Supporting Information

Hydrogen-Bonded Anionic Host Lattices Constructed with Isocyanurate and Thiourea/Urea

Chi-Keung Lam,[†,‡,*] Sam Chun-Kit Hau,[†] Chung-Wah Yau[†] and Thomas C. W. Mak[†]

[†]Department of Chemistry and Centre of Novel Functional Molecules, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong SAR, People's Republic of China

[‡]School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China

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1. IR data for complexes (1)~(7)

$(CH_3)_4N^+C_3H_2N_3O_3^-\cdot 3(NH_2)_2CS\cdot H_2O$ (**1**). IR/cm^{-1} (KBr): 3345 (m), 3265 (m), 3170 (m), 3010 (w), 2833 (m), 1717 (vs), 1650 (vs), 1488 (vs), 1451 (s), 1289 (w), 1176 (w), 1151 (w), 1079 (s), 1004 (s), 856 (w), 790 (s), 761 (m), 737 (m), 695 (m), 620 (w), 533 (s).

$(CH_3)_4N^+C_3H_2N_3O_3^-\cdot (NH_2)_2CS$ (**2**). IR/cm^{-1} (KBr): 3390 (m), 3173 (m), 3021 (w), 2832 (vs), 1720 (vs), 1654 (s), 1485 (vs), 1441 (s), 1435 (m), 1293 (w), 1261 (m), 1060 (w), 949 (vs), 789 (s), 760 (m), 618 (w), 531 (m), 463 (w).

$(C_2H_5)_4N^+C_3H_2N_3O_3^-\cdot (NH_2)_2CS$ (**3**). IR/cm^{-1} (KBr): 3453 (m), 3411 (m), 3179 (w), 2965 (s), 2871 (m), 2839 (m), 1759 (m), 1726 (vs), 1691 (m), 1648 (w), 1637 (w), 1438 (m), 1287 (w), 1246 (w), 1169 (m), 1139 (s), 1060 (w), 1031 (m), 1011 (s),881 (m), 827 (w), 796 (w), 762 (m), 688 (w), 619 (w), 549 (s), 528 (m), 515 (w).

$(n\text{-}C_3H_7)_4N^+C_3H_2N_3O_3^-\cdot (NH_2)_2CS\cdot H_2O$ (**4**). IR/cm^{-1} (KBr): 3287 (m), 3163 (s), 3030 (m), 2997 (vs), 2976 (vs), 2934 (s), 2874 (vs), 1727 (vs), 1663 (m), 1656 (m), 1623 (m), 1452 (m), 1289 (w), 1261 (m), 1152 (m), 1085 (w), 1035 (w), 1012 (m), 973 (m), 910 (w), 856 (w),797 (w), 769 (m), 761 (m), 729(w), 699 (w), 613 (w), 529 (m).

$3[(n\text{-}C_4H_9)_4N^+C_3H_2N_3O_3^-]\cdot 5(NH_2)_2CS\cdot 3H_2O$ (**5**). IR/cm^{-1} (KBr): 3351 (s), 3143 (m), 2959 (s), 2870 (s), 1719 (vs), 1648 (m), 1452 (m), 1289 (w), 1151 (w), 1011 (w), 878 (w), 789 (w), 754 (m), 749 (w), 697 (w), 620 (w), 529 (s).

$(C_2H_5)_4N^+C_3H_2N_3O_3^-\cdot (NH_2)_2CO$ (**6**). IR/cm^{-1} (KBr): 3397 (m), 3161 (w), 3032 (s), 2981 (s), 2882 (vs), 2841 (s), 1732 (vs), 1649 (m), 1632 (m), 1451 (vs), 1429(w), 1228(w), 1192 (s), 1152 (w), 1032 (w), 966 (s), 858 (w), 789 (m), 762 (m), 692 (w), 620 (w), 559 (s), 530 (s).

(n-$C_3H_7)_4N^+C_3H_2N_3O_3^-$ · $2(NH_2)_2CO$ · H_2O (**7**). IR/cm^{-1} (KBr): 3432, 3371 (m), 3180 (w), 2983 (s), 1690, 1651 (m), 1629 (m), 1492 (s), 1439 (w), 1389 (s), 1179 (w), 1057 (w), 998 (w), 789 (w), 708 (w), 616 (w), 521 (s).

2. Powder XRD patterns.

To confirm the phase purity of the seven inclusion complexes, the PXRD patterns were recorded for complexes (**1**)~(**7**). All the peaks displayed in the measured patterns are similar to those in the simulated ones calculated from the single-crystal diffraction data, indicating a pure phase of each bulky sample.

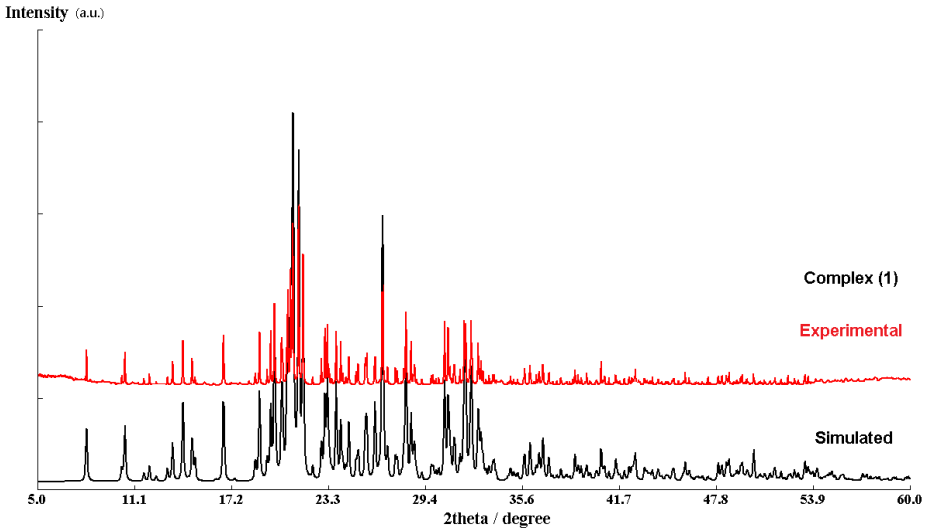


Figure S1. Experimental and simulated powder X-ray diffraction (PXRD) patterns of **1**.

