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Second sphere coordination in fluoroanion binding: Synthesis, spectroscopic and X-ray structural study of $[Co(phen)_2CO_3](Pfbz)\cdot 6H_2O$

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ABSTRACT

To explore the anion receptor potential of $[Co(phen)_2(CO)_3]^+$ for the pentafluorobenzoate ion, $[Co(phen)_2(CO)_3](Pfbz)\cdot 6H_2O$ (where phen = 1,10-phenanthroline and Pfbz = pentafluorobenzoate) was synthesized by reacting appropriate salts in aqueous medium. A detailed packing analysis has been undertaken to delineate the role of second sphere C–H···F interactions amid other heteroatom interactions. The complex salt has been characterized by elemental analyses, spectroscopic studies (IR, UV/Vis, multinuclear NMR) and solubility product measurement. The complex salt crystallizes in the monoclinic crystal system with space group $P2_1/n$ having the cell dimensions $a = 13.377(3)$ Å, $b = 17.204(3)$ Å, $c = 15.408(3)$ Å, $\beta = 108.11(3)^\circ$, $V = 3370.1(12)$ Å^3 and $Z = 4$. Single crystal X-ray structure determination revealed ionic structure consisting of complex cation, $[Co(phen)_2(CO)_3]^+$, Pfbz anion and six lattice water molecules. In the crystal lattice, discrete ions $[Co(phen)_2CO_3]^+$ are forming rectangular voids in which the Pfbz anions are entrapped. Crystal lattice is stabilized by electrostatic forces of attraction and hydrogen bonding interactions, i.e. O–H···O, C–H···O, and C–H···F, involving second sphere coordination besides π···π interactions.

1. Introduction

Recognition and sensing of anions is of considerable current interest due to their biological and environmental effects. Tools to achieve the required selectivity and specificity in anion recognition mostly hinge upon the utilization of non-covalent interactions, notably their directionality and cooperativity. In this direction, binding of anions by metal-complex based anion receptors has utilized the power of second sphere coordination through a multitude of weak interactions, particularly hydrogen bonds involving heteroatoms such as O–H···O, O–H···N, N–H···O, N–H···N, etc., besides C–H···π and π···π aromatic interactions. Such endeavors directly or indirectly bring the design and synthesis of anion receptors close to the realm of supramolecular chemistry and profitably utilize the understanding that has been gathered through decades of research on the "chemistry beyond molecules" [1–10]. We [11–16] and others [17–22] have used these interactions towards anion binding, yet harnessing all the knowledge associated with the binding features of anions is in its incipient stage compared to their cationic counterparts. This inherent difficulty is due to the varied size, shape and pH sensitivity of anions as compared with metal ions.

Other than the above mentioned heteroatom interactions, intermolecular interactions involving heavier halogens (Cl, Br, I) have also become an effective tool in preorganising molecules in the crystalline state [23–31]. The role of lightest of the halogens, namely fluorine, in engineering molecules is still debatable as it has been argued that organic fluorine does not accept interactions involving hydrogen atom [32–37]. However notable studies taking the center stage of C–H···F interactions and F···F interactions has started furnishing concrete evidence towards the participation of fluorine in lattice stabilizing interactions [38–42], especially in the absence of any other strong intermolecular forces such as strong O–H···O/N hydrogen bonding.

In this backdrop it is worth mentioning that we have undertaken an extensive research programme to exploit cationic cobalt(III) complex, $[Co(phen)_2CO_3]^+$ as anion receptor and the initial results show that the aromatic hydrogen atoms of the phenanthroline moiety (hydrogen bond donor) and the carbonato group (hydrogen bond acceptor) take part in extensive second sphere coordination in all the compounds studied [43–45]. We thus envisaged that if we can identify a simple anion with high F/C ratio and virtually devoid of any hydrogen atom, then that would facilitate multiple C–H···F_{anion} interactions that may be decisive in crystal packing. Pentaflurobenboate (Pfbz) became the chosen candidate as it is stable and has no hydrogen in it and also has an

