

Supplementary information

for

Reactivity of 4-Amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole, Structures and Magnetic Properties of Polynuclear and Polymeric Mn(II), Cu(II) and Cd(II) Complexes

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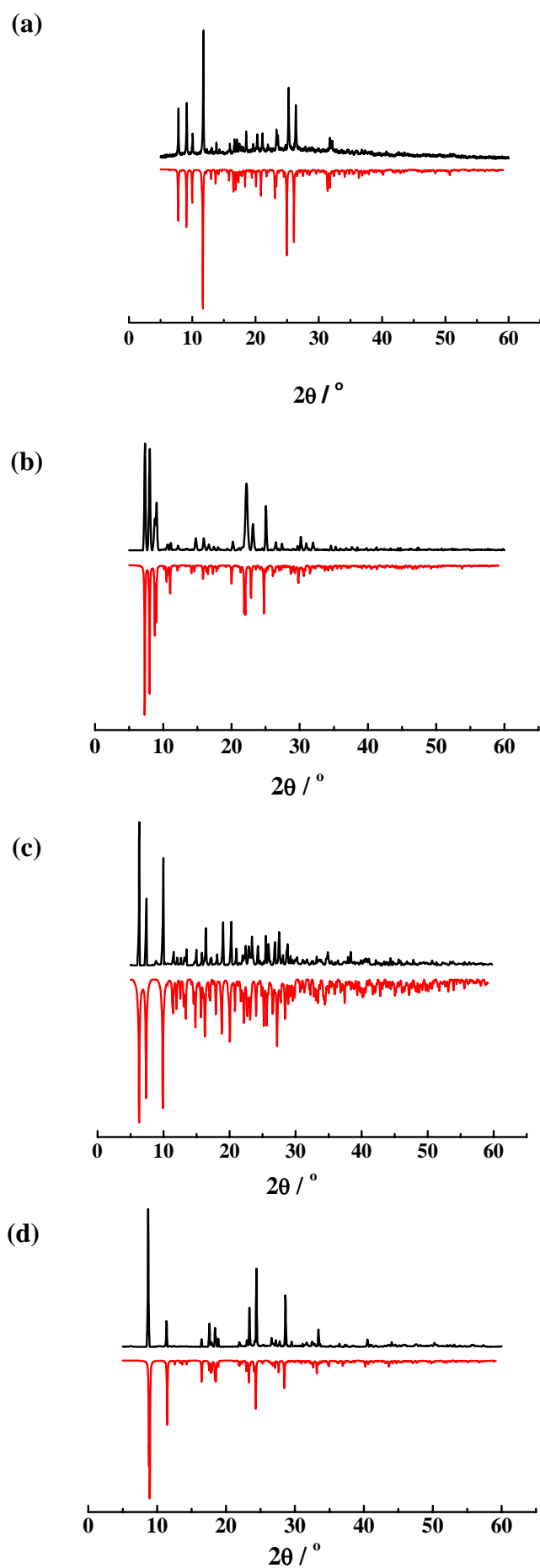


Figure S1. Simulated (red) & experimental (black) XRPD data for **2** (a), **3** (b), **4** (c) and **5** (d).

