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# Synthesis, Crystal Structure and Thermodynamic Properties of *Tris*(8-Quinolinolato-N,O)cobalt(III) Methanol

WEN-YAN DAN, YOU-YING DI*, DONG-MEI ZHANG, DONG-HUA HE and YU-PU LIU

College of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, Shandong Province, P.R. China

*Corresponding author: Fax: +86 635 8239121; Tel: +86 635 8230645; E-mail: diyouying@126.com; yydi@lcu.edu.cn

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*Tris*(8-quinolinolato-N,O)cobalt(III) methanol ($Co(C_9H_6NO)_3{\cdot}CH_3OH$) solvate, which may be a kind of potential organic light-emittings material was synthesized by solvonthermal synthesis. X-Ray crystallography, elemental analysis and chemical analysis were applied to characterize the structure and composition of the complex. Lattice energy of the complex was derived from its crystal data. Low-temperature heat capacities of $Co(C_9H_6NO)_3{\cdot}CH_3OH(s)$ were measured by a small sample precision automated adiabatic calorimeter over the temperature range from 78-370 K. A polynomial equation of the heat capacities as a function of temperature was fitted by the least square method. Based on the fitted polynomial, the smoothed heat capacities and thermodynamic functions of the compound relative to the standard reference temperature 298.15 K were calculated and tabulated at intervals of 5 K.

**Key Words: *Tris*(8-quinolinolato-N,O)cobalt(III) methanol solvate, Organic light-emittings devices, Thermodynamic functions.**

## INTRODUCTION

8-Hydroxyquinoline has been used in large-scale industrial application. For example, some intermediate products of dyestuffs and drugs were prepared using 8-hydroxyquinoline. In addition, some 8-hydroxyquinoline metal complexes have used as organic electroluminescent devices. For example, *tris*(8-hydroxyquinolinato)aluminium(III) is an important part of organic light-emittings devices (OLEDs) due to its advantages in quantum efficiency, carrier mobility and thermal stability. Among this research a variety of 8-hydroxyquinoline metal coordination compounds have been explored for the design of OLEDs[1]. The present cobalt(III) compound may be a kind of potential light-emittings material.

Li *et al.*[2] synthesized the present compound and investigated its crystal structure. However, lattice energy and some important thermodynamic properties of the present compound have not been found in the literature, which restricted the progress of relevant theoretical studies and application development of the compounds used as the light-emittings material. Lattice energy has an important role in evaluating the stability of new materials. Heat capacity is one of the most fundamental thermodynamic properties and closely related to other physical, biological, physiological and chemical properties[3,4]. The purpose of the present work is to measure low temperature heat capacities of the compound by an adiabatic calorimetry and thermodynamic functions of the title compound were derived from these experimental results.

## EXPERIMENTAL

Cobalt acetate and 8-hydroxyquinoline used as the reactants were of analytical grade with a labeled mass percent purity of 99.5 %. The reactants were accurately weighed at the molar ratio of $n[Co(CH_3COO)_2{\cdot}4H_2O]:n[C_9H_7NO] = 1:3$. A solution of 8-hydroxyquinoline (6.6559 g, 0.045 mol) in methanol and another solution of $Co(CH_3COO)_2{\cdot}4H_2O$ (3.8064 g, 0.015 mol) in the certain amount of methanol were mixed together in a flask of 250 mL. The solution was heated and stirred under reflux for 10 h. The final solution was naturally cooled to room temperature, filtered and the crude product was washed three times by anhydrous methanol. The solid product was recrystallized using anhydrous methanol and brown crystals were obtained. Finally, the sample was placed in a vacuum desiccator to dry for 6 h at 303 K. Theoretical contents of Co, C, H and N in the compound have been calculated as, 11.26, 64.25, 4.23 and 8.03 %, respectively. Chemical analysis and elemental analysis (model: PE-2400, Perkin Elmer, USA) have shown that the practical contents of Co, C, H and N in the compound have been measured to be 11.24, 64.26, 4.21 and 8.05 %, respectively. This showed the mass per cent purity of the sample prepared was higher than 99.50 %. The content of cobalt in the sample was measured by $Na_2EDTA$ complex titration. It was demonstrated from results of chemical and elemental analysis that one solvent molecule $CH_3OH$ exists in the coordination compound.