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aromatic core. There are very limited examples in the literature in which this anion is reported (e.g. Na, Er(III), benzylammonioun, Xe(II), Zn(II) and Cu(II) pentafluorobenzoates) [46–50]. There is also an added advantage as cobalt(III) salts are easier to synthesize in excellent yields from readily available materials, they are stable at room temperature for months and do not decay under X-ray exposure. Moreover, the cationic complex cation, $[Co(phen)_2CO_3]^+$ fulfils all the basic criteria [51,52] to be an anion receptor, it has (i) unit positive charge for electrostatic interaction, (ii) large number (16) of C–H hydrogen bond donor groups and (iii) stable framework onto which the anionic group can be assembled. In all probabilities, these chosen ions would form an intricate network of weak interactions which may enable us to examine the role of weak C–H···F and F···F interactions as a synthetic strategy to generate molecular networks. In addition, this structural study would also enable us to evaluate the role of these interactions amidst the possible charge assisted C–H···O [53] and $\pi\cdots\pi$ interactions between the chosen anion and cation. Thus, this paper reports the synthesis, spectroscopic studies and detailed packing analyses of the complex formed between $[Co(phen)_2(CO)_3]Cl{\cdot}5H_2O$ and sodium salt of pentafluorobenzoic acid.

2. Results and discussion

The complex salt $[Co(phen)_2CO_3](Pfbz){\cdot}6H_2O$ was obtained by reaction of $[Co(phen)_2(CO)_3]Cl{\cdot}5H_2O$ and sodium salt of pentafluorobenzoic acid in 1:1 molar ratio in the aqueous medium (Scheme 1). The newly formed complex salt is soluble in methanol, ethanol, DMSO, partially soluble in water and insoluble in acetone. The melting/decomposition point of complex salt is 96 °C. The complex salt has been characterized by elemental analyses, spectroscopic studies (IR,UV/Vis, ^1H, ^{13}C, ^{19}F and ^{59}Co-NMR) and solubility product measurements. The crystal structure has been unambiguously established by single-crystal X-ray crystallography.

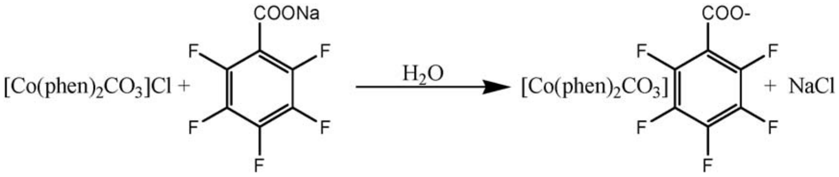
2.1. Measurements of solubility products

Solubility of ionic salts in water differs to a great extent and on the basis of solubility criterion the salts are classified into three categories: soluble, sparingly soluble and insoluble. The solubility product was measured as 5.66×10^{-5} compared to 9.80×10^{-3} of $[Co(phen)_2CO_3]Cl{\cdot}5H_2O$ which gave an idea that the affinity or binding of cationic complex, $[Co(phen)_2CO_3]^+$ is greater for Pfbz anion as compared to chloride ion. Although nearly 100-fold decrease in the solubility product points towards this affinity, it is to be mentioned that hydration influences the solubility product, especially in the cases of different sizes of concerned ions.

2.2. Spectroscopic characterization

IR spectrum of newly synthesized complex salt has been recorded in the region 400–4000 cm^{-1}. The IR spectral bands at 3381, 1665, 1613 and 478 cm^{-1} were assigned to ν(O–H) of H_2O, ν(C═O), ν(C═C)/ν(C═N) and ν(Co–N) respectively. These peaks are characteristic for the carbonato and 1,10-phenanthroline ligands attached to the cobalt(III) center. The bands at 1479, 1354, 987 and 851 cm^{-1} were assigned to ν_{as}(COO), ν_s (COO), ν(C–F) and δ(C═C) respectively. These bands indicated the presence of ionic Pfbz. Similar bands at 1650, 1490, 1320, 940 and 1638, 1495, 1284, 987 were observed in $Er(Pfbz)_3$[47] and $[Zn(phen)_2(Pfbz)(H_2O)](Pfbz)(H_2O)_2$ [50], respectively, which were assigned to ν(CO), ν_{as}(COO), ν_s (COO) and ν(C–F) vibrations. The peak assignments have been made in consultation with literature values [54,55]. The FT-IR spectrum of the title complex salt is shown in Fig. 1.

