

Structural characterization of the *trans*-equatorial isomer of (aqua)(ethylenediamine-*N,N,N'*-tripropionato)chromium(III) trihydrate, [Cr(edtrp)(H₂O)] · 3H₂O

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Abstract

The structure of *trans*-equatorial [Cr(edtrp)(H₂O)] · 3H₂O (edtrp³⁻ is the anion of ethylenediamine-*N,N,N'*-tripropionic acid) was determined by single crystal X-ray diffraction. The chromium(III) ion is surrounded octahedrally by the two nitrogen and three oxygen atoms of the quinquedentate edtrp³⁻, forming a five-membered diamine ring and the three six-membered β -propionato chelate rings. The remaining coordination position is occupied by the H₂O ligand. The crystal structure conformation is compared to the result of recent molecular mechanics analysis. The ring strain of R and G chelate rings was found to be in agreement with the previously proposed mechanisms for the C–N bond cleavage and recombination.

Introduction

The focus of activity in the coordination chemistry of edta-type complexes is gradually changing from fundamental to various areas of applied chemistry. This is due to a growing interest in the sequestering abilities of (poly)amino(poly)carboxylato ligands towards toxic metals in edta chelation therapy [1] and in wastewater treatment [2, 3], to the use of edta-type complexes in speciation of metals in environmental and plant [4, 5] research, and to development of the corresponding analytical methods [5–7].

Nevertheless, basic research into the coordination chemistry of edta-type ligands continues to be a fertile area, as exemplified by recent studies of metal–edta-peroxide complexes [8, 9], the use of edta complexes in selective cleavage of DNA [8, 10] and as radiotherapeutic agents [11], as well as in studies of the chelating behavior of edta in silica-gel matrices [12].

From a stereochemical point of view, edta-type complexes provide a wide range of structures suitable for studying isomerism and chelate ring conformations.

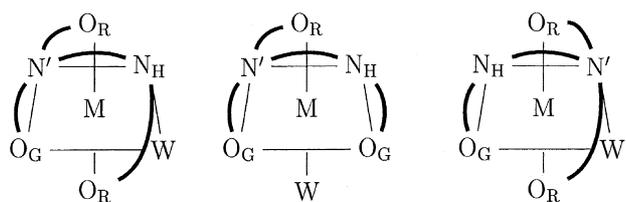
Series of compounds with various denticities, chelate ring sizes, and the branching patterns of edta-type ligands are synthetically readily accessible. Such structures facilitate systematic studies of fine-tuned flexibilities of individual chelate rings in fused multidentate structures, and the effects of ring conformations, the changes in coordination number, as well as the size and d-electron count of the central metal atoms on their physical properties and chemical reactivity.

In spite of the rich stereochemistry of edta-type complexes, their conformational studies are surprisingly rare [13, 14]. We have recently completed an extensive study [15] of the conformations of [Cr(edtrp)(H₂O)] isomers. The [Cr(edtrp)(H₂O)] species was chosen due to its key role in the former studies, by some of us, of anomalous C–N bond cleavage [16–18] and unprecedented C–N bond recombination [19]. In these structures the ethylenediamine-*N,N,N'*-tripropionato (edtrp) anion acts as a quinquedentate ligand, theoretically forming three geometrical isomers: *cis*-polar, *cis*-equatorial and *trans*-equatorial with respect to the coordination site of the unidentate ligand (in this case, a molecule of water), as shown in Figure 1. So far, their assignment on the basis of p.m.r. and c.d. spectra did not give unequivocal results [17]. Using a newly developed force field [15], parametrized for edta-type complexes, molecular mechanics (MM) showed the *trans*-equatorial isomer to be the most stable one. Furthermore,

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trans (H₂O, N') *trans* (H₂O, O) *trans* (H₂O, N_H)
(*cis*-Equatorial) (*cis*-Polar) (*trans*-Equatorial)

Fig. 1. Three geometric isomers of [Cr(edtp)(H₂O)] common labels, used in this paper, are shown in parentheses.

the calculated minimum energy conformation of the *trans*-eq isomer corresponded closely to that found in structurally analogous [Cr(pdtrp)(H₂O)] and [Cr(cydrtp)(H₂O)] complexes¹ characterized previously by X-ray diffraction analysis [17].