A single crystal with dimensions of 0.33 mm × 0.21 mm × 0.19 mm suitable for X-ray analysis was mounted on a fiber. All diffraction data for the compound were collected on a Bruker Smart-1000 CCD area-detector diffractometer with graphite monochromated $MoK_\alpha$ radiation ($\lambda = 0.71073$ Å) at 298(2) K. The structure was solved by direct methods and expanded using Fourier techniques with the SHELXL-97 program[5] and refined with a full-matrix least-squares technique on $F^2$. All non-hydrogen atoms were refined anisotropically. All H-atoms were located theoretically and refined. Absorption corrections were applied by SADABS. Crystal data and refinement details are summarized in Table-1.

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT FOR THE PRESENT COMPOUND

| Crystallographic data | Structure refinement |
|---|---|
| Empirical formula | $C_{28}H_{22}N_3O_4Co$ |
| Formula weight | 523.42 |
| Temperature | 298(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | $P2_1/n$ |
| Unit cell dimensions | a = 10.8759 (12) Å, b = 13.1334 (14) Å, c = 16.700(2) Å; α = 90°, β = 97.7310 (10)°, γ = 90° |
| Volume | 2363.6 (5) $Å^3$ |
| Z | 4 |
| Calculated density | 1.471 $g/cm^3$ |
| Absorption coefficient | 0.767 $mm^{-1}$ |
| F(000) | 1080 |
| Crystal size | 0.33 mm × 0.21 mm × 0.19 mm |
| θ range for data collection | 1.98-25.02° |
| Limiting indices | $-6 \le h \le 12$, $-15 \le k \le 15$, $-19 \le l \le 19$ |
| Reflections collected/unique | 11705/4156 [R(int) = 0.0358] |
| Completeness to θ = 25.02 | 99.7 % |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data/restraints/parameters | 4156/1/326 |
| Goodness-of-fit on $F^2$ | 1.000 |
| Final R indices [I > 2σ(I)] | $R_1 = 0.0407$, $wR_2 = 0.0837$ |
| R indices (all data) | $R_1 = 0.0738$ $wR_2 = 0.1052$ |
| Largest diff. peak and hole | 0.406 and -0.361 $eÅ^{-3}$ |

**Detection method:** A precise automatic adiabatic calorimeter was used to measure heat capacities of the compound over the temperature range $78 \le (T/K) \le 370$. The calorimeter was established in the Thermochemistry Laboratory of Liaocheng University, Shandong Province, China. The principle and structure of the adiabatic calorimeter have been described in detail elsewhere [6,7]. Briefly, the calorimeter mainly comprised a sample cell, a platinum resistance thermometer, an electric heater, inner, middle and outer adiabatic shields, three sets of six-junction chromel-constantan thermopiles installed between the calorimetric cell and the inner shield, between the inner and middle shields and between the middle and outer shields, respectively and a high vacuum can. The miniature platinum resistance thermometer (IPRT No. 2, produced by the Shanghai Institute of Industrial Automatic Meters, 16 mm in length, 1.6 mm in diameter and a nominal resistance of 100 Ω) was applied to measure the temperature of the sample. The thermometer was calibrated on the basis of ITS-90 by the station of low-temperature Metrology and Measurements, Academia Sinica. The electrical energy introduced into the sample cell and the equilibrium temperature of the cell after the energy input were automatically recorded by use of a Data Acquisition/Switch Unit (Model 34970A, Agilent, USA) and processed on line by a computer.

To verify the performance of the calorimeter, the heat capacities of the reference standard material ($\alpha$-$Al_2O_3$) were measured over the temperature range $78 \le (T/K) \le 400$. The sample mass used was 1.7143 g, which was equivalent to 0.0168 mol based on its molar mass, $M(Al_2O_3) = 101.9613$ g $mol^{-1}$. The experimental molar heat capacities of $\alpha$-$Al_2O_3$ were fitted by a least squares method to a polynomial equation. Relative deviations of the experimental results from those of the smooth curve lie within ± 0.29 %, while the uncertainty is ± 0.30 %, as compared with the values given by the former National Bureau of Standards[8] over the whole temperature range.