The ^1H, ^{13}C, ^{19}F and ^{59}Co NMR spectra of the title complex salt were recorded in DMSO-d_6. The numbering scheme employed for the spectral assignment is shown in Fig. 2. In the ^1H NMR spectrum, doublets at 9.26, 9.21, 8.91 and 8.42 ppm were assigned to protons H9, H7, H2 and H8, multiplets at 8.50 and 7.80 were assigned to



Scheme 1. Schematic representation of chemical reaction.

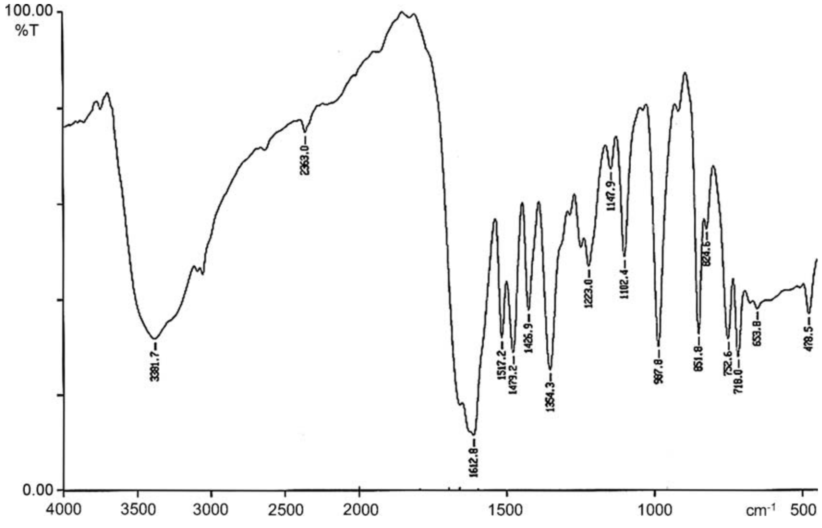


Fig. 1. FT-IR spectrum of complex salt $[Co(phen)_2CO_3](Pfbz){\cdot}6H_2O$.

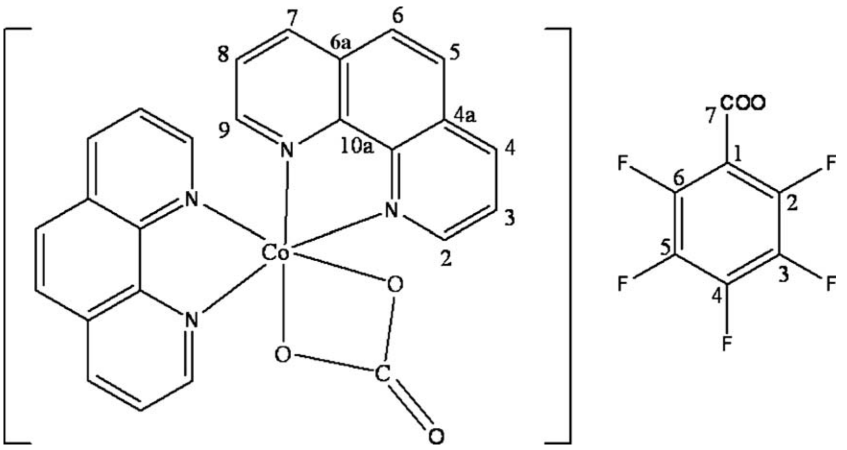


Fig. 2. Numbering scheme employed for the spectral assignment in NMR.

protons H5,6 and H3,4 of the ligand 1,10-phenanthroline coordinated to Co(III).

