*Supplementary Material*

# A Versatile Polyoxovanadate in Diverse Cation Matrices: A Supramolecular Perspective

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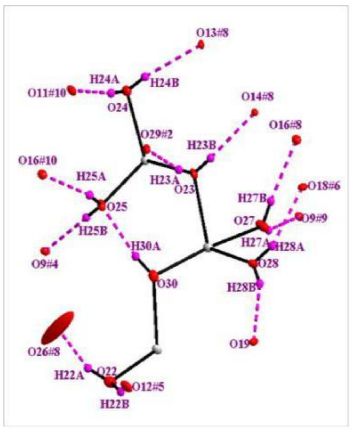
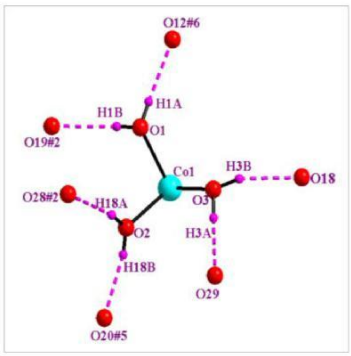
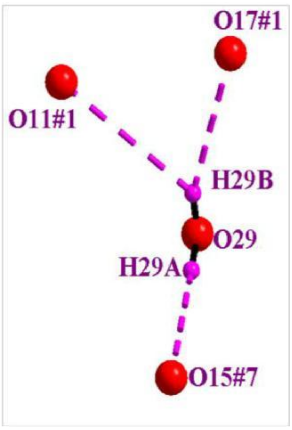
## 1 Supplementary Figures and Tables

## 1.1 Supplementary Figures

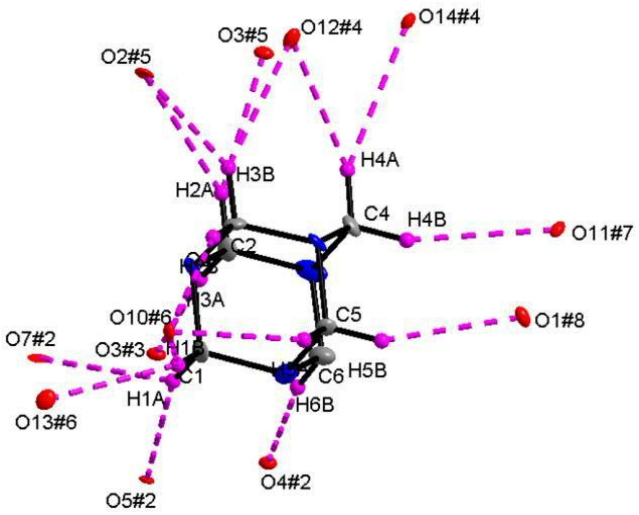


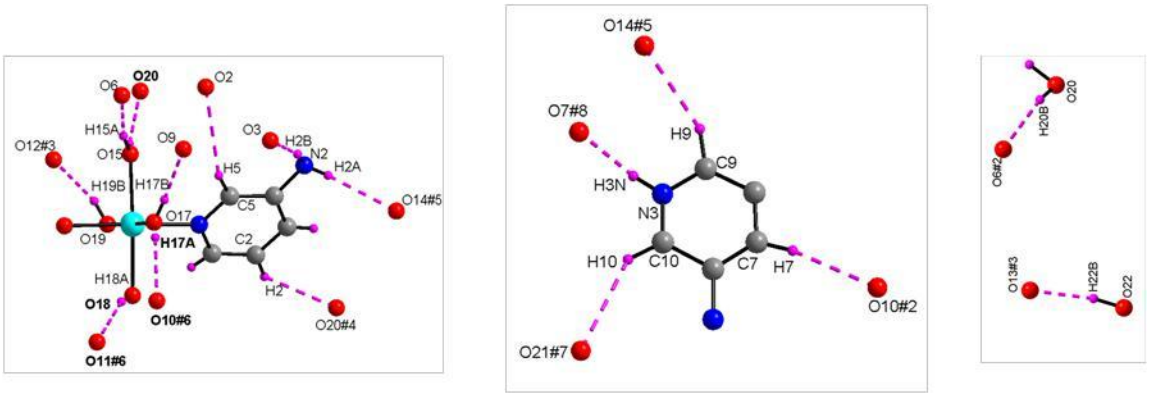




**SF1a** **SF1b** **SF1c**

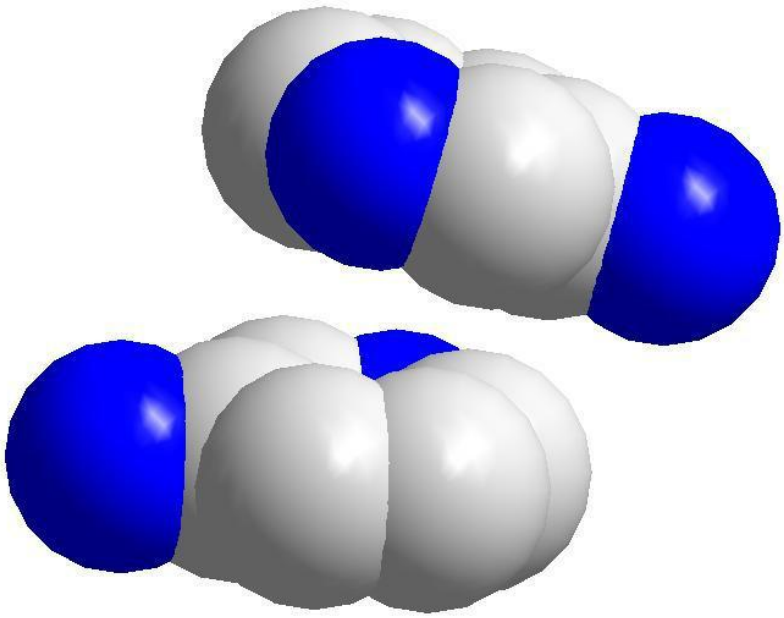
**Supplementary Figure 1.** Hydrogen bonding situation around {Na}, {Co} and water motifs in compound $[Co(H_2O)_6][\{Na_4(H_2O)_{14}\}\{V_{10}O_{28}\}]\cdot 4H_2O$ (**1**). Color codes: Na, grey, Co, green; O, red, H, purple. symmetry codes: Symmetry codes: #1, -x+2, -y+1, -z+1; #2, -x+1, -y+1, -z; #3, -x+1, -y, - z-1, #4 -x+1, -y, -z; #5 x-1, y, z; #6 -x+2, -y+1, -z; #7 -x+1, -y+1, -z+1, #8 x, y, z-1; #9, -x+2, -y, - z; #10 x-1, y, z-1.



