	0
6	89	3	-0	2	73	2	-2	-8	73	2	4	7	117	3	3	-3	242	4	3
	H,K=	4,	8	3	39	8	-5	-7	62	6	4	8	67	3	-6	-2	51	2	5
-9	66	3	4	4	74	6	1	-6	102	2	6	9	78	2	2	-1	311	5	5
-8	95	4	1	5	100	3	-1	-5	67	4	1	10	25	6	-1	0	195	3	4
-7	64	2	5	6	30	6	-0	-4	91	2	2		H,K=	5,	-4	1	238	4	-0

OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	152	3	2	1	37	4	1	-7	109	3	3	-8	20	24	5*	0	76	4	-1
3	263	4	1	2	155	3	-2	-6	148	4	4	-7	89	3	5	1	41	14	1
4	249	4	6	3	175	3	-1	-5	109	2	1	-6	96	3	1	2	82	3	-2
5	124	2	3	4	77	2	1	-4	203	3	1	-5	52	4	7	3	34	4	4
6	159	3	-2	5	65	2	0	-3	130	2	3	-4	90	3	1	4	31	6	-7
7	149	3	1	6	144	3	3	-2	29	4	-3	-3	80	3	-1	5	87	3	-5
8	108	4	1	7	71	3	2	-1	252	4	1	-2	139	3	3	6	61	2	5
9	83	2	-4	8	83	3	2	0	143	2	1	-1	63	2	1	H,K= 6,-10			
10	54	3	1	9	69	4	-2	1	151	3	-2	0	137	3	1	-5	56	3	-2
H,K= 5,			-1	H,K= 5,			2	2	53	2	-3	1	88	3	-1	-4	40	11	-3
-11	24	11	6	-11	37	5	-6	3	184	3	1	2	75	2	3	-3	64	3	1
-10	64	3	1	-10	71	6	-1	4	58	5	-1	3	108	2	2	-2	113	4	1
-9	113	2	3	-9	77	2	1	5	42	3	3	4	69	4	-2	-1	86	2	3
-8	116	2	1	-8	112	3	-2	6	132	4	4	5	75	5	1	0	94	3	0
-7	152	3	-0	-7	107	2	0	7	47	3	-2	H,K= 5,			8	1	139	3	4
-6	127	2	-2	-6	97	2	0	8	63	4	-0	-9	69	3	2	2	54	3	1
-5	239	4	0	-5	154	3	-2	H,K= 5,			5	-8	67	3	2	3	89	5	3
-4	219	3	-1	-4	191	3	-5	-11	57	4	-3	-7	56	3	-2	4	114	4	1
-3	188	3	1	-3	86	3	4	-10	79	2	3	-6	121	3	2	5	92	2	3
-2	321	5	3	-2	262	4	-2	-9	73	4	4	-5	114	3	-1	6	47	4	-6
-1	365	6	-1	-1	269	4	2	-8	110	2	4	-4	60	3	-1	7	86	6	3
0	137	2	7	0	178	3	2	-7	70	4	-4	-3	100	2	-0	H,K= 6,-9			
1	192	3	-5	1	161	3	2	-6	109	2	2	-2	70	2	1	-6	61	3	-1
2	385	6	-3	2	261	4	-1	-5	143	3	3	-1	122	3	5	-5	58	11	-2
3	264	4	4	3	275	4	2	-4	92	2	2	0	79	2	-1	-4	147	3	4
4	239	4	1	4	159	3	1	-3	186	4	2	1	49	4	-1	-3	124	3	-3
10	60	6	-0	5	144	2	3	-2	118	2	2	2	92	3	2	-2	51	2	3
H,K= 5,			0	6	106	2	-1	-1	168	3	-3	3	58	3	1	-1	92	2	-1
-11	55	5	-2	7	64	2	4	0	90	2	0	4	70	4	3	0	147	5	2
-10	127	3	5	8	87	3	0	1	66	5	2	H,K= 5,			9	1	77	2	-1
-9	129	3	2	9	70	3	-3	2	86	2	5	-7	37	6	2	2	74	3	1
-8	82	3	-3	H,K= 5,			3	3	149	3	0	-6	70	5	-1	3	151	3	5
-7	129	2	1	-11	38	6	-2	4	36	4	-1	-5	53	4	-2	4	101	2	2
-6	261	4	5	-10	71	3	3	5	75	3	3	-4	64	3	-1	5	77	9	-0
-5	170	3	-2	-9	136	3	0	6	35	5	-2	-3	45	4	-5	6	53	3	3
-4	248	4	4	-8	111	2	4	7	30	14	1	-2	45	6	2	7	52	4	-3
-3	313	5	1	-7	84	2	0	H,K= 5,			6	-1	76	3	-1	8	46	4	-0
-2	291	4	-4	-6	74	2	2	-10	70	3	-0	0	0	31	-8*	H,K= 6,-8			
-1	239	4	6	-5	358	5	4	-9	91	3	0	1	37	10	2	-7	82	3	-1
