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Four new Cu_6S_6 cluster-based coordination compounds: synthesis, crystal structure and fluorescent properties.

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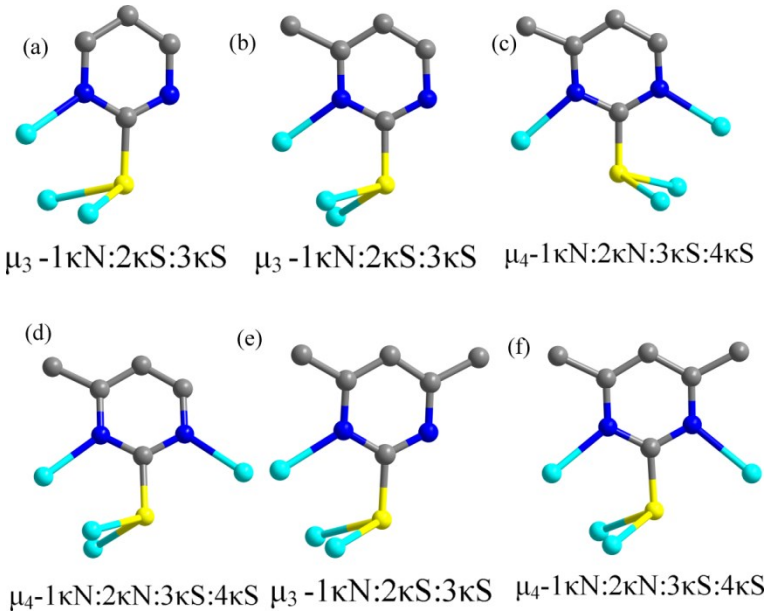

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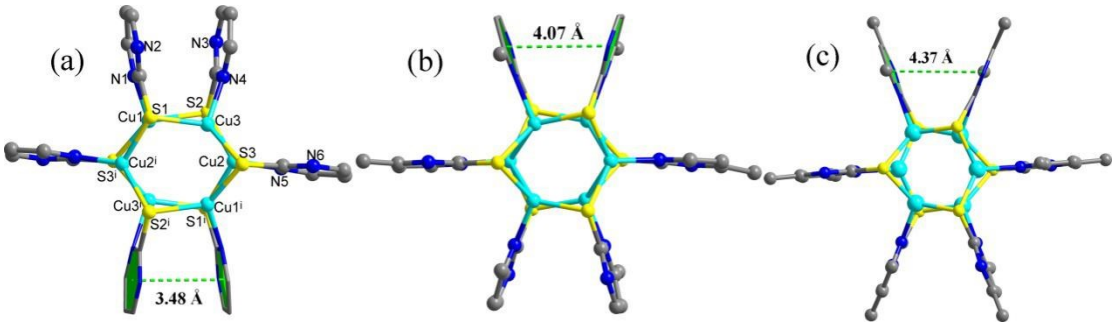

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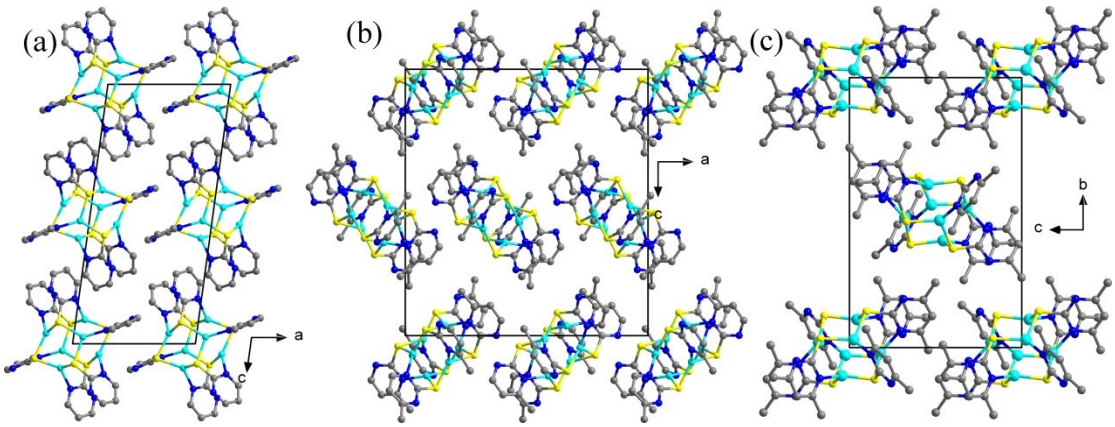