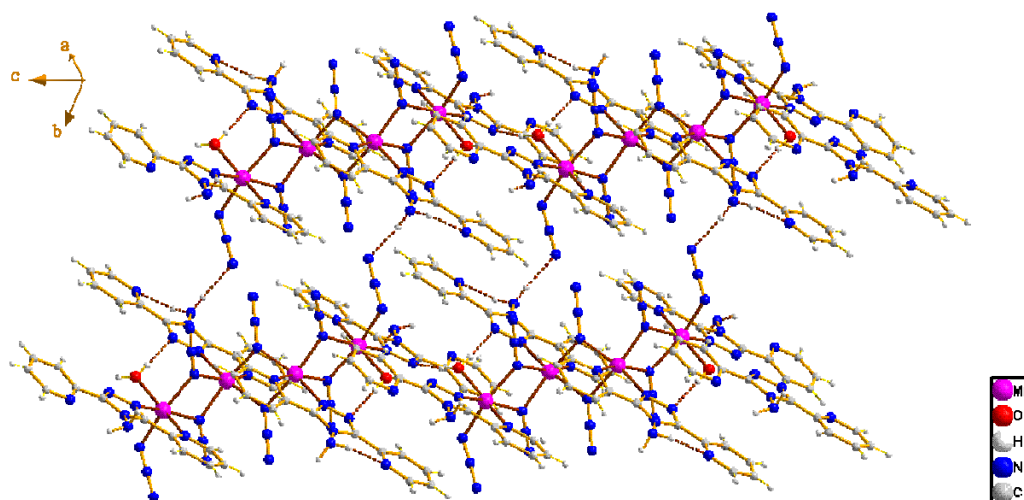


Figure S2. The 2D hydrogen-bonded layer in **2**.

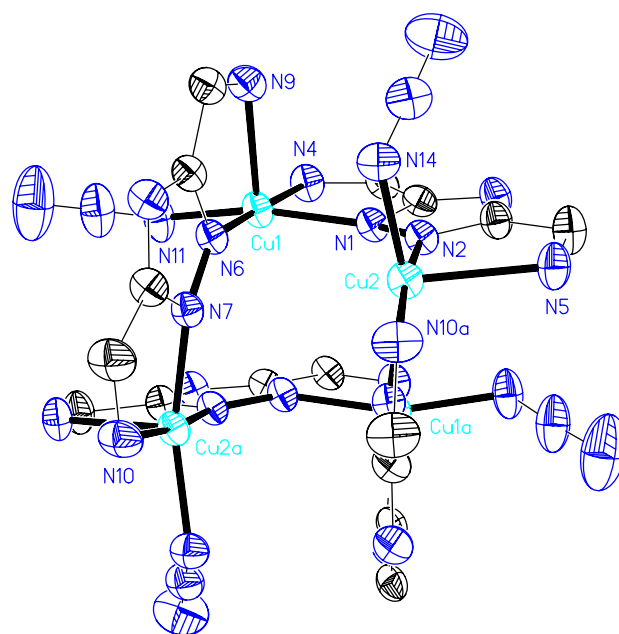


Figure S3. ORTEP drawing of the coordination environments of the Cu^{2+} ions in **3** with thermal ellipsoids at 50% probability.