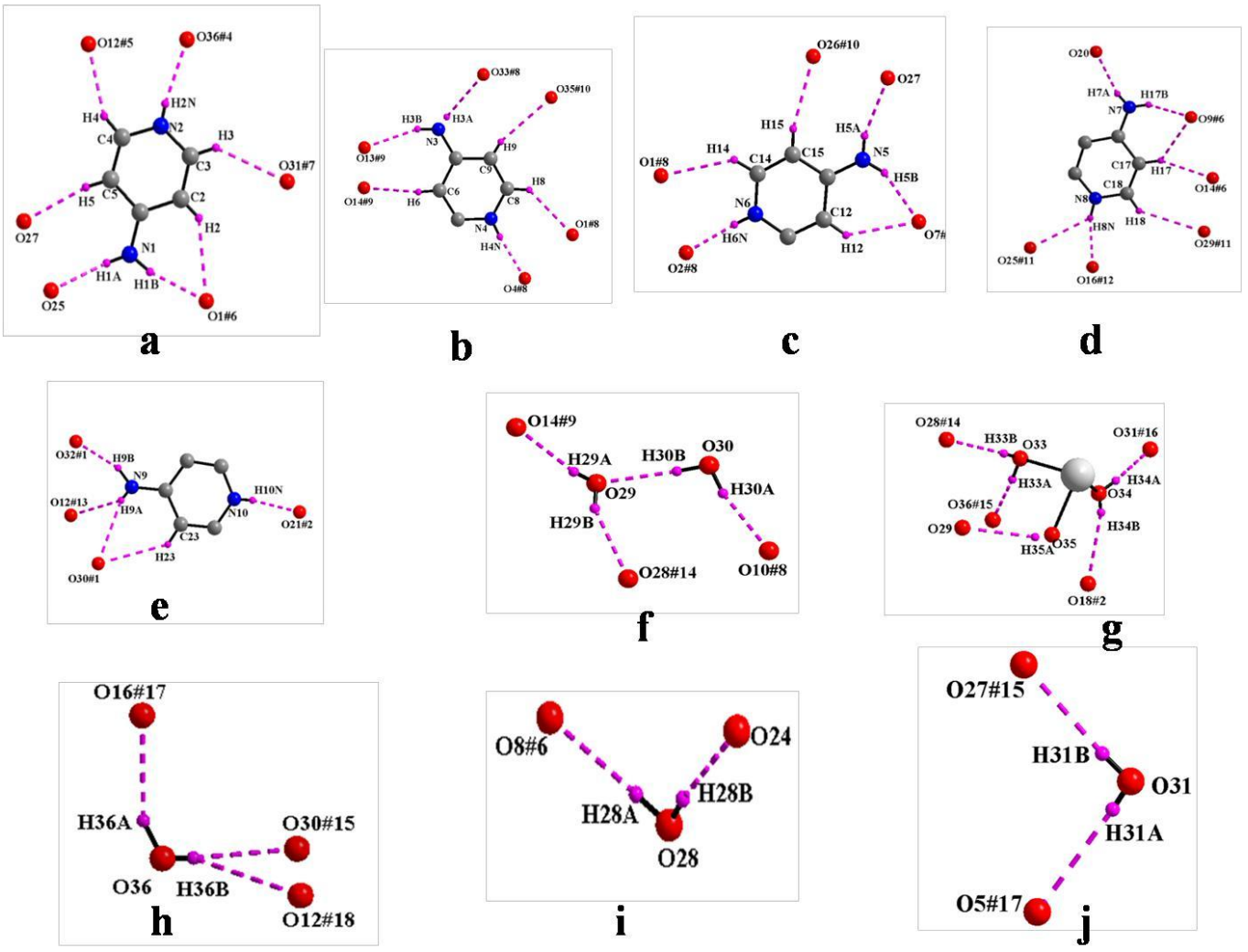

**Supplementary Figure 2.** Hydrogen bonding environment around the organic cation $[HMATAH]^{1+}$ in $[HMTAH]_2[\{Zn(H_2O)_4\}_2\{V_{10}O_{28}\}]\cdot 2H_2O$ (**3**). Symmetry codes: #1, -x+1,-y+1,-z; #2, x,-y+3/2,z+1/2; #3, x,-y+3/2,z-1/2; #4, x+1,-y+3/2,z+3/2; #5, -x+2,y+1/2,-z+3/2; #6, x, y, z+1, #7 -x+1, y, z+1; #8, x+2,-y+1,-z+1. Color codes: O, red; C, grey; H, purple; N, blue.



