Supporting Information for:

An addition to the oxoacid family: $\text{H}_2\text{B}_{12}(\text{OH})_{12}$

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The acid, $\text{H}_2\text{B}_{12}(\text{OH})_{12}$, can be isolated as a crystalline solid by protonation of the hydroxylated borane anion, $\text{B}_{12}(\text{OH})_{12}^{2-}$. This acidic compound has low solubility in water, conducts protons in the solid state and has thermal stability to a temperature of 400°C. The conductivity mechanism is a Grotthuss mechanism with a low activation enthalpy (9-13 kcal/mol). This new acid represents an addition to the class of oxoacids of which sulfuric and phosphoric acid are the most prominent examples.

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General

All reagents were purchased from Aldrich or Fisher unless otherwise noted. The $\text{Cs}_2\text{B}_{12}(\text{OH})_{12}$ and $(\text{NH}_4)_2\text{B}_{12}(\text{OH})_{12}$ were synthesized according to literature procedure (Ref. 4a in article). No attempt to control humidity or oxygen was attempted unless otherwise noted.

Synthesis of $\text{H}_2\text{B}_{12}(\text{OH})_{12}$

Generation of fine inhomogeneous powders of the material can be undertaken using methods described in Ref 4a for the compound described as $(\text{H}_3\text{O})_2\text{B}_{12}(\text{OH})_{12}$. Highly crystalline samples can be prepared using the following hydrothermal method.

In an acid digestion bomb (Parr, 23 mL total vol) was placed without stirring 500 mg of $\text{Cs}_2\text{B}_{12}(\text{OH})_{12}$ (0.83 mmol) and 5 mL of conc. HCl. The bomb was sealed, transferred to an oven, and heated for 3 days at 150°C . The pressure inside the bomb should rise to no more than 125 psi under these conditions, though no measure of internal pressure was attempted. The bomb assembly was cooled to room temperature and dismantled, the excess acid decanted from the white crystalline solid. This product was collected by filtration, washed with water and dried in air to yield 240 mg of $\text{H}_2\text{B}_{12}(\text{OH})_{12}$ (85% yield).

Infrared spectra were recorded both as KBr pellets and using a single pass ATR cell on a Spectrum GX-FTIR. While the relative intensities of the peaks were marginally different, the peak positions were unchanged. Only the spectrum in KBr is shown below.

Fig S1

FTIR (KBr, cm^{-1}) 3372 (br, s, OH), 3326 (shoulder, s, OH), 3194 (m, br, OH), 1578 (br), 1419 (br), 1188 (s), 1122 (s), 761 (w), 715 (s), 644 (w), 550 (w), 501 (w).

NMR

The ^1H NMR spectra were recorded on a Varian Inova 600 spectrometer operating at 599.9 MHz. The sample was centered inside the NMR coil of a Varian 5mm $^1\text{H}[\text{X}]$ z-pfg probe with sample spinning turned off. The 90° pulse width was $\sim 11.5\ \mu\text{s}$ and the spectra width was 500 kHz. Due to long T_1 relaxation time, a recycle delay time of 200 s was used in the acquisition of proton variable temperature spectra.

Fig. S2 ^1H solid state NMR spectrum with spin-echo pulse sequence.

Fig. S3 ^1H linewidth for solid state sample of $\text{H}_2\text{B}_{12}(\text{OH})_{12}$ as a function of temperature.

Using the T_2 relaxation rates derived from the ^1H NMR linewidth data between 21 °C and 60 °C, we obtain an activation enthalpy of ~3 kcal/mol. This can be obtained graphically from a plot of $\text{Log } T_2$ vs $1000/\text{K}$ or using the method of Chandra et al. by examining the ‘jump frequency’ in a similar manner. (Ref 18 and 19 in manuscript)

The jump frequency, ν_c , is obtained from the following equation:

$$\nu_c = \frac{1}{\tau_c} = \frac{\alpha \gamma \Delta \omega}{\tan\left[\frac{1}{2} \pi (\Delta \omega^2 - B^2) / (A^2 - B^2)\right]}$$

where α is a constant (assumed 1), γ is the gyromagnetic ratio of the nuclei, $\Delta\omega$ is the linewidth (in Gauss), A is the unnarrowed linewidth (taken as 68kHz), and B is the fully narrowed linewidth (taken as 6 kHz at the high temperature limit). Fitting the jump frequency with the Arrhenius expression, the activation enthalpy was found to be ~3 kcal/mol.

