

Supporting information of

Hydrogen-bonded assembly of aminophosphonic anions: Different 1D, 2D and 3D supramolecular architectures

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Figure S1: 1D zigzag supramolecular chain formed by AEDPH₂²⁻ anions in compound **9**;

Figure S2: The ORTEP of compound **1** with thermal ellipsoids at the 30% probability level;

Figure S3: The ORTEP of compound **2** with thermal ellipsoids at the 30% probability level;

Figure S4: The ORTEP of compound **3** with thermal ellipsoids at the 30% probability level;

Figure S5: The ORTEP of compound **4** with thermal ellipsoids at the 30% probability level;

Figure S6: The ORTEP of compound **5** with thermal ellipsoids at the 30% probability level;

Figure S7: The ORTEP of compound **6** with thermal ellipsoids at the 30% probability level;

Figure S8: The ORTEP of compound **7** with thermal ellipsoids at the 30% probability level;

Figure S9: The ORTEP of compound **8** with thermal ellipsoids at the 30% probability level;

Figure S10: The 1(1)3(1)R4 water cluster in compound **4** and its connections to the host;

Figure S11. IR spectra of compounds **1-8**;

Figure S12: TG curves of compounds **1-8**;

Table S13: Hydrogen bonds of compounds **1-8** [Å and °].

Figure S1. 1D zigzag supramolecular chain formed by AEDPH₂²⁻ anions in compound **9**.

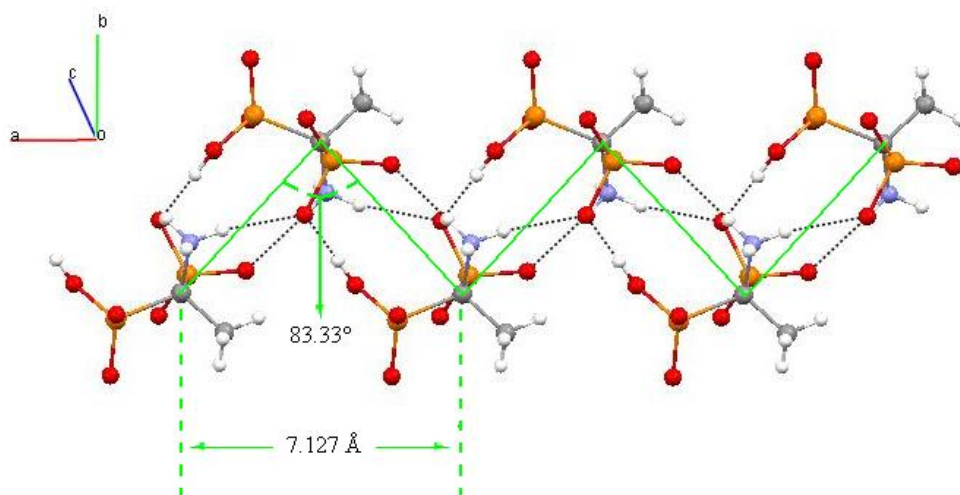


Figure S2. The ORTEP of compound **1** with thermal ellipsoids at the 30% probability level.

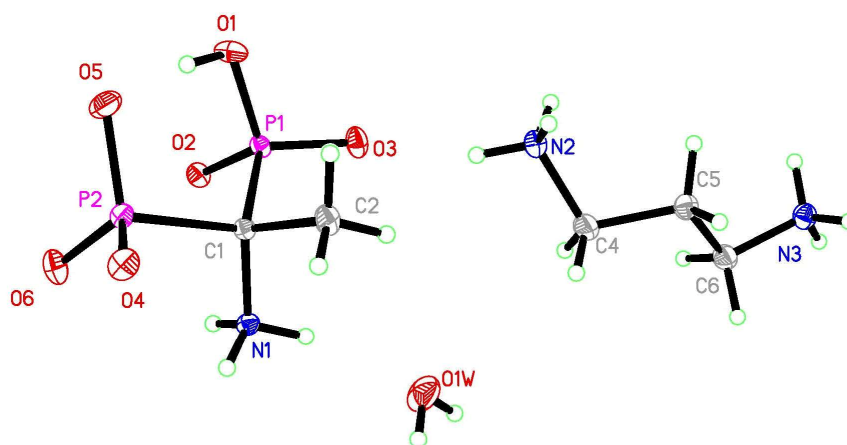


Figure S3. The ORTEP of compound **2** with thermal ellipsoids at the 30% probability level.