We report here the X-ray structure of the parent [Cr(edtp)(H₂O)]·3H₂O complex. X-ray analysis confirms the *trans*-equatorial configuration of the complex and reveals an agreement between the conformation of the ligand in the solid state and in the two lowest-energy *trans*-equatorial forms. The X-ray structure, together with the MM results [15], also substantiates that the anomalous C—N bond cleavage, observed in two of the three possible diastereoisomers of [Cr(edtp)][−] complexes², occurs at the R (out-of-plane) ring, but not at the G (in-plane) ring [17]. Moreover, the strain analysis shows that one of the β-propionato R rings in the [Cr(edtp)(H₂O)] complex is more strained than the G ring, which explains its greater reactivity in C—N bond formation [19].

Experimental

Syntheses and isomer separation

When the reaction solution of [Cr(edtp)][−] (the complex was prepared according to the published procedures [16, 18]) was poured onto a column of QAE-Sephadex C-25 anion exchanger, a portion was not adsorbed. This red solution was concentrated and passed through a column of Dowex 50W-X8 cation-exchange resin in the H⁺ form. After washing with H₂O a neutral complex was obtained whose elemental analysis showed it to contain quinquedentate ethylenediamine-*N,N,N'*-tripropionate together with one water molecule. (Found: C, 33.15; H, 6.35; N, 6.95. C₁₁H₁₉O₇N₂Cr·3H₂O: calcd. C, 33.25; H, 6.35; N, 7.05%).

Structure determination

Single crystals suitable for the X-ray diffraction study were obtained by adding acetone to an aqueous solution

of [Cr(edtp)(H₂O)]. The single crystals selected for X-ray measurements were loaded into glass capillaries.

Measurements were made on a Rigaku AFC5R diffractometer using graphite monochromated MoK_α radiation. The calculations were performed using the TEXAN crystallographic software package of Molecular Structure Corporation [20] on a VAX computer.

The data were collected at 296 ± 1 K using the ω − 2θ scan technique. Three representative reflections were monitored every 100 scans and their intensities showed no decay.

The structure was solved by direct methods. The positional and thermal parameters were refined by the block-diagonal least-squares refinement. The non-hydrogen atoms were refined anisotropically. All hydrogen atoms except, those of the waters of crystallization, were found in the difference Fourier map, and were refined isotropically. The complex is found to be resolved spontaneously having the S absolute configuration on the secondary N atom.

Crystallographic data are listed in Table 1. The selected bond distances, angles, and torsion angles are summarized in Tables 2–6, respectively. Molecular diagrams were produced with *Ortep-3 for Windows* V1.073 [21].

Results and discussion

X-ray structure determination of [Cr(edtp)(H₂O)]·3H₂O

The trihydrate of [Cr(edtp)(H₂O)] crystallizes as dark red rod-like crystals in the P3₁ space group (no. 144). The asymmetric unit is comprised of a monomeric species containing a six-coordinate chromium(III) center with an almost regular octahedral [CrN₂O₄] geometry (Figure 2).

Table 1. Crystallographic data for *trans*-eq [Cr(edtp)(H₂O)]·3H₂O

Chemical formula	C ₁₁ H ₁₉ O ₇ N ₂ Cr·3H ₂ O
Formula weight	397.32
Space group	P3 ₁
Crystal system	Trigonal
a (Å)	11.920(3)
b (Å)	11.920(3)
c (Å)	10.397(2)
α = β(°)	90.0
γ(°)	120.0
V(Å ³)	1279.2(5)
Z	3
D _{calc.} (g cm ^{−3})	1.547
Crystal size (mm)	0.2 × 0.2 × 0.7
λ(MoK _α) (Å)	0.7107
μ (cm ^{−1})	7.03
<i>hkl</i> range	−14 ≤ <i>h</i> ≤ 14, 0 ≤ <i>k</i> ≤ 15, 0 ≤ <i>l</i> ≤ 14
No. of unique reflections	2522
No. of observed reflections	2258
R = ∑(F _o − F _c)/ F _o	0.037
R _w = [∑w(F _o − F _c) ² /∑wF _o ²] ^{1/2}	0.051