Fig S4. Jump frequency as a function of temperature (Arrhenius plot)

As temperature increases the intensity of the broad component decreases while the intensity of the narrower component increases.

Above 60°C the data linewidth does not change with temperature and may indicate a phase change or be due to the addition of intensity from the exchange with the remaining 12 protons per molecule. In the slow motion regime, T_1 should decrease as the proton mobility increases. The spin-lattice relaxation times at 19°C, 65°C and 104°C are 57 s, 34 s and 24 s respectively.

DTA/TGA

Fig. S5 DTA/TGA of H₂A in air, 10°C/min.

DTA/TGA was performed under both air and nitrogen at a 100 ml/min flow rate on a TA Instruments DTA/TGA (SDT 2960). The mass loss in air with an onset of 450°C was 13.8 %. The compound had a 16.6% change in mass also with an onset of 450°C under a nitrogen stream. This corresponds to loss of 2 and ½ molecules of water and 3 water molecules per formula unit for air and inert atmosphere respectively. Extended heating at 300 °C for 1hr in air resulted in less than 1% mass loss.

Conductivity

Conductivity measurements were performed using a PG&E PARSTAT Impedance analyzer and the PowerSine control software using AC voltage frequencies between 1mHz and 1MHz and a amplitude between 10mV or 1V. The measurements were performed directly on isostatically pressed pellets of the sample using stainless steel electrodes. The effective d.c. resistivity of the sample was taken as the high frequency intercept of the data when plotted on a complex plane (Nyquist plot) or as the minimum resistance where the real component of the impedance is dominant. Values were also obtained by fitting the impedance data to an equivalent circuit (using the ZSimpWin program and circuit that consisted of a constant phase element in series with another constant phase element which is in parallel with a resistor) and the results were consistent with those obtained for the graphical method. These resistivities were converted into geometry independent conductivities using the known area of the electrode and the measured thickness of the sample. Where possible, conductive silver paint (Ted Pella) could be applied directly to the pellets and used as an electrode but no difference in bulk conductivity was observed with different electrode configurations or materials. Variable temperature measurements were performed in a modified GC oven with a temperature stability of ± 0.5 °C.

Fig. S6 Typical impedance measurements as a function of temperature (Cole-Cole plot)

Fig. S7 Plot of Log Conductivity ($\Omega^{-1}\text{cm}^{-1}$) vs $1000/\text{K}$

X-Ray diffraction

Powder Diffraction: Powder X-ray diffraction data were collected on a Scintag XDS-2000 diffractometer with a Ge solid-state detector. Slit sizes were chosen so that the entire X-ray beam footprint would stay on the sample at the lowest angle.

Peak positions were extracted by individual profile fitting in DMSNT. A zero point correction was applied using the harmonics method. The corrected peak positions were used for indexing runs with the Crysfire suite of indexing programs. The data were then subjected to a Le Bail fit using the program FullProf. Finally, a Rietveld structural refinement was carried out in FullProf using either literature or single crystal data as a starting model.

For $(\text{NH}_4)_2\text{B}_{12}(\text{OH})_{12}$, data were collected from 12 to $100^\circ 2\theta$ at a scan rate of $0.1^\circ/\text{min}$. Indexing with several programs showed a clear preference for a monoclinic unit cell with $a = 9.25 \text{ \AA}$, $b = 10.40 \text{ \AA}$, $c = 7.13 \text{ \AA}$ and $\beta = 93.0^\circ$. Systematic absences suggested space group $P 2_1/n$, which was confirmed by a Le Bail fit. Comparison with the literature suggested that the compound is isostructural to $\text{K}_2\text{B}_{12}(\text{OH})_{12}$. Rietveld refinement assuming the $\text{K}_2\text{B}_{12}(\text{OH})_{12}$ structure as a starting model gave a good fit with $R_F = 8.1\%$ (see Fig. S8). The refinement was carried out with soft constraints on the interatomic distances within the $\text{B}_{12}(\text{OH})_{12}$ cage. All positional parameters were varied independently, while only one thermal parameter was assigned to all boron and all oxygen atoms. The thermal parameters of the hydrogen atoms were not varied. The final crystal structure parameters are listed in Table S1.