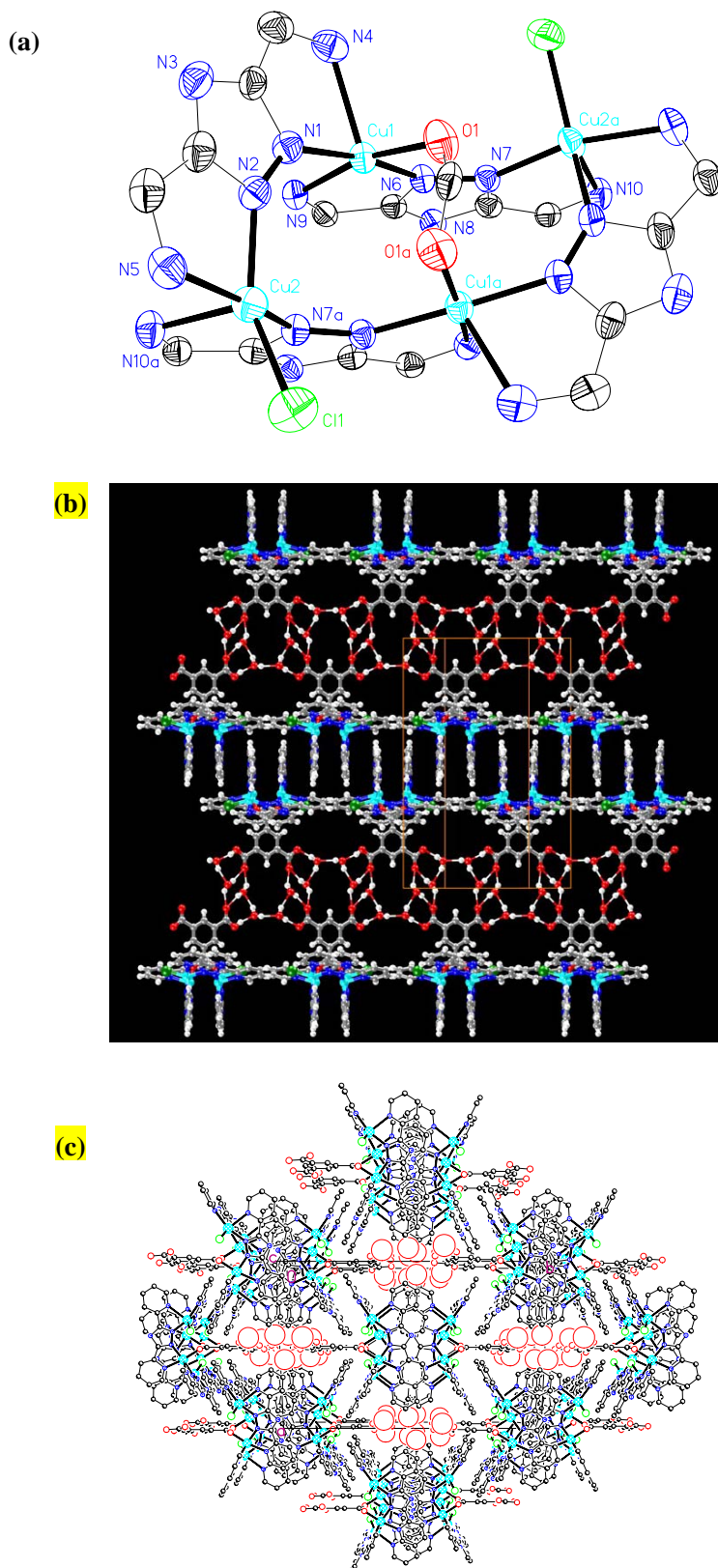


Figure S4. The crystal structure of **4**: ORTEP drawings of the coordination environments of the Cu^{2+} ions (a), the 2D supramolecular layer (b) and the 3D supramolecular architecture (c) viewed along the *c*-axis.

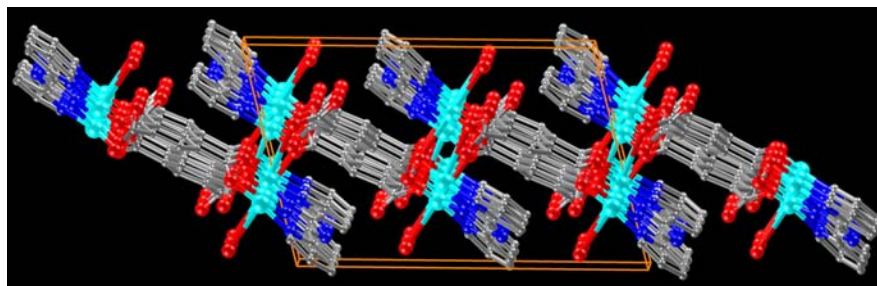


Figure S5. The 2D coordination layer in **5**.

Table S1. Bond lengths (Å) and angles (°) for **1-5**.