Heat-capacity measurements were continuously and automatically carried out by means of the standard method of intermittently heating the sample and alternately measuring the temperature. The heating rate and temperature increments were generally controlled at (0.1-0.4) K $min^{-1}$ and (1-3) K. The heating duration was 10 min and the temperature drift rates of the sample cell measured in an equilibrium period were always kept within ($10^{-3}$-$10^{-4}$) K $min^{-1}$ during the acquisition of all heat-capacity data. The data of heat capacities and corresponding equilibrium temperature have been corrected for heat exchange of the sample cell with its surroundings[7]. The sample mass used in the calorimetric measurements was 1.81251 g, which is equivalent to 0.0035 mol in terms of its molar mass, 523.42 g $mol^{-1}$.

## RESULTS AND DISCUSSION

**Crystal structure:** The molecular structure of $Co(C_9H_6NO)_3\cdot CH_3OH(s)$ is shown in Fig. 1. The selected bond lengths and angles of the compound are listed in Table-2. Hydrogen bonds are listed in Table-3. Unit cell parameters are a = 10.8759 (12) Å, b = 13.1334 (14) Å, c = 16.700(2) Å, α = 90°, β = 97.7310 (10)° and γ = 90°, respectively. It was found that the crystal system of the coordination compound is monoclinic and the space group is $P2_1/n$, as shown in Table-1. Three 8-quinolinolate monoanions chelate to the cobalt atom with an octahedral coordination geometry. The packing of the