0	336	5	-2	-4	63	2	1	-8	129	3	3	2	46	4	0	-6	40	7	1
1	346	5	-4	-3	129	2	3	-7	28	13	0	H,K= 5,			10	-5	77	3	2
2	66	2	-4	-2	368	6	2	-6	51	4	1	-5	43	4	0	-4	98	2	-1
3	227	4	1	-1	163	3	1	-5	140	3	-0	-4	17	20	-8*	-3	45	4	-1
10	57	3	3	0	189	3	3	-4	50	3	3	-3	24	11	-9	-2	38	6	2
H,K= 5,			1	1	184	3	1	-3	86	2	3	-2	51	4	-6	-1	143	3	-0
-11	64	3	-0	2	168	3	3	-2	137	2	0	-1	38	4	2	0	86	4	1
-10	103	4	-2	3	122	2	0	-1	105	2	-1	0	17	14	3	1	101	2	-5
-9	97	2	-1	4	210	3	5	0	63	5	1	H,K= 6,-12			2	121	2	-1	
-8	104	2	-2	5	56	3	2	1	70	3	6	0	30	8	-3	3	28	5	6
-7	141	2	5	6	40	4	4	2	92	2	4	1	50	4	-2	4	125	2	2
-6	214	4	0	7	115	2	0	3	50	3	2	2	46	3	4	5	50	3	-2
-5	109	2	-2	8	78	2	7	4	90	2	-2	3	35	7	-1	6	58	2	5
-4	301	5	3	H,K= 5,			4	5	59	4	4	4	53	3	-2	7	102	2	7
-3	60	3	1	-11	43	4	-3	6	0	23	-16*	H,K= 6,-11			8	62	3	-0	
-2	43	2	-1	-10	60	3	-1	H,K= 5,			7	-3	46	5	-1	9	0	18	-17*
-1	238	4	1	-9	91	2	3	-10	50	5	6	-2	37	4	-0	H,K= 6,-7			
0	119	2	-1	-8	82	2	1	-9	81	4	-1	-1	65	5	-1	-8	73	3	-2

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-7	17	26	1*	10	23	12	-7	1	138	3	1	-9	125	3	0	5	109	3	0
-6	49	3	-2					2	114	2	-0	-8	43	2	1	6	53	2	6
-5	105	2	1	-10	35	12	3	3	282	4	-1	-7	51	5	-5	7	78	3	-0
-4	37	3	-6	-9	89	3	7	4	125	2	-1	-6	141	3	-0	8	47	5	-8
-3	93	2	4	-8	142	3	3	5	62	2	-2	-5	144	3	1				
-2	113	3	-2	-7	98	2	-4	6	120	2	1	-4	139	2	0	H,K=	6,	4	
-1	141	2	1	-6	92	2	1	7	100	4	1	-3	144	2	-1	-10	56	7	-5
0	115	2	-1	-5	212	4	-1	8	76	6	-3	-2	128	2	0	-9	100	2	5
1	101	2	3	-4	182	3	-1	9	57	3	2	-1	51	2	1	-8	101	2	1
2	47	3	-3	-3	111	3	1	10	40	4	4	0	199	3	1	-7	82	2	1
3	57	2	1	-2	102	2	0					1	180	3	1	-6	120	2	-3
4	153	3	1	-1	376	6	-2	H,K=	6,	-1	1	2	97	2	5	-5	138	2	3
5	75	4	3	0	208	3	0	-11	72	3	4	3	140	3	-7	-4	133	3	3
6	49	2	-1	1	181	3	-5	-10	51	3	1	4	118	2	1	-3	149	3	-1
7	83	4	-1	2	42	3	3	-9	61	6	-4	5	21	7	4	-2	118	2	0
8	85	2	3	3	106	2	-4	-8	108	3	1	6	53	3	-2	-1	69	3	3
9	45	12	2	4	120	2	-3	-7	124	2	2	7	86	4	-2	0	109	3	-2
	H,K=	6,	-6	5	76	2	3	-6	78	2	1	8	63	2	1	1	157	3	1
-9	83	3	2	6	114	2	1	-5	129	3	3	9	34	6	-7	2	102	3	-1
-8	9	17	-7*	7	70	2	1	-4	300	5	-6					3	90	2	-1
-7	56	3	0	8	58	5	-2	-3	83	2	-1	H,K=	6,	2	4	4	96	4	-4
-6	117	3	-2	9	49	4	2	-2	180	3	5	-11	35	7	-5	5	3	18	-9*
-5	13	15	-2*	10	0	20	-14*	-1	237	4	1	-10	40	4	-0	6	40	5	0
-4	122	2	0					0	335	5	-0	-9	58	3	-2	7	66	4	-1
-3	138	3	3	H,K=	6,	-3	1	1	134	2	-2	-8	41	3	4				
-2	84	2	1	-10	46	6	-2	2	108	2	-0	-7	59	2	1	-10	79	4	-1