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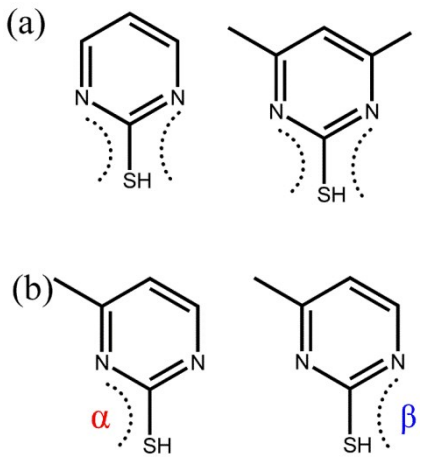

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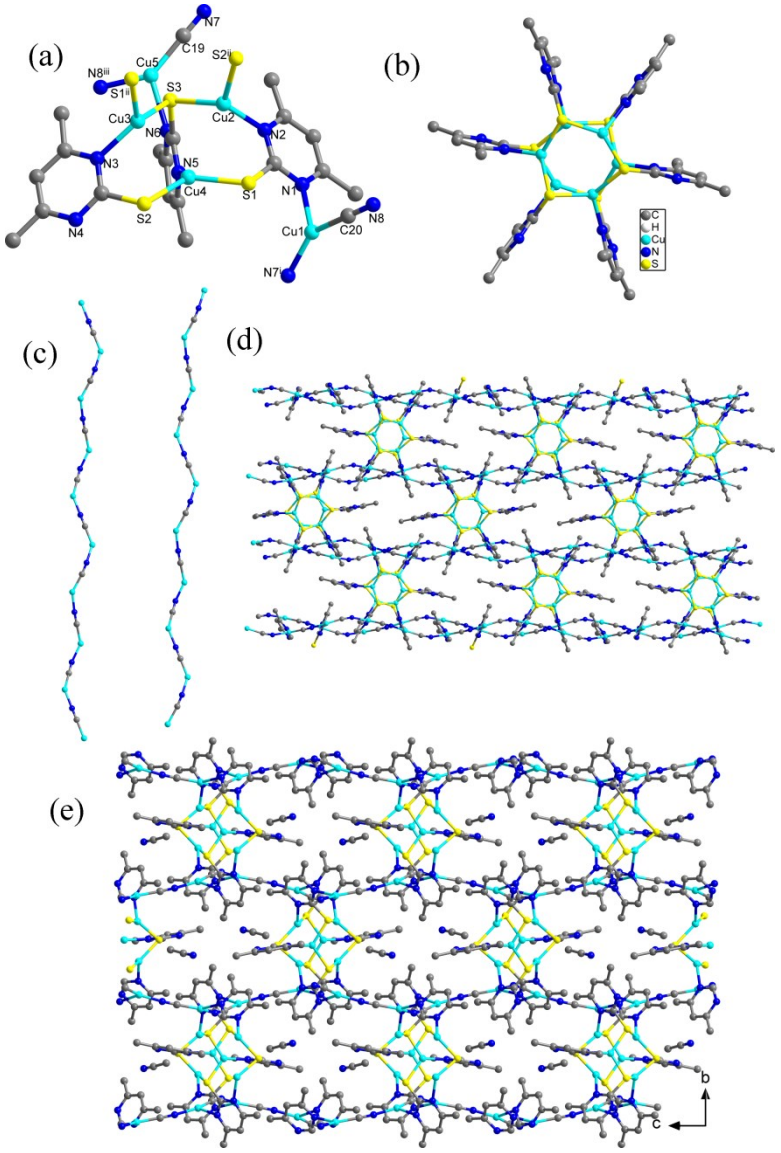

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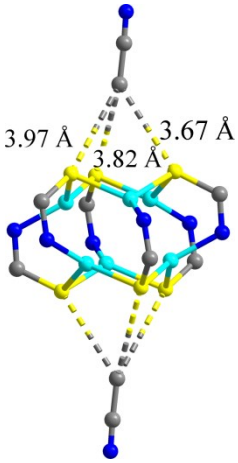