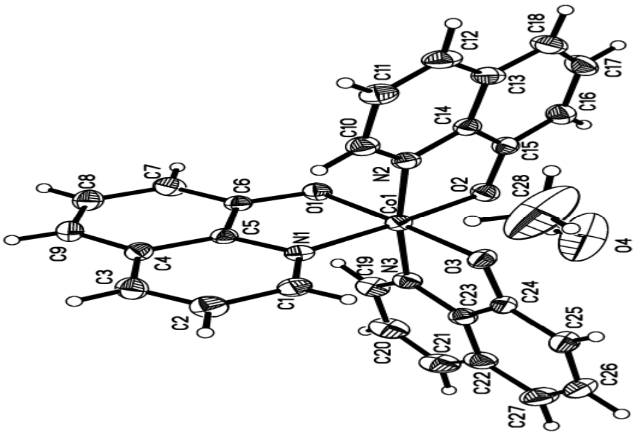

Fig. 1. Structure of the title compound $Co(C_9H_6NO)_3\cdot CH_3OH(s)$

TABLE-2
SELECTED BOND LENGTHS (Å) AND ANGLES (°)
FOR THE PRESENT COMPOUND

| | | | |
|---|---|---|---|
| Co(1)-O(2) | 1.896(2) | O(2)-Co(1)-O(1) | 89.64(10) |
| Co(1)-N(3) | 1.922(3) | O(1)-Co(1)-N(3) | 93.04(11) |
| Co(1)-O(3) | 1.905(2) | O(1)-Co(1)-N(1) | 85.66 (11) |
| Co(1)-N(2) | 1.935(3) | O(2)-Co(1)-O(3) | 92.46(10) |
| Co(1)-O(1) | 1.898(2) | O(3)-Co(1)-N(3) | 85.70(11) |
| Co(1)-N(1) | 1.928(3) | O(3)-Co(1)-N(1) | 92.22(11) |
| N(1)-C(1) | 1.320(4) | O(1)-Co(1)-N(2) | 91.69(10) |
| N(2)-C(14) | 1.372(4) | N(1)-Co(1)-N(2) | 94.25(11) |
| O(1)-C(6) | 1.332(4) | C(5)-N(1)-Co(1) | 110.6(2) |
| O(4)-C(28) | 1.339(5) | C(14)-N(2)-Co(1) | 109.5(2) |
| N(2)-C(10) | 1.318(4) | C(23)-N(3)-Co(1) | 110.7(2) |
| N(3)-C(23) | 1.367(4) | C(24)-O(3)-Co(1) | 111.3(2) |
| O(3)-C(24) | 1.328(4) | O(2)-Co(1)-N(2) | 86.27(11) |
| N(1)-C(5) | 1.372(4) | N(3)-Co(1)-N(2) | 172.47(12) |
| N(3)-C(19) | 1.320(4) | C(1)-N(1)-Co(1) | 130.4(2) |
| O(2)-C(15) | 1.325(4) | C(10)-N(2)-Co(1) | 131.2(2) |
| O(4)-H(4) | 0.8200 | C(19)-N(3)-Co(1) | 129.3(3) |
| C(1)-H(1) | 0.9300 | C(15)-O(2)-Co(1) | 111.3(2) |
| C(1)-C(2) | 1.406(5) | N(1)-C(1)-C(2) | 121.5(3) |
| C(2)-H(2) | 0.9300 | N(1)-C(1)-H(1) | 119.2 |
| C(4)-C(9) | 1.405(5) | O(1)-C(6)-C(7) | 124.9(3) |
| C(6)-C(7) | 1.377(5) | O(1)-C(6)-C(5) | 117.1(3) |
| C(8)-C(9) | 1.366(5) | N(1)-C(5)-C(4) | 123.0(3) |
| C(10)-C(11) | 1.405(5) | N(1)-C(5)-C(6) | 114.7(3) |
| C(11)-H(11) | 0.9300 | N(2)-C(10)-C(11) | 121.8(3) |
| C(13)-C(18) | 1.413(5) | N(2)-C(10)-H(10) | 119.1 |
| C(15)-C(16) | 1.384(5) | N(2)-C(14)-C(13) | 122.3(3) |
| C(17)-C(18) | 1.361(5) | N(2)-C(14)-C(15) | 115.2(3) |
| C(19)-C(20) | 1.410(5) | O(2)-C(15)-C(16) | 124.7(3) |
| C(20)-H(20) | 0.9300 | O(2)-C(15)-C(14) | 117.5(3) |
| C(22)-C(27) | 1.408(6) | N(3)-C(19)-C(20) | 120.6(4) |
| C(24)-C(25) | 1.385(5) | N(3)-C(19)-H(19) | 119.7 |
| C(26)-C(27) | 1.362(6) | C(3)-C(2)-C(1) | 120.1(3) |
| C(28)-H(28A) | 0.9600 | C(9)-C(8)-C(7) | 123.0(4) |

TABLE-3
HYDROGEN BONDS FOR $Co(C_9H_6NO)_3{\cdot}CH_3OH(s)$

| D–H···A | d(D–H) (Å) | d(H···A) (Å) | < DHA (°) | d(D···A) (Å) |
|---|---|---|---|---|
| O(4)-H(4)···O(3) | 0.82 | 2.06 | 147.7 | 2.785(4) |
| C(1)-H(1)···O(3) | 0.93 | 2.53 | 111.0 | 2.996(4) |
| C(19)-H(19)···O(1) | 0.93 | 2.53 | 111.0 | 2.992(4) |

complex was shown in Fig. 2. The quinoline plane containing atom N3 parallels to another quinoline plane containing atom N3 (1-x, 1-y, 1-z). The vertical distance of two planes is 3.427 Å and the rectilineal distance of the center of two planes is 3.728 Å. The above findings indicates the existence of π-π stacking between the neighboring complex molecules. The crystal data and the structure of the title compound determined was almostly consistent with the previously reported results[2].