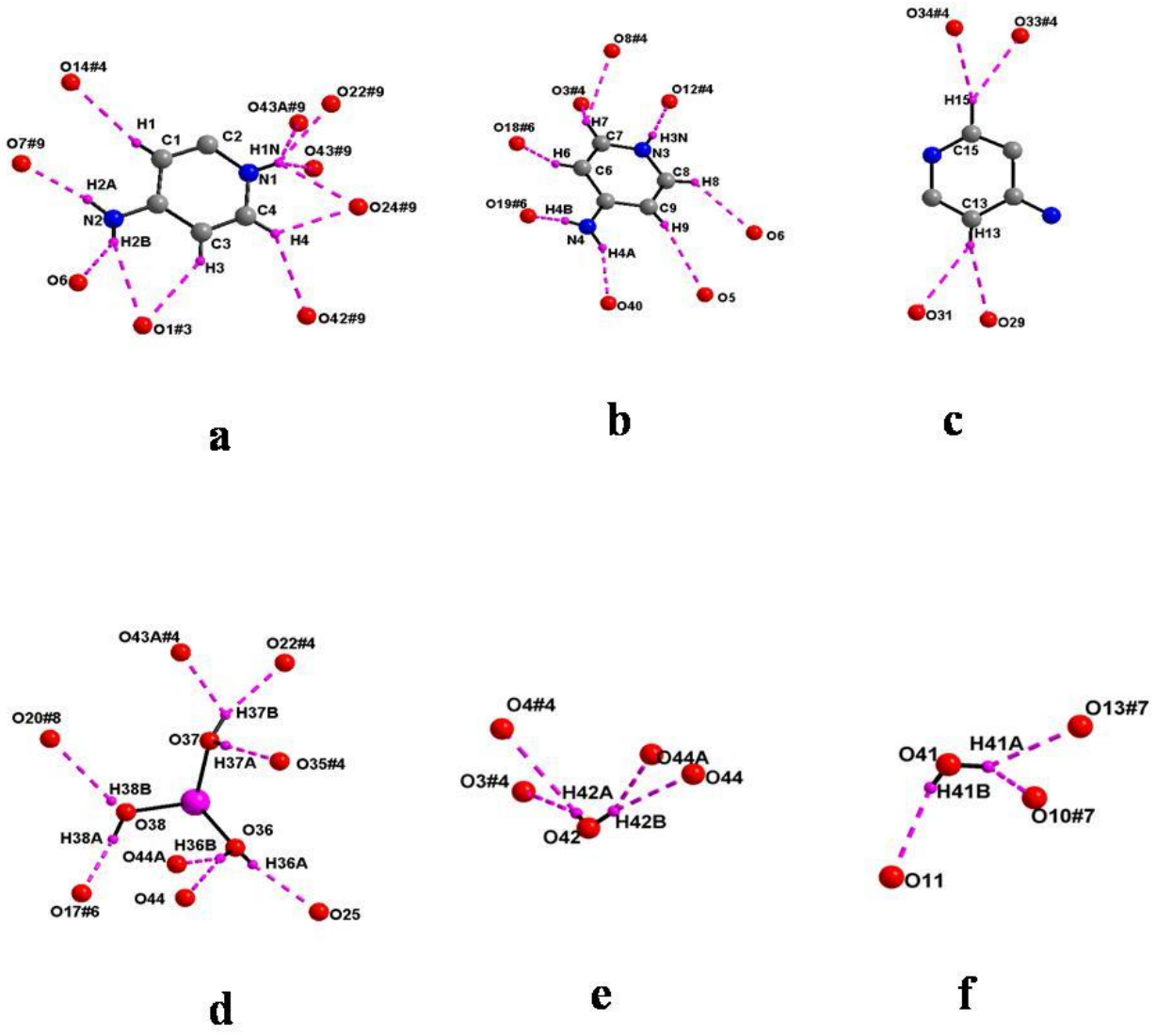

**Supplementary Figure 3.** Hydrogen bonding environment around 3-aminopyridines and water moieties in compound $[\{Co(3\text{-amp})(H_2O)_5\}_2\{3\text{-ampH}\}_2][V_{10}O_{28}]\cdot 6H_2O$ (**4**). Symmetry codes. #1, - x+1,-y+2,-z+2; #2, -x+1,-y+1,-z+2; #3, x,y-1,z; #4, -x+1,-y+1,-z+1; #5, -x+1,-y+2,-z+1; #6, - x+2,-y+2,-z+2; #7, -x+2,-y+1,-z+1; #8, x,y,z-1. Color codes: O, red; C, grey; H, purple; N, blue.



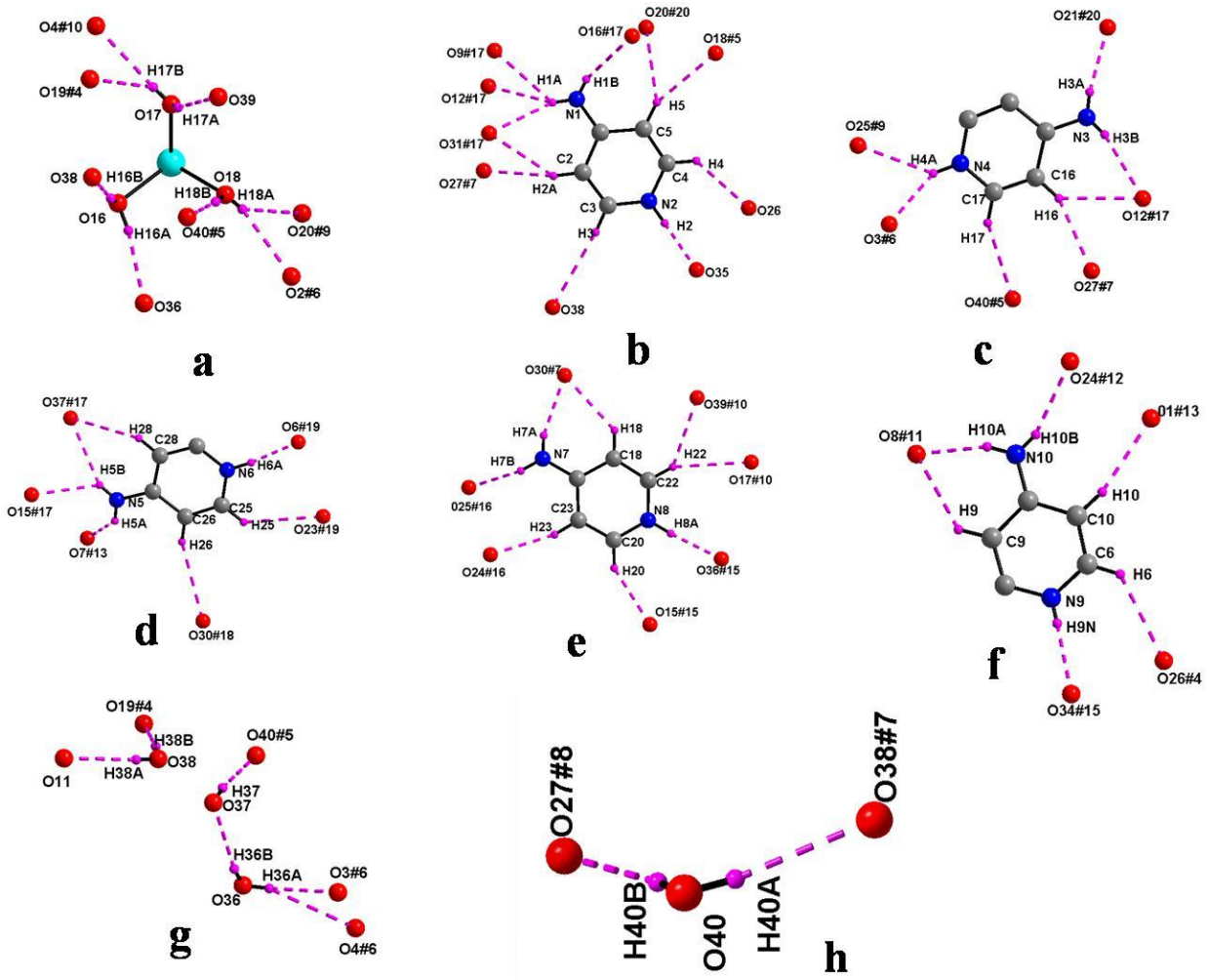
**Supplementary Figure 4.** Arrangement (space filling presentation) between two 3-aminopyridine molecules due to π–π interactions (3.718 Å) in the crystal structure of compound $[\{Co(3amp)(H_2O)_5\}_2\{3\text{-ampH}\}_2][V_{10}O_{28}]\cdot 6H_2O$ (**4**) (hydrogen atoms are omitted for clarity). Color codes: C, medium grey; N, blue.




**Supplementary Figure 5.** Hydrogen bonding environment around (a) {N1N2}, (b) {N3N4}, (c) {N5N6}, (d) {N7N8}, (e) {N9N10} and (f-j) water moieties in the crystal structure of compound [4-ampH]$_{10}$[{Na(H$_2$O)$_6$} {HV$_{10}$O$_{28}$}] [V$_{10}$O$_{28}$] ·15H$_2$O (**5**). Symmetry codes: #1, -x,-y,-z; #2, -x+1,-y+1,-z; #3, -x,-y+1,-z; #4,x,-y+3/2,z-1/2; #5, x+1,y+1,z; #6, -x+1,y+1/2,-z+1/2; #7, -x+1,y+1/2,-z+3/2; #8, -x,y+1/2,-z+1/2; #9, x,y+1,z; #10, x,-y+3/2,z+1/2; #11, -x+1,y-1/2,-z+1/2; #12, x,-y+1/2,z+1/2; #13, x+1,y,z; #14, x-1,y,z; #15, -x+1,-y+1,-z+1; #16, x,y,z-1; #17, x,y,z+1; #18, x+1,-y+1/2,z+1/2; Color codes: O, red; C, grey; H, purple, N, blue.