-1	73	3	-1	-9	101	3	0	3	140	2	0	-6	77	2	-1	-9	89	2	-0
0	220	4	-1	-8	43	4	-3	4	30	3	-0	-5	83	2	-2	-8	38	4	2
1	130	3	0	-7	50	2	-1	5	147	3	2	-4	134	2	2	-7	96	2	3
2	22	5	2	-6	92	2	4	6	85	2	2	-3	57	2	-1	-6	125	2	4
3	224	4	1	-5	138	3	-2	7	29	5	-6	-2	37	2	5	-5	112	4	2
4	118	3	3	-4	36	4	5	8	71	5	-0	-1	179	3	-1	-4	100	2	2
5	96	2	1	-3	137	3	1	9	37	4	2	0	48	2	3	-3	64	2	0
6	84	3	-2	-2	68	2	1	H,K=	6,	0	1	1	80	2	1	-2	93	2	-3
7	75	4	-2	-1	78	2	1	-11	24	30	-7*	2	105	2	-3	-1	78	5	-2
8	102	3	2	0	178	3	-1	-10	79	5	-1	3	127	3	-1	0	121	2	1
9	55	5	-0	1	93	2	0	-9	129	2	1	4	49	3	-6	1	24	8	0
	H,K=	6,	-5	2	112	2	-2	-8	110	2	-1	5	70	2	2	2	79	2	0
-9	42	4	2	3	155	3	-0	-7	70	3	0	6	104	2	5	3	97	3	-3
-8	65	2	9	4	72	2	-2	-6	134	4	1	7	43	6	1	4	33	4	-0
-7	98	3	-2	5	108	2	2	-5	229	4	2	8	52	5	1	5	4	19	-7*
-6	64	6	-0	6	25	5	-5	-4	90	2	-0					6	47	4	1
-5	189	3	3	7	117	3	1	-3	182	3	-3	H,K=	6,	3	3				
-4	194	3	1	8	85	4	0	-11	20	20	-5*					H,K=	6,	6	
-3	102	2	1	9	53	3	3	-2	186	3	-3	-10	33	6	-3	-10	69	4	2
-2	127	2	1	10	44	4	-1	-1	187	3	0	-9	80	3	-5	-9	17	11	10
-1	222	4	1					0	182	3	-2	-8	96	2	1	-8	80	5	5
0	203	3	1	H,K=	6,	-2	1	1	102	3	3	-7	48	3	3	-7	44	11	-2
1	152	3	-1	-10	71	9	-2	2	267	4	-1	-6	89	2	-2	-6	57	5	1
2	185	3	-4	-9	31	4	2	3	108	2	0	-5	163	3	1	-5	80	3	-2
3	155	3	4	-8	51	3	-2	4	146	3	-1	-4	138	2	-2	-4	65	3	-0
4	188	3	0	-7	33	5	-8	5	104	2	2	-3	41	3	3	-3	45	4	0
5	88	2	1	-6	125	2	-2	6	28	4	-0	-2	177	3	3	-2	77	6	0
6	143	3	1	-5	77	2	2	7	90	3	-1	-1	225	4	1	-1	118	3	-1
7	125	2	-2	-4	214	3	0	8	79	2	1	0	63	3	3	0	56	3	1
8	93	3	3	-3	47	2	-2	9	32	5	0	1	66	2	-5	1	64	3	-1
9	59	2	3	-2	117	2	-0					H,K=	6,	1	2	2	84	2	1
				-1	153	2	-0	-11	34	23	-4	3	62	2	1	3	75	2	3
				0	226	4	-2	-10	60	2	1	4	80	2	-6	4	78	4	3

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	36	13	-7	2	41	4	4	7	66	3	7	3	79	2	-1	-3	163	3	-1
	H,K=	6,	7	3	105	2	-1	8	66	2	3	4	85	4	-2	-2	173	3	-2
-9	68	6	2	4	108	3	1	9	62	3	-5	5	95	2	1	-1	279	4	-2
-8	30	5	4	5	75	2	1		H,K=	7,	-5	6	73	2	-2	0	113	2	3
-7	58	3	5	6	24	15	-3	-9	80	2	-2	7	82	3	-1	1	105	2	4
-6	99	3	1	7	38	4	5	-8	27	29	0*	8	20	21	-8*	2	133	2	0
-5	76	4	1		H,K=	7,	-8	-7	82	2	5	9	56	5	0	3	95	2	0
4	56	3	3	-7	57	8	1	-6	72	2	-4		H,K=	7,	-2	4	72	2	4
	H,K=	6,	8	-6	50	4	-4	-5	61	3	-3	-10	76	3	2	5	120	3	-2
-8	20	14	-11	-5	31	14	-2	-4	145	3	0	-9	51	4	2	6	60	3	0
-7	60	4	0	-4	100	3	-3	-3	138	2	1	-8	73	2	1	7	54	4	-4
-6	84	5	4	-3	105	2	1	-2	144	2	-0	-7	95	2	0	8	50	3	2