In the ^{13}C NMR spectrum, the signals at 163.84, 154.51, 152.06, 147.29 & 147.26, 141.32, 140.27, 130.76 & 130.63, 128.47, 128.26, 127.29, and 127.16 ppm were assigned to Cco$_3$, C2, C9, C10a, C4, C7, C4a,6a, C5, C6, C3, and C8 of the coordinated phenanthroline group. The other signals at 165.36, 144.65, 141.32, 136.72, and 112.75 ppm were assigned to C7, C2,6, C4, C3,5, and C1 of the Pfbz ion. Also in ^{19}F NMR spectrum of complex salt, the signals observed at −144.12, −155.73, and −161.89 were assigned to fluorine atoms attached to C2,6, C4, and C3,5 of the anion Pfbz. Similar signals have been also observed at −146.6, −158.2, −164.4 and −141.59, 154.39, −162.43 in sodium pentafluorobenzoate and pentafluorophenylxenon(II) pentafluorobenzoate. ^{19}F NMR spectrum of complex salt is shown in Fig. 3. In ^{59}Co NMR, the signal was observed at 8362 ppm. The signals observed in the NMR spectra are in good agreement with reported values in the literature [46,49,56–59].

The electronic spectrum of the title complex salt was recorded in water. For Co(III) complexes, two types of transitions, i.e. $^1A_{1g} \rightarrow T_{1g}$ and $^1A_{1g} \rightarrow {}^1T_{2g}$ are expected. In the $[Co(phen)_2CO_3]^+$ complexes, these transitions were observed around 500 and 360 nm as reported in the literature [60]. In the title complex salt, these transitions were observed at 511 and 357 nm. Characteristic peaks due to 1,10-phenanthroline groups coordinated to the Co(III) were observed around 272 and 224 nm as in other related complex salts reported in the literature [61].

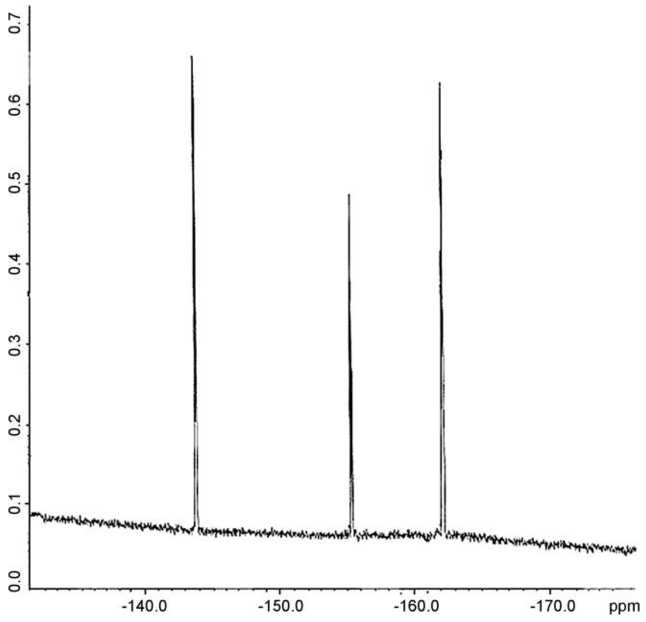


Fig. 3. ^{19}F NMR of the complex salt $[Co(phen)_2CO_3](Pfbz){\cdot}6H_2O$.