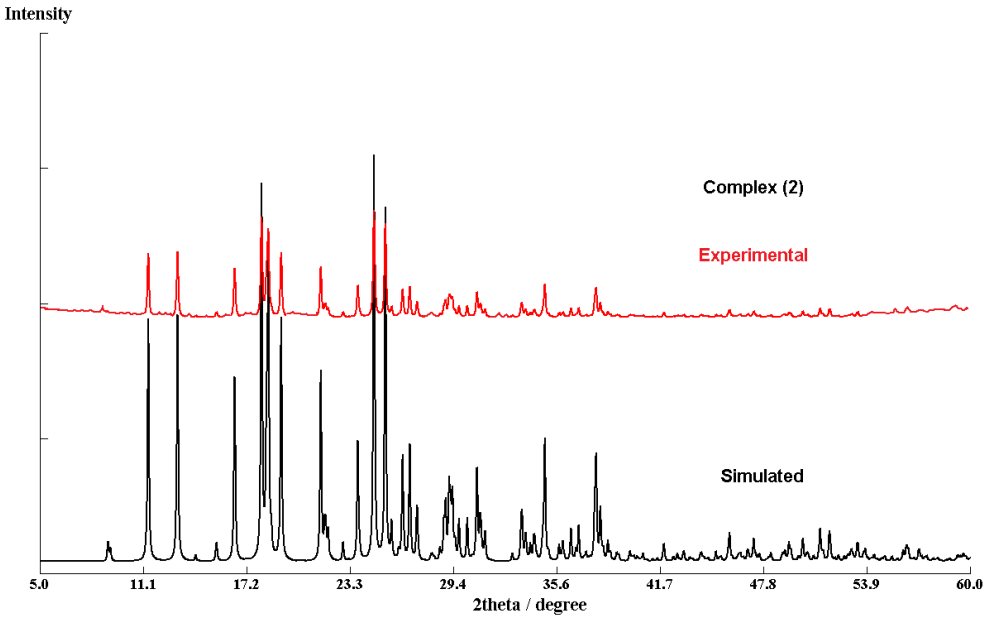


Figure S2. Experimental and simulated powder X-ray diffraction (PXRD) patterns of **2**.

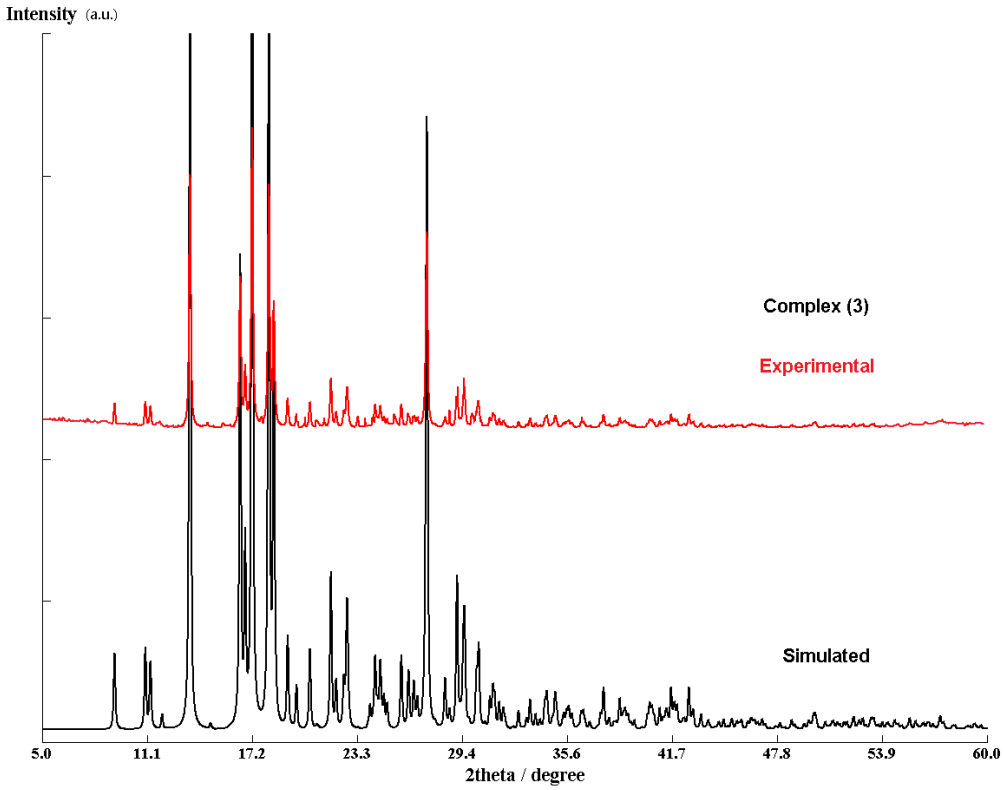


Figure S3. Experimental and simulated powder X-ray diffraction (PXRD) patterns of **3**.