-5	106	3	3	-2	31	4	-4	-1	172	4	0	-6	81	2	3		H,K=	7,	1
-4	26	5	5	-1	69	2	1	0	123	2	-3	-5	139	2	-4	-10	67	5	-1
-3	66	3	3	0	119	3	-1	1	147	2	5	-4	104	2	-4	-9	105	5	1
-2	71	3	1	1	42	3	4	2	95	2	-2	-3	128	2	-1	-8	69	3	0
2	58	6	0	2	52	2	1	3	152	3	1	-2	221	4	1	-7	29	7	5
3	44	7	-2	3	80	2	2	4	112	3	2	-1	243	4	3	-6	115	2	3
	H,K=	6,	9	4	43	9	1	5	57	3	2	0	168	3	-5	-5	189	4	-2
-6	56	4	-1	5	52	3	-1	6	18	11	-0	1	173	3	0	-4	45	2	5
-5	55	3	1	6	28	5	9	7	79	2	-0	2	122	2	3	-3	76	2	-5
-4	49	4	-3	7	34	4	1	8	30	7	-4	3	99	2	1	-2	127	2	-2
-3	50	3	1	8	35	7	2	9	38	6	-1	4	225	4	-2	-1	82	2	-0
-2	61	6	-1		H,K=	7,	-7		H,K=	7,	-4	5	15	16	-2*	0	121	2	0
-1	53	8	-6	-7	52	2	2	-9	33	9	0	6	47	9	-2	1	93	2	-1
0	28	30	-6*	-6	17	12	4	-8	93	2	1	7	78	3	1	2	92	2	2
1	14	21	-6*	-5	92	2	-1	-7	87	2	2	8	92	3	-3	3	48	6	1
	H,K=	7,	-11	-4	69	3	-1	-6	34	4	-6	9	50	3	0	4	85	3	0
-2	66	3	-2	-3	0	18	-8*	-5	46	5	2		H,K=	7,	-1	5	70	2	2
-1	45	6	-1	-2	17	9	-5	-4	243	4	-4	-10	51	5	-2	6	31	5	-2
0	94	3	1	-1	137	2	1	-3	57	2	1	-9	81	3	1	7	57	5	6
1	8	25	-14*	0	63	2	3	-2	59	3	-1	-8	34	12	3	8	72	3	0
2	47	4	-1	1	44	3	7	-1	226	4	-4	-7	128	2	3		H,K=	7,	2
3	61	3	-1	2	60	2	-2	0	58	2	1	-6	104	2	-1	-10	57	7	-5
4	37	4	1	3	23	7	10	1	34	2	-0	-5	94	2	1	-9	66	3	4
5	54	4	-5	4	81	2	0	2	60	3	2	-4	225	4	1	-8	20	8	-2
	H,K=	7,	-10	5	87	2	2	3	80	2	2	-3	120	2	-1	-7	32	4	1
-4	58	9	1	6	54	3	1	4	25	5	7	-2	168	3	-2	-6	97	2	2
-3	26	27	-1*	7	65	4	1	5	70	3	-0	-1	178	3	2	-5	132	2	-0
-2	38	7	1	8	78	6	-0	6	88	2	2	0	277	5	-2	-4	28	4	-6
-1	93	3	2	9	42	4	5	7	39	4	-4	1	133	2	3	-3	128	3	-0
0	36	13	-3		H,K=	7,	-6	8	46	5	-2	2	40	3	0	-2	123	2	-2
1	77	3	1	-8	57	3	-4	9	32	10	-3	3	228	4	-1	-1	45	2	-2
2	51	3	1	-7	29	5	13		H,K=	7,	-3	4	72	2	-1	0	191	3	-3
3	82	3	5	-6	68	3	-4	-10	16	18	-4*	5	95	5	-5	1	79	2	1
4	87	4	1	-5	88	5	-0	-9	65	2	1	6	126	3	0	2	89	2	-5
5	51	4	1	-4	69	2	1	-8	102	2	5	7	81	2	2	3	145	3	3
6	56	4	-3	-3	121	2	0	-7	46	5	-4	8	69	5	-1	4	108	2	1
7	37	9	-7	-2	109	2	-1	-6	89	2	-1	9	32	7	-1	5	26	12	-7
	H,K=	7,	-9	-1	97	2	3	-5	130	3	2		H,K=	7,	0	6	94	2	3
-5	46	6	0	0	138	2	-1	-4	68	2	-2	-10	30	7	-12	7	105	3	2
-4	57	6	1	1	178	3	1	-3	67	2	1	-9	58	5	-4		H,K=	7,	3
-3	63	3	-1	2	123	2	2	-2	191	3	0	-8	121	2	3	-10	60	4	1
-2	92	2	1	3	129	2	-4	-1	99	2	1	-7	106	3	1	-9	74	2	2
-1	22	6	4	4	161	3	1	0	128	2	0	-6	150	3	-2	-8	63	3	-2
0	125	3	-4	5	127	3	1	1	188	3	0	-5	198	3	-2	-7	96	2	3
1	67	2	3	6	83	2	1	2	143	2	-3	-4	73	2	1	-6	159	3	0