2.3. X-ray crystallography

2.3.1. Coordination geometry and bonding

In $[Co(phen)_2CO_3](Pfbz){\cdot}6H_2O$, the central metal atom Co(III) is hexacoordinated with a distorted octahedral environment in which the bite angle of carbonato group is deviated to the extent of 20.51° (ideal value = 90°). The two 1,10-phenanthroline ligands are coordinated to metal ion in a bidentate fashion and are almost orthogonal to each other making an angle of 88.04° with each other (angle between the best least square planes). The pyridyl rings of each of the phenanthroline moieties are nearly coplanar. The isobidentate coordination (1.886(2) and 1.888(2) Å) of the carbonato group to the metal ion has reduced the higher D_{3h} symmetry of the carbonato group to nearly C_{2V} in which the non-coordinated >C=O distance is much smaller (1.211(4) Å) than the other two (1.303(4) and 1.332(4) Å). In addition, the carbonato group is also highly strained in its coordination as O(2)–C(1)–O(3) angle is 109.35° whereas the other two angles subtended around C1 is 125.11(3)° and 125.54(3)°, respectively. It is also evident that there is significant π-electron donation from carbonato group to the metal center which resulted in shorter Co–O (1.887 Å), average bond length as compared to the Co–O bond distance (1.947 and 1.942 Å) observed in case of $[Co(NH_3)_5H_2O]_2[Zr_3F_{18}]{\cdot}6H_2O$ [62] and $[cis\text{-}Co(en)_2(H_2O)Cl]$ [63]. The carboxylate moiety of the Pfbz anion is significantly deviated (C31–C26–C32–O5 torsion angle = 46.29°) from the phenyl ring to minimize the steric crowding from the adjacent fluorine atoms. The average Co–O and Co–N bond distances in the title complex salt are 1.887 and 1.944 Å, which are in agreement with those in similar reported complex salts [64–70] containing the complex cation $[Co(phen)_2CO_3]^+$. Selected bond lengths and bond angles of the complex salt are given in Table 1.

2.3.2. Crystal packing

The complex salt $[Co(phen)_2CO_3](Pfbz){\cdot}6H_2O$ crystallizes in monoclinic crystal system (space group $P2_1/n$). The asymmetric unit consists of one complex cation; $[Co(phen)_2CO_3]^+$, one anion; Pfbz and six lattice water molecules (Fig. 4) out of which two water molecules are found disordered over two positions (due to this disorder any interaction involving these oxygen atoms (O6 and O11) are not presented here).

Table 1
Selected bond lengths and bond angles (Å, °) for complex salt $[Co(phen)_2CO_3](Pfbz)\cdot 6H_2O$.

Cation			
Co(1)–O(2)	1.886(2)	Co(1)–N(4)	1.956(2)
Co(1)–O(3)	1.888(2)	O(1)–C(1)	1.211(4)
Co(1)–N(1)	1.928(2)	O(2)–C(1)	1.303(4)
Co(1)–N(2)	1.960(2)	O(3)–C(1)	1.332(4)
Co(1)–N(3)	1.935(2)		
O(2)–Co(1)–O(3)	69.49(9)	N(1)–Co(1)–N(4)	175.55(11)
N(1)–Co(1)–N(3)	92.79(10)	N(1)–Co(1)–N(2)	83.92(9)
Anion			
O(4)–C(32)	1.250(4)	F(5)–C(30)	1.340(4)
O(5)–C(32)	1.214(4)	C(26)–C(32)	1.542(4)
F(1)–C(27)	1.340(4)	O(5)–C(32)–O(4)	127.6(3)
F(2)–C(28)	1.337(4)	O(5)–C(32)–C(26)	116.5(3)
F(3)–C(31)	1.344(3)	O(4)–C(32)–C(26)	115.8(3)
F(4)–C(29)	1.335(4)		

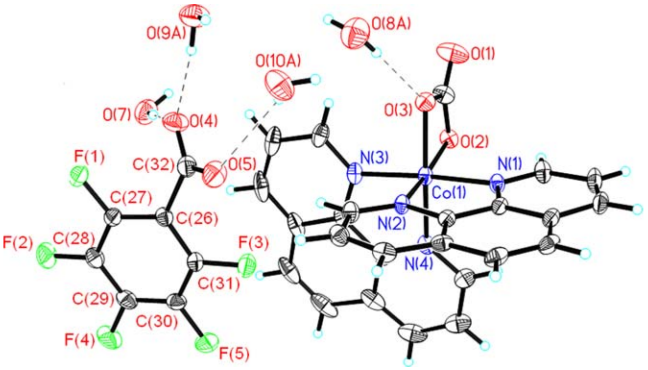


Fig. 4. ORTEP diagram of the complex salt $[Co(phen)_2CO_3](Pfbz)\cdot 6H_2O$ (disordered water molecules are not shown for clarity).