**Supplementary Figure 6.** Hydrogen bonding environment around (a) {N1N2}, (b) {N3N4}, (c) {N5N6}, (d) {Co} and (e-f) water moieties in the crystal structure of compound [{4-ampH}$_6${Co(H$_2$O)$_6$}$_3$][V$_{10}$O$_{28}$]$_2$·10H$_2$O (**6**). Symmetry codes: #1, -x,-y,-z; #2, -x+1,-y+1,-z; #3, -x,-y+1,-z; #4,x,-y+3/2,z-1/2; #5, x+1,y+1,z; #6, -x+1,y+1/2,-z+1/2; #7, -x+1,y+1/2,-z+3/2; #8, -x,y+1/2,-z+1/2; #9, x,y+1,z; #10, x,-y+3/2,z+1/2; #11, -x+1,y-1/2,-z+1/2; #12, x,-y+1/2,z+1/2; #13, x+1,y,z; #14, x-1,y,z; #15, -x+1,-y+1,-z+1; #16, x,y,z-1; #17, x,y,z+1; #18, x+1,-y+1/2,z+1/2; Color codes: O, red; C, grey; H, purple, N, blue.




**Supplementary Figure 7.** Hydrogen bonding environment around (a) {Zn}, (b) {N1N2}, (c) {N3N4}, (d) {N5N6}, (e) {N7N8}, (f) {N9N10} and (g-h) water moieties in the crystals [{4-ampH}$_{10}${Zn($H_2O$)$_6$}][$V_{10}O_{28}$]$_2$ ·10$H_2O$ (**7**). Symmetry codes: #1, -x,-y,-z; #2,-x+1,-y+1,-z; #3, -x,-y+1,-z; #4,x,-y+3/2,z-1/2; #5, x+1,y+1,z; #6, -x+1,y+1/2,-z+1/2; #7, -x+1,y+1/2,-z+3/2; #8, -x,y+1/2,-z+1/2;#9, x,y+1,z; #10, x,-y+3/2,z+1/2; #11,-x+1,y-1/2,-z+1/2; #12, x,-y+1/2,z+1/2; #13, x+1,y,z; #14, x-1,y,z; #15, -x+1,-y+1,-z+1; #16, x,y,z-1; #17, x,y,z+1; #18, x+1,-y+1/2,z+1/2; Color codes: O, red; C, grey; H, purple; N, blue.

## 1.2 Supplementary Tables

**Table S1.** Crystal data and structure refinement for compound **1**

| Entry | **1** |
|---|---|
| Molecular formula | $CoH_{44}Na_4O_{52}V_{10}$ |
| Formula weight | 1536.64 |
| Temperature (K) | 298(2) |
| Wavelength (Å) | 0.71073 |
| Crystal system | Triclinic |
| Space group | *P*-1 |
| a (Å) | 8.9888(5) |
| b (Å) | 11.2680 (17) |
| c (Å) | 11.6587(15) |
| α (deg) | 105.292(15) |
| β (deg) | 97.570(2) |
| γ (deg) | 100.77(3) |
| Volume ($Å^3$) | 1098.4(3) |
| Z | 1 |
| ρ (g $cm^{-3}$) | 2.323 |
| μ ($mm^{-1}$) | 2.567 |
| F (000) | 761 |
| Crystal size ($mm^3$) | 0.24x0.18x0.14 |
| Θ range for data collection (º) | 2.24 to 25.93 |
| Reflections collected/unique | 11396/4243 |
| R(int) | 0.0205 |
| Data/restraints/parameters | 4243/0/395 |
| Goodness of fit on $F^2$ | 1.234 |
| Final R indices [ I > 2 sigma(I)] | 0.0430,0.0969 |
| R indices (all data) | 0.0450/0.0977 |
| Largest diff. Peak and hole (e.$Å^{-3}$) | 1.418/-1.524 |

**Table S2.** Bond lengths [Å] and angles [˚] for decavanadate cluster of compound **1**

| Bond Lengths (Å) | | | |
|---|---|---|---|
| V(7)-O(16) | 1.617(3) | V(7)-O(9) | 1.800(3) |
| V(7)-O(11) | 1.845(3) | V(7)-O(14) | 1.965(3) |
| V(7)-O(17) | 2.009(3) | V(7)-O(10) | 2.238(3) |
| V(8)-O(18) | 1.618(3) | V(8)-O(20) | 1.791(3) |
| V(8)-O(19) | 1.846(3) | V(8)-O(10) | 2.237(3) |
| V(9)-O(15) | 1.685(3) | V(9)-O(13) | 1.687(3) |
| V(9)-O(14) | 1.951(3) | V(9)-O(10) | 2.098(3) |
| V(10)-O(8) | 1.594(3) | V(10)-O(7) | 1.827(3) |
| V(10)-O(19) | 1.862(3) | V(10)-O(9) | 1.890(3) |
| V(10)-O(13) | 2.039(3) | V(10)-O(10) | 2.296(3) |
| V(11)-O(12) | 1.614(3) | V(11)-O(7) | 1.822(3) |
| V(11)-O(11) | 1.836(3) | V(11)-O(20) | 1.899(3) |
| V(11)-O(10) | 2.291(3) | | |

| Bond angles [˚] | | | |
|---|---|---|---|
| O(16)-V(7)-O(9) | 103.89(15) | O(16)-V(7)-O(11) | 101.89(14) |
| O(9)-V(7)-O(11) | 94.39(14) | O(16)-V(7)-O(14) | 100.54(14) |
| O(9)-V(7)-O(14) | 91.39(13) | O(11)-V(7)-O(14) | 154.73(12) |
| O(16)-V(7)-O(17) | 99.41(14) | O(9)-V(7)-O(17) | 155.36(13) |

| | | | |
|---|---|---|---|
| O(11)-V(7)-O(17) | 88.53(13) | O(14)-V(7)-O(17) | 76.42(12) |
| O(16)-V(7)-O(10) | 174.48(14) | O(9)-V(7)-O(10) | 80.91(12) |
| O(11)-V(7)-O(10) | 80.24(12) | O(14)-V(7)-O(10) | 76.41(11) |
| O(17)-V(7)-O(10) | 75.48(11) | | |