OBSERVED STRUCTURES FACTORS (CONT) FOR  
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-5	149	3	-1	0	76	2	2	H,K=	8,	-8	-2	157	3	-3	-2	184	3	-2	
-4	190	3	-1	1	53	2	6	-6	60	5	0	-1	142	3	2	-1	243	4	1
-3	70	2	1	2	93	2	-1	-5	49	5	-13	0	118	3	-1	0	89	2	-1
-2	128	3	-2	3	56	5	1	-4	43	3	4	1	87	2	0	1	161	3	-3
-1	291	5	0	4	66	4	-8	-3	133	3	7	2	132	3	-3	2	178	3	-1
0	149	3	1	H,K=	7,	7	7	-2	62	2	0	3	98	2	-3	3	108	4	-1
1	45	3	-1	-8	51	4	-4	-1	52	9	-4	4	149	3	1	4	210	4	1
2	169	3	0	-7	62	4	-2	0	79	2	2	5	70	2	3	5	109	2	0
3	130	2	4	-6	87	4	-0	1	54	2	4	6	45	4	-0	6	65	2	5
4	85	2	2	-5	51	6	5	2	19	22	4*	7	63	4	2	7	103	3	2
5	98	3	-2	-4	91	2	6	3	95	2	-1	8	71	2	5	8	97	2	5
6	89	3	-0	-3	40	6	2	4	100	3	4	H,K=	8,	-4	H,K=	8,	-1		
7	49	4	-2	-2	95	2	2	5	30	7	-2	-9	109	4	2	-10	75	3	2
H,K=	7,	4	-1	105	3	4	4	6	42	4	-6	-8	72	2	4	-9	118	3	2
-10	66	5	4	0	57	4	-1	7	55	5	-9	-7	69	4	2	-8	66	2	3
-9	116	2	8	1	96	3	4	H,K=	8,	-7	-6	124	3	-2	-7	90	2	-5	
-8	121	3	1	2	67	3	1	-7	67	3	2	-5	89	4	2	-6	98	3	-2
-7	80	2	4	3	80	3	-3	-6	49	4	-1	-4	185	3	1	-5	172	3	2
-6	144	3	0	H,K=	7,	8	8	-5	47	3	3	-3	145	3	-1	-4	191	4	-1
-5	133	3	4	-6	96	4	-1	-4	118	2	0	-2	66	2	1	-3	206	3	-3
-4	148	3	1	-5	106	2	4	-3	50	3	-2	-1	185	3	-1	-2	197	3	1
-3	75	4	3	-4	52	9	0	-2	25	5	-1	0	143	2	-2	-1	151	3	1
-2	119	2	0	-3	86	3	6	-1	92	2	1	1	75	2	4	0	157	3	1
-1	175	3	2	-2	100	3	-1	0	126	2	-1	2	123	3	-1	1	189	3	3
0	85	3	0	-1	80	3	-2	1	38	4	-5	3	177	3	-1	2	94	2	2
1	116	2	1	0	80	2	3	2	93	2	-1	4	118	3	3	3	171	3	-1
2	98	2	4	1	77	3	-2	3	186	3	3	5	75	4	2	4	172	3	-3
3	70	2	1	H,K=	8,-11	4	4	4	54	4	-1	6	80	4	-0	5	74	2	0
4	79	3	3	-1	16	17	4*	5	84	3	-1	7	56	3	-2	6	43	3	-2
5	58	3	-2	0	83	3	-4	6	57	4	-1	8	84	4	-1	7	88	3	4
6	35	9	1	1	11	30	-11*	7	65	4	-3	H,K=	8,	-3	8	62	5	-1	
H,K=	7,	5	2	8	18	-11*	8	98	3	-1	-9	74	3	2	H,K=	8,	0		
-9	85	2	1	3	62	3	2	H,K=	8,	-6	-8	104	3	5	-10	99	3	1	
-8	7	17	0*	4	43	4	-2	-8	94	4	-0	-7	103	4	2	-9	82	3	3
-7	75	2	5	H,K=	8,-10	-7	15	19	-4*	-6	50	2	2	-8	102	2	2		
-6	89	2	2	-3	25	28	-7*	-6	33	10	2	-5	144	3	0	-7	107	2	-1
-5	108	2	3	-2	31	5	8	-5	153	3	2	-4	161	3	-0	-6	168	3	0
-4	32	4	4	-1	78	7	-4	-4	92	4	-1	-3	76	2	-4	-5	127	2	-1
-3	107	2	-0	0	53	3	-2	-3	29	11	-8	-2	146	3	-0	-4	96	2	1
-2	97	3	-1	1	76	2	2	-2	155	3	1	-1	189	3	-0	-3	151	3	-1
-1	28	5	0	2	91	2	0	-1	138	3	-1	0	168	3	-2	-2	116	3	0
0	133	2	3	3	81	4	1	0	111	2	-2	1	114	2	-1	-1	126	3	5
1	74	4	-6	4	77	3	0	1	129	2	-2	2	125	3	-2	0	158	3	-1