The powder data collected on the initial sample of “ $(\text{H}_3\text{O})_2\text{B}_{12}(\text{OH})_{12}$ ” could not be indexed, suggesting the presence of an impurity phase. This was confirmed by the disappearance of several peaks after hydrothermal treatment. While indexing of the data (14 to $80^\circ 2\theta$, $0.12^\circ/\text{min}$) for the hydrothermal sample was not unambiguous, the most likely cells appeared to be monoclinic or orthorhombic with a volume of $567 \text{ \AA}^3$. Le Bail fits using either cell looked satisfactory, with the monoclinic cell giving slightly better statistics. It was not possible to solve the structure using the extracted structure factors and a rigid body model of the hydroxyborane cage for either cell choice. Collection of single crystal data confirmed the monoclinic setting as the correct cell and provided a starting model for subsequent Rietveld analysis. An excellent fit was obtained with $R_F = 2.1\%$ and $\chi^2 = 2.2$ (see Fig. S9). All positional parameters could be varied without constraints, and a thermal parameter for each element was refined. The final crystal structure parameters are in good agreement with the single crystal data, confirming that the single crystals chosen for data collection were representative of the bulk sample.

Fig.S8: Final Rietveld fit for $(\text{NH}_4)_2\text{B}_{12}(\text{OH})_{12}$: Data (dotted line), calculated profile (solid line), and difference curve. The tick marks represent calculated Bragg peak positions.

Fig.S9: Final Rietveld fit for $\text{H}_2\text{B}_{12}(\text{OH})_{12}$: Data (dotted line), calculated profile (solid line), and difference curve. The tick marks represent calculated Bragg peak positions.

Table S1: Atom positions and isotropic thermal displacement parameters for $(\text{NH}_4)_2\text{B}_{12}(\text{OH})_{12}$.

Atom	x	y	z	U_{iso}	Occupancy	Atom type
N1	0.7780	0.5475	0.5155	0.006	1.000	N
B1	0.6971	0.5239	0.1129	0.005	1.000	B
O1	0.8592	0.5408	0.2093	0.041	1.000	O
B2	0.4567	0.5581	0.1667	0.005	1.000	B
O2	0.4241	0.6063	0.3188	0.041	1.000	O
B3	0.5592	0.6542	0.0362	0.005	1.000	B
O3	0.5974	0.7970	0.0602	0.041	1.000	O
B4	0.6930	0.5596	-0.0863	0.005	1.000	B
O4	0.8586	0.6068	-0.1444	0.041	1.000	O
B5	0.6741	0.3853	-0.0184	0.005	1.000	B
O5	0.8444	0.3208	-0.0246	0.041	1.000	O
B6	0.5377	0.3922	0.1396	0.005	1.000	B
O6	0.5748	0.3063	0.2708	0.041	1.000	O
H1	0.9691	0.5345	0.1966	0.041	1.000	H
H2	0.2980	0.6179	0.3171	0.041	1.000	H
H3	0.7117	0.7996	0.0683	0.041	1.000	H
H4	0.9715	0.5991	-0.1424	0.041	1.000	H
H5	0.9567	0.3219	-0.0257	0.041	1.000	H
H6	0.4627	0.2918	0.2479	0.041	1.000	H

Single Crystal Data collection

A small (20 micron) crystal was mounted with oil on a glass fiber and diffraction data were collected at room temperature using synchrotron radiation ($\lambda = 0.4959 \text{ \AA}$) at the Advanced Photon Source at Argonne National Labs beamline 15-ID-B. The data were integrated using SAINT V6.45A followed by oblique incidence correction (G. Wu, B. L. Rodrigues and P. Coppens, J. Appl. Crystallogr. 35, 356-359 (2002)) and absorption/decay correction using SADABS. A starting model for the structure was provided by direct methods. The final structure model contained anisotropic displacement factors for all non-hydrogen atoms. Hydrogen atoms were located and included in the refinement with isotropic displacement factors. Refinement was accomplished by the full matrix least-squares technique on F^2 using all data.