**Table S3.** Hydrogen bond distances and angles for compound **1** [Å and º].

| D–H···A | d(D–H) | d(H···A) | d(D···A) | <(DHA) |
|---|---|---|---|---|
| O(3)-H(3B)... O(18) | 0.87(8) | 2.00(8) | 2.839(5) | 162(7) |
| O(3)-H(3A)... O(29) | 0.86(7) | 1.87(7) | 2.720(5) | 172(6) |
| O(2)-H(18B)... O(20)#5 | 0.77(7) | 1.93(7) | 2.688(5) | 168(6) |
| O(2)-H(18A)... O(28)#2 | 0.82(6) | 1.97(6) | 2.778(5) | 169(5) |
| O(1)-H(1B)... O(19)#2 | 0.72(7) | 1.98(7) | 2.707(5) | 178(7) |
| O(1)-H(1A)... O(12)#6 | 0.82(7) | 1.95(7) | 2.766(5) | 172(6) |
| O(29)-H(29A)... O(15)#7 | 0.73(7) | 2.07(7) | 2.801(5) | 178(7) |
| O(29)-H(29B)... O(17)#1 | 0.64(7) | 2.27(7) | 2.872(5) | 159(8) |
| O(29)-H(29B)... O(11)#1 | 0.64(7) | 2.64(7) | 3.123(5) | 135(8) |
| O(30)-H(30A)... O(25) | 0.86(6) | 2.03(6) | 2.881(5) | 169(5) |
| O(23)-H(23A)... O(29)#2 | 0.78(5) | 2.11(5) | 2.874(5) | 169(5) |
| O(23)-H(23B)... O(14)#8 | 0.74(6) | 2.06(6) | 2.801(4) | 176(6) |

| | | | | |
|---|---|---|---|---|
| O(27)-H(27B)...O(16)#8 | 0.79(7) | 2.07(7) | 2.858(5) | 174(7) |
| O(27)-H(27A)...O(9)#9 | 0.65(8) | 2.55(8) | 3.162(5) | 159(9) |
| O(28)-H(28B)...O(19) | 0.70(6) | 2.23(6) | 2.861(5) | 152(6) |
| O(28)-H(28A)...O(18)#6 | 0.82(7) | 2.03(7) | 2.817(5) | 159(6) |
| O(22)-H(22A)...O(26)#8 | 0.85(6) | 1.95(6) | 2.591(7) | 131(5) |
| O(22)-H(22B)...O(12)#5 | 0.90(8) | 2.07(8) | 2.877(5) | 150(7) |
| O(25)-H(25B)...O(9)#4 | 0.73(7) | 2.00(7) | 2.732(5) | 180(8) |
| O(25)-H(25A)...O(16)#10 | 0.77(6) | 2.16(6) | 2.907(5) | 165(5) |
| O(24)-H(24A)...O(11)#10 | 0.67(6) | 2.23(7) | 2.874(5) | 162(7) |
| O(24)-H(24B)...O(13)#8 | 0.81(6) | 2.22(6) | 3.017(5) | 171(5) |

Symmetry transformations used to generate equivalent atoms: #1, -x+2,-y+1,-z+1; #2, -x+1,-y+1,-z ; #3, -x+1,-y,-z-1; #4, -x+1,-y,-z; #5, x-1,y,z; #6, -x+2,-y+1,-z; #7, -x+1,-y+1,-z+1; #8, x,y,z-1; #9, -x+2,-y,-z; #10, x-1,y,z-1;

**Table S4.** Hydrogen bonds and angles for compound **3** [Å and º].

| D-H···A | d(D-H) | d(H···A) | d(D···A) | <(DHA) |
|---|---|---|---|---|
| C(4)-H(4A)... O(14)#4 | 0.97 | 2.81 | 3.705(16) | 153.8 |
| C(4)-H(4A)... O(12)#4 | 0.97 | 2.60 | 3.418(16) | 141.6 |
| C(3)-H(3B)... O(3)#5 | 0.97 | 2.53 | 3.450(16) | 157.8 |
| C(2)-H(2A)... O(12)#4 | 0.97 | 2.46 | 3.319(16) | 147.1 |
| C(2)-H(2B)... O(10)#6 | 0.97 | 2.40 | 3.286(17) | 151.7 |
| C(5)-H(5A)... O(10)#6 | 0.97 | 2.68 | 3.495(18) | 141.5 |
| C(1)-H(1B)... O(10)#6 | 0.97 | 2.51 | 3.358(16) | 146.3 |
| C(1)-H(1B)... O(13)#6 | 0.97 | 2.51 | 3.297(17) | 138.6 |
| C(1)-H(1A)... O(5)#2 | 0.97 | 2.45 | 3.381(16) | 160.0 |
| C(1)-H(1A)... O(7)#2 | 0.97 | 2.77 | 3.528(17) | 136.0 |
| C(3)-H(3A)... O(3)#2 | 0.97 | 2.31 | 3.273(16) | 170.1 |
| C(6)-H(6B)... O(4)#2 | 0.97 | 2.56 | 3.501(17) | 164.6 |
| C(2)-H(2A)... O(2)#5 | 0.97 | 2.45 | 3.263(16) | 140.7 |
| C(3)-H(3B)... O(2)#5 | 0.97 | 2.72 | 3.453(17) | 132.8 |
| C(4)-H(4B)... O(11)#7 | 0.97 | 2.62 | 3.542(17) | 159.5 |
| C(5)-H(5B)... O(1)#8 | 0.97 | 2.45 | 3.359(17) | 156.7 |

Symmetry transformations used to generate equivalent atoms:

#1, -x+1,-y+1,-z; #2, x,-y+3/2,z+1/2; #3, x,-y+3/2,z-1/2; #4, x+1,-y+3/2,z+3/2; #5, -x+2,y+1/2,-z+3/2; #6, x,y,z+1; #7, x+1,y,z+1; #8, -x+2,-y+1,-z+1; **Table S5.**

Hydrogen bond distance and angles for compound **4** [Å and º]

| D–H···A | d(D–H) | d(H···A) | d(D···A) | <(DHA) |
|---|---|---|---|---|
| O(20)-H(20B)... O(6)#2 | 0.86(9) | 2.01(9) | 2.846(6) | 164(8) |
| O(22)-H(22B)... O(13)#3 | 0.92(8) | 1.85(8) | 2.767(5) | 171(7) |
| O(19)-H(19B)...O(12)#3 | 0.80(8) | 1.93(8) | 2.705(5) | 162(8) |
| C(2)-H(2)... O(20)#4 | 0.93(8) | 2.53(8) | 3.272(8) | 138(6) |
| N(2)-H(2A)... O(14)#5 | 0.82(8) | 2.27(8) | 3.056(8) | 162(7) |
| O(17)-H(17B)... O(9) | 0.82(7) | 1.95(7) | 2.750(5) | 166(6) |
| N(2)-H(2B)... O(3) | 0.66(8) | 2.37(8) | 2.991(7) | 157(8) |
| O(17)-H(17B)... O(9) | 0.82(7) | 1.95(7) | 2.750(5) | 166(6) |
| O(15)-H(15B)... O(20) | 0.59(6) | 2.24(6) | 2.804(8) | 163(8) |
| O(15)-H(15A) ...O(6) | 0.91(10) | 1.92(10) | 2.816(5) | 169(8) |
| O(18)-H(18A) ...O(11)#6 | 0.54(8) | 2.13(8) | 2.650(5) | 160(12) |
| O(17)-H(17A)... O(10)#6 | 0.56(6) | 2.26(6) | 2.811(6) | 174(9) |
| O(17)-H(17B)... O(9) | 0.82(7) | 1.95(7) | 2.750(5) | 166(6) |
| C(7)-H(7)... O(10)#6 | 0.96(9) | 2.37(9) | 3.307(8) | 166(7) |
| C(7)-H(7)... O(8)#6 | 0.96(9) | 2.88(8) | 3.301(8) | 108(6) |

| | | | | |
|---|---|---|---|---|
| C(10)-H(10)...O(21)#7 | 1.01(6) | 2.88(7) | 3.745(13) | 144(5) |
| N(3)-H(3N)...O(7)#8 | 0.90(12) | 1.77(12) | 2.662(5) | 172(11) |
| C(9)-H(9)...O(14)#5 | 1.04(10) | 2.49(10) | 3.437(9) | 152(7) |

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+2; #2 -x+1,-y+1,-z+2; #3 x,y-1,z; #4 -x+1,-y+1,-z+1; #5 -x+1,-y+2,-z+1 #6 - x+2,-y+2,-z+2; #7 -x+2,-y+1,-z+1; #8, x,y,z-1.