2	48	12	-5	5	0	19	-8*	2	135	2	0	3	147	3	-3	1	79	2	-2
3	93	2	4	H,K=	8,	-9	3	3	93	2	-1	4	56	3	3	2	110	2	-3
4	66	3	1	-5	96	5	1	4	87	2	-1	5	100	2	1	3	112	2	-0
5	34	5	-0	-4	77	2	-1	5	75	3	-2	6	59	2	2	4	83	2	0
H,K=	7,	6	-3	71	2	5	6	51	4	-4	7	96	4	-3	5	43	3	1	
-9	37	11	1	-2	86	4	0	7	66	7	-0	8	78	5	-1	6	86	2	7
-8	34	5	-1	-1	93	2	0	8	73	3	4	H,K=	8,	-2	7	76	3	-1	
-7	72	3	1	0	74	4	1	H,K=	8,	-5	-9	79	2	1	H,K=	8,	1		
-6	51	3	2	1	111	3	3	-8	81	5	-2	-8	82	5	2	-10	55	3	1
-5	87	2	4	2	56	3	5	-7	43	4	2	-7	38	3	0	-9	94	3	0
-4	82	2	1	3	62	3	-2	-6	114	2	3	-6	97	2	-1	-8	97	3	3
-3	68	5	3	4	67	4	-3	-5	116	2	1	-5	161	3	2	-7	58	2	4
-2	51	3	5	5	41	7	1	-4	72	3	2	-4	76	3	2	-6	102	3	0
-1	115	2	-0	6	15	19	-13*	-3	152	3	-0	-3	122	2	-2	-5	106	2	1

OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	147	3	-0	0	111	3	-1	3	91	3	-1	2	154	3	1	7	86	3	5
-3	21	12	2	1	47	4	1	4	36	19	1	3	72	2	-1		H,K=	9,	-1
-2	189	3	-1	2	92	3	3	5	75	3	3	4	94	2	2	-9	131	3	4
-1	192	3	-2	3	103	3	0		H,K=	9,	-8	5	93	4	-3	-8	57	4	-4
0	58	4	-1	4	24	25	-3*	-5	101	3	1	6	72	3	4	-7	56	3	0
1	139	2	-1	5	57	3	1	-4	37	10	3	7	81	3	-2	-6	170	3	1
2	110	2	3		H,K=	8,	5	-3	77	3	1		H,K=	9,	-4	-5	90	3	3
3	130	2	2	-8	76	6	1	-2	80	3	2	-8	85	3	2	-4	109	3	-2
4	99	2	3	-7	42	3	2	-1	82	2	0	-7	56	3	-0	-3	136	2	-1
5	105	2	2	-6	107	3	4	0	70	3	-4	-6	122	3	2	-2	150	3	-1
6	78	4	-2	-5	84	3	4	1	102	3	-3	-5	115	3	-3	-1	91	2	-4
7	50	4	1	-4	46	3	-1	2	73	3	-2	-4	40	3	-1	0	124	3	-1
	H,K=	8,	2	-3	82	3	1	3	27	11	4	-3	163	3	-3	1	119	2	-4
-10	61	5	2	-2	137	3	-0	4	119	3	-1	-2	52	4	-6	2	103	3	1
-9	77	4	-0	-1	51	2	4	5	65	9	4	-1	113	2	-3	3	119	2	2
-8	93	3	1	0	25	6	2	6	53	4	-1	0	160	3	-3	4	97	2	3
-7	74	5	-2	1	77	3	0		H,K=	9,	-7	1	64	2	-2	5	83	8	-4
-6	81	5	-1	2	50	5	1	-6	67	3	-3	2	65	2	2	6	25	8	-7
-5	162	3	1	3	71	4	4	-5	53	4	1	3	135	3	3	7	59	5	2
-4	99	2	3	4	64	3	2	-4	74	3	3	4	101	2	-1		H,K=	9,	0
-3	180	3	-3		H,K=	8,	6	-3	46	9	-7	5	42	4	1	-9	77	3	-4
-2	220	4	-5	-7	53	3	-0	-2	81	2	-1	6	64	7	-8	-8	67	3	-2
-1	65	2	1	-6	86	4	2	-1	111	2	-1	7	62	3	3	-7	81	3	-5
0	127	2	-3	-5	63	3	5	0	95	2	-2		H,K=	9,	-3	-6	104	3	0
1	134	3	-2	-4	54	3	-1	1	86	2	2	-8	55	5	4	-5	136	3	-4
2	127	3	1	-3	81	3	1	2	40	3	-1	-7	50	5	2	-4	44	3	-0
3	141	3	-2	-2	67	2	1	3	110	2	-1	-6	90	2	2	-3	162	3	-0
4	149	3	3	-1	71	3	-1	4	85	2	2	-5	74	3	-4	-2	112	2	-2
5	71	3	-3	0	82	3	-6	5	46	7	-1	-4	85	3	1	-1	94	2	-5
6	56	8	2	1	53	3	4	6	81	2	2	-3	112	4	-2	0	126	3	-4