**Lattice energy:** The lattice energy ($U_{POT}$) is calculated by the following formula[9],

$$U_{POT} = \gamma\left(\frac{\rho_m}{M_m}\right)^{1/3} + \delta \qquad (1)$$

where $M_m$/g (or Mg) is the chemical formula mass of the ionic material; $\rho_m$/g cm$^{-3}$ (or Mg m$^{-3}$) is the density of the substance; coefficients γ and δ take the following values for $M_pX_q$ (q:p), $\gamma = 2342.6$ I kJ mol$^{-1}$ cm and $\delta = 55.2$ I kJ mol$^{-1}$ [9]; where I is the ionic strength term [$I = 1/2(pq^2 + qp^2)$]. The values of $\rho_m$ and $M_m$ are found in Table-1. The lattice energy of the complex is calculated to be 2314.72 kJ mol$^{-1}$, which reveals that its structure is very stable.

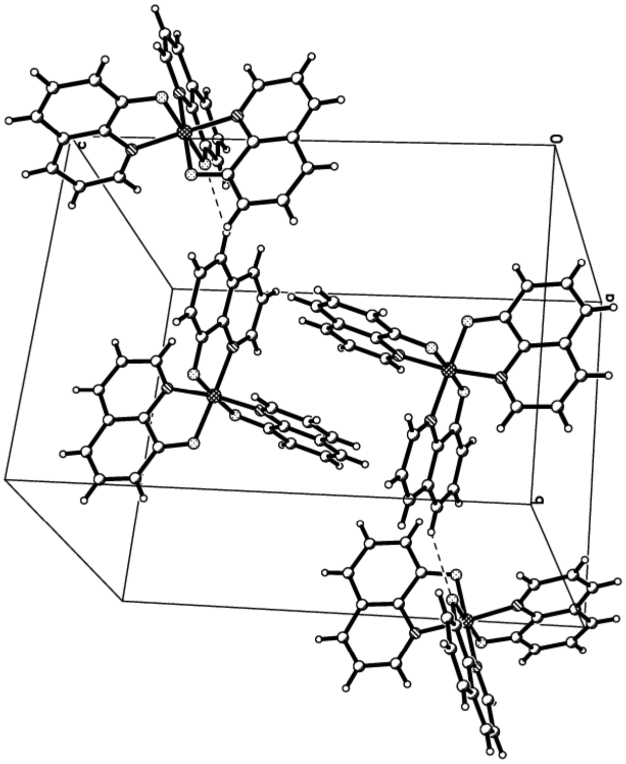

Fig. 2. Packing of structure of the title compound $Co(C_9H_6NO)_3{\cdot}CH_3OH(s)$ in unit cell

**Low-temperature heat capacities:** The experimental molar heat capacities of the coordination compound are listed in Table-4 and plotted in Fig. 3, which showed that the heat capacity curve of the compound smoothly increased with temperature. The present compound was thermally stable over the temperature range between T = 78 and 370 K, no phase change, association and thermal decomposition occurred. The experimental points in the temperature region between T = 78 and 370 K were fitted by the least square method and a polynomial equation of the experimental molar heat capacities ($C_{p,m}$) *versus* reduced temperature (X), X = f(T ), have been obtained by eqn. 2:

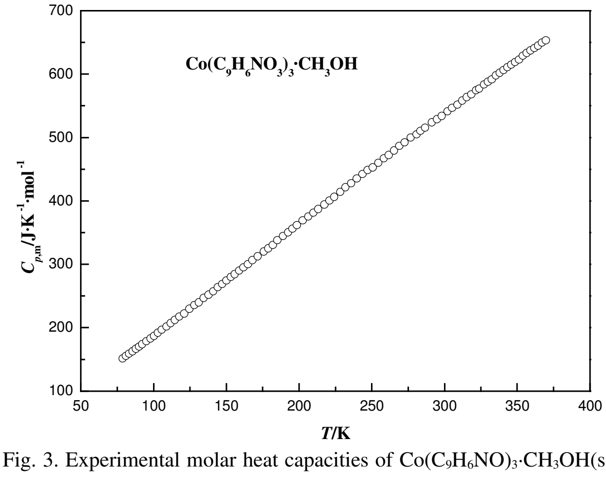

Fig. 3. Experimental molar heat capacities of $Co(C_9H_6NO)_3{\cdot}CH_3OH(s)$

TABLE-4
EXPERIMENTAL MOLAR HEAT CAPACITIES
OF $Co(C_9H_6NO)_3{\cdot}CH_3OH(s)$

| T (K) | $C_{p,m}$ (J $K^{-1}$ $mol^{-1}$) | T (K) | $C_{p,m}$ (J $K^{-1}$ $mol^{-1}$) | T (K) | $C_{p,m}$ (J $K^{-1}$ $mol^{-1}$) |
|---|---|---|---|---|---|
| 78.697 | 151.35 | 168.03 | 306.38 | 280.82 | 504.94 |
| 80.990 | 155.42 | 171.60 | 312.64 | 283.52 | 510.34 |
| 83.282 | 158.97 | 175.72 | 319.95 | 286.69 | 515.40 |
| 85.574 | 162.80 | 178.88 | 325.02 | 291.27 | 523.91 |
| 87.866 | 166.63 | 181.99 | 330.49 | 294.85 | 528.98 |
| 90.159 | 169.99 | 185.15 | 337.87 | 298.08 | 534.04 |
| 92.114 | 173.73 | 189.00 | 344.49 | 302.13 | 541.40 |
| 95.148 | 178.40 | 192.44 | 350.17 | 305.30 | 546.80 |
| 97.845 | 182.93 | 195.54 | 356.00 | 308.94 | 551.87 |
| 100.41 | 186.98 | 198.64 | 361.68 | 312.11 | 558.24 |
| 102.97 | 191.81 | 202.55 | 369.09 | 315.28 | 563.47 |
| 105.60 | 196.65 | 206.39 | 375.24 | 318.51 | 568.05 |
| 108.83 | 201.66 | 209.83 | 381.23 | 321.68 | 574.36 |
| 111.80 | 207.13 | 213.27 | 387.05 | 323.91 | 576.88 |
| 114.70 | 212.18 | 217.45 | 394.08 | 327.14 | 583.42 |
| 117.67 | 217.49 | 221.02 | 400.62 | 329.84 | 587.67 |
| 121.10 | 222.28 | 224.12 | 406.35 | 332.54 | 591.60 |
| 124.68 | 229.77 | 228.30 | 414.03 | 335.23 | 597.81 |
| 127.98 | 235.54 | 232.01 | 421.23 | 337.93 | 602.06 |
| 131.08 | 239.80 | 235.92 | 427.93 | 340.56 | 606.31 |
| 134.52 | 246.90 | 239.77 | 435.29 | 343.19 | 610.56 |
| 137.76 | 252.10 | 243.61 | 442.32 | 345.89 | 614.81 |
| 141.06 | 257.46 | 247.18 | 448.53 | 348.51 | 618.90 |
| 144.16 | 263.77 | 250.69 | 452.81 | 351.21 | 622.99 |
| 147.13 | 268.65 | 254.46 | 460.06 | 353.84 | 628.88 |
| 150.16 | 274.54 | 258.37 | 467.31 | 356.47 | 633.29 |
| 153.13 | 279.89 | 261.68 | 472.20 | 359.10 | 637.21 |
| 155.62 | 284.15 | 265.38 | 479.43 | 361.73 | 640.98 |
| 158.93 | 289.91 | 269.03 | 486.79 | 364.29 | 644.90 |
| 161.89 | 295.14 | 272.67 | 492.19 | 366.99 | 649.31 |
| 164.86 | 300.21 | 276.71 | 499.87 | 369.75 | 653.05 |

$$C_{p,m}/(J\ K^{-1}\ mol^{-1}) = 406.669 + 58.949X - 10.757\ X^2 - 6.900X^3 + 6.701\ X^4 \quad (2)$$

in which X = (T(K) - 224)/146. The correlation coefficient for the fitting $R^2$ equaled 0.99999. The value, 224, is half of the upper limit 370 K plus the lower limit 78 K in the temperature range of (78-370) K, while 146 is half of the upper limit 370 K minus the lower limit 78 K in the same range. The reduced temperature (X) obtained using the method are between +1 and -1 and relative deviations of the smooth heat capacities from the experimental values will become smaller and smaller with the increase of the power of X in the fitted polynomial equation according to the principle in statistics.