¹ pdtrp = S-propane-1,2-diamine-*N,N,N'*-tripropionate; cydrtp = 1S, 2S-*trans*-cyclohexane-1,2-diamine-*N,N,N'*-tripropionate.

² edtp = ethylenediamine-*N,N,N',N'*-tetrapropionate.

Table 2. Selected bond distances (Å) in *trans*-eq [Cr(edtrp)(H₂O)]

Cr(1)—O(1)	1.947(3)
Cr(1)—O(3)	1.958(4)
Cr(1)—O(5)	1.954(4)
Cr(1)—O(7)	1.976(4)
Cr(1)—N(1)	2.048(4)
Cr(1)—N(2)	2.088(3)
O(1)—C(3)	1.285(5)
O(2)—C(3)	1.222(6)
O(3)—C(6)	1.268(6)
O(4)—C(6)	1.237(7)
O(5)—C(9)	1.261(6)
O(6)—C(9)	1.236(8)
N(1)—C(1)	1.484(5)
N(1)—C(10)	1.468(5)
N(2)—C(4)	1.509(7)
N(2)—C(7)	1.494(7)
N(2)—C(11)	1.484(6)
C(1)—C(2)	1.512(6)
C(2)—C(3)	1.525(8)
C(4)—C(5)	1.520(9)
C(5)—C(6)	1.511(6)
C(7)—C(8)	1.512(8)
C(8)—C(9)	1.536(6)
C(10)—C(11)	1.525(6)

Table 3. Selected valence angles (°) in *trans*-eq [Cr(edtrp)(H₂O)]

O(1)—Cr(1)—N(1)	93.7(1)
O(3)—Cr(1)—N(2)	92.7(1)
O(5)—Cr(1)—N(2)	91.6(1)
N(1)—Cr(1)—N(2)	83.4(1)
Cr(1)—O(1)—C(3)	132.2(3)
Cr(1)—O(3)—C(6)	134.7(3)
Cr(1)—O(5)—C(9)	134.7(3)
Cr(1)—N(1)—C(1)	114.8(3)
Cr(1)—N(1)—C(10)	107.7(3)
C(1)—N(1)—C(10)	111.4(3)
Cr(1)—N(2)—C(4)	111.0(3)
Cr(1)—N(2)—C(7)	109.7(3)
Cr(1)—N(2)—C(11)	109.5(2)
C(4)—N(2)—C(7)	104.6(3)
C(4)—N(2)—C(11)	110.5(4)
C(7)—N(2)—C(11)	111.4(4)
N(1)—C(1)—C(2)	112.6(4)
C(1)—C(2)—C(3)	116.2(4)
O(1)—C(3)—O(2)	121.6(5)
O(1)—C(3)—C(2)	118.0(4)
O(2)—C(3)—C(2)	120.3(4)
N(2)—C(4)—C(5)	115.5(4)
C(4)—C(5)—C(6)	117.2(5)
O(3)—C(6)—O(4)	122.1(4)
O(3)—C(6)—C(5)	119.8(5)
O(4)—C(6)—C(5)	118.1(5)
N(2)—C(7)—C(8)	116.9(4)
C(7)—C(8)—C(9)	114.7(4)
O(5)—C(9)—O(6)	123.5(4)
O(5)—C(9)—C(8)	119.0(5)
O(6)—C(9)—C(8)	117.4(5)
N(1)—C(10)—C(11)	108.9(4)
N(2)—C(11)—C(10)	111.3(4)

The chromium center is coordinated by a quinque-dentate edtrp³⁻ ligand chelating the metal through two N donors and three O donors. The H₂O molecule occupies