	H,K=	8,	3	2	88	3	2	7	51	3	6	-2	71	2	-3	1	109	2	-3
-9	89	4	-1	3	85	3	-3		H,K=	9,	-6	-1	69	2	0	2	134	3	-4
-8	61	6	4		H,K=	8,	7	-7	70	3	3	0	165	3	-6	3	97	2	-2
-7	113	5	2	-6	86	3	1	-6	48	4	4	1	134	2	-4	4	98	3	1
-6	130	4	1	-5	50	3	2	-5	90	3	4	2	99	2	-1	5	40	8	-5
-5	133	3	2	-4	83	3	1	-4	154	3	0	3	135	2	4	6	41	5	-3
-4	76	2	1	-3	82	3	0	-3	61	3	-2	4	71	3	-2		H,K=	9,	1
-3	166	3	-1	-2	104	6	2	-2	73	2	4	5	46	4	2	-9	64	4	-2
-2	116	2	2	-1	115	2	1	-1	93	2	0	6	67	3	-2	-8	26	6	-3
-1	139	3	-1	0	100	3	-2	0	166	3	1	7	116	3	4	-7	77	3	-2
0	157	3	-2	1	63	4	2	1	105	3	-0		H,K=	9,	-2	-6	103	2	4
1	90	2	-2		H,K=	9,-10	2	2	121	3	3	-9	16	20	-9*	-5	104	2	1
2	108	4	-1	-2	51	9	-4	3	113	2	-1	-8	59	4	-1	-4	129	2	-4
3	154	3	3	-1	105	3	-0	4	70	2	4	-7	63	3	1	-3	69	2	-0
4	99	4	-3	0	82	3	1	5	74	4	-4	-6	83	3	-5	-2	30	4	2
5	31	5	0	1	94	2	5	6	66	3	3	-5	136	3	-1	-1	160	3	-3
6	92	4	5	2	78	3	-0	7	83	3	-2	-4	161	3	-1	0	88	2	-1
	H,K=	8,	4	3	73	3	1		H,K=	9,	-5	-3	43	3	0	1	51	3	-3
-9	64	3	3	4	80	3	5	-7	56	5	-3	-2	97	2	-3	2	89	2	-4
-8	83	3	0		H,K=	9,	-9	-6	84	3	3	-1	186	3	-4	3	123	3	2
-7	113	3	2	-4	147	3	4	-5	202	5	0	0	92	2	-3	4	51	3	3
-6	83	4	-3	-3	33	7	-3	-4	111	2	1	1	70	2	-3	5	30	13	7
-5	77	4	-1	-2	41	5	-4	-3	64	3	-1	2	157	3	-1	6	101	3	1
-4	127	3	5	-1	120	3	3	-2	197	3	-1	3	123	3	5		H,K=	9,	2
-3	100	2	-2	0	101	2	5	-1	163	3	1	4	66	3	2	-9	63	4	-3
-2	74	4	-0	1	54	5	2	0	67	2	2	5	57	5	-5	-8	47	12	-5
-1	189	3	5	2	81	2	2	1	160	3	0	6	86	5	-1	-7	48	5	1



OBSERVED STRUCTURES FACTORS (CONT) FOR  
D-CO(C2H8N2)3 CL (D-C4H4O6) 5H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	67	3	-3	H,K= 10,	10	-9	6	35	6	-7	1	104	2	-0	2	64	3	-1	
-5	100	2	2	-2	53	12	-4	H,K= 10,	10	-4	2	59	3	-0	3	20	26	12*	
-4	102	2	-0	-1	54	3	4	-7	22	11	-7	3	99	3	-2	H,K= 10,	10	4	
-3	4	15	-12*	0	87	3	-0	-6	49	4	-5	4	30	6	-4	-6	70	4	-4
-2	110	2	-1	1	26	14	-3	-5	88	4	-3	5	66	3	-6	-5	61	3	2
-1	106	2	-3	2	27	13	-5	-4	4	27	-10*	H,K= 10,	10	0	-4	50	4	-2	
0	36	3	2	3	97	3	0	-3	40	4	2	-8	59	5	-3	-3	39	4	-1
1	78	5	-3	H,K= 10,	10	-8	-2	117	3	-1	-7	51	4	-2	-2	62	4	1	
2	121	2	4	-4	43	5	-9	-1	80	2	-3	-6	69	6	-3	-1	16	17	-8*
3	88	5	-1	-3	18	28	0*	0	72	2	-2	-5	79	3	-3	0	45	10	-2
4	62	3	2	-2	50	4	-1	1	63	6	-4	-4	26	4	5	1	42	13	-6
5	89	3	1	-1	71	3	3	2	41	5	7	-3	70	2	3	H,K= 10,	10	5	
H,K= 9,	9	3	0	48	3	-4	3	49	4	-3	-2	101	2	-6	-4	25	11	-2	
-8	60	3	1	1	0	22	-17*	4	55	3	2	-1	47	3	1	-3	29	5	-3
-7	30	17	-8	2	78	3	1	5	50	3	4	0	57	3	-2	-2	14	17	-5*