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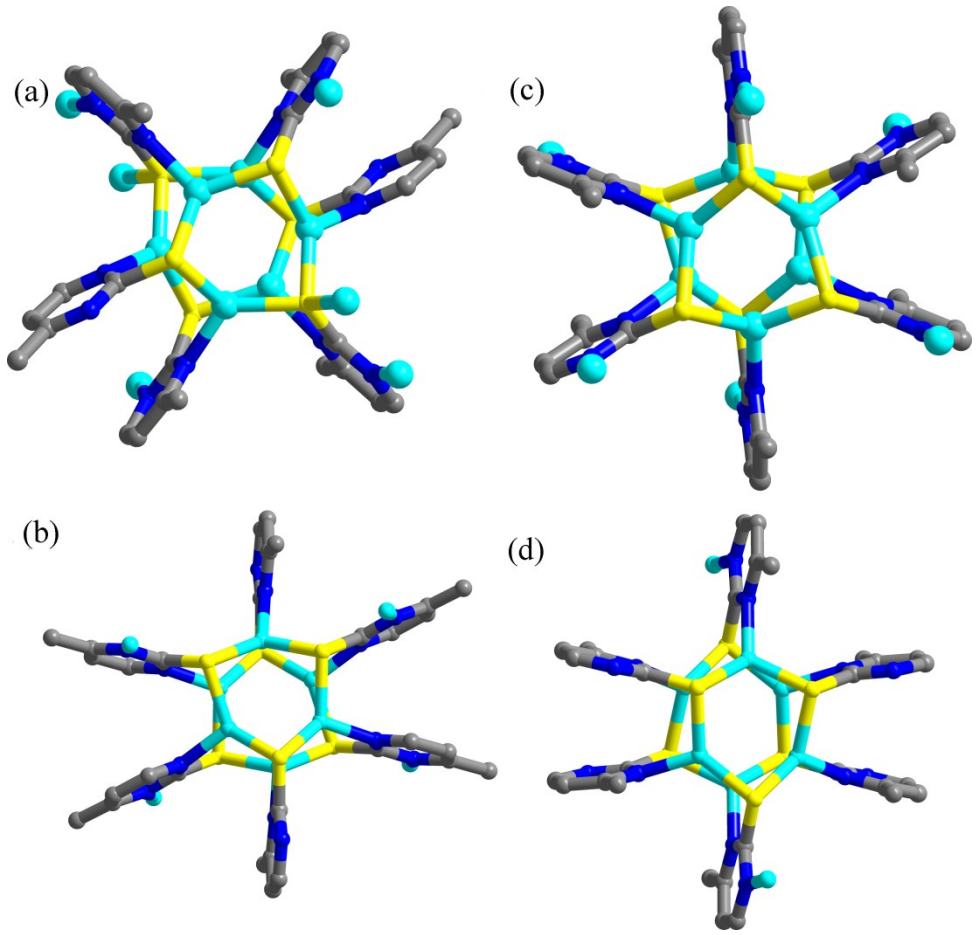