Table 4. Selected torsional angles (°) in *trans*-eq [Cr(edtrp)(H₂O)]

Cr(1)—O(1)—C(3)—O(2)	-166.6(5)
Cr(1)—O(1)—C(3)—C(2)	17.3(8)
Cr(1)—O(3)—C(6)—O(4)	-176.4(3)
Cr(1)—O(3)—C(6)—C(5)	3.0(7)
Cr(1)—O(5)—C(9)—O(6)	-163.2(4)
Cr(1)—O(5)—C(9)—C(8)	19.9(7)
Cr(1)—N(1)—C(1)—C(2)	-57.0(6)
Cr(1)—N(1)—C(10)—C(11)	45.6(5)
Cr(1)—N(2)—C(4)—C(5)	60.7(5)
Cr(1)—N(2)—C(7)—C(8)	-63.9(5)
Cr(1)—N(2)—C(11)—C(10)	21.7(6)
O(1)—Cr(1)—N(1)—C(1)	27.1(4)
O(1)—C(3)—C(2)—C(1)	-44.3(7)
O(2)—C(3)—C(2)—C(1)	139.4(6)
O(3)—Cr(1)—N(2)—C(4)	-28.8(3)
O(3)—C(6)—C(5)—C(4)	25.3(6)
O(4)—C(6)—C(5)—C(4)	-155.3(5)
O(5)—Cr(1)—N(2)—C(7)	35.8(3)
O(5)—C(9)—C(8)—C(7)	-35.0(6)
O(6)—C(9)—C(8)—C(7)	148.0(5)
N(1)—Cr(1)—O(1)—C(3)	-8.6(6)
N(1)—Cr(1)—N(2)—C(11)	2.6(4)
N(1)—C(1)—C(2)—C(3)	67.2(7)
N(1)—C(10)—C(11)—N(2)	-45.0(7)
N(2)—Cr(1)—O(3)—C(6)	-0.6(4)
N(2)—Cr(1)—O(5)—C(9)	-19.4(4)
N(2)—Cr(1)—N(1)—C(10)	-26.9(3)
N(2)—C(4)—C(5)—C(6)	-61.5(6)
N(2)—C(7)—C(8)—C(9)	63.0(6)

Table 5. Dimensions of hydrogen bonds in the structure of *trans*-eq [Cr(edtrp)(H₂O)]·3H₂O

Atoms involved	D···A (Å)	H···A (Å)	D—H···A (°)
O(11)—H(112)···O(1)	3.066	2.433	130.97
O(11)—H(112)···O(2)	3.109	2.328	151.09
O(12)—H(123)···O(4)	2.772	1.932	152.67
N(1)—H(1)···O(4) ^a	2.897	1.939	169.27
O(7)—H(72)···O(6) ^b	2.631	1.906	154.39
O(7)—H(72)···O(5) ^b	3.560	2.891	145.27
O(11)—H(111)···O(6) ^b	2.829	1.945	154.12

Equivalent positions: ^a $-x + y - 1$, $-x + 1$, $+z - 1/3$; ^b $-y + 1$, $+x - y + 1$, $+z + 1/3$.

the remaining octahedral position *trans* to the secondary N donor atom. The geometric configuration is therefore *trans*-equatorial, with one equatorial (in-plane) β -propionato chelate ring stemming from the secondary nitrogen and two (out-of-plane) β -propionato rings, attached to the tertiary nitrogen, which are coordinated meridionally.

As indicated in Figure 1, two out-of-plane β -propionato rings stemming from the tertiary N donor, on the same and on opposite side with respect to the axially oriented proton of the secondary N donor, are denoted as R and R', respectively. The in-plane β -propionato ring is labeled G.