-6	82	5	-1	3	29	5	1	6	42	4	-1	1	39	3	1	-1	36	11	-4
-5	85	3	0	4	52	6	-3	H,K= 10,	10	-3	2	51	3	4	H,K= 11,	11	-8	-8	-8
-4	75	2	-4	H,K= 10,	10	-7	-7	43	4	2	3	44	12	-2	-1	33	5	4	
-3	78	3	-5	-5	47	8	-3	-6	53	4	-6	4	29	6	-5	0	49	9	-2
-2	112	2	-1	-4	22	11	8	-5	36	9	-5	5	46	5	-4	1	19	10	5
-1	100	4	-3	-3	38	3	7	-4	36	5	-5	H,K= 10,	10	1	2	32	6	-1	
0	60	5	-5	-2	89	2	1	-3	58	5	-8	-8	24	7	5	H,K= 11,	11	-7	
1	108	3	-1	-1	84	3	-1	-2	43	4	-5	-7	6	16	-8*	-3	17	20	-9*
2	75	4	1	0	49	10	-6	-1	39	13	-5	-6	59	5	-0	-2	54	4	-2
3	91	3	3	1	96	3	-1	0	105	4	-3	-5	42	4	0	-1	74	3	0
4	74	3	4	2	17	21	-3*	1	29	3	-1	-4	48	3	3	0	0	25	-19*
H,K= 9,	9	4	3	50	5	-1	2	0	30	-12*	-3	19	7	4	1	31	7	-10	
-8	43	4	-1	4	96	3	-0	3	60	2	-2	-2	31	8	-1	2	53	11	-5
-7	73	4	-2	5	47	8	2	4	79	2	2	-1	43	7	-5	3	51	4	-2
-6	76	3	-0	H,K= 10,	10	-6	5	0	19	-20*	0	24	8	-12	H,K= 11,	11	-6	-6	-6
-5	85	3	-2	-6	69	3	4	6	49	3	3	1	39	6	2	-4	5	17	0*
-4	93	3	-1	-5	78	2	2	H,K= 10,	10	-2	2	43	18	-1	-3	61	4	-0	
-3	78	3	-3	-4	64	4	-4	-8	23	8	3	3	62	3	-3	-2	58	11	-6
-2	56	3	-2	-3	105	3	-1	-7	74	2	-1	4	32	12	0	-1	36	5	-4
-1	57	3	-5	-2	55	4	-5	-6	57	3	2	H,K= 10,	10	2	0	78	4	-3	
0	101	3	1	-1	112	2	-0	-5	80	2	-3	-7	43	5	-1	1	31	5	0
1	11	16	-4*	0	107	3	-1	-4	80	2	-0	-6	28	8	-1	2	53	4	-2
2	46	4	-1	1	52	7	-3	-3	70	3	0	-5	75	2	-1	3	62	4	4
3	74	5	1	2	56	3	-4	-2	38	3	2	-4	51	4	-4	4	67	5	-4
H,K= 9,	9	5	3	97	3	-1	-1	113	2	-4	-3	30	6	-6	H,K= 11,	11	-5	-5	-5
-7	59	4	-8	4	89	3	-1	0	71	2	-5	-2	51	3	-3	-5	10	17	5*
-6	39	4	4	5	54	3	3	1	63	2	-1	-1	84	3	4	-4	65	3	-1
-5	80	3	0	6	35	9	-8	2	97	2	0	0	89	3	-4	-3	81	4	-6
-4	61	5	1	H,K= 10,	10	-5	3	80	3	-4	1	34	5	-2	-2	28	4	7	
-3	33	6	3	-7	82	5	0	4	73	4	-1	2	92	3	1	-1	78	2	-6
-2	62	3	0	-6	50	7	-4	5	28	5	5	3	52	8	-3	0	45	3	5
-1	64	11	-3	-5	72	2	1	6	68	4	-3	4	12	29	-12*	1	53	4	1
0	14	16	-3*	-4	127	4	-3	H,K= 10,	10	-1	H,K= 10,	10	3	2	70	2	2	2	2
1	43	3	5	-3	33	9	-1	-8	59	4	-2	-7	46	4	4	3	63	5	-1
2	80	4	-3	-2	41	4	-0	-7	64	3	-0	-6	83	2	2	4	42	7	2
H,K= 9,	9	6	-1	121	4	0	-6	78	2	0	-5	69	5	-8	H,K= 11,	11	-4	-4	-4
-5	53	3	0	0	60	6	-5	-5	113	2	1	-4	60	3	-2	-6	16	17	0*
-4	38	6	-2	1	45	6	-6	-4	92	2	-5	-3	66	3	1	-5	69	3	-1
-3	57	3	1	2	80	3	-8	-3	39	4	-1	-2	94	4	-3	-4	65	4	-2
-2	78	3	-1	3	80	3	-1	-2	84	2	-4	-1	105	4	-5	-3	0	19	-14*
-1	61	3	1	4	54	5	4	-1	143	3	-4	0	32	9	5	-2	49	3	-1
0	32	6	-4	5	36	13	-3	0	110	3	-2	1	50	5	-6	-1	75	4	-7



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