The near orthogonal arrangement of the two phenanthroline moieties around the metal ion, when placed centrosymmetrically, generates rectangular voids in which Pfbz anions reside. One such arrangement is shown in Fig. 5.

The crystal lattice is stabilized by composite interplay of O–H···O, C–H···O and C–H···F hydrogen bonding interactions whose parameters are recorded in Table 2. If the lattice is viewed down the *ab* plane (down *c* axis), as shown in Fig. 6, it is clear that the "box-like" arrangement of cations is placed along the diagonal of this plane and all the four sides having extensive hydrogen bonding interactions.

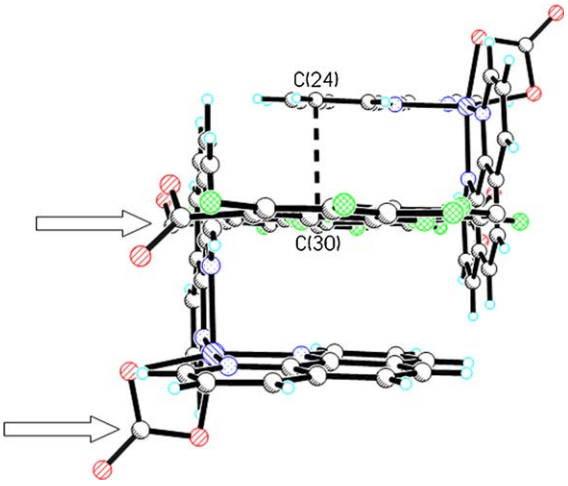


Fig. 5. The rectangular voids generated by cations when placed across $\bar{1}$ and the position of Pfbz anions in these voids. The protruded carboxylate and carbonato groups are marked with arrows at the left hand side of the figure.

Water molecules in the lattice are extensively involved in O–H···O bonding to the carboxylate part of the anion as well as to the carbonato part (first six entries in Table 2). This help positioning the anions as shown in Fig. 6. As expected, a large number of aromatic hydrogen atoms (as high as eight) of the phenanthroline ligand take part in C–H···O/F type hydrogen bonding (last eight entries) towards the lattice stabilization, in which notably two are with fluorine. Both the ortho fluorine atoms (F1 and F3) are involved in C–H···F interactions even in the presence of a large number of O–H···O hydrogen bonds. It is noteworthy that no F···F interaction is observed in the lattice (the minimal F···F distance is 3.166 Å in the lattice). The lattice derives its stabilization through two different types of $\pi\cdots\pi$ interactions, one is between the phenanthroline ligands (the average distance between rings involved is 3.41 Å). It is also observed that the two phenanthroline rings that are juxtaposed each other are sheered to each other also. In the second $\pi\cdots\pi$ interaction, the Pfbz ring is placed close to the phenanthroline ring. Here also the aromatic rings are displaced in such a manner that the C(24)···C(30) distance is 3.33 Å (shown in Fig. 5 with the help of dotted line).

The packing analyses of complex salt $[Co(phen)_2CO_3](Pfbz)\cdot 6H_2O$ brings to the light that even in packing of charged species $[Co(phen)_2CO_3]^+$ and Pfbz, the role of second sphere coordination involving O–H···O and C–H···O along with C–H···F are significant in the total lattice stabilization.

2.4. Conclusions

The potential of second sphere interactions in fluoroanion binding by cationic cobalt(III) complex, $[Co(phen)_2CO_3]^+$ has been

Table 2
Hydrogen bonding parameters (Å, °) for complex salt $[Co(phen)_2CO_3](Pfbz)\cdot 6H_2O$ (only those interactions are considered significant where the distance between two atoms is less than sum of their van der Waals radii).

