Crystal structure of aquabis(4-methyl-5-formyl-imidazolfuranoylhydrazone)-(trinitrato)praseodymium(III) monohydrate, $\text{Pr}(\text{H}_2\text{O})(\text{C}_9\text{H}_{10}\text{O}_2\text{N}_4)_2(\text{NO}_3)_3 \cdot \text{H}_2\text{O}$

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Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	<i>U</i> _{iso}
H(3)	4e	0.2765	−0.1377	1.1679	0.15(3)
H(20A)	4e	0.514(3)	0.246(6)	1.244(3)	0.09(2)
H(20C)	4e	0.585(3)	0.232(6)	1.310(2)	0.08(1)
H(10A)	4e	−0.157(4)	0.520(7)	0.828(3)	0.11(2)
H(10B)	4e	−0.110(5)	0.42(1)	0.812(4)	0.17(3)
H(6)	4e	0.036(2)	0.338(4)	0.897(2)	0.038(8)
H(13)	4e	0.404(2)	0.498(4)	0.870(2)	0.039(8)
H(16)	4e	0.368(2)	−0.052(4)	1.094(2)	0.031(8)
H(2)	4e	0.074(2)	0.161(4)	1.043(2)	0.05(1)
H(19)	4e	0.344(2)	0.510(5)	1.307(2)	0.06(1)
H(6A)	4e	0.475(2)	0.135(3)	1.035(2)	0.025(8)
H(15)	4e	0.626(2)	0.390(5)	0.970(2)	0.05(1)

Table 2. Continued.

Atom	Site	x	y	z	<i>U</i> _{iso}
H(14)	4e	0.541(2)	0.572(5)	0.882(2)	0.05(1)
H(2A)	4e	0.037(3)	−0.424(6)	0.802(2)	0.08(2)
H(2B)	4e	0.070(3)	−0.308(7)	0.837(3)	0.09(2)
H(1A)	4e	0.158(2)	0.456(5)	0.885(2)	0.05(1)
H(9)	4e	−0.119(2)	0.302(5)	1.031(2)	0.06(1)
H(1B)	4e	0.228(2)	0.478(5)	0.907(2)	0.05(1)
H(4)	4e	0.242(5)	−0.142(9)	1.259(4)	0.15(3)
H(20B)	4e	0.564(4)	0.379(8)	1.255(3)	0.13(2)
H(5)	4e	0.129(4)	0.03(1)	1.249(4)	0.18(3)
H(10C)	4e	−0.080(5)	0.56(1)	0.851(4)	0.17(4)
H(8A)	4e	0.387(2)	0.373(5)	1.240(2)	0.06(1)
H(4A)	4e	−0.178(3)	0.433(6)	0.930(2)	0.07(1)