1			
Cd(1)-N(10)	2.2953(19)	Cd(1)-N(7 <i>a</i>)	2.3446(19)
Cd(1)-N(7)	2.3010(19)	Cd(1)-N(10 <i>b</i>)	2.3800(19)
Cd(1)-N(1)	2.328(2)	Cd(1)-N(5)	2.4167(19)
N(4)···N(6)	2.844(3)	N(4)···N(9 <i>c</i>)	3.029(3)
N(10)-Cd(1)-N(7)	111.75(7)	N(1)-Cd(1)-N(10 <i>b</i>)	100.19(7)
N(10)-Cd(1)-N(1)	95.80(7)	N(7 <i>a</i>)-Cd(1)-N(10 <i>b</i>)	168.74(7)
N(7)-Cd(1)-N(1)	150.71(7)	N(10)-Cd(1)-N(5)	151.46(7)
N(10)-Cd(1)-N(7 <i>a</i>)	101.14(7)	N(7)-Cd(1)-N(5)	88.77(7)
N(7)-Cd(1)-N(7 <i>a</i>)	75.48(8)	N(1)-Cd(1)-N(5)	69.61(6)
N(1)-Cd(1)-N(7 <i>a</i>)	90.05(6)	N(7 <i>a</i>)-Cd(1)-N(5)	103.19(7)
N(10)-Cd(1)-N(10 <i>b</i>)	73.36(8)	N(10 <i>b</i>)-Cd(1)-N(5)	84.93(6)
N(7)-Cd(1)-N(10 <i>b</i>)	97.17(7)	N(4)-H(4B)···N(9 <i>c</i>)	117.6
N(4)-H(4B)···N(6)	136.3		
2			
Mn(1)-N(7)	2.136(5)	Mn(2)-N(4)	2.192(4)
Mn(1)-O(1w)	2.163(3)	Mn(2)-N(10)	2.210(4)
Mn(1)-N(1)	2.205(4)	Mn(2)-N(1)	2.219(4)
Mn(1)-N(13)	2.246(4)	Mn(2)-N(10 <i>a</i>)	2.222(4)
Mn(1)-N(4)	2.312(4)	Mn(2)-N(19)	2.258(4)
Mn(1)-N(17)	2.327(4)	Mn(2)-N(23)	2.346(4)
O(1w)···N(20)	2.871(5)	O(1w)···N(14 <i>b</i>)	2.853(5)
N(16)···N(18)	2.854(6)	N(16)···N(6 <i>c</i>)	3.032(7)
N(22)···N(24)	2.839(6)	N(22)···N(9 <i>d</i>)	2.967(7)
N(7)-Mn(1)-O(1w)	95.59(16)	N(4)-Mn(2)-N(10)	161.99(16)
N(7)-Mn(1)-N(1)	163.44(17)	N(4)-Mn(2)-N(1)	78.43(14)
O(1w)-Mn(1)-N(1)	85.70(14)	N(10)-Mn(2)-N(1)	92.27(15)
N(7)-Mn(1)-N(13)	95.63(17)	N(4)-Mn(2)-N(10 <i>a</i>)	90.80(15)
O(1w)-Mn(1)-N(13)	87.62(13)	N(10)-Mn(2)-N(10 <i>a</i>)	77.98(15)
N(1)-Mn(1)-N(13)	100.93(14)	N(1)-Mn(2)-N(10 <i>a</i>)	110.72(15)
N(7)-Mn(1)-N(4)	87.61(17)	N(4)-Mn(2)-N(19)	96.90(15)
O(1w)-Mn(1)-N(4)	105.93(14)	N(10)-Mn(2)-N(19)	98.00(14)
N(1)-Mn(1)-N(4)	76.20(14)	N(1)-Mn(2)-N(19)	87.03(13)
N(13)-Mn(1)-N(4)	165.74(14)	N(10 <i>a</i>)-Mn(2)-N(19)	161.80(14)
N(7)-Mn(1)-N(17)	96.35(17)	N(4)-Mn(2)-N(23)	103.32(15)
O(1w)-Mn(1)-N(17)	156.42(14)	N(10)-Mn(2)-N(23)	91.21(15)
N(1)-Mn(1)-N(17)	88.59(14)	N(1)-Mn(2)-N(23)	157.44(14)

