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# Hemipotassium hemirubidium digallium(III) manganese(II) tris(phosphate) dihydrate

**Jing Zhang,[a] Ping Li,[a] Zhi-Hong Liu[a] and Seik Weng Ng[b]***

[a]School of Chemistry and Materials Science, Shaanxi Normal University, Xi'an 710062, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(Mn–O) = 0.002 Å; disorder in solvent or counterion; $R$ factor = 0.023; $wR$ factor = 0.065; data-to-parameter ratio = 13.1.

The title manganese(II) substituted gallophosphate, $K_{0.5}Rb_{0.5}[Ga_2Mn(PO_4)_3(H_2O)_2]$, features a three-dimensional network built of $PO_4$ tetrahedra, $GaO_5$ trigonal bipyramids and $MnO_6$ octahedra. The $Rb^I$ and $K^I$ ions, which are disordered with respect to each other in a 1:1 ratio, occupy sites within the channels of the framework. The $Rb^I/K^I$ and $Mn^{II}$ atoms occupy positions of 2 symmetry, as does one of the two P atoms. The $Rb^I/K^I$ site is surrounded by six O atoms [2.996 (2)–3.178 (4) Å] in an irregularly-shaped coordination environment. O—H···O hydrogen bonds between the water molecules and phosphate O atoms consolidate the crystal packing.

## Related literature

For isotypic $NH_4[Ga_2Mn(PO_4)_3(H_2O)_2]$, see: Chippindale *et al.* (1998).

## Experimental

### Crystal data

$K_{0.5}Rb_{0.5}[Ga_2Mn(PO_4)_3(H_2O)_2]$
$M_r$ = 577.61
Monoclinic, $C2/c$
$a$ = 13.5504 (12) Å
$b$ = 10.2965 (9) Å
$c$ = 8.9072 (8) Å
$\beta$ = 108.527 (1)°
$V$ = 1178.34 (18) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 8.31 mm$^{-1}$
$T$ = 295 K
0.45 × 0.40 × 0.35 mm

### Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.118, $T_{max}$ = 0.159
6267 measured reflections
1348 independent reflections
1239 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.065
$S$ = 1.04
1348 reflections
103 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.75 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$w$—H1···O3$^{i}$ | 0.84 (3) | 1.97 (2) | 2.790 (3) | 166 (4) |
| O1$w$—H2···O6$^{ii}$ | 0.84 (3) | 2.10 (2) | 2.913 (3) | 165 (4) |

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Shaanxi Normal University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2164).

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# supporting information

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## Hemipotassium hemirubidium digallium(III) manganese(II) tris(phosphate) dihydrate

**Jing Zhang, Ping Li, Zhi-Hong Liu and Seik Weng Ng**

### S1. Comment

Microporous aluminium phosphates are readily synthesized by using the hydrothermal route; studies on these compounds have led to improvements in the synthesis of the related gallophosphates. The structure of $NH_4[Ga_2Mn(PO_4)_3(H_2O)_2]$ features $PO_4$ tetrahedra, $GaO_5$ trigonal bipyramids and $MnO_6$ octahedra that are linked together to form a three-dimensional network (Chippindale *et al.*, 1998). The title compound has a similar structure (Fig. 1); however, the rubidium and potassium atoms that occupy the channels within the network rattle in the cavities, as noted from the irregular nature of the polyhedron surrounding the atoms. The coordination number is much higher when longer interactions are considered.

### S2. Experimental

The compound was synthesized from a mixture of gallium oxide (0.037 g), boric acid (0.035 g), rubidium carbonate (0.023 g), potassium carbonate (0.138 g), manganese dichloride tetrahydrate (0.397 g), phosphoric acid (0.15 ml) and water (1.8 ml) (molar ratio of 2:5:1:10:20:20:1000). This mixture was sealed in 25 ml, Teflon-lined, stainless-steel Parr bomb. The bomb was heated at 468 K for 7 days. Colorless block-shaped crystals were isolated.

### S3. Refinement

The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H 0.84±0.01 Å; their temperature factors were tied to those of the O atom by a factor of 1.5 times.

The potassium and rubidium atoms share the same site, a special position of *2* site symmetry. As the occupancy of each refined to nearly 1/2, the occupancies were then fixed as exactly 1/2. The temperature factors of K1 and Rb1 were restrained to be identical.

