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**Tris(1,10-Phenanthroline)Cobalt(II) Triiodide**

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Tris(1,10-phenanthroline)cobalt(II) triiodide

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Key indicators
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.008 Å
R factor = 0.038
wR factor = 0.087
Data-to-parameter ratio = 18.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The asymmetric unit of the title compound, [Co(C12H8N2)3]2+ (I)2, contains one [Co(1,10-phenanthroline)3]2+ cation, half each of two centrosymmetric triiodide anions, and one complete triiodide anion. The title compound was synthesized solvothermally from Co(NO3)2, 1,10-phenanthroline, and SnI2, where the SnI2 reagent serves only as a source of I atoms.

Comment

Single crystals of the coordination compound tris(1,10-phenanthroline)cobalt(II) triiodide, (I), were isolated from the solvothermal reaction of Co(NO3)2, 1,10-phenanthroline (phen), and SnI2. Though the synthesis includes tin(II) iodide as a reagent, the resultant product contains no tin. However, it is a well known phenomenon that tin(II) compounds are air-sensitive (Ryan & Xu, 2004), and since an inert environment was not used in the present synthesis, the absence of tin in the resulting compound is not surprising. Thus, the SnI2starting material functions only as a source of I atoms.

![Diagram](I)

The asymmetric unit of (I) contains a [Co(phen)3]2+ cation in addition to three crystallographically distinct I3- anions, two of which are located about inversion centers (Fig. 1). For the non-centrosymmetric anion (I5—I6—I7), one I–I bond is slightly longer than the other and the anion deviates slightly from linearity. Both the cation and the anion of this compound have been observed in numerous other compounds, and the bond angles and distances for both species are typical (Table 1). The present compound is isostructural with [Ni(phen)3]2+ (Freckmann & Tebbe, 1981). Additionally, the title compound is related to several other compounds having the same basic formula, [M(phen)3]2+ (M = Mn or Fe; Horn et al., 2002; Ramalakshmi et al., 1999). However, these compounds crystallized in a different space group, and most of them contain solvents of crystallization.

Experimental

SnI2 (0.3 mmol, 110 mg), Co(NO3)2·6H2O (0.1 mmol, 29 mg), and 1,10-phenanthroline (0.3 mmol, 70 mg) were weighed and placed in a 23 ml Teflon-lined autoclave with absolute ethanol (10 ml) as the reaction solvent. The autoclave was subsequently sealed and heated...
at a rate of 1 K min⁻¹ to 433 K. The temperature was held at 433 K for 3 d before it was decreased at a rate of 0.1 K min⁻¹ to 353 K, where it was then held for 6 h. Finally, the temperature was decreased at a rate of 0.1 K min⁻¹ to room temperature. Orange–brown crystals were isolated from the reaction and a suitable single crystal was selected for the X-ray diffraction experiment.

table 1

<table>
<thead>
<tr>
<th>Selected geometric parameters (Å, °)</th>
<th>11−12</th>
<th>12−11</th>
<th>12−13</th>
<th>13−12</th>
<th>13−14</th>
<th>14−13</th>
<th>14−15</th>
<th>15−14</th>
<th>15−16</th>
<th>16−15</th>
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<tbody>
<tr>
<td>I1−I2</td>
<td>2.9414 (4)</td>
<td>180</td>
<td>1.0556</td>
<td>1.0556</td>
<td>1.0556</td>
<td>1.0556</td>
<td>1.0556</td>
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<td>0.8634</td>
<td>1.0556</td>
<td>1.0556</td>
<td>1.0556</td>
<td>1.0556</td>
<td>1.0556</td>
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<tr>
<td>I2−I1</td>
<td>2.9280 (5)</td>
<td>0.8634</td>
<td>1.0556</td>
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<td>1.0556</td>
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<tr>
<td>I6−I5</td>
<td>2.8855 (5)</td>
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<td>1.0556</td>
<td>1.0556</td>
<td>1.0556</td>
<td>1.0556</td>
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<tr>
<td>I5−I6</td>
<td>2.9280 (5)</td>
<td>0.8634</td>
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<tr>
<td>I4−I3</td>
<td>2.8855 (5)</td>
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</tr>
<tr>
<td>I3−I4</td>
<td>2.9236 (4)</td>
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<td>1.0556</td>
<td>1.0556</td>
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<tr>
<td>Symmetry codes: (i) −x+1, −y−1, z; (ii) x+1, y, z</td>
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</table>

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C−H = 0.95 Å and Uiso(H) = 1.2Ueq(C). The highest peak and depest hole are located 0.88 and 0.74 Å, respectively, from atom I7.

Data collection: SMART-NT (Bruker, 2001); cell refinement: SAINT-Plus-NT (Bruker, 2001); data reduction: SAINT-Plus-NT; program(s) used to solve structure: SHELX97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 2000); software used to prepare material for publication: SHELXTL.

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References