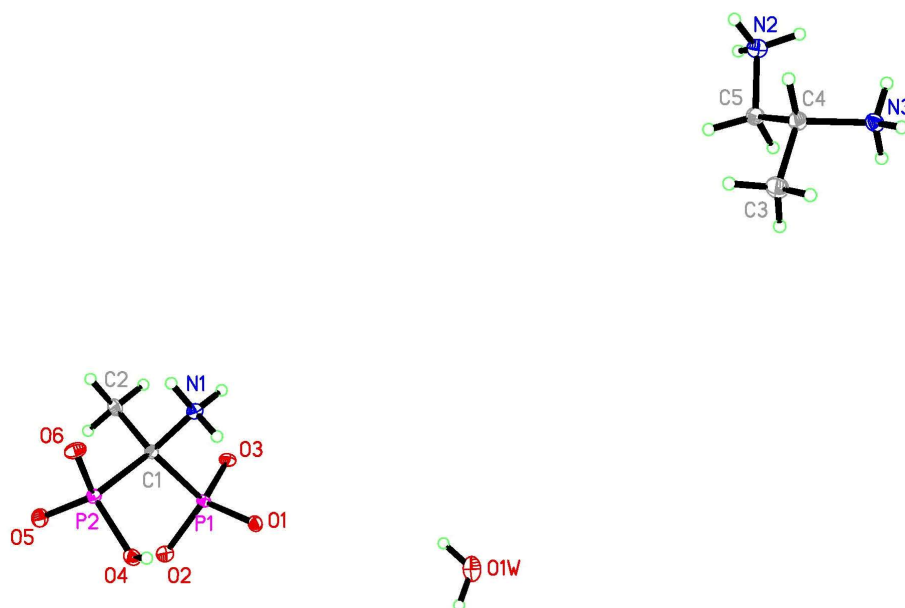


Figure S4. The ORTEP of compound **3** with thermal ellipsoids at the 30% probability level.



Figure S5. The ORTEP of compound **4** with thermal ellipsoids at the 30% probability level.

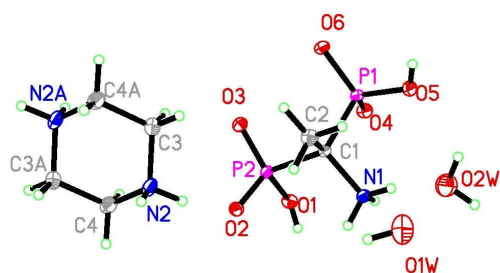


Figure S6. The ORTEP of compound **5** with thermal ellipsoids at the 30% probability level.