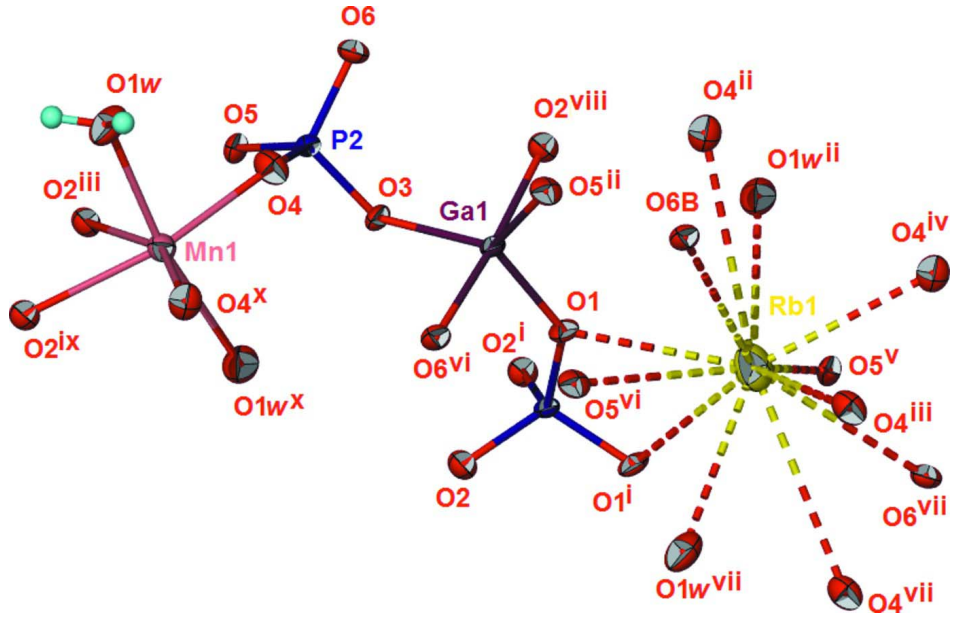


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of a portion of the polymeric structure of $K_{0.5}Rb_{0.5}[Ga_2Mn(PO_4)_3(H_2O)_2]$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The potassium atoms are disordered with respect to the rubidium atoms in a 1:1 ratio. Symmetry codes: (i) *x* + 1/2, -*y* + 3/2, *z* + 1/2; (ii) -*x* + 1/2, -*y* + 3/2, -*z* + 1; (iii) -*x* + 1, *y*, -*z* + 3/2; (iv) -*x* + 1/2, *y* + 1/2, -*z* + 1/2; (v) *x* + 1/2, *y* + 1/2, *z* + 1; (vi) *x*, -*y* + 1, *z* + 1/2; (vii) -*x* + 1, -*y* + 1, -*z* + 1; (viii) *x*, -*y* + 1, *z* - 1/2; (ix) -*x*, *y*, -*z* + 1/2; (*x*) *x* - 1/2, -*y* + 1/2, *z* - 1/2.

## Hemipotassium hemirubidium digallium(III) manganese(II) tris(phosphate) dihydrate

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*b* = 10.2965 (9) Å
*c* = 8.9072 (8) Å
*β* = 108.527 (1)°
*V* = 1178.34 (18) Å$^3$
*Z* = 4
*F*(000) = 1104
$D_x$ = 3.256 Mg m$^{-3}$
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4099 reflections
*θ* = 2.5–28.6°
*μ* = 8.31 mm$^{-1}$
*T* = 295 K
Block, colorless
0.45 × 0.40 × 0.35 mm

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
*ω* scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.118, $T_{max}$ = 0.159
6267 measured reflections
1348 independent reflections
1239 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.5°
*h* = −17→17
*k* = −13→13
*l* = −11→11

