# Crystal structure of caesium(I) hydrogen maleate, $Cs(C_4H_3O_4)$

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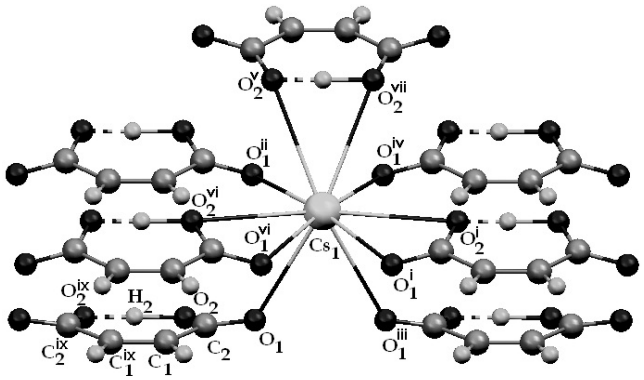


**Abstract**

$C_4H_3CsO_4$, orthorhombic, *Pnma* (no. 62), $a = 5.597(2)$ Å, $b = 8.775(1)$ Å, $c = 12.572(2)$ Å, $V = 617.4$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.029$, $wR_{ref}(F^2) = 0.080$, $T = 298$ K.

**Source of material**

$Cs_2CO_3$ (652 mg, 2 mmol) was carefully added to an aqueous solution (15 ml) containing maleic acid (464 mg, 4 mmol), until no further bubbles formed. The reaction mixture produced a colourless and clear solution which was stirred at 323 K for 2 h until it solidified. The solid product was re-dissolved in water (5 ml) and allowed to stand for three days at ambient temperature, after which transparent fine crystals were harvested.

**Experimental details**

The H1 atom was positioned geometrically and refined using riding model, with $d$(C—H) = 0.93 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C). The H2 atom was found in difference Fourier map and refined.

**Discussion**

Multidendate carboxylic acids are found to be excellent ligands for the synthesis of coordination polymers giving the structures with a diverse range of topologies and conformations, due to the carboxylate groups being able to coordinate to a metal centre as a mono-, bi-, or multidentate ligand [1,2]. Although most of the studies conducted in this area is primarily focused on coordination polymers containing transition metals as connectors, such as Zn, Ni and Co [3,4], there is little attention on the Group I metal [5,6]. As part of ongoing studies on Group I dicarboxylates [7-9], we present here the caesium complex formed with maleic acid. The asymmetric unit of the title compound contains one caesium cation, one hydrogen maleate anion. The Cs atom is ten-coordinated by ten O atoms from seven different hydrogen maleate ions. The anion is linked to two caesium cations, while the $Cs^+$ cation is surrounded by seven organic ligands, three of which are coordinated by employing both O atoms and the other four are coordinated solely by O atoms. The Cs—O distances are in the range from 3.196 (2) to 3.466 (2) Å, which are well within the range reported in the literature for other caesium complexes [10-12]. In the crystal structure, intramolecular hydrogen bonds occur, linking carboxylate O atoms. The H2 atom is involved in this bond and maintains the charge balance by sharing between two carboxylate groups within the structure.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | colorless prism, size 0.03 × 0.12 × 0.40 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71069 Å) |
| $\mu$: | 59.33 cm$^{-1}$ |
| Diffractometer, scan mode: | Rigaku AFC-7S, $\omega/2\theta$ |
| $2\theta_{max}$: | 79.98° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 2000, 2000 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 1137 |
| $N(param)_{refined}$: | 46 |
| Programs: | SHELXS-97 [13], SHELXL-97 [14] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(1) | 8*d* | –0.2824 | 0.1297 | 0.6338 | 0.042 |
| H(2) | 4*c* | 0.29(1) | ¼ | 0.606(4) | 0.07(2) |

**Table 3.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Cs(1) | 4*c* | –0.02295(4) | ¼ | 0.12835(2) | 0.0297(1) | 0.0331(1) | 0.0419(1) | 0 | –0.0019(1) | 0 |
| O(1) | 8*d* | 0.0272(4) | –0.0714(3) | 0.6471(2) | 0.042(1) | 0.0259(8) | 0.079(2) | 0.0017(8) | –0.000(1) | 0.005(1) |
| C(1) | 8*d* | –0.1316(4) | 0.1741(3) | 0.6311(2) | 0.0212(9) | 0.030(1) | 0.053(2) | –0.0027(7) | –0.001(1) | –0.001(1) |
| O(2) | 8*d* | 0.2818(3) | 0.1122(2) | 0.6048(2) | 0.0250(8) | 0.0349(9) | 0.062(1) | 0.0047(7) | 0.0051(8) | –0.0014(9) |
| C(2) | 8*d* | 0.0718(5) | 0.0632(3) | 0.6275(2) | 0.029(1) | 0.0263(9) | 0.040(1) | 0.0026(8) | –0.002(1) | –0.003(1) |

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