N(13)-Mn(1)-N(17)	71.03(13)	N(10a)-Mn(2)-N(23)	91.81(14)
N(4)-Mn(1)-N(17)	94.83(14)	N(19)-Mn(2)-N(23)	70.41(13)
O(1w)-H(1wa)···N(20)	177.4	O(1w)-H(1wa)···N(14b)	159.1
N(16)-H(16A)···N(18)	119.7	N(16)-H(16B)···N(6c)	155.7
N(22)-H(22A)···N(24)	133.2	N(22)-H(22B)···N(9d)	171.4
3			
Cu(1)-N(11)	1.932(5)	Cu(2)-N(14)	1.968(5)
Cu(1)-N(1)	1.990(4)	Cu(2)-N(7a)	1.984(4)
Cu(1)-N(6)	1.991(4)	Cu(2)-N(2)	1.995(4)
Cu(1)-N(4)	2.043(4)	Cu(2)-N(10a)	2.046(4)
Cu(1)-N(9)	2.303(5)	Cu(2)-N(5)	2.308(5)
O(1w)···N(3)	2.942(7)	O(1w)···N(14c)	3.029(7)
O(2w)···N(8)	3.114(9)	O(2w)···O(1wd)	2.807(10)
N(11)-Cu(1)-N(1)	162.0(2)	N(14)-Cu(2)-N(7a)	158.85(19)
N(11)-Cu(1)-N(6)	94.05(18)	N(14)-Cu(2)-N(2)	95.19(18)
N(1)-Cu(1)-N(6)	96.70(16)	N(7a)-Cu(2)-N(2)	95.44(16)
N(11)-Cu(1)-N(4)	89.8(2)	N(14)-Cu(2)-N(10a)	91.08(19)
N(1)-Cu(1)-N(4)	79.64(17)	N(7a)-Cu(2)-N(10a)	79.58(17)
N(6)-Cu(1)-N(4)	176.14(18)	N(2)-Cu(2)-N(10a)	173.04(18)
N(11)-Cu(1)-N(9)	102.0(2)	N(14)-Cu(2)-N(5)	98.97(19)
N(1)-Cu(1)-N(9)	94.61(17)	N(7a)-Cu(2)-N(5)	101.32(17)
N(6)-Cu(1)-N(9)	76.15(17)	N(2)-Cu(2)-N(5)	76.00(16)
N(4)-Cu(1)-N(9)	102.80(18)	N(10a)-Cu(2)-N(5)	100.07(19)
O(1w)-H(1wa)···N(3)	172.9	O(1w)-H(1wb)···N(14c)	177.6
O(2w)-H(2wa)···N(8)	138.5	O(2w)-H(2wb)···O(1wd)	165.9
4			
Cu(1)-N(6)	1.950(4)	Cu(2)-N(7a)	1.989(4)
Cu(1)-N(1)	1.970(4)	Cu(2)-N(2)	2.003(4)
Cu(1)-O(1)	1.980(4)	Cu(2)-N(5)	2.039(4)
Cu(1)-N(9)	2.073(4)	Cu(2)-Cl(1)	2.2520(18)
Cu(1)-N(4)	2.273(5)	Cu(2)-N(10a)	2.343(4)
O(2)···O(1w)	2.643(8)	O(1w)···O(2w)	2.754(8)
O(1w)···O(2)	2.643(8)	O(1w)···O(1wb)	2.903(13)
O(2w)···O(3c)	2.865(9)	O(2w)···O(3)	2.946(10)
N(6)-Cu(1)-N(1)	171.17(17)	N(7a)-Cu(2)-N(2)	96.32(17)
N(6)-Cu(1)-O(1)	94.73(16)	N(7a)-Cu(2)-N(5)	162.43(18)
N(1)-Cu(1)-O(1)	91.44(17)	N(2)-Cu(2)-N(5)	79.70(18)
N(6)-Cu(1)-N(9)	80.43(16)	N(7a)-Cu(2)-Cl(1)	96.89(13)
N(1)-Cu(1)-N(9)	92.22(17)	N(2)-Cu(2)-Cl(1)	146.86(14)

O(1)-Cu(1)-N(9)	167.26(17)	N(5)-Cu(2)-Cl(1)	95.54(15)
N(6)-Cu(1)-N(4)	108.06(17)	N(7 <i>a</i>)-Cu(2)-N(10 <i>a</i>)	76.07(16)
N(1)-Cu(1)-N(4)	77.34(18)	N(2)-Cu(2)-N(10 <i>a</i>)	98.47(17)
O(1)-Cu(1)-N(4)	97.19(17)	N(5)-Cu(2)-N(10 <i>a</i>)	87.52(17)
N(9)-Cu(1)-N(4)	95.52(17)	Cl(1)-Cu(2)-N(10 <i>a</i>)	114.18(13)
O(2)-H(2O)···O(1w)	166.4	O(1w)-H(1wa)···O(2w)	158.5
O(1w)-H(1wb)···O(2)	173.7	O(1w)-H(1wc)···O(1wb)	166.4
O(2w)-H(2wa)···O(3c)	150.4	O(2w)-H(2wb)···O(3)	168.7