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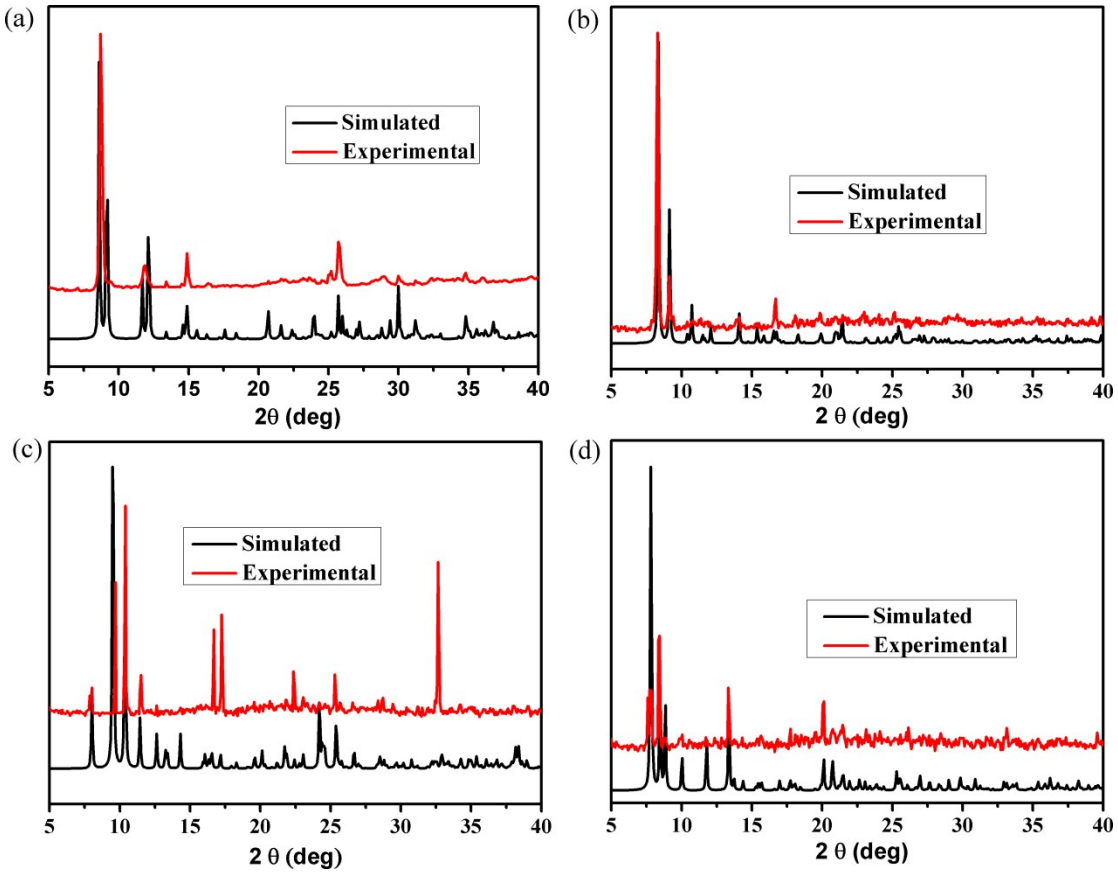

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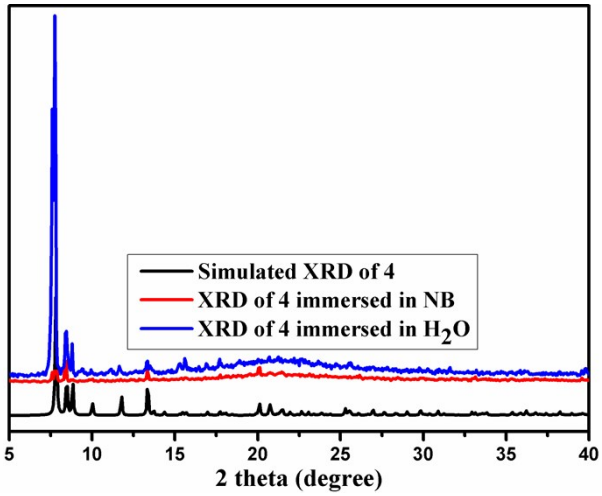

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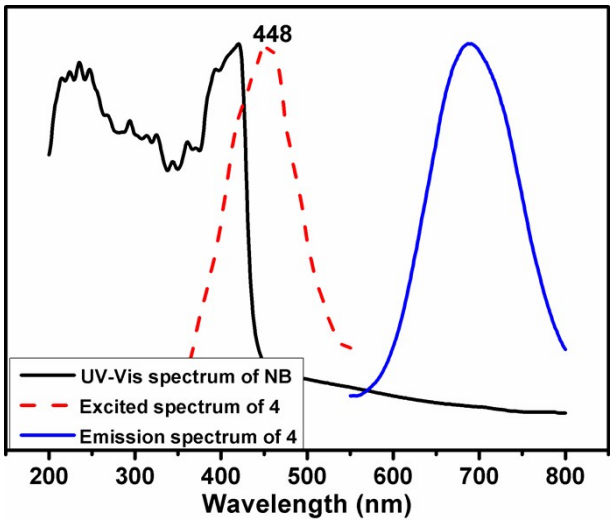