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Pr(1)	4e	0.230207(8)	0.14174(2)	0.950186(7)	0.02417(9)	0.0304(1)	0.02439(9)	0.00122(6)	0.00877(6)	0.00213(6)
O(5)	4e	0.2737(1)	0.3561(3)	1.0472(1)	0.055(1)	0.051(1)	0.030(1)	−0.003(1)	0.008(1)	−0.005(1)
O(8)	4e	0.2627(1)	−0.1793(3)	0.9602(1)	0.047(1)	0.038(1)	0.040(1)	0.005(1)	0.017(1)	0.0009(9)
O(1)	4e	0.2192(1)	0.0178(3)	1.0461(1)	0.035(1)	0.048(1)	0.036(1)	0.0072(9)	0.0187(9)	0.0092(9)
O(3)	4e	0.3342(1)	0.2741(3)	0.9280(1)	0.029(1)	0.040(1)	0.038(1)	0.0031(9)	0.0124(8)	0.0108(9)
O(11)	4e	0.1128(1)	0.1557(3)	0.8320(1)	0.055(1)	0.047(1)	0.043(1)	−0.004(1)	0.007(1)	0.008(1)
O(13)	4e	0.0300(2)	−0.0405(4)	0.7860(2)	0.077(2)	0.086(2)	0.062(2)	−0.025(2)	−0.027(2)	−0.001(2)
O(6)	4e	0.2904(2)	0.4814(5)	1.1364(2)	0.081(2)	0.167(4)	0.059(2)	0.068(2)	−0.006(2)	−0.046(2)
O(12)	4e	0.1160(1)	−0.0642(3)	0.8861(1)	0.043(1)	0.047(1)	0.044(1)	−0.004(1)	0.010(1)	0.005(1)
O(9)	4e	0.2655(1)	−0.0511(3)	0.8759(1)	0.063(1)	0.040(1)	0.055(1)	0.001(1)	0.037(1)	0.001(1)
O(4)	4e	0.5384(1)	0.2993(3)	0.9773(1)	0.029(1)	0.039(1)	0.040(1)	0.0008(9)	0.0130(9)	0.0034(9)
O(10)	4e	0.2899(2)	−0.3126(3)	0.8876(1)	0.062(2)	0.043(1)	0.067(2)	0.005(1)	0.029(1)	−0.017(1)
O(7)	4e	0.3522(2)	0.2614(3)	1.1435(1)	0.091(2)	0.062(2)	0.039(1)	0.021(2)	0.004(1)	−0.003(1)
O(2)	4e	0.1259(2)	0.0576(6)	1.1563(2)	0.102(3)	0.164(4)	0.072(2)	0.022(3)	0.059(2)	0.010(2)
OW(1)	4e	0.1966(2)	0.4243(3)	0.9065(1)	0.034(1)	0.040(1)	0.060(2)	0.001(1)	0.008(1)	0.014(1)
OW(2)	4e	0.0660(2)	−0.4049(4)	0.8363(2)	0.062(2)	0.049(2)	0.063(2)	0.010(1)	0.007(2)	0.006(2)
N(9)	4e	0.3050(1)	0.3618(4)	1.1097(1)	0.028(1)	0.060(2)	0.037(1)	−0.004(1)	0.010(1)	−0.013(1)
N(2)	4e	0.1089(2)	0.1505(3)	1.0319(1)	0.033(1)	0.050(2)	0.035(1)	0.004(1)	0.019(1)	0.005(1)
N(11)	4e	0.0849(2)	0.0171(4)	0.8335(1)	0.040(1)	0.052(2)	0.042(2)	−0.002(1)	0.003(1)	−0.004(1)
N(7)	4e	0.4550(1)	0.5386(3)	1.3733(1)	0.032(1)	0.049(2)	0.035(1)	0.001(1)	0.011(1)	−0.003(1)
N(4)	4e	−0.1379(2)	0.3975(4)	0.9436(2)	0.036(2)	0.063(2)	0.069(2)	0.014(2)	0.024(2)	0.003(2)
N(5)	4e	0.3772(1)	0.0724(3)	1.0288(1)	0.027(1)	0.035(1)	0.031(1)	0.000(1)	0.0118(9)	0.005(1)
N(6)	4e	0.4321(2)	0.1480(3)	1.0120(1)	0.025(1)	0.037(1)	0.032(1)	−0.000(1)	0.009(1)	0.005(1)