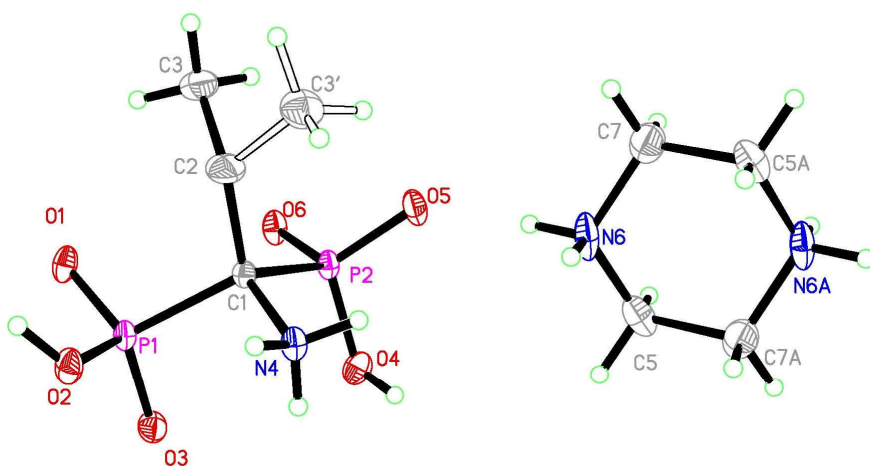


Figure S7. The ORTEP of compound **6** with thermal ellipsoids at the 30% probability level.

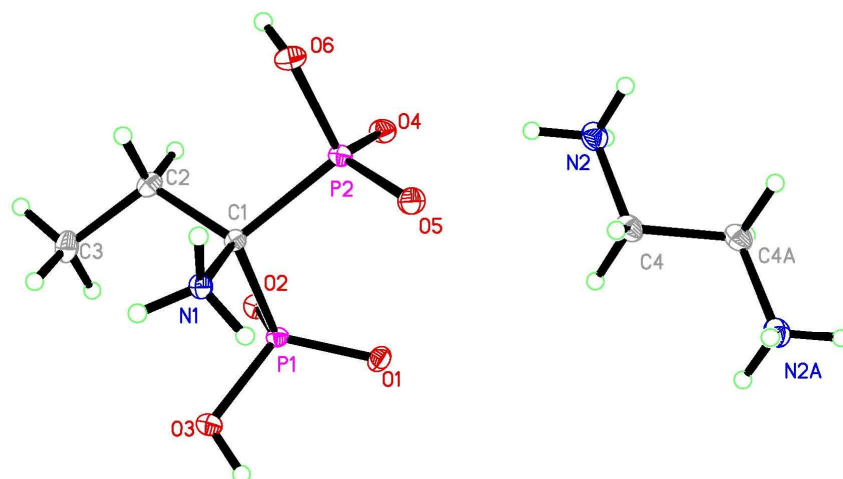


Figure S8. The ORTEP of compound **7** with thermal ellipsoids at the 30% probability level.

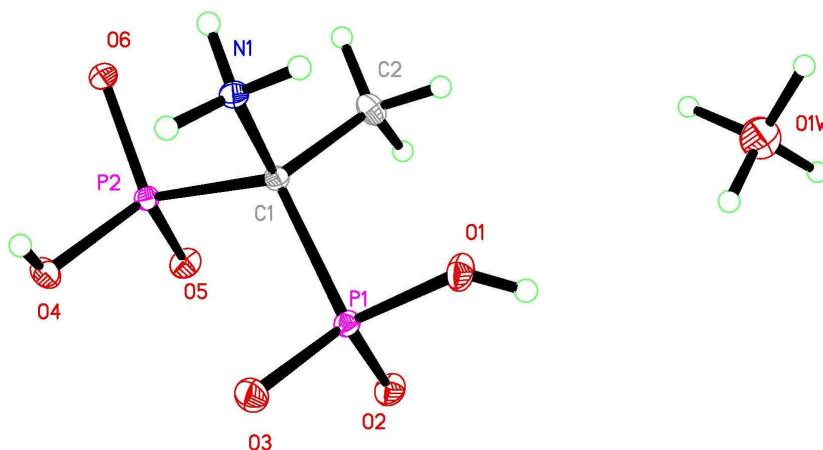


Figure S9. The ORTEP of compound **8** with thermal ellipsoids at the 30% probability level.

