# Structure of $[Co(meen)_2(en)]Br_3 \cdot H_2O$*

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(Received April 4, 1989)

The crystal structure of this compound (meen = *N*-methylethane-1,2-diamine) has recently been described as monoclinic, space group $I2/a$, with $a$ = 12.626(5), $b$ = 22.977(5), $c$ = 12.619(6) Å, $\beta$ = 97.84(4)°, $Z$ = 8 [1]. It is properly described as orthorhombic, space group *Fddd*, with $a$ = 19.030, $b$ = 22.977, $c$ = 16.589 Å, $Z$ = 16. The orthorhombic cell can be derived from the vectors $[10\bar{1}]$, [010] and [101]; the corresponding coordinate transformations are: $x' = \frac{1}{2}(x - z)$, $y' = y$, $z' = \frac{1}{2}(x + z)$. After averaging over appropriate pairs of atoms and shifting the origin by $\Delta x' = 0.25$, $\Delta z' = 0.25$ (in order to place the origin at the conventional center in *Fddd*), the coordinates in Table 1 result. No atom neeeded to be shifted by more than its e.s.d. in order to comply with the symmetry of *Fddd*.

*Contribution No. 7926 from the Arthur Amos Noyes Laboratory.

TABLE 1. Coordinates for the space group *Fddd*

| Atom | Site | $x$ | $y$ | $z$ |
|---|---|---|---|---|
| Br(1) | 16(e) | 0.47214 | 0.12500 | 0.12500 |
| Br(2) | 32(h) | 0.57255 | 0.02094 | 0.36028 |
| Co | 16(f) | 0.37500 | 0.12282 | 0.37500 |
| N(1) | 32(h) | 0.3328 | 0.1826 | 0.4452 |
| N(2) | 32(h) | 0.2840 | 0.1258 | 0.3152 |
| N(3) | 32(h) | 0.4107 | 0.0598 | 0.3051 |
| C(1) | 32(h) | 0.2577 | 0.1899 | 0.4248 |
| C(2) | 32(h) | 0.2485 | 0.1814 | 0.3359 |
| C(3) | 32(h) | 0.2814 | 0.1170 | 0.2268 |
| C(4) | 32(h) | 0.3762 | 0.0039 | 0.3297 |
| O | 16(f) | 0.3750 | 0.2958 | 0.3750 |

Since the required shifts are so small, there are no significant changes in the bond lengths and angles reported earlier [1]. The two molecules a and **b**, which were independent in the earlier description, now become equivalent by symmetry.

## Reference

1 G. H. Searle and E. R. T. Tiekink, *Inorg. Chim. Acta, 156* (1989) 57.

0020-1693/89/3.50