5

Cu(1)-O(3 <i>a</i>)	1.936(5)	Cu(2)-O(5 <i>c</i>)	1.957(5)
Cu(1)-O(1)	1.942(5)	Cu(2)-O(2)	1.957(5)
Cu(1)-N(2)	1.955(5)	Cu(2)-N(5)	2.046(6)
Cu(1)-N(1)	2.034(6)	Cu(2)-O(3 <i>d</i>)	2.785(6)
Cu(1)-O(2 <i>b</i>)	2.550(5)	Cu(1)···Cu(2)	4.2924(14)
Cu(1)-O(1w)	2.581(7)	Cu(1)···Cu(2 <i>b</i>)	3.5122(13)
Cu(2)-N(3)	1.946(6)	O(1w)···O(4 <i>a</i>)	2.632(8)
O(1w)···N(4 <i>e</i>)	2.887(8)	C(10)···O(1w <i>d</i>)	3.379(10)
C(4)···O(1w <i>e</i>)	3.198(10)		

O(3 <i>a</i>)-Cu(1)-O(1)	89.3(2)	N(1)-Cu(1)-O(1w)	86.8(2)
O(3 <i>a</i>)-Cu(1)-N(2)	168.9(2)	O(2 <i>b</i>)-Cu(1)-O(1w)	178.31(18)
O(1)-Cu(1)-N(2)	98.2(2)	N(3)-Cu(2)-O(5 <i>c</i>)	167.3(2)
O(3 <i>a</i>)-Cu(1)-N(1)	92.4(2)	N(3)-Cu(2)-O(2)	96.8(2)
O(1)-Cu(1)-N(1)	174.7(2)	O(5 <i>c</i>)-Cu(2)-O(2)	92.1(2)
N(2)-Cu(1)-N(1)	80.8(2)	N(3)-Cu(2)-N(5)	79.8(2)
O(3 <i>a</i>)-Cu(1)-O(2 <i>b</i>)	82.7(2)	O(5 <i>c</i>)-Cu(2)-N(5)	92.7(2)
O(1)-Cu(1)-O(2 <i>b</i>)	93.5(2)	O(2)-Cu(2)-N(5)	170.4(2)
N(2)-Cu(1)-O(2 <i>b</i>)	88.6(2)	N(3)-Cu(2)-O(3 <i>d</i>)	106.2(2)
N(1)-Cu(1)-O(2 <i>b</i>)	91.7(2)	O(5 <i>c</i>)-Cu(2)-O(3 <i>d</i>)	84.57(19)
O(3 <i>a</i>)-Cu(1)-O(1w)	96.5(2)	O(2)-Cu(2)-O(3 <i>d</i>)	76.25(18)
O(1)-Cu(1)-O(1w)	88.0(2)	N(5)-Cu(2)-O(3 <i>d</i>)	95.94(19)
N(2)-Cu(1)-O(1w)	92.0(2)	O(6 <i>c</i>)-Cu(2)-O(3 <i>d</i>)	138.67(16)
O(1w)-H(1wb)···O(4 <i>a</i>)	137.6	O(1w)-H(1wa)···N(4 <i>e</i>)	151.5
C(10)-H(10)···O(1w <i>d</i>)	169.9	C(4)-H(4)···O(1w <i>e</i>)	153.2

Symmetry codes: *a*) -x+1, y, -z+1/2; *b*) -x+1, -y-2, -z+1; *c*) x, y+1, z for **1**; *a*) -x+2, -y+2, -z; *b*) -x+2, -y+1, -z+1; *c*) x+1, y, z; *d*) x, y-1, z for **2**; *a*) -x+2, y, -z+3/2; *c*) -x+5/2, y-1/2, -z+3/2; *d*) -x+5/2, y+1/2, -z+3/2 for **3**; *a*) -x, y, -z-1/2; *b*) -x, y, -z-3/2; *c*) -x, -y+1, -z-1 for **4**; *a*) -x+1, y-1/2, -z-1/2; *b*) -x+1, -y+1, -z; *c*) -x+1, y+1/2, -z-1/2; *d*) x, -y+3/2, z+1/2; *e*) -x, -y+1, -z for **5**.