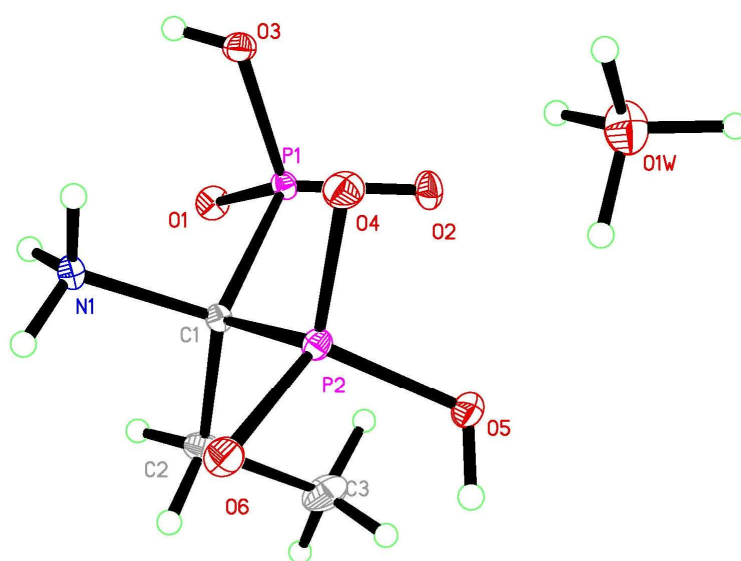


Figure S10. The 1(1)3(1)R4 water cluster in compound **4** and its connections to the host.

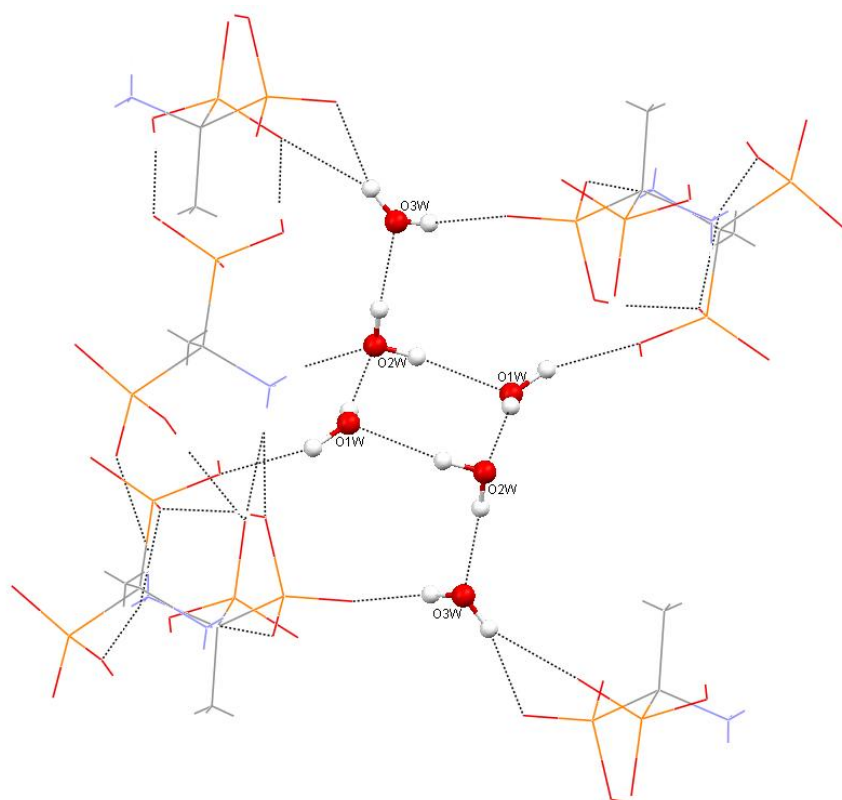


Figure S11. IR spectra of compounds **1-8**.