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Table S2. Crystal data and structure refinement for **H₂A, H₂B₁₂(OH)₁₂**.

Empirical formula	H ₁₄ B ₁₂ O ₁₂	
Formula weight	335.83	
Temperature	571(2) K	
Wavelength	0.49590 Å	
Crystal system	monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 8.2370(5) Å	α = 90°.
	b = 8.2930(5) Å	β = 90.143(2)°.
	c = 8.3553(4) Å	γ = 90°.
Volume	570.74(6) Å ³	
Z	2	
Density (calculated)	1.954 Mg/m ³	
Absorption coefficient	0.100 mm ⁻¹	
F(000)	340	
Crystal size	0.02 x 0.02 x 0.005 mm ³	
Theta range for data collection	2.41 to 18.17°.	
Index ranges	-9<=h<=9, -9<=k<=9, -9<=l<=10	
Reflections collected	2428	
Independent reflections	807 [R(int) = 0.0543]	
Completeness to theta = 18.17°	67.5 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	807 / 0 / 137	
Goodness-of-fit on F ²	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0577, wR2 = 0.1395	
R indices (all data)	R1 = 0.0656, wR2 = 0.1494	
Largest diff. peak and hole	0.399 and -0.441 e.Å ⁻³	

Fig. S10. Ortep (50%) of H₂A (2 views)

Figure S11 Hydrogen bonding arrangement of H₂A

Table S3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for H_2A . $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
B(1)	-1724(4)	9970(4)	3876(4)	13(1)
B(2)	-84(4)	11300(4)	3417(4)	13(1)
B(3)	1761(4)	10302(4)	3974(4)	13(1)
B(4)	1267(4)	8359(4)	4818(4)	13(1)
B(5)	-900(4)	8157(4)	4752(4)	14(1)
B(6)	139(4)	9150(4)	3119(4)	14(1)
O(1)	-3217(2)	9950(2)	2959(2)	17(1)
O(2)	-199(2)	12417(2)	2094(2)	17(1)
O(3)	3242(2)	10467(2)	3088(2)	19(1)
O(4)	2420(2)	7065(2)	4709(2)	17(1)
O(5)	-1667(3)	6596(2)	4576(2)	17(1)
O(6)	319(3)	8477(2)	1540(2)	18(1)

Table S4. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **H₂A**.

B(1)-O(1)	1.447(4)
B(1)-B(2)	1.786(4)
B(1)-B(6)	1.795(4)
B(1)-B(4)#1	1.803(4)
B(1)-B(5)	1.804(4)
B(1)-B(3)#1	1.810(4)
B(2)-O(2)	1.444(4)
B(2)-B(5)#1	1.788(4)
B(2)-B(3)	1.792(4)
B(2)-B(4)#1	1.792(4)
B(2)-B(6)	1.810(4)
B(3)-O(3)	1.435(4)
B(3)-B(6)	1.791(4)
B(3)-B(4)	1.805(4)
B(3)-B(5)#1	1.809(4)
B(3)-B(1)#1	1.810(4)
B(4)-O(4)	1.437(4)
B(4)-B(2)#1	1.792(4)
B(4)-B(5)	1.793(5)
B(4)-B(1)#1	1.803(4)
B(4)-B(6)	1.817(4)
B(5)-O(5)	1.447(4)
B(5)-B(2)#1	1.788(4)
B(5)-B(3)#1	1.809(4)
B(5)-B(6)	1.811(4)
B(6)-O(6)	1.440(4)
O(1)-H(1A)	1.04(7)
O(1)-H(1B)	0.99(5)
O(2)-H(2)	0.89(4)
O(3)-H(3)	0.95(5)
O(4)-H(4)	0.87(4)
O(5)-H(5)	0.80(5)
O(6)-H(6)	0.86(4)