**Table S6.** Hydrogen bonds and angles for compound **5** [Å and º].

| D–H···A | d(D–H) | d(H···A) | d(D···A) | <(DHA) |
|---|---|---|---|---|
| N(2)-H(2N)...O(36)#4 | 0.69(5) | 2.12(5) | 2.801(5) | 167(5) |
| C(4)-H(4)...O(12)#5 | 0.89(5) | 2.33(5) | 3.123(5) | 148(5) |
| C(5)-H(5)...O(27) | 0.87(5) | 2.30(5) | 3.161(5) | 168(5) |
| N(1)-H(1A)...O(25) | 0.79(5) | 2.29(5) | 3.036(4) | 156(5) |
| N(1)-H(1B)...O(6)#6 | 0.88(5) | 2.05(5) | 2.897(4) | 162(4) |
| C(2)-H(2)...O(6)#6 | 0.84(4) | 2.56(4) | 3.245(4) | 140(3) |
| C(3)-H(3)...O(31)#7 | 0.89(4) | 2.62(4) | 3.333(6) | 138(4) |
| N(3)-H(3A)...O(33)#8 | 0.59(5) | 2.65(5) | 3.177(5) | 150(6) |
| N(3)-H(3B)...O(13)#9 | 0.85(4) | 2.36(4) | 3.166(6) | 158(4) |

| | | | | |
|---|---|---|---|---|
| C(6)-H(6)...O(14)#9 | 0.87(4) | 2.58(4) | 3.354(4) | 148(3) |
| N(4)-H(4N)...O(4)#8 | 0.79(4) | 1.91(4) | 2.702(4) | 174(4) |
| C(8)-H(8)...O(1)#8 | 0.88(4) | 2.60(4) | 3.264(4) | 133(4) |
| C(9)-H(9)...O(35)#10 | 0.76(4) | 2.75(4) | 3.471(5) | 159(4) |
| C(15)-H(15)...O(26)#10 | 0.85(4) | 2.50(4) | 3.328(4) | 164(4) |
| N(5)-H(5A)...O(27)#10 | 0.79(4) | 2.24(5) | 2.976(4) | 154(4) |
| N(5)-H(5B)...O(7)#6 | 0.87(5) | 2.13(5) | 2.933(4) | 155(4) |
| C(12)-H(12)...O(7)#6 | 0.92(5) | 2.62(5) | 3.336(5) | 135(4) |
| N(6)-H(6N)...O(2)#8 | 0.80(6) | 1.91(6) | 2.685(4) | 163(6) |
| C(14)-H(14)...O(1)#8 | 0.92(4) | 2.64(4) | 3.352(4) | 135(3) |
| N(7)-H(7A)...O(20) | 0.76(4) | 2.12(5) | 2.844(4) | 162(4) |
| N(7)-H(17B)...O(9)#6 | 0.81(5) | 2.31(5) | 3.033(4) | 150(5) |
| C(17)-H(17)...O(9)#6 | 0.93(5) | 2.63(5) | 3.347(4) | 134(4) |
| C(17)-H(17)...O(14)#6 | 0.93(5) | 2.41(5) | 3.268(4) | 154(4) |
| C(18)-H(18)...O(29)#11 | 0.87(4) | 2.76(4) | 3.477(6) | 140(4) |
| N(8)-H(8N)...O(16)#12 | 0.85(5) | 2.05(5) | 2.855(4) | 159(5) |
| N(8)-H(8N)...O(25)#11 | 0.85(5) | 2.70(5) | 3.319(4) | 131(4) |
| N(10)-H(10N)...O(21)#2 | 0.72(5) | 1.97(5) | 2.677(4) | 168(5) |
| C(23)-H(23)...O(30)#11 | 0.91(5) | 2.81(5) | 3.516(5) | 135(4) |
| N(9)-H(9A)...O(30)#11 | 0.65(7) | 2.63(7) | 3.216(9) | 152(9) |
| N(9)-H(9A)...O(12)#13 | 0.65(7) | 2.43(7) | 2.934(5) | 136(9) |

| | | | | |
|---|---|---|---|---|
| N(9)-H(9B)...O(32)#11 | 0.93(7) | 2.06(7) | 2.937(5) | 159(5) |
| O(33)-H(33B)... O(28)#14 | 0.63(4) | 2.18(4) | 2.807(4) | 177(5) |
| O(33)-H(33A)... O(36)#15 | 0.88(4) | 1.92(4) | 2.795(4) | 173(3) |
| O(35)-H(35A)... O(29) | 0.53(4) | 2.32(4) | 2.829(5) | 160(7) |
| O(34)-H(34B)... O(18)#2 | 0.61(6) | 2.41(6) | 2.967(4) | 153(7) |
| O(34)-H(34A)... O(31)#16 | 0.71(5) | 2.13(5) | 2.790(6) | 156(6) |
| O(28)-H(28A)... O(8)#6 | 0.80(5) | 2.11(6) | 2.906(4) | 174(5) |
| O(28)-H(28B)... O(24) | 0.72(5) | 1.97(5) | 2.686(4) | 170(5) |
| O(36)-H(36A)... O(16)#17 | 0.82(5) | 2.06(5) | 2.824(4) | 154(5) |
| O(36)-H(36B)... O(30)#15 | 0.61(6) | 2.27(6) | 2.841(5) | 157(8) |
| O(36)-H(36B)... O(12)#18 | 0.61(6) | 2.82(6) | 3.254(4) | 132(7) |
| O(29)-H(29A)... O(14)#9 | 0.71(5) | 2.04(5) | 2.746(4) | 170(5) |
| O(29)-H(29B)... O(28)#14 | 0.72(5) | 2.15(5) | 2.815(5) | 154(5) |
| O(30)-H(30B)... O(29) | 0.82(6) | 2.06(6) | 2.866(5) | 169(5) |
| O(30)-H(30A)... O(10)#8 | 0.87(5) | 1.98(5) | 2.837(4) | 168(4) |
| O(31)-H(31B)... O(27)#15 | 0.73(6) | 2.17(6) | 2.903(5) | 176(6) |
| O(31)-H(31A)... O(5)#17 | 0.61(5) | 2.37(5) | 2.976(5) | 170(7) |

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x+1,-y+1,-z #3 -x,-y+1,-z; #4 x,-y+3/2,z-1/2; #5 x+1,y+1,z; #6, -x+1,y+1/2,-z+1/2; #7, -x+1,y+1/2,-z+3/2; #8, -x,y+1/2,-z+1/2; #9, x,y+1,z; #10, x,-y+3/2,z+1/2; #11, -

x+1,y-1/2,-z+1/2; #12, x,-y+1/2,z+1/2; #13, x+1,y,z; #14, x-1,y,z; #15, -x+1,-y+1,-z+1; #16, x,y,z-1; #17, x,y,z+1; #18, x+1,-y+1/2,z+1/2.