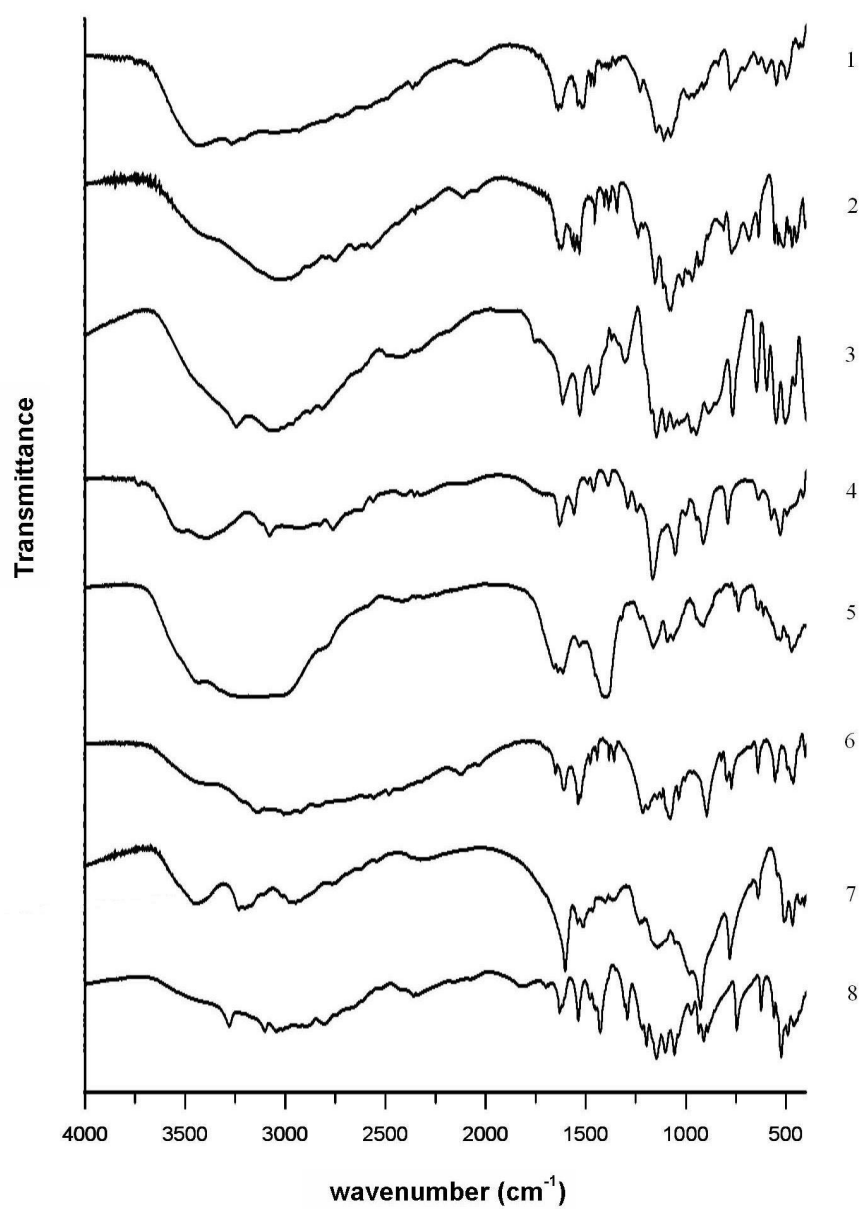


Figure S12. TG curves of compounds **1-8**.