S-Fig. 10 The UV-vis absorption spectrum (black line); the excited spectrum of **4** (red dot line); the emission spectrum (blue line)

S-Table 1 Bond lengths (Å) and Angles (deg) for compounds **1-4.**

Compound 1			
Cu(1)-N(1)	2.034(3)	S(1)-Cu(2)#1	2.2546(10)
Cu(1)-S(3)#1	2.2365(10)	S(3)-Cu(1)#1	2.2365(10)
Cu(1)-S(2)	2.2791(10)	N(1)-Cu(1)-S(3)#1	128.60(9)
Cu(1)-Cu(2)#1	2.8439(7)	N(1)-Cu(1)-S(2)	106.72(9)
Cu(1)-Cu(3)#1	2.9814(7)	S(3)#1-Cu(1)-S(2)	121.48(4)
Cu(2)-N(5)	2.004(3)	N(5)-Cu(2)-S(1)#1	121.25(8)
Cu(2)-S(1)#1	2.2546(10)	N(5)-Cu(2)-S(2)	132.20(8)
Cu(2)-S(2)	2.2571(9)	S(1)#1-Cu(2)-S(2)	103.24(4)
Cu(2)-Cu(3)	2.7168(7)	N(4)-Cu(3)-S(3)	126.63(9)
Cu(3)-N(4)	2.031(3)	N(4)-Cu(3)-S(1)	107.24(9)
Cu(3)-S(3)	2.2242(10)	S(3)-Cu(3)-S(1)	118.81(4)
Cu(3)-S(1)	2.2692(11)		
Compound 2			
C(17)-Cu(5)	1.854(11)	Cu(5)-N(4)	2.079(9)
Cu(1)-N(1)	2.041(9)	C(17)-N(8)	1.187(14)
Cu(1)-S(3)	2.233(3)	C(16)-N(7)	1.141(14)
Cu(1)-S(2)	2.267(3)	C(16)-Cu(4)	1.886(11)
Cu(1)-Cu(2)#1	2.8199(18)	N(1)-Cu(1)-S(3)	119.0(3)
Cu(1)-Cu(3)#1	2.9881(18)	N(1)-Cu(1)-S(2)	110.6(3)
Cu(1)-Cu(3)	3.0534(19)	S(3)-Cu(1)-S(2)	123.79(11)
Cu(2)-N(6)#1	2.030(9)	N(6)#1-Cu(2)-S(2)	127.6(3)
Cu(2)-S(2)	2.254(3)	N(6)#1-Cu(2)-S(1)#1	112.8(3)
Cu(2)-S(1)#1	2.267(3)	S(2)-Cu(2)-S(1)#1	110.83(11)
Cu(2)-Cu(3)	2.7275(18)	N(3)-Cu(3)-S(3)#1	125.9(3)
Cu(2)-Cu(1)#1	2.8199(18)	N(3)-Cu(3)-S(1)	109.6(3)
Cu(3)-N(3)	2.012(8)	S(3)#1-Cu(3)-S(1)	117.61(11)
Cu(3)-S(3)#1	2.203(3)	N(8)#2-Cu(4)-C(16)	138.3(4)
Cu(3)-S(1)	2.254(3)	N(8)#2-Cu(4)-N(2)	113.6(4)
Cu(3)-Cu(1)#1	2.9881(18)	C(16)-Cu(4)-N(2)	107.7(4)
Cu(4)-N(8)#2	1.879(12)	C(17)-Cu(5)-N(7)#3	132.8(4)
Cu(4)-N(2)	2.077(8)	C(17)-Cu(5)-N(4)	117.7(4)
Cu(5)-N(7)#3	1.911(11)	N(7)#3-Cu(5)-N(4)	104.1(4)
Compound 3			
Cu(1)-N(1)#1	1.895(3)	S(2)-Cu(3)#2	2.2599(7)
Cu(1)-N(6)	2.030(2)	S(3)-Cu(4)#2	2.2659(7)
Cu(1)-S(1)	2.2337(10)	N(1)#1-Cu(1)-N(6)	120.71(11)
Cu(2)-N(7)	2.0157(19)	N(1)#1-Cu(1)-S(1)	126.24(9)
Cu(2)-S(3)	2.2329(6)	N(6)-Cu(1)-S(1)	112.39(7)