N(8)	4e	0.4184(2)	0.4044(4)	1.2786(1)	0.038(1)	0.060(2)	0.027(1)	−0.009(1)	0.003(1)	−0.003(1)
N(1)	4e	0.1037(1)	0.2109(3)	0.9715(1)	0.033(1)	0.043(1)	0.033(1)	0.004(1)	0.016(1)	0.006(1)
N(3)	4e	−0.0332(2)	0.2619(3)	1.0066(1)	0.039(1)	0.051(2)	0.047(2)	0.004(1)	0.023(1)	0.001(1)
N(10)	4e	0.2730(1)	−0.1845(3)	0.9079(1)	0.033(1)	0.034(1)	0.048(2)	−0.001(1)	0.015(1)	−0.005(1)
C(1)	4e	0.8305(2)	−0.0568(4)	0.9333(1)	0.034(2)	0.043(2)	0.033(2)	−0.003(1)	0.014(1)	0.002(1)
C(16)	4e	0.4025(2)	−0.0071(4)	1.0841(1)	0.030(1)	0.035(2)	0.033(2)	0.001(1)	0.013(1)	0.005(1)
C(11)	4e	0.4053(2)	0.2495(3)	0.9602(1)	0.031(1)	0.028(1)	0.032(1)	−0.001(1)	0.013(1)	−0.003(1)
C(17)	4e	0.5195(2)	0.4721(4)	1.3669(1)	0.031(1)	0.034(2)	0.031(1)	−0.003(1)	0.010(1)	0.001(1)
C(6)	4e	0.0401(2)	0.2890(4)	0.9360(2)	0.036(2)	0.044(2)	0.037(2)	0.003(1)	0.015(1)	0.006(1)
C(7)	4e	−0.0265(2)	0.3181(4)	0.9497(2)	0.034(2)	0.041(2)	0.044(2)	0.002(1)	0.016(1)	−0.001(1)
C(19)	4e	0.3961(2)	0.4946(5)	1.3190(2)	0.032(2)	0.063(2)	0.036(2)	−0.000(2)	0.008(1)	−0.001(2)
C(13)	4e	0.4522(2)	0.4522(4)	0.8970(2)	0.038(2)	0.044(2)	0.042(2)	0.004(1)	0.017(1)	0.010(1)
C(18)	4e	0.4969(2)	0.3891(4)	1.3079(1)	0.038(2)	0.037(2)	0.030(1)	−0.003(1)	0.009(1)	0.001(1)
C(14)	4e	0.5280(2)	0.4931(4)	0.9040(2)	0.048(2)	0.043(2)	0.050(2)	−0.006(2)	0.027(2)	0.004(2)
C(2)	4e	0.1773(2)	0.0041(5)	1.1321(2)	0.049(2)	0.061(2)	0.042(2)	0.002(2)	0.027(2)	0.008(2)
C(8)	4e	−0.0920(2)	0.4038(4)	0.9102(2)	0.036(2)	0.051(2)	0.059(2)	0.008(2)	0.019(2)	0.004(2)
C(9)	4e	−0.1012(2)	0.3130(5)	1.0001(2)	0.043(2)	0.058(2)	0.059(2)	0.003(2)	0.030(2)	−0.005(2)
C(20)	4e	0.5422(3)	0.2983(6)	1.2773(2)	0.059(2)	0.073(3)	0.040(2)	0.004(2)	0.017(2)	−0.019(2)
C(3)	4e	0.2346(2)	−0.0885(6)	1.1741(2)	0.059(2)	0.089(3)	0.042(2)	0.014(2)	0.010(2)	0.022(2)
C(10)	4e	−0.1144(3)	0.4890(9)	0.8452(3)	0.056(3)	0.099(4)	0.073(3)	0.029(3)	0.025(2)	0.032(3)
C(4)	4e	0.2167(7)	−0.095(1)	1.2316(3)	0.158(8)	0.178(8)	0.048(3)	−0.018(6)	0.006(4)	0.055(4)
C(5)	4e	0.1545(6)	−0.012(2)	1.2193(3)	0.148(7)	0.26(1)	0.060(4)	−0.021(7)	0.069(5)	0.019(5)
C(12)	4e	0.4611(2)	0.3339(3)	0.9421(1)	0.030(1)	0.034(2)	0.033(1)	0.002(1)	0.013(1)	−0.001(1)
C(15)	4e	0.5772(2)	0.3990(4)	0.9522(2)	0.034(2)	0.045(2)	0.048(2)	−0.005(1)	0.020(2)	−0.003(2)

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