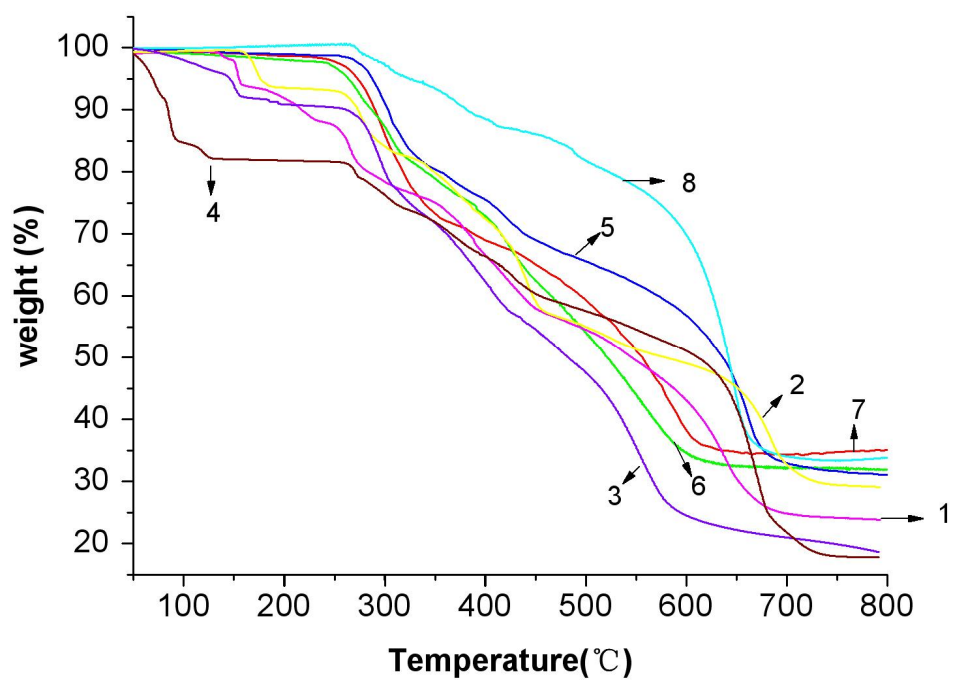


Table S13. Hydrogen bonds of compounds **1-8** [Å and °].

Donor–H···Acceptor	D(Donor···Acceptor)	<(Donor–H···Acceptor)
Compound 1 ^{a)}		
O(1W)-H(1W1)...O(3)#1	2.850(2)	163(3)
O(1)-H(1)...O(5)	2.479(2)	172(3)
O(1W)-H(2W1)...O(5)#2	2.800(2)	166(2)
N(2)-H(2F)...O(2)#3	2.8494(17)	171.3
N(2)-H(2E)...O(3)	2.766(2)	159.4
N(2)-H(2D)...O(4)#4	2.6877(17)	161.5
N(3)-H(3C)...O(6)#5	2.7430(18)	160.1
N(3)-H(3B)...O(6)#6	2.8141(19)	174.2
N(3)-H(3A)...O(3)#3	3.1000(19)	167.2
N(1)-H(1C)...O(2)#1	2.7718(16)	167.1
N(1)-H(1B)...O(2)	2.9867(16)	113.8
N(1)-H(1B)...O(4)#7	2.8433(17)	147.9
N(1)-H(1A)...O(1W)	2.765(2)	157.6
Compound 2 ^{b)}		
N(3)-H(3F)...O(2)#1	2.9061(15)	167.7
N(3)-H(3E)...O(4)#2	3.0563(15)	113.5
N(3)-H(3E)...O(2)#2	2.8680(15)	157.1
N(3)-H(3D)...O(3)#3	2.7653(14)	179.9
N(2)-H(2F)...O(2)#2	2.8479(16)	169.3
N(2)-H(2E)...O(1W)#4	2.7136(16)	152.2
N(2)-H(2D)...O(5)#2	2.7453(15)	116.2
N(2)-H(2D)...O(5)#5	2.8055(16)	146.7
N(1)-H(1C)...O(1W)#6	2.9669(17)	170.5
N(1)-H(1B)...O(3)#7	2.9573(14)	160.7
N(1)-H(1A)...O(4)#8	3.0254(15)	110.9
N(1)-H(1A)...O(1)#8	2.8147(14)	160.1

O(4)-H(3)...O(1)#7	2.5223(13)	174(3)
O(1W)-H(2W1)...O(6)#9	2.6174(14)	164(2)
O(1W)-H(1W1)...O(6)#8	2.6576(15)	167(2)