Cu(2)-S(2)	2.2396(6)	N(7)-Cu(2)-S(3)	126.07(6)
Cu(2)-Cu(4)	2.7251(4)	N(7)-Cu(2)-S(2)	119.49(6)
Cu(2)-Cu(3)	2.7580(4)	S(3)-Cu(2)-S(2)	107.19(2)
Cu(3)-N(4)	2.022(2)	N(4)-Cu(3)-S(4)	127.18(6)
Cu(3)-S(4)	2.2245(7)	N(4)-Cu(3)-S(2)#2	110.41(6)
Cu(3)-S(2)#2	2.2599(7)	S(4)-Cu(3)-S(2)#2	116.58(2)
Cu(3)-Cu(4)	3.0599(5)	N(2)-Cu(4)-S(4)	126.98(6)
Cu(4)-N(2)	2.018(2)	N(2)-Cu(4)-S(3)#2	109.05(6)
Cu(4)-S(4)	2.2341(7)	S(4)-Cu(4)-S(3)#2	117.56(3)
Cu(4)-S(3)#2	2.2659(7)	C(1)-N(1)	1.138(4)
Compound 4			
C(19)-Cu(5)	1.848(5)	Cu(3)-Cu(2)#2	2.8341(8)
C(20)-N(8)	1.146(7)	Cu(4)-N(5)	2.028(4)
C(20)-Cu(1)	1.866(6)	Cu(4)-S(1)	2.2422(13)
Cu(1)-N(7)#1	1.894(5)	Cu(4)-S(2)	2.2490(12)
Cu(1)-N(1)	2.151(4)	Cu(4)-Cu(2)#2	3.0485(9)
Cu(2)-N(2)	2.042(4)	Cu(5)-N(8)#3	1.923(5)
Cu(2)-S(2)#2	2.2363(13)	Cu(5)-N(6)	2.117(4)
Cu(2)-S(3)	2.2562(13)	N(7)-Cu(1)#4	1.894(5)
Cu(2)-Cu(3)#2	2.8341(8)	N(8)-Cu(5)#5	1.923(5)
Cu(2)-Cu(4)	2.9332(9)	S(1)-Cu(3)#2	2.2309(12)
Cu(2)-Cu(4)#2	3.0485(9)	S(2)-Cu(2)#2	2.2363(13)
Cu(3)-N(3)	2.013(4)	C(20)-Cu(1)-N(7)#1	142.6(2)
Cu(3)-S(1)#2	2.2309(12)	C(20)-Cu(1)-N(1)	103.7(2)
Cu(3)-S(3)	2.2470(12)	N(7)#1-Cu(1)-N(1)	112.6(2)
Cu(3)-Cu(4)	2.7378(8)	N(2)-Cu(2)-S(2)#2	121.63(11)
N(5)-Cu(4)-S(2)	117.94(11)	N(2)-Cu(2)-S(3)	111.58(11)
S(1)-Cu(4)-S(2)	119.87(5)	S(2)#2-Cu(2)-S(3)	118.88(5)
C(19)-Cu(5)-N(8)#3	138.1(2)	N(3)-Cu(3)-S(1)#2	120.93(11)
C(19)-Cu(5)-N(6)	124.1(2)	N(3)-Cu(3)-S(3)	117.09(11)
N(8)#3-Cu(5)-N(6)	96.40(18)	S(1)#2-Cu(3)-S(3)	113.67(5)
N(5)-Cu(4)-S(1)	114.76(11)		

Symmetry code: For compound **1**, #1 –x + 2, -y + 1, -z + 1. For compound **2**: #1 –x + 1, -y, -z; #2 x, y, z+1; #3 x - 1/2, -y + 1/2, z - 1/2; #4 x + 1/2, -y + 1/2, z+1/2; #5 x, y, z-1. For compound **3**: #1 –x + 1/2, y - 1/2, -z + 3/2; #2 -x, -y, -z + 2. For compound **4**: #1 x - 1/2, -y + 1/2, z + 1/2; #2 –x + 1, - y, - z; #3 x + 1, y, z; #4 x + 1/2, - y + 1/2, z - 1/2; #5 x-1, y, z.