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.065$
$S = 1.04$
1348 reflections
103 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 2.8102P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.63$ e Å$^{-3}$
$\Delta\rho_{min} = -0.75$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Rb1 | 0.5000 | 0.86132 (6) | 0.7500 | 0.03306 (18) | 0.50 |
| Ga1 | 0.32950 (2) | 0.57498 (3) | 0.42741 (3) | 0.01061 (11) | |
| Mn1 | 0.0000 | 0.28198 (6) | 0.2500 | 0.01443 (15) | |
| K1 | 0.5000 | 0.86132 (6) | 0.7500 | 0.03306 (18) | 0.50 |
| P1 | 0.5000 | 0.49997 (9) | 0.7500 | 0.0106 (2) | |
| P2 | 0.21012 (6) | 0.37336 (7) | 0.17422 (8) | 0.01171 (16) | |
| O1 | 0.44106 (16) | 0.59068 (19) | 0.6149 (2) | 0.0150 (4) | |
| O2 | 0.42851 (16) | 0.40472 (19) | 0.8014 (2) | 0.0154 (4) | |
| O3 | 0.29213 (16) | 0.41300 (18) | 0.3344 (2) | 0.0146 (4) | |
| O4 | 0.10038 (17) | 0.3988 (2) | 0.1749 (3) | 0.0198 (4) | |
| O5 | 0.23416 (16) | 0.22845 (19) | 0.1603 (2) | 0.0156 (4) | |
| O6 | 0.22740 (16) | 0.45222 (19) | 0.0373 (2) | 0.0148 (4) | |
| O1w | −0.11223 (19) | 0.3043 (2) | 0.0069 (3) | 0.0263 (5) | |
| H1 | −0.146 (3) | 0.237 (3) | −0.033 (5) | 0.039* | |
| H2 | −0.154 (3) | 0.366 (3) | −0.001 (5) | 0.039* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Rb1 | 0.0418 (4) | 0.0181 (3) | 0.0425 (4) | 0.000 | 0.0179 (3) | 0.000 |
| Ga1 | 0.01323 (18) | 0.01036 (17) | 0.00716 (17) | 0.00043 (10) | 0.00172 (12) | 0.00000 (10) |
| Mn1 | 0.0166 (3) | 0.0129 (3) | 0.0145 (3) | 0.000 | 0.0059 (2) | 0.000 |
| K1 | 0.0418 (4) | 0.0181 (3) | 0.0425 (4) | 0.000 | 0.0179 (3) | 0.000 |
| P1 | 0.0127 (4) | 0.0117 (4) | 0.0067 (4) | 0.000 | 0.0021 (3) | 0.000 |
| P2 | 0.0142 (4) | 0.0121 (3) | 0.0088 (3) | −0.0013 (3) | 0.0036 (3) | −0.0006 (2) |
| O1 | 0.0181 (10) | 0.0163 (10) | 0.0072 (9) | −0.0007 (8) | −0.0010 (7) | 0.0015 (7) |
| O2 | 0.0182 (10) | 0.0134 (9) | 0.0165 (10) | −0.0009 (8) | 0.0081 (8) | 0.0005 (8) |
| O3 | 0.0213 (11) | 0.0110 (9) | 0.0101 (9) | −0.0030 (8) | 0.0028 (8) | −0.0027 (7) |
| O4 | 0.0176 (10) | 0.0203 (10) | 0.0232 (11) | 0.0004 (8) | 0.0088 (9) | 0.0042 (9) |
| O5 | 0.0202 (10) | 0.0115 (9) | 0.0147 (9) | −0.0038 (8) | 0.0048 (8) | −0.0038 (7) |
| O6 | 0.0196 (10) | 0.0146 (9) | 0.0118 (9) | 0.0006 (8) | 0.0072 (8) | 0.0026 (7) |
| O1w | 0.0286 (13) | 0.0226 (11) | 0.0204 (11) | 0.0018 (10) | −0.0025 (9) | −0.0040 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Rb1—O1 | 3.040 (2) | Mn1—O2$^{ix}$ | 2.264 (2) |
| Rb1—O1$^{i}$ | 3.040 (2) | Mn1—O2$^{x}$ | 2.264 (2) |
| Rb1—O4$^{ii}$ | 3.613 (2) | Mn1—O4 | 2.079 (2) |
| Rb1—O4$^{iii}$ | 2.996 (2) | Mn1—O4$^{xi}$ | 2.079 (2) |
| Rb1—O4$^{iv}$ | 2.996 (2) | Mn1—O1w | 2.228 (2) |
| Rb1—O5$^{v}$ | 3.555 (2) | Mn1—O1w$^{xi}$ | 2.228 (2) |
| Rb1—O5$^{vi}$ | 3.555 (2) | P1—O1 | 1.532 (2) |
| Rb1—O6$^{vii}$ | 3.451 (2) | P1—O1$^{i}$ | 1.532 (2) |
| Rb1—O6$^{ii}$ | 3.451 (2) | P1—O2 | 1.546 (2) |
| Rb1—O4$^{vii}$ | 3.613 (2) | P1—O2$^{i}$ | 1.546 (2) |
| Rb1—O1w$^{ii}$ | 3.178 (3) | P2—O4 | 1.512 (2) |
| Rb1—O1w$^{vii}$ | 3.178 (3) | P2—O5 | 1.541 (2) |
| Ga1—O1 | 1.870 (2) | P2—O6 | 1.543 (2) |
| Ga1—O2$^{viii}$ | 2.015 (2) | P2—O3 | 1.558 (2) |
| Ga1—O3 | 1.860 (2) | O1w—H1 | 0.84 (3) |
| Ga1—O5$^{ii}$ | 1.850 (2) | O1w—H2 | 0.84 (3) |
| Ga1—O6$^{vi}$ | 1.952 (2) | | |