The eqn. 2 is valid in the temperature range of (78-370) K. The relative deviations of the smoothed heat capacities obtained by the above equation from experimental heat capacities were within ± 0.30 %, as shown in Fig. 4.

**Thermodynamic functions of the compound:** The smoothed molar heat capacities and thermodynamic functions of the sample were calculated based on the fitted polynomial of the heat capacity as a function of the reduced temperature (X) according to the following thermodynamic equations,

$$H_{(T)} - H_{(298.15\,K)} = \int_{298.15\,K}^{T} C_{p,m} dT \quad (3)$$

$$S_{(T)} - S_{(298.15\,K)} = \int_{298.15\,K}^{T} C_{p,m} T^{-1} dT \quad (4)$$

TABLE-5
SMOOTHED HEAT CAPACITIES AND THERMODYNAMIC
FUNCTIONS OF $Co(C_9H_6NO)_3{\cdot}CH_3OH$

| T (K) | $C_{p,m}$ (J $K^{-1}$ $mol^{-1}$) | $H_T - H_{298.15\,K}$ (kJ $mol^{-1}$) | $S_T - S_{298.15\,K}$ (J $K^{-1}$ $mol^{-1}$) | $G_T - G_{298.15\,K}$ (kJ $mol^{-1}$) |
|---|---|---|---|---|
| 80 | 153.77 | -75.042 | -398.51 | -43.162 |
| 85 | 161.85 | -74.253 | -388.95 | -41.193 |
| 90 | 170.03 | -73.424 | -379.46 | -39.272 |
| 95 | 178.32 | -72.553 | -370.05 | -37.398 |
| 100 | 186.69 | -71.640 | -360.69 | -35.572 |
| 105 | 195.16 | -70.686 | -351.37 | -33.791 |
| 110 | 203.69 | -69.688 | -342.10 | -32.058 |
| 115 | 212.30 | -68.648 | -332.85 | -30.370 |
| 120 | 220.97 | -67.565 | -323.64 | -28.729 |
| 125 | 229.70 | -66.439 | -314.44 | -27.134 |
| 130 | 238.48 | -65.268 | -305.26 | -25.584 |
| 135 | 247.31 | -64.054 | -296.10 | -24.081 |
| 140 | 256.17 | -62.795 | -286.94 | -22.623 |
| 145 | 265.07 | -61.492 | -277.80 | -21.211 |
| 150 | 274.00 | -60.144 | -268.66 | -19.845 |
| 155 | 282.95 | -58.752 | -259.53 | -18.525 |
| 160 | 291.92 | -57.315 | -250.40 | -17.250 |
| 165 | 300.90 | -55.833 | -241.28 | -16.021 |
| 170 | 309.90 | -54.306 | -232.17 | -14.837 |
| 175 | 318.90 | -52.734 | -223.05 | -13.699 |
| 180 | 327.90 | -51.117 | -213.94 | -12.607 |
| 185 | 336.90 | -49.455 | -204.84 | -11.560 |
| 190 | 345.89 | -47.748 | -195.73 | -10.559 |
| 195 | 354.87 | -45.996 | -186.63 | -9.6028 |
| 200 | 363.85 | -44.199 | -177.53 | -8.6923 |
| 205 | 372.81 | -42.357 | -168.44 | -7.8273 |
| 210 | 381.75 | -40.471 | -159.35 | -7.0078 |
| 215 | 390.67 | -38.540 | -150.26 | -6.2336 |
| 220 | 399.57 | -36.564 | -141.18 | -5.5049 |
| 225 | 408.44 | -34.544 | -132.10 | -4.8216 |
| 230 | 417.29 | -32.480 | -123.03 | -4.1836 |
| 235 | 426.12 | -30.371 | -113.96 | -3.5911 |
| 240 | 434.91 | -28.219 | -104.90 | -3.0439 |
| 245 | 443.67 | -26.022 | -95.838 | -2.5420 |
| 250 | 452.41 | -23.782 | -86.786 | -2.0854 |
| 255 | 461.11 | -21.498 | -77.741 | -1.6742 |
| 260 | 469.79 | -19.171 | -68.703 | -1.3082 |
| 265 | 478.43 | -16.800 | -59.672 | -0.98733 |
| 270 | 487.04 | -14.387 | -50.648 | -0.71167 |
| 275 | 495.62 | -11.930 | -41.632 | -0.48112 |
| 280 | 504.17 | -9.4306 | -32.625 | -0.29562 |
| 285 | 512.68 | -6.8884 | -23.626 | -0.15512 |
| 290 | 521.17 | -4.3038 | -14.635 | -0.059568 |
| 295 | 529.63 | -1.6767 | -5.6537 | -0.0089000 |
| 298.15 | 534.95 | 0 | 0 | 0 |
| 300 | 538.07 | 0.99254 | 3.3187 | -0.0030669 |
| 302 | 541.44 | 2.0721 | 6.9051 | -0.013275 |
| 310 | 554.86 | 6.4573 | 21.236 | -0.12571 |
| 315 | 563.23 | 9.2526 | 30.180 | -0.25410 |
| 320 | 571.58 | 12.090 | 39.115 | -0.42715 |
| 325 | 579.91 | 14.968 | 48.041 | -0.64485 |
| 330 | 588.22 | 17.889 | 56.957 | -0.90718 |
| 335 | 596.53 | 20.851 | 65.865 | -1.2141 |
| 340 | 604.83 | 23.854 | 74.764 | -1.5656 |
| 345 | 613.12 | 26.899 | 83.654 | -1.9617 |
| 350 | 621.42 | 29.985 | 92.536 | -2.4024 |
| 355 | 629.71 | 33.113 | 101.41 | -2.8875 |
| 360 | 638.02 | 36.283 | 110.28 | -3.4170 |
| 365 | 646.33 | 39.494 | 119.13 | -3.9907 |
| 370 | 654.66 | 42.746 | 127.99 | -4.6084 |