Compound 3 ^{c)}

N(3)-H(3B)...O(3)#1	3.1583(15)	123.2
N(3)-H(3B)...O(2)#1	2.8096(15)	152.5
N(3)-H(3A)...O(5)#2	3.1673(15)	129.1
N(3)-H(3A)...O(4)#2	2.6841(15)	158.3
N(2)-H(2E)...O(6)#3	2.5581(14)	173.5
N(2)-H(2D)...O(1W)#4	2.7944(15)	163.8
O(1W)-H(2W1)...O(2)	2.6412(14)	175(2)
O(1W)-H(1W1)...O(1)#5	2.7043(14)	158.9(18)
O(3)-H(3)...O(5)#6	2.5303(14)	173(3)
N(1)-H(1C)...O(1)#5	2.8520(15)	156.9
N(1)-H(1B)...O(5)#7	2.7695(14)	137.9
N(1)-H(1A)...O(6)#5	2.8138(14)	139.1

Compound 4 ^{d)}

O(1)-H(1)...O(4)#2	2.5388(18)	173(4)
O(5)-H(5)...O(6)#3	2.5141(19)	172(4)
O(1W)-H(1W1)...O(5)#4	2.879(2)	152(4)
O(1W)-H(2W1)...O(2W)	2.821(3)	153(4)
O(2W)-H(1W2)...O(3W)#5	2.757(3)	171(5)
O(2W)-H(2W2)...O(1W)#6	2.797(3)	167(5)
O(3W)-H(1W3)...O(3)#7	3.007(2)	156(2)
O(3W)-H(1W3)...O(6)#7	2.982(2)	123(2)
O(3W)-H(2W3)...O(3)#8	2.854(2)	174(3)
N(1)-H(1A)...O(2W)	2.786(2)	167.2

N(1)-H(1B)...O(2)#9	2.7891(18)	160.4
N(1)-H(1C)...O(1)#2	2.951(2)	157.6
N(1)-H(1C)...O(4)#2	3.078(2)	118.2
N(2)-H(2D)...O(2)	2.781(2)	149.5
N(2)-H(2D)...O(4)#4	2.953(2)	119.6
N(2)-H(2E)...O(3)#4	2.926(2)	145.8
N(2)-H(2E)...O(6)#4	3.037(2)	129.3

Compound 5 ^{e)}

N(6)-H(6B)...O(5)	2.6030(19)	169.2
N(6)-H(6A)...O(6)#2	2.7053(19)	160.8
N(4)-H(4C)...O(3)#3	3.0971(18)	122.7
N(4)-H(4C)...O(4)#3	2.8469(19)	134.9
N(4)-H(4B)...O(6)#2	2.8043(18)	153.4
N(4)-H(4A)...O(1)#2	2.8425(17)	147
O(4)-H(4)...O(3)#3	2.5141(19)	167(3)
O(2)-H(2)...O(1)#4	2.5527(16)	172(4)

Compound 6 ^{f)}

O(3)-H(3)...O(5)#2	2.6603(17)	165(3)
O(6)-H(6)...O(4)#3	2.6624(19)	173(3)
N(1)-H(1A)...O(4)#4	3.0417(19)	155.4
N(1)-H(1B)...O(1)#2	2.6930(18)	169.2
N(1)-H(1C)...O(2)#4	2.8267(18)	149
N(2)-H(2C)...O(2)#5	2.738(2)	168.5
N(2)-H(2D)...O(4)	2.984(2)	167.9
N(2)-H(2E)...O(5)#6	2.821(2)	158

Compound 7 ^{g)}

N(1)-H(4)...O(2)#1	2.811(2)	161(2)
N(1)-H(6)...O(5)#1	2.714(2)	159(2)
N(1)-H(5)...O(3)#2	2.824(2)	154(2)
O(4)-H(7)...O(3)#2	2.591(2)	174(3)
O(1)-H(8)...O(6)#3	2.549(2)	172(3)
O(1W)-H(9)...O(5)#4	2.804(2)	159(3)
O(1W)-H(10)...O(3)#5	3.040(2)	145(3)
O(1W)-H(11)...O(2)#6	2.828(2)	173(3)
O(1W)-H(12)...O(6)#3	2.816(2)	173(3)