| | | | |
|---|---|---|---|
| O4$^{iv}$—Rb1—O4$^{iii}$ | 68.95 (8) | O4$^{iii}$—Rb1—O4$^{ii}$ | 95.69 (5) |
| O4$^{iv}$—Rb1—O1 | 138.43 (6) | O1—Rb1—O4$^{ii}$ | 73.69 (5) |
| O4$^{iii}$—Rb1—O1 | 139.75 (6) | O1$^{i}$—Rb1—O4$^{ii}$ | 118.48 (5) |
| O4$^{iv}$—Rb1—O1$^{i}$ | 139.75 (6) | O1w$^{ii}$—Rb1—O4$^{ii}$ | 51.14 (5) |
| O4$^{iii}$—Rb1—O1$^{i}$ | 138.43 (6) | O1w$^{vii}$—Rb1—O4$^{ii}$ | 131.83 (5) |
| O1—Rb1—O1$^{i}$ | 47.11 (7) | O6$^{vii}$—Rb1—O4$^{ii}$ | 134.28 (5) |
| O4$^{iv}$—Rb1—O1w$^{ii}$ | 68.68 (6) | O6$^{ii}$—Rb1—O4$^{ii}$ | 40.88 (5) |
| O4$^{iii}$—Rb1—O1w$^{ii}$ | 131.90 (6) | O5$^{vi}$—Rb1—O4$^{ii}$ | 77.00 (5) |
| O1—Rb1—O1w$^{ii}$ | 70.81 (6) | O5$^{v}$—Rb1—O4$^{ii}$ | 106.30 (5) |
| O1$^{i}$—Rb1—O1w$^{ii}$ | 89.44 (6) | O4$^{iv}$—Rb1—O4$^{vii}$ | 95.69 (5) |
| O4$^{iv}$—Rb1—O1w$^{vii}$ | 131.90 (6) | O4$^{iii}$—Rb1—O4$^{vii}$ | 74.01 (6) |
| O4$^{iii}$—Rb1—O1w$^{vii}$ | 68.68 (6) | O1—Rb1—O4$^{vii}$ | 118.48 (5) |
| O1—Rb1—O1w$^{vii}$ | 89.44 (6) | O1$^{i}$—Rb1—O4$^{vii}$ | 73.69 (5) |
| O1$^{i}$—Rb1—O1w$^{vii}$ | 70.81 (6) | O1w$^{ii}$—Rb1—O4$^{vii}$ | 131.83 (5) |
| O1w$^{ii}$—Rb1—O1w$^{vii}$ | 158.73 (9) | O1w$^{vii}$—Rb1—O4$^{vii}$ | 51.14 (5) |
| O4$^{iv}$—Rb1—O6$^{vii}$ | 65.17 (5) | O6$^{vii}$—Rb1—O4$^{vii}$ | 40.88 (5) |
| O4$^{iii}$—Rb1—O6$^{vii}$ | 88.43 (6) | O6$^{ii}$—Rb1—O4$^{vii}$ | 134.28 (5) |
| O1—Rb1—O6$^{vii}$ | 127.06 (5) | O5$^{vi}$—Rb1—O4$^{vii}$ | 106.30 (5) |
| O1$^{i}$—Rb1—O6$^{vii}$ | 83.95 (5) | O5$^{v}$—Rb1—O4$^{vii}$ | 77.00 (5) |
| O1w$^{ii}$—Rb1—O6$^{vii}$ | 93.74 (5) | O4$^{ii}$—Rb1—O4$^{vii}$ | 167.72 (7) |
| O1w$^{vii}$—Rb1—O6$^{vii}$ | 92.00 (5) | O5$^{ii}$—Ga1—O3 | 123.61 (9) |
| O4$^{iv}$—Rb1—O6$^{ii}$ | 88.43 (6) | O5$^{ii}$—Ga1—O1 | 116.06 (9) |
| O4$^{iii}$—Rb1—O6$^{ii}$ | 65.17 (5) | O3—Ga1—O1 | 120.26 (9) |
| O1—Rb1—O6$^{ii}$ | 83.95 (5) | O5$^{ii}$—Ga1—O6$^{vi}$ | 91.40 (9) |
| O1$^{i}$—Rb1—O6$^{ii}$ | 127.06 (5) | O3—Ga1—O6$^{vi}$ | 87.64 (9) |
| O1w$^{ii}$—Rb1—O6$^{ii}$ | 92.00 (5) | O1—Ga1—O6$^{vi}$ | 93.74 (9) |
| O1w$^{vii}$—Rb1—O6$^{ii}$ | 93.74 (5) | O5$^{ii}$—Ga1—O2$^{viii}$ | 88.85 (8) |
| O6$^{vii}$—Rb1—O6$^{ii}$ | 148.53 (7) | O3—Ga1—O2$^{viii}$ | 88.85 (9) |