D(donor)–H···A(acceptor)	D···A	H···A	Angle D–H–A
O7–H7B···O4	2.865(4)	1.996(3)	175.9(2)
O8–H8C···O3 (−*x* + 1/2, +*y* − 1/2, −*z* + 1/2 + 1)	2.868(4)	2.022(2)	173.5(3)
O9–H9C···O10 (*x*, +*y*, +*z* − 1)	3.330(5)	2.648(3)	137.9(2)
O9–H9B···O4 (*x* − 1/2, *y* + 1/2 + 1, +*z* + 1/2)	2.709(4)	1.839(3)	165.1(2)
O10–H10B···O5 (−*x* + 1/2, +*y* − 1/2, −*z* + 1/2 + 1)	2.851(3)	2.385(4)	116.3(2)
O10–H10C···O8	2.749(5)	2.241(4)	119.7(2)
C2–H2A···O2	2.978(4)	2.517(2)	110.8(2)
C13–H13A···F3	3.171(3)	2.538(2)	125.7(2)
C14–H14A···O3	2.982(4)	2.529(2)	110.3(2)
C25–H25A···O9 (−*x*, −*y* + 1, −*z* + 1)	3.328(5)	2.614(4)	134.0(2)
C4 –H4A···F1 (*x*, +*y*, +*z* + 1)	3.501(4)	2.662(2)	150.2(2)
C10–H10A···O2 (*x* + 1/2, −*y* + 1/2 + 1, +*z* + 1/2)	3.255(3)	2.544(2)	133.6(2)
C11–H11A···O1 (−*x* + 1/2, +*y* + 1/2, −*z* + 1/2 + 1)	3.280(4)	2.379(3)	162.9(2)
C22–H22A···O3 (*x* − 1/2, −*y* + 1/2 + 1, +*z* − 1/2)	3.367(4)	2.684(8)	130.9(3)

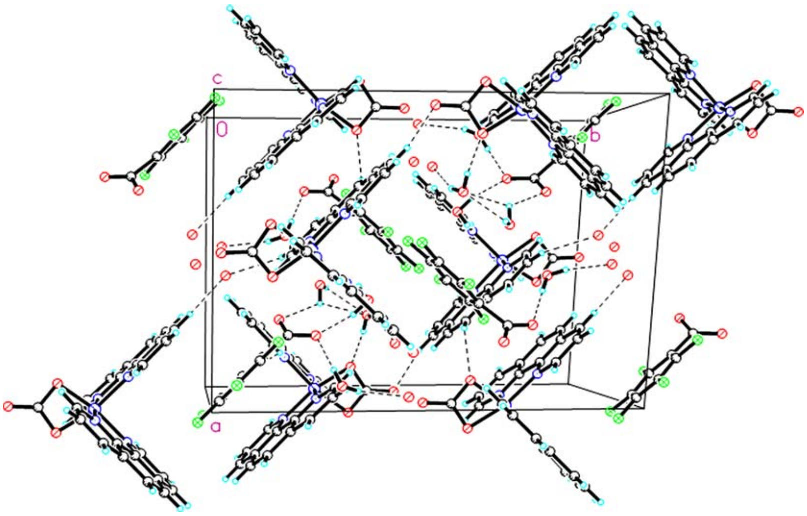


Fig. 6. Packing of $[Co(phen)_2CO_3](Pfbz)\cdot6H_2O$ view down *c* axis. Note the arrangement of the rectangular voids (Fig. 5) along the diagonal of the unit cell.

explored by isolating and characterizing the new Co(III) complex salt, $[Co(phen)_2CO_3](Pfbz)\cdot6H_2O$. Single-crystal X-ray structure determination revealed ionic structures consisting of discrete ions: one complex cation, one Pfbz and six lattice water molecules in the asymmetric unit. The packing analyses of complex salt reveal that C–H···F interactions can manifest even in ionic compounds having a large number of heteroatom interactions like O–H···O, C–H···O and $\pi\cdots\pi$ stacking interactions. Thus, it is important to consider the possibility of C–H···F interactions in compounds that have a relatively high fluorine substitution and in such cases, probably other than the individual strength, their cooperative interplay would be substantial in the lattice stabilization.

3. Experimental

3.1. Materials

Analytical grade reagents were used without any further purification. $[Co(phen)_2CO_3]Cl\cdot5H_2O$ has been prepared by the reaction between $CoCl_2\cdot6H_2O$, 1,10-phenanthroline and sodium bicarbonate [70].