O(1)-B(1)-B(2)	122.4(2)
O(1)-B(1)-B(6)	122.3(2)
B(2)-B(1)-B(6)	60.70(17)
O(1)-B(1)-B(4)#1	120.4(2)
B(2)-B(1)-B(4)#1	59.92(17)
B(6)-B(1)-B(4)#1	109.1(2)
O(1)-B(1)-B(5)	121.6(2)
B(2)-B(1)-B(5)	108.5(2)
B(6)-B(1)-B(5)	60.40(16)
B(4)#1-B(1)-B(5)	108.5(2)
O(1)-B(1)-B(3)#1	120.5(2)
B(2)-B(1)-B(3)#1	107.8(2)
B(6)-B(1)-B(3)#1	108.6(2)
B(4)#1-B(1)-B(3)#1	59.95(17)
B(5)-B(1)-B(3)#1	60.08(16)
O(2)-B(2)-B(1)	120.8(2)
O(2)-B(2)-B(5)#1	121.5(2)
B(1)-B(2)-B(5)#1	108.2(2)
O(2)-B(2)-B(3)	123.3(2)
B(1)-B(2)-B(3)	107.5(2)
B(5)#1-B(2)-B(3)	60.72(17)
O(2)-B(2)-B(4)#1	119.6(2)
B(1)-B(2)-B(4)#1	60.50(17)
B(5)#1-B(2)-B(4)#1	60.11(17)
B(3)-B(2)-B(4)#1	108.7(2)
O(2)-B(2)-B(6)	122.2(2)
B(1)-B(2)-B(6)	59.89(17)
B(5)#1-B(2)-B(6)	108.7(2)
B(3)-B(2)-B(6)	59.62(17)
B(4)#1-B(2)-B(6)	108.9(2)
O(3)-B(3)-B(6)	118.6(2)
O(3)-B(3)-B(2)	122.9(2)
B(6)-B(3)-B(2)	60.68(17)
O(3)-B(3)-B(4)	118.6(2)
B(6)-B(3)-B(4)	60.71(17)
B(2)-B(3)-B(4)	108.7(2)

O(3)-B(3)-B(5)#1	124.9(3)
B(6)-B(3)-B(5)#1	108.6(2)
B(2)-B(3)-B(5)#1	59.53(17)
B(4)-B(3)-B(5)#1	108.2(2)
O(3)-B(3)-B(1)#1	122.7(2)
B(6)-B(3)-B(1)#1	108.4(2)
B(2)-B(3)-B(1)#1	107.4(2)
B(4)-B(3)-B(1)#1	59.81(16)
B(5)#1-B(3)-B(1)#1	59.80(16)
O(4)-B(4)-B(2)#1	122.0(2)
O(4)-B(4)-B(5)	125.9(2)
B(2)#1-B(4)-B(5)	59.82(17)
O(4)-B(4)-B(1)#1	118.4(2)
B(2)#1-B(4)-B(1)#1	59.58(17)
B(5)-B(4)-B(1)#1	107.3(2)
O(4)-B(4)-B(3)	119.5(2)
B(2)#1-B(4)-B(3)	107.7(2)
B(5)-B(4)-B(3)	107.3(2)
B(1)#1-B(4)-B(3)	60.23(16)
O(4)-B(4)-B(6)	123.9(2)
B(2)#1-B(4)-B(6)	108.0(2)
B(5)-B(4)-B(6)	60.20(17)
B(1)#1-B(4)-B(6)	107.5(2)
B(3)-B(4)-B(6)	59.25(16)
O(5)-B(5)-B(2)#1	120.6(2)
O(5)-B(5)-B(4)	121.4(2)
B(2)#1-B(5)-B(4)	60.06(17)
O(5)-B(5)-B(1)	122.7(3)
B(2)#1-B(5)-B(1)	107.8(2)
B(4)-B(5)-B(1)	107.9(2)
O(5)-B(5)-B(3)#1	121.3(2)
B(2)#1-B(5)-B(3)#1	59.75(16)
B(4)-B(5)-B(3)#1	107.9(2)
B(1)-B(5)-B(3)#1	60.12(16)
O(5)-B(5)-B(6)	122.5(2)
B(2)#1-B(5)-B(6)	108.4(2)