**Table S7.** Hydrogen bonds and angles for compound **6** [Å and º].

| D-H···A | d(D–H) | d(H···A) | d(D···A) | <(DHA) |
|---|---|---|---|---|
| O(42)-H(42A)···O(3)#4 | 0.58(8) | 2.46(8) | 2.987(6) | 154(10) |
| O(42)-H(42A)···O(4)#4 | 0.58(8) | 2.53(8) | 2.958(6) | 134(10) |
| O(42)-H(42B)···O(44A) | 0.70(8) | 1.83(8) | 2.481(12) | 155(8) |
| O(42)-H(42B)···O(44) | 0.70(8) | 2.17(8) | 2.849(8) | 165(8) |
| O(35)-H(35A)···O(4) | 0.68(7) | 2.89(7) | 3.341(5) | 126(6) |
| O(35)-H(35A)···O(42)#5 | 0.68(7) | 2.25(7) | 2.900(6) | 160(7) |
| O(35)-H(35B)···O(39) | 0.87(6) | 1.84(6) | 2.697(5) | 168(5) |
| O(39)-H(39A)···O(16)#5 | 0.73(6) | 2.03(7) | 2.753(5) | 173(7) |
| O(39)-H(39B)···O(21) | 0.84(7) | 1.88(8) | 2.701(5) | 167(7) |
| O(40)-H(40B)···O(20)#6 | 0.79(8) | 2.34(8) | 2.989(6) | 140(7) |
| O(40)-H(40A)···O(4) | 0.86(8) | 1.93(8) | 2.761(5) | 163(7) |
| O(41)-H(41A)···O(10)#7 | 0.87(7) | 2.23(6) | 2.941(5) | 140(5) |
| O(41)-H(41A)···O(13)#7 | 0.87(7) | 2.12(6) | 2.743(5) | 128(5) |

| | | | | |
|---|---|---|---|---|
| O(41)-H(41B)···O(11) | 0.67(8) | 2.09(8) | 2.710(5) | 153(9) |
| O(38)-H(38B)···O(20)#8 | 0.48(8) | 2.32(9) | 2.777(6) | 158(14) |
| O(38)-H(38A)···O(17)#6 | 0.84(7) | 1.86(7) | 2.685(6) | 167(6) |
| O(36)-H(36B)···O(44A) | 0.71(6) | 2.14(6) | 2.812(13) | 160(6) |
| O(36)-H(36B)···O(44) | 0.71(6) | 2.09(6) | 2.788(6) | 171(6) |
| O(36)-H(36A)···O(25) | 0.68(7) | 2.11(7) | 2.754(5) | 158(8) |
| O(37)-H(37A)···O(35)#4 | 0.79(7) | 1.95(8) | 2.722(5) | 165(7) |
| O(37)-H(37B)···O(22)#4 | 0.90(10) | 2.16(10) | 3.030(5) | 163(8) |
| O(37)-H(37B)···O(43A)#4 | 0.90(10) | 2.12(9) | 2.700(12) | 122(7) |
| C(13)-H(13)···O(29) | 0.83(5) | 2.76(5) | 3.416(6) | 137(4) |
| C(13)-H(13)···O(31) | 0.83(5) | 2.73(6) | 3.462(7) | 147(5) |
| C(15)-H(15)···O(33)#4 | 1.07(7) | 2.57(7) | 3.518(8) | 148(5) |
| C(15)-H(15)···O(34)#4 | 1.07(7) | 2.67(7) | 3.526(8) | 136(5) |
| C(6)-H(6)···O(18)#6 | 0.86(7) | 2.54(8) | 3.228(6) | 138(6) |
| N(4)-H(4B)···O(19)#6 | 0.71(6) | 2.39(6) | 2.869(6) | 126(6) |
| N(4)-H(4A)···O(40) | 0.90(9) | 2.05(9) | 2.884(8) | 155(8) |
| C(9)-H(9)···O(5) | 0.82(6) | 2.69(6) | 3.411(6) | 147(5) |
| C(8)-H(8)···O(6) | 0.92(5) | 2.49(5) | 3.192(6) | 134(4) |
| N(3)-H(3N)···O(12)#4 | 0.83(6) | 1.87(6) | 2.704(5) | 175(6) |
| C(7)-H(7)···O(8)#4 | 0.95(6) | 2.67(6) | 3.392(6) | 134(4) |

| | | | | |
|---|---|---|---|---|
| C(7)-H(7)···O(3)#4 | 0.95(6) | 2.63(6) | 3.305(6) | 129(4) |
| C(4)-H(4)···O(42)#9 | 0.92(7) | 2.61(7) | 3.377(7) | 141(5) |
| N(1)-H(1N)···O(43)#9 | 0.87(7) | 2.83(7) | 3.390(7) | 124(5) |
| N(2)-H(2B)···O(1)#3 | 0.75(9) | 2.52(9) | 3.189(6) | 151(9) |
| C(1)-H(1)···O(14)#4 | 0.81(6) | 2.58(6) | 3.331(6) | 155(5) |
| N(2)-H(2A)···O(7)#9 | 0.88(5) | 2.01(6) | 2.875(6) | 171(5) |
| N(2)-H(2B)···O(6) | 0.75(9) | 2.48(9) | 3.094(6) | 141(9) |
| C(3)-H(3)···O(1)#3 | 0.88(6) | 2.48(6) | 3.243(6) | 145(5) |
| C(4)-H(4)···O(24)#9 | 0.92(7) | 2.39(7) | 3.026(6) | 127(5) |
| N(1)-H(1N)···O(24)#9 | 0.87(7) | 2.43(7) | 3.018(6) | 126(5) |
| N(1)-H(1N)···O(22)#9 | 0.87(7) | 2.18(7) | 2.952(6) | 147(6) |
| N(1)-H(1N)···O(43A)#9 | 0.87(7) | 2.88(7) | 3.444(12) | 124(5) |

Symmetry transformations used to generate equivalent atoms:

#1, -x+1, -y+2, -z; #2, -x+2, -y+1, -z #3, -x+1, -y, -z+1 #4, x, y+1, z; #5, x, y-1, z #6 x-1,y,z #7 -x,-y,-z+1 #8 x-1,y+1,z #9 -x+1,-y+1,-z+1.