3.2. Synthesis of $[Co(phen)_2CO_3](Pfbz)\cdot6H_2O$

To a 10 mL solution of $[Co(phen)_2CO_3]Cl\cdot5H_2O$ (0.5 g, 0.8 mmol) in water, 10 mL solution of sodium salt of pentafluorobenzoic acid (prepared by the reaction of 0.316 g (0.8 mmol) of pentafluorobenzoic acid and 0.033 g (0.8 mmol) sodium hydroxide in 10 mL of water) was added. Pink coloured crystals were obtained after 6 days when the reaction mixture was allowed to evaporate slowly at room temperature. Yield was 75%. It decomposed at 96 °C. The composition was established by elemental analyses; $[Co(phen)_2CO_3](Pfbz)\cdot6H_2O$, found (%): C, 47.98; H, 3.42; N, 7.30; Co, 7.15. Calculated (%): C, 48.12; H, 3.50; N, 7.01; Co, 7.39.

3.3. Instruments and measurements

C, H and N were estimated microanalytically by automatic PERKIN ELMER 2400 CHN elemental analyzer. Cobalt was estimated by volumetric method [71]. UV/Visible spectrum was recorded using HITACHI 330 spectrophotometer in water. Infrared spectrum of the title complex salt was recorded using PERKIN ELMER spectrum RX FT-IR system using KBr pellet. ^1H-, ^{13}C-, ^{19}F- and ^{59}Co NMR spectra of title complex salt were run in the solvent DMSO-d_6 by using BRUKER AC 400 F (400 MHz) spectrometer. The chemical shift values are expressed as δ value (ppm) down field from tetramethylsilane as an internal standard. In ^{19}F NMR, chemical shift values are expressed as δ value (ppm) with respect to CCl_3F. In ^{59}Co NMR, chemical shift values are expressed as δ value (ppm) with respect to $K_3[Co(CN)_6]$.

Table 3

Crystal data and refinement parameters of $[Co(phen)_2CO_3](Pfbz)\cdot6H_2O$.

Empirical formula	$C_{32}H_{28}CoN_4O_{11}F_5$
M_w	798.51 g/mol
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 13.377(3) Å, b = 17.204(3) Å, c = 15.408(3) Å, β = 108.11(3)°
V	3370.1(12) $Å^3$
Z	4
Calculated density	1.574 Mg/m^3
Absorption coefficient (μ)	0.604 mm^{-1}
Reflections (measured/unique/observed)	24,899/6610/4624
R_{int}	0.028
Data/parameters	6610/498
R_1, wR_2 [$I > 2\sigma(I)$]	R_1 = 0.050, wR_2 = 0.152
R_1, wR_2 (all data)	R_1 = 0.077, wR_2 = 0.166

3.4. X-ray crystallography

The X-ray diffraction data were collected on a Bruker X8 APEX II KAPPA CCD diffractometer (at the Scientific and Technological Research Equipment Centre of Chulalongkorn University) at 298 K using graphite monochromatized Mo Kα radiation (λ = 0.71073 Å). The crystal was positioned at 40 mm from the CCD and the diffraction spots were measured using a counting time of 10 s. Data reduction and multi-scan absorption were carried out using the APEX II program suite [72]. The structure was solved using SHELXS-97 [73] and refined using full-matrix least squares with SHELXL-97 [73]. Anisotropic thermal parameters were used for all non-H atoms. The hydrogen atoms C–H groups were riding with isotropic thermal parameters equivalent to 1.2 times those of the atom to which they were attached. The residual electronic density was within the expected values (0.33/−0.33 e $Å^{-3}$). Final *R*-values together with selected refinement details are given in Table 3.

4. Supplementary data

Crystallographic data of the title complex salt have been deposited with the Cambridge Crystallographic Data Center allocated with the deposit number CCDC 722529. Copy of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, fax: +44 1223 336033, e-mail: deposit@ccdc.cam.ac.uk.

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