B(4)-B(5)-B(6)	60.56(17)
B(1)-B(5)-B(6)	59.55(17)
B(3)#1-B(5)-B(6)	108.0(2)
O(6)-B(6)-B(3)	119.6(2)
O(6)-B(6)-B(1)	124.1(2)
B(3)-B(6)-B(1)	107.2(2)
O(6)-B(6)-B(2)	121.2(2)
B(3)-B(6)-B(2)	59.69(17)
B(1)-B(6)-B(2)	59.40(17)
O(6)-B(6)-B(5)	124.3(2)
B(3)-B(6)-B(5)	107.2(2)
B(1)-B(6)-B(5)	60.05(17)
B(2)-B(6)-B(5)	107.2(2)
O(6)-B(6)-B(4)	121.5(2)
B(3)-B(6)-B(4)	60.05(16)
B(1)-B(6)-B(4)	107.3(2)
B(2)-B(6)-B(4)	107.5(2)
B(5)-B(6)-B(4)	59.24(17)
B(1)-O(1)-H(1A)	120(3)
B(1)-O(1)-H(1B)	119(3)
H(1A)-O(1)-H(1B)	115(4)
B(2)-O(2)-H(2)	117(2)
B(3)-O(3)-H(3)	111(3)
B(4)-O(4)-H(4)	106(3)
B(5)-O(5)-H(5)	113(4)
B(6)-O(6)-H(6)	115(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1

Table S5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for H_2A . The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	18(2)	5(2)	18(2)	-1(1)	0(1)	2(1)
B(2)	17(2)	2(2)	19(2)	-2(1)	-2(1)	1(1)
B(3)	13(2)	5(2)	20(2)	0(1)	-4(1)	3(1)
B(4)	15(2)	7(2)	18(2)	-1(1)	-2(1)	0(1)
B(5)	16(2)	7(2)	19(2)	-3(1)	-2(1)	1(1)
B(6)	18(2)	4(2)	21(2)	-1(1)	-2(1)	0(1)
O(1)	18(1)	10(1)	23(1)	2(1)	-5(1)	-2(1)
O(2)	21(1)	7(1)	22(1)	3(1)	2(1)	3(1)
O(3)	19(1)	13(1)	25(1)	0(1)	4(1)	-3(1)
O(4)	22(1)	7(1)	22(1)	-3(1)	-1(1)	4(1)
O(5)	22(1)	5(1)	25(1)	-3(1)	1(1)	-4(1)
O(6)	24(1)	11(1)	19(1)	-4(1)	-2(1)	3(1)

Table S6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **H₂A**.

	x	y	z	U(eq)
H(1A)	-3960(70)	8940(80)	2970(80)	120(20)
H(1B)	-3290(60)	10620(60)	1980(60)	66(14)
H(2)	710(50)	12610(50)	1550(50)	37(10)
H(3)	3920(50)	11280(60)	3540(50)	54(13)
H(4)	2050(50)	6410(50)	3980(50)	44(12)
H(5)	-2480(60)	6510(60)	5090(60)	60(15)
H(6)	-570(50)	8370(50)	1000(50)	49(13)

Table S7. Hydrogen bonds for **H₂A** [$\text{\AA}$ and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
O(1)-H(1A)...O(2)#2	1.04(7)	1.44(7)	2.473(3)	172(6)
O(1)-H(1B)...O(5)#3	0.99(5)	1.53(5)	2.521(3)	177(4)
O(2)-H(2)...O(4)#4	0.89(4)	1.92(4)	2.759(3)	155(4)
O(2)-H(2)...O(3)#4	0.89(4)	2.54(4)	3.004(3)	113(3)
O(3)-H(3)...O(6)#4	0.95(5)	1.93(5)	2.781(3)	148(4)
O(4)-H(4)...O(3)#5	0.87(4)	1.91(4)	2.740(3)	158(4)
O(5)-H(5)...O(6)#6	0.80(5)	2.18(6)	2.980(3)	175(5)
O(6)-H(6)...O(4)#7	0.86(4)	2.01(4)	2.868(3)	175(4)

Symmetry transformations used to generate equivalent atoms:

#1 $-x, -y+2, -z+1$ #2 $-x-1/2, y-1/2, -z+1/2$ #3 $-x-1/2, y+1/2, -z+1/2$

#4 $-x+1/2, y+1/2, -z+1/2$ #5 $-x+1/2, y-1/2, -z+1/2$

#6 $x-1/2, -y+3/2, z+1/2$ #7 $x-1/2, -y+3/2, z-1/2$