**Table S8.** Hydrogen bond distances and angles for compound **7** [Å and º ].

| D–H···A | d(D–H) | d(H···A) | d(D···A) | <(DHA) |
|---|---|---|---|---|
| O(38)-H(38B)... O(19)#4 | 0.69(6) | 2.01(6) | 2.683(5) | 168(7) |
| O(38)-H(38A)... O(11) | 0.69(5) | 2.21(6) | 2.902(5) | 176(6) |
| O(37)-H(37)...O(40)#5 | 0.74(7) | 2.12(7) | 2.853(6) | 171(8) |
| O(36)-H(36B)... O(37) | 0.70(5) | 2.16(5) | 2.837(6) | 163(6) |
| O(36)-H(36A)... O(3)#6 | 0.74(5) | 2.11(5) | 2.828(5) | 165(5) |
| O(36)-H(36A)... O(4)#6 | 0.74(5) | 2.79(5) | 3.235(5) | 121(4) |
| O(40)-H(40A)... O(38)#7 | 0.74(6) | 2.11(6) | 2.788(6) | 151(6) |
| O(40)-H(40B)... O(27)#8 | 0.73(6) | 2.02(6) | 2.746(5) | 171(6) |
| O(18)-H(18B)... O(40)#5 | 0.81(6) | 2.00(6) | 2.804(6) | 176(6) |
| O(18)-H(18A)... O(20)#9 | 0.65(5) | 2.59(6) | 3.113(6) | 139(6) |
| O(18)-H(18A)... O(2)#6 | 0.65(5) | 2.30(6) | 2.852(5) | 144(6) |
| O(16)-H(16A)... O(36) | 0.79(5) | 2.01(5) | 2.793(5) | 171(5) |
| O(16)-H(16B)... O(38) | 0.66(5) | 2.13(5) | 2.795(6) | 175(6) |

| | | | | |
|---|---|---|---|---|
| O(17)-H(17B)...O(19)#4 | 0.68(6) | 2.53(7) | 2.981(5) | 127(7) |
| O(17)-H(17B)...O(4)#10 | 0.68(6) | 2.30(7) | 2.963(5) | 165(7) |
| O(17)-H(17A)...O(39) | 0.73(6) | 2.12(6) | 2.806(6) | 158(6) |
| C(9)-H(9)...O(8)#11 | 0.95 | 2.61 | 3.328(6) | 132.6 |
| N(10)-H(10A)...O(8)#11 | 0.83(7) | 2.13(7) | 2.910(6) | 157(6) |
| N(10)-H(10B)...O(24)#12 | 0.76(5) | 2.28(5) | 2.976(6) | 152(5) |
| C(10)-H(10)...O(1)#13 | 0.95 | 2.40 | 3.327(5) | 166.3 |
| C(6)-H(6)...O(26)#14 | 0.95 | 2.63 | 3.344(5) | 132.2 |
| N(9)-H(9N)...O(34)#15 | 0.73(5) | 1.96(5) | 2.684(5) | 176(5) |
| C(22)-H(22)...O(39)#10 | 0.95 | 2.56 | 3.332(7) | 138.3 |
| C(22)-H(22)...O(17)#10 | 0.95 | 2.76 | 3.645(6) | 154.6 |
| N(8)-H(8A)...O(36)#15 | 0.88 | 1.93 | 2.795(5) | 169.4 |
| C(20)-H(20)...O(15)#15 | 0.95 | 2.31 | 3.107(6) | 141.4 |
| C(23)-H(23)...O(24)#16 | 0.95 | 2.25 | 3.159(6) | 158.6 |
| N(7)-H(7B)...O(25)#16 | 0.87(6) | 2.17(6) | 3.002(5) | 161(5) |
| N(7)-H(7A)...O(30)#7 | 0.78(5) | 2.14(5) | 2.892(5) | 163(5) |
| C(18)-H(18)...O(30)#7 | 0.95 | 2.47 | 3.223(5) | 135.9 |
| C(28)-H(28)...O(37)#17 | 0.95 | 2.82 | 3.523(7) | 131.3 |
| N(5)-H(5B)...O(37)#17 | 0.78(8) | 2.47(8) | 3.176(10) | 150(8) |
| N(5)-H(5B)...O(15)#17 | 0.78(8) | 2.34(8) | 2.924(6) | 132(8) |
| N(5)-H(5A)...O(7)#13 | 0.81(6) | 2.33(6) | 2.935(6) | 133(5) |

| | | | | |
|---|---|---|---|---|
| C(26)-H(26)...O(30)#18 | 0.95 | 2.82 | 3.700(6) | 154.3 |
| C(25)-H(25)...O(23)#19 | 0.95 | 2.83 | 3.532(5) | 131.2 |
| N(6)-H(6A)...O(6)#19 | 0.88 | 1.79 | 2.670(4) | 173.8 |
| N(4)-H(4A)...O(25)#9 | 0.88 | 2.63 | 3.331(5) | 137.4 |
| N(4)-H(4A)...O(3)#6 | 0.88 | 2.04 | 2.846(5) | 151.3 |
| C(17)-H(17)...O(40)#5 | 0.95 | 2.65 | 3.466(7) | 143.7 |
| C(16)-H(16)...O(27)#7 | 0.95 | 2.39 | 3.263(5) | 153.1 |
| N(3)-H(3B)...O(12)#17 | 0.76(5) | 2.36(5) | 3.020(5) | 146(5) |
| N(3)-H(3A)...O(21)#20 | 0.77(5) | 2.10(5) | 2.833(5) | 161(5) |
| C(5)-H(5)...O(20)#20 | 0.95 | 2.77 | 3.474(5) | 131.3 |
| C(5)-H(5)...O(18)#5 | 0.95 | 2.54 | 3.428(6) | 155.2 |
| C(4)-H(4)...O(26) | 0.95 | 2.56 | 3.248(5) | 129.2 |
| N(2)-H(2)...O(35) | 0.88 | 1.82 | 2.697(4) | 174.6 |
| C(3)-H(3)...O(38) | 0.95 | 2.81 | 3.756(6) | 173.5 |
| C(2)-H(2A)...O(27)#7 | 0.95 | 2.50 | 3.348(5) | 148.4 |
| C(2)-H(2A)...O(31)#17 | 0.95 | 2.81 | 3.535(5) | 134.1 |
| N(1)-H(1A)...O(31)#17 | 0.79(5) | 2.42(5) | 3.158(6) | 156(4) |
| N(1)-H(1A)...O(12)#17 | 0.79(5) | 2.48(5) | 3.111(5) | 138(4) |
| N(1)-H(1A)...O(9)#17 | 0.79(5) | 2.74(5) | 3.287(5) | 128(4) |
| N(1)-H(1B)...O(16)#17 | 0.73(6) | 2.45(6) | 3.128(6) | 154(6) |

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Symmetry transformations used to generate equivalent atoms:

#1, -x+1,-y,-z+1; #2, -x,-y+2,-z+1; #3, -x+1,-y,-z; #4, x+1,y-1,z; #5, x,-y+1/2,z-1/2; #6, x,y-1,z;#7, x,-y+1/2,z+1/2; #8, x,y,z+1; #9, -x,-y+1,-z+1; #10, -x+1,-y+1,-z+1; #11, x+1,y+1,z; #12, x+1,-y+3/2,z-1/2; #13, -x+1,y-1/2,-z+1/2; #14, -x+1,-y+1,-z; #15, x,y+1,z; #16, x,-y+3/2,z-1/2; #17, -x+1,y+1/2,-z+1/2; #18, x+1,-y+1/2,z+1/2; #19, x+1,y,z; #20, -x,y-1/2,-z+1/2.

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##################End of the Supplementary Information#######################

Supplementary Material