| | | | |
|---|---|---|---|
| O4$^{iv}$—Rb1—O5$^{vi}$ | 131.58 (5) | O1—Ga1—O2$^{viii}$ | 89.78 (9) |
| O4$^{iii}$—Rb1—O5$^{vi}$ | 76.41 (5) | O6$^{vi}$—Ga1—O2$^{viii}$ | 175.95 (8) |
| O1—Rb1—O5$^{vi}$ | 63.43 (5) | O4—Mn1—O4$^{xi}$ | 109.28 (12) |
| O1$^{i}$—Rb1—O5$^{vi}$ | 88.32 (5) | O4—Mn1—O1w | 86.67 (9) |
| O1w$^{ii}$—Rb1—O5$^{vi}$ | 118.20 (5) | O4$^{xi}$—Mn1—O1w | 86.48 (9) |
| O1w$^{vii}$—Rb1—O5$^{vi}$ | 55.36 (5) | O4—Mn1—O1w$^{xi}$ | 86.48 (9) |
| O6$^{vii}$—Rb1—O5$^{vi}$ | 147.08 (4) | O4$^{xi}$—Mn1—O1w$^{xi}$ | 86.67 (9) |
| O6$^{ii}$—Rb1—O5$^{vi}$ | 45.70 (4) | O1w—Mn1—O1w$^{xi}$ | 168.14 (13) |
| O4$^{iv}$—Rb1—O5$^{v}$ | 76.41 (5) | O4—Mn1—O2$^{x}$ | 157.23 (8) |
| O4$^{iii}$—Rb1—O5$^{v}$ | 131.58 (6) | O4$^{xi}$—Mn1—O2$^{x}$ | 93.49 (8) |
| O1—Rb1—O5$^{v}$ | 88.32 (5) | O1w—Mn1—O2$^{x}$ | 94.61 (8) |
| O1$^{i}$—Rb1—O5$^{v}$ | 63.43 (5) | O1w$^{xi}$—Mn1—O2$^{x}$ | 95.46 (8) |
| O1w$^{ii}$—Rb1—O5$^{v}$ | 55.36 (5) | O4—Mn1—O2$^{ix}$ | 93.49 (8) |
| O1w$^{vii}$—Rb1—O5$^{v}$ | 118.20 (5) | O4$^{xi}$—Mn1—O2$^{ix}$ | 157.23 (8) |
| O6$^{vii}$—Rb1—O5$^{v}$ | 45.70 (4) | O1w—Mn1—O2$^{ix}$ | 95.46 (8) |
| O6$^{ii}$—Rb1—O5$^{v}$ | 147.08 (4) | O1w$^{xi}$—Mn1—O2$^{ix}$ | 94.61 (8) |
| O5$^{vi}$—Rb1—O5$^{v}$ | 149.86 (6) | O2$^{x}$—Mn1—O2$^{ix}$ | 63.75 (10) |
| O4$^{iv}$—Rb1—O4$^{ii}$ | 74.01 (6) | | |

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2; (ii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iii) −*x*+1/2, −*y*+3/2, −*z*+1; (iv) *x*+1/2, −*y*+3/2, *z*+1/2; (v) −*x*+1, −*y*+1, −*z*+1; (vi) *x*, −*y*+1, *z*+1/2; (vii) *x*+1/2, *y*+1/2, *z*+1; (viii) *x*, −*y*+1, *z*−1/2; (ix) −*x*+1/2, −*y*+1/2, −*z*+1; (x) *x*−1/2, −*y*+1/2, *z*−1/2; (xi) −*x*, *y*, −*z*+1/2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*w*—H1···O3$^{x}$ | 0.84 (3) | 1.97 (2) | 2.790 (3) | 166 (4) |
| O1*w*—H2···O6$^{xii}$ | 0.84 (3) | 2.10 (2) | 2.913 (3) | 165 (4) |

Symmetry codes: (x) *x*−1/2, −*y*+1/2, *z*−1/2; (xii) −*x*, −*y*+1, −*z*.