Compound 8 ^{h)}

N(1)-H(1C)...O(2)#1	2.7932(17)	149.9
N(1)-H(1B)...O(1)#2	2.8461(18)	161.9
N(1)-H(1A)...O(4)#3	3.1336(18)	121
N(1)-H(1A)...O(3)#3	2.9102(17)	154.4
O(1W)-H(4W1)...O(1)#4	2.792(2)	170(3)
O(1W)-H(3W1)...O(6)#5	2.810(2)	165(3)
O(1W)-H(2W1)...O(2)	2.882(2)	147(3)
O(1W)-H(1W1)...O(5)	3.013(2)	153(3)
O(5)-H(5)...O(6)#6	2.5686(17)	176(2)
O(3)-H(3)...O(4)#3	2.5240(17)	169(3)

Symmetry transformations used to generate equivalent atoms: ^{a)}: #1 $x+1/2, -y+3/2, z$; #2 $-x+1/2, y+1/2, z+1/2$; #3 $-x, -y+1, z+1/2$; #4 $-x+1, -y+1, z+1/2$; #5 $x, y, z+1$; #6 $x-1/2, -y+3/2, z+1$; #7 $x-1/2, -y+3/2, z$. ^{b)}: #1 $-x+1, -y+1, -z+1$; #2 $x, y-1, z+1$; #3 $x, y, z+1$; #4 $x+1/2, -y+1/2, z+1/2$; #5 $-x+2, -y+1, -z+1$; #6 $x+1, y, z$; #7 $-x+3/2, y+1/2, -z+1/2$; #8 $-x+3/2, y-1/2, -z+1/2$; #9 $x-1, y, z$. ^{c)}: #1 $-x+1, -y+1, -z+1$; #2 $x, y+1, z-1$; #3 $x+1/2, -y+1/2, z-1/2$; #4 $-x+1/2, y+1/2, -z+1/2$; #5 $x+1, y, z$; #6 $-x, -y, -z+2$; #7 $-x+1, -y, -z+2$. ^{d)}: #1 $-x+1/2, -y+3/2, -z$; #2 $-x+1/2, y+1/2, -z+1/2$; #3 $-x+1, y, -z+1/2$; #4 $x, y+1, z$; #5 $x+1/2, -y+1/2, z-1/2$; #6 $-x+1, -y+1, -z+1$; #7 $-x+1/2, -y+1/2, -z+1$; #8 $x, y, z+1$; #9 $-x+1/2, y-1/2, -z+1/2$. ^{e)}: #1 $-x, -y+2, -z$; #2 $x, y+1, z$; #3 $-x+1/2, y+1/2, -z+1/2$; #4 $-x+1/2, -y+1/2, -z+1$.

^{f)}: #1 $-x, -y, -z+1$; #2 $-x+1, -y+1, -z+1$; #3 $-x+1, -y+1, -z$; #4 $x+1, y, z$; #5 $x, y-1, z$; #6 $x-1, y, z$. ^{g)}: #1 $x-1/2, -y+3/2, z-1/2$; #2 $-x+1/2, y-1/2, -z+1/2$; #3 $-x+1/2, y+1/2, -z+1/2$; #4 $x, y-1, z$; #5 $x+1/2, -y+1/2, z+1/2$; #6 $-x+1, -y+1, -z$. ^{h)}: #1 $-x+2, y+1/2, -z+1/2$; #2 $-x+2, -y+1, -z$; #3 $x-1, y, z$; #4 $-x+2, -y+1, -z+1$; #5 $-x+1, y+1/2, -z+1/2$; #6 $-x+1, -y+1, -z+1$.