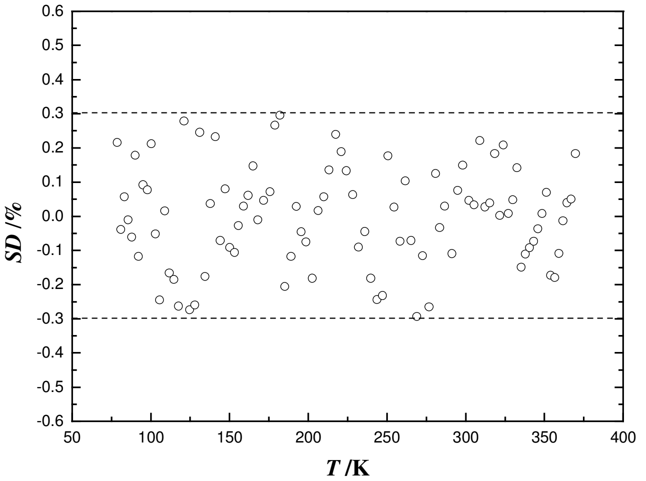

Fig. 4. Plot of the relative deviations, SD (%) = [($C_{smo} - C_{exp}$)/$C_{exp}$] × 100 %, of the smoothed molar heat capacities of the compound from the experimental values against the absolute temperature. In which $C_{smo}$ and $C_{exp}$ represent the smoothed and experimental molar heat capacities of the compound

$$G_{(T)} - G_{(298.15\,K)} = \int_{298.15\,K}^{T} C_{p,m}\,dT - T\cdot\int_{298.15\,K}^{T} C_{p,m}\,T^{-1}\,dT \quad (5)$$

The polynomial fitted values of the molar heat capacities and fundamental thermodynamic functions of the sample relative to the standard reference temperature 298.15 K are tabulated in Table-5 at intervals of 5 K.

## Conclusion

The crystal structure, lattice energy, low-temperature heat capacities and some basic thermodynamic functions of *tris*(8-quinolinolato-N,O)cobalt(III) methanol solvate, were reported. These results are instructive to the applications of 8-hydroxyquinoline metal coordination compounds.

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