Disregarding the non-planarity of the chelate rings, their pairing in the octahedron is symmetrical, therefore the only source of dissymmetry in [Cr(edtrp)(H₂O)] is the secondary N atom. Its absolute configuration was found

Table 6. Strain analysis of *trans*-eq [Cr(edtrp)(H₂O)]

Complex	[Cr(edtrp)]
$\sum \Delta(O_h)S^a$	24
$\Delta\Sigma(en)^b$	-7
$\Delta\Sigma(R)^c$	+32
$\Delta\Sigma(R')^c$	+28
$\Delta\Sigma(G)^d$	+29
$\Delta\{M-O-C\}(R)^e$	+14.7
$\Delta\{M-O-C\}(G)^f$	+12.2
$\sum \Delta(N)^g$	6

^a $\sum \Delta(O_h)$ is the sum of the absolute values of the deviations from 90° of the twelve L-M-L' angles; ^b $\Delta\Sigma(en)$ the deviation of the ethylenediamine ring bond angle sum from the ideal value (528°); ^c $\Delta\Sigma(R)$ the deviation of the axial β -propionato ring bond angle sum from the ideal value (658.5°); Standard value for the Cr—O—C angle was taken as 120.0°; ^d $\Delta\Sigma(G)$ the deviation of the equatorial β -propionato ring bond angle sum from the ideal value (658.5°); Standard value for the Cr—O—C angle was taken as 120.0°; ^e $\Delta\{M-O-C\}(R)$ the mean value of deviation of M—O—C bond angles from 120.0° for R rings; ^f $\Delta\{M-O-C\}(G)$ the deviation of the M—O—C bond angle from 120.0° for the G ring; ^g $\sum \Delta(N)$ the sum of the mean absolute values of the six bond angles on the nitrogen atoms.

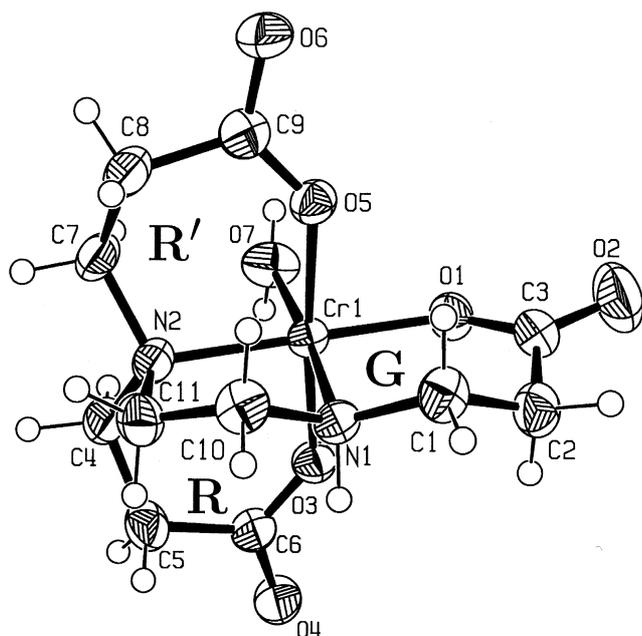


Fig. 2. ORTEP [21] representation of the molecular structure of [Cr(edtrp)(H₂O)] with the atom and ring labelling scheme adopted. Ellipsoids are drawn at 30% probability level.

to be S on the basis of the anomalous dispersion in the final cycle of refinement.

All bond distances and valence angles in the present structure are remarkably similar to those observed [17] in the crystal structures of [Cr(pdtrp)(H₂O)] and [Cr(cydrp)(H₂O)]. This shows that substitutions on the diamine backbone of edtrp³⁻ have a negligible perturbation on the geometry of the coordination sphere.

The atomic groups O(1), N(1), N(2), O(7); O(1), O(3), O(5), N(2); and N(1), O(3), O(5), O(7) separately define the three basal planes of the [CrN₂O₄] octahedron. They have r.m.s. deviations of 0.008, 0.028, and 0.084 Å,

respectively. The displacement of the Cr center from these least-squares planes is only -0.0155, -0.0192, and 0.0009 Å, respectively. All basal planes are mutually orthogonal (dihedral angle av. 88.8°) which altogether shows that the coordination octahedron in [Cr(edtrp)(H₂O)] is insignificantly distorted.

Shapes of chelate rings

The G, R' and R six-membered β -propionato chelate rings adopt irregular conformations close to or intermediate between half-boats and half-chairs, and are best described by the values of θ_2 and φ_2 Cremer-Pople angles [15, 22]. Thus the G ring is closest to a half-boat ($\theta_2 = 42.5^\circ$ and $\varphi_2 = 130.4^\circ$); the R ring is a slightly puckered half-chair ($\theta_2 = 35.0^\circ$ and $\varphi_2 = 101.5^\circ$), and the other R' ring has a slightly flattened conformation, intermediate between a half-chair and a half-boat ($\theta_2 = 52.3^\circ$ and $\varphi_2 = 109.8^\circ$). Therefore, the conformations of these rings comply with the universal feature [15] of six-membered β -propionato chelates; they are markedly flat in the 'carboxylato' part and puckered in the 'amino' (or 'ethylenic') part. On this basis the conformations of β -propionato chelate rings have been sometimes (e.g., Ref. [17]) described using δ/λ labels with respect to their 'ethylenic *gauche* conformations' reflecting merely the sign of the N—CH₂—CH₂—C' torsional angle. In the present structure G, R' and R rings are δ , δ , and λ , respectively.

The ethylenediamine backbone adopts the asymmetrical envelope conformation (with the apex at the methylene C center) which differs from the usual ethylenic *gauche* conformation by having a decreased value for the torsional angle N—C—C—N (-45.0° comparing to av. 60° as found in the isolated five-membered diamine chelates).

Comparison with MM results

The conformation of [Cr(edtrp)(H₂O)], observed in the solid state, is in agreement with the conformations obtained from the MM analysis [15]. The lowest energy structures were found among *trans*-equatorial isomers, of which the global minimum (I) and the next to global conformation (II) together have a population of 90% at 298 K [15]. Both of these two lowest energy conformations closely match the crystallographic conformation in certain fragments of the structure, and most of the observed bond distance values, valence angles and torsional angles are found to be bracketed by the corresponding values found in the two MM optimized conformations. Upon closer inspection of all the four minima (I, II, III, IV) obtained by MM for the *trans*-equatorial configuration [15] it becomes evident that they span a range of accessible points on a conjectured conformational interconversion path between the two highest-energy forms (III) and (IV) which bracket two lowest-energy minima (I and II) as well as the X-ray conformation. The collating sequence (III, II, X-ray, I,

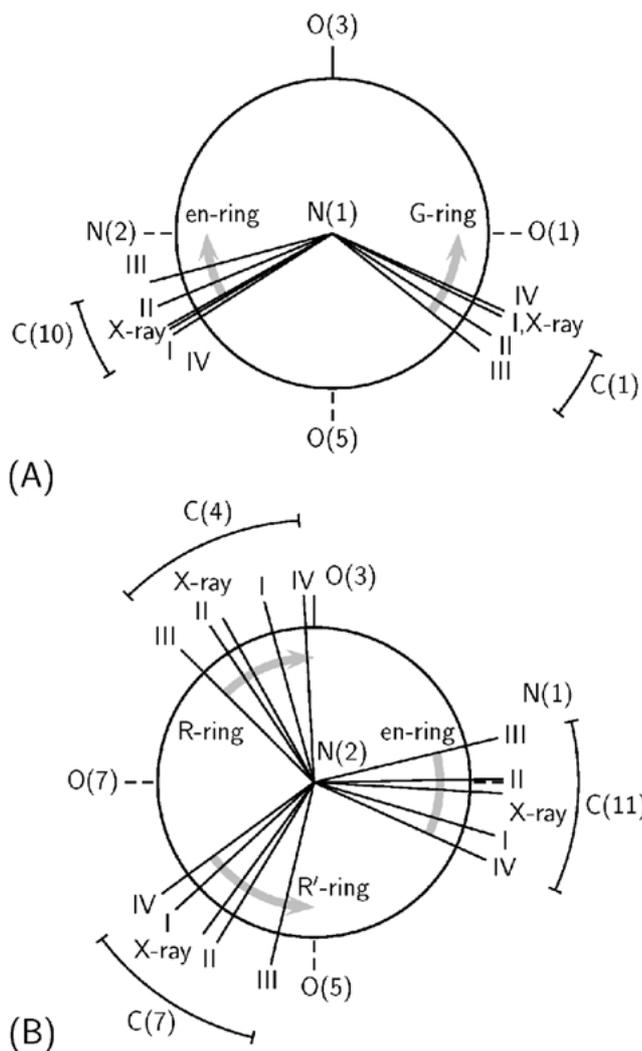
Hydrogen bonding in $[Cr(edtp)(H_2O)]$ crystal structure

Fig. 3. Newman projections for the bonds between Cr and: (A) secondary nitrogen, and (B) tertiary nitrogen. All torsional angles are drawn to scale with respect to O(3) atom. Positions of O(1), N(2) and O(5) in (A), as well as N(1), O(5) and O(7) in (B) are approximate. Hydrogen was omitted from secondary nitrogen N(1) for clarity. Roman numerals indicate four MM calculated equilibrium conformers [15] for the *trans*-eq isomer in the order of increasing energy.

IV) is clearly seen in the Newman projections along both Cr—N bonds (Figure 3) which also shows that the range of torsional angles is almost twice as large for the Cr—N_{tert} bond in comparison with the Cr—N_{sec} bond. This may provide an additional reason for the facile rearrangement of the R β -propionato rings after C—N bond formation (see below).

The greatest differences between the crystal structure conformation and the MM calculations are found exclusively in the flattened ‘carboxylato’ parts of β -propionato chelate rings. This is understandable considering the fact that very small changes in atomic positions of the coordinated carboxylate atoms can easily produce changes in the values of the endocyclic torsional angles that are sufficient to flip the ring from one local minimum to the neighboring one in the torsional subspace.

Another source of discrepancy between the observed and calculated conformations of $[Cr(edtp)(H_2O)]$ is the isolated molecule treatment used in MM. In this crystal structure we found a network of hydrogen bonds involving carbonyl O atoms and O donors of the β -propionato chelates. These perturbations (which are neglected in MM) are precisely responsible for modifying the conformations of the easily deformable ‘carboxylato’ moieties of the six-membered rings. Possible hydrogen bonds are listed in Table 5 and shown in Figure 4. They involve the lattice water molecule, O(11), which bridges G and R rings of two neighboring $[Cr(edtp)(H_2O)]$ complex units (Figure 4). This bridging is further reinforced by the interaction between coordinated water, O(7), and the carboxylate of the neighboring R ring via O—H...O hydrogen bonds. Secondary nitrogen, N(1), as well as another independent lattice water molecule, O(12), are involved concomitantly in hydrogen bond with the R’ ring of a neighboring complex. In conclusion, practically all three carboxylates (from G, R’ and R rings) participate in hydrogen bonding, which clearly explains the inability of MM to fully reproduce the conformational details of β -propionato chelate rings in the isolated $[Cr(edtp)(H_2O)]$ structure.

Strain analysis of *trans*-equatorial $[Cr(edtp)(H_2O)]$

In describing the molecular structure of edta-type complexes it has become customary [23] to comment on various angular deformations in terms of the so-called strain analysis. This approach is undoubtedly informative and useful when comparing two or more structures in a series of closely related edta-type complexes. Since the geometry of the structure of $[Cr(edtp)(H_2O)]$ does not deviate significantly from other similar structures, we do not expect the strain analysis to reveal any unusual results.

As indications of ring strain for this complex, we considered: (i) the 12 octahedral angles around the central ion, (ii) the endocyclic angle sums for the various kinds of rings, (iii) the M—O—C valence angles, and (iv) the bond angles that the chelating nitrogen atoms make with their connectors [23].

Strain analysis performed on the *trans*-equatorial $[Cr(edtp)(H_2O)]$ complex (see Table 6) shows that one of the β -propionato R rings is more strained in comparison with the G ring, and that the strain about the tertiary N atom is great, which is consistent with the facile rearrangement after C—N bond formation in the reaction of the *trans*-equatorial $[Cr(edtp)(H_2O)]$ with 3-hydroxypropionic acid [19].

Finally, the results presented in this work together with the recent MM analysis [15] are in complete agreement with the previous experimental studies of anomalous C—N bond cleavage [16–18] and recombination [19]. Namely, the greater stability of the *trans*-eq

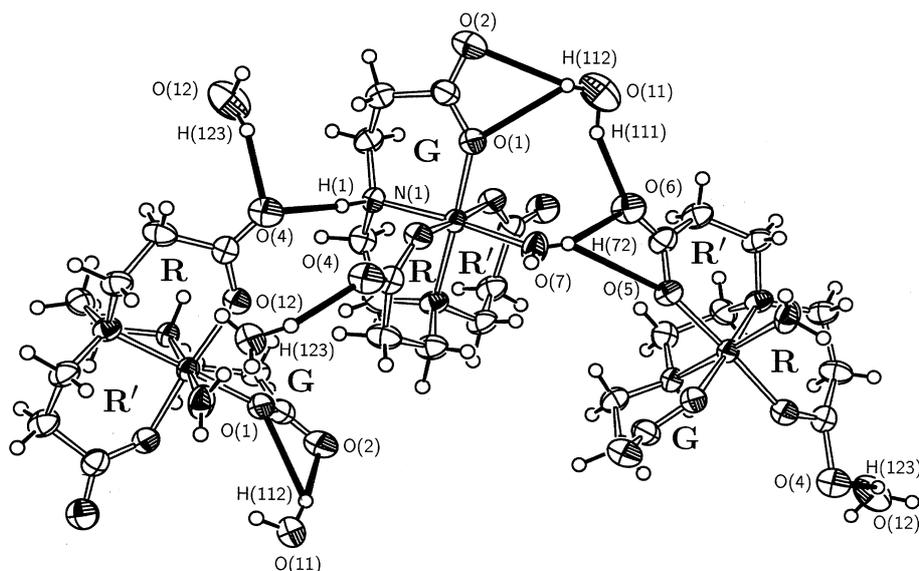


Fig. 4. Crystallographic motive based on hydrogen bonds in the structure of $[\text{Cr}(\text{edtrp})(\text{H}_2\text{O})] \cdot 3\text{H}_2\text{O}$. Possible hydrogen bonds are emphasized with heavy black lines, and the atoms involved in hydrogen bonding are labelled for clarity.

isomer of $[\text{Cr}(\text{edtrp})(\text{H}_2\text{O})]$ may explain the conjectured isomerization of *cis*-polar into *trans*-eq form after C–N bond rupture of the β -propionato R-ring having *ob* conformation in sexidentate $[\text{Cr}(\text{edtrp})]$ [16–18]. In addition, the more strained β -propionato R-ring, in comparison to the G-ring, in $[\text{Cr}(\text{edtrp})(\text{H}_2\text{O})]$ explains the facile rearrangement after C–N bond formation in the reaction of the *trans*-eq isomer with 3-hydroxypropionic acid [19]. This is supported by the fact that a partial sum of energy contributions due to endocyclic bonds (and angles) appears to be generally always greater for the rings involving tertiary N center (e.g., R-rings in the case of the *trans*-eq $[\text{Cr}(\text{edtrp})(\text{H}_2\text{O})]$ isomer), although this may not be reflected in the total energy which includes all nonbonded contributions and the strain due to the diamine ring as well.

The investigation of the strain in the edtrp complexes and geometrical structure around the coordinated secondary amine may provide clues for understanding the fundamental conditions governing the anomalous reactivity in the chromium(III) complexes. The reactions found in this type of metal complex are of interest as models for the enzymatic reversible deamination related to the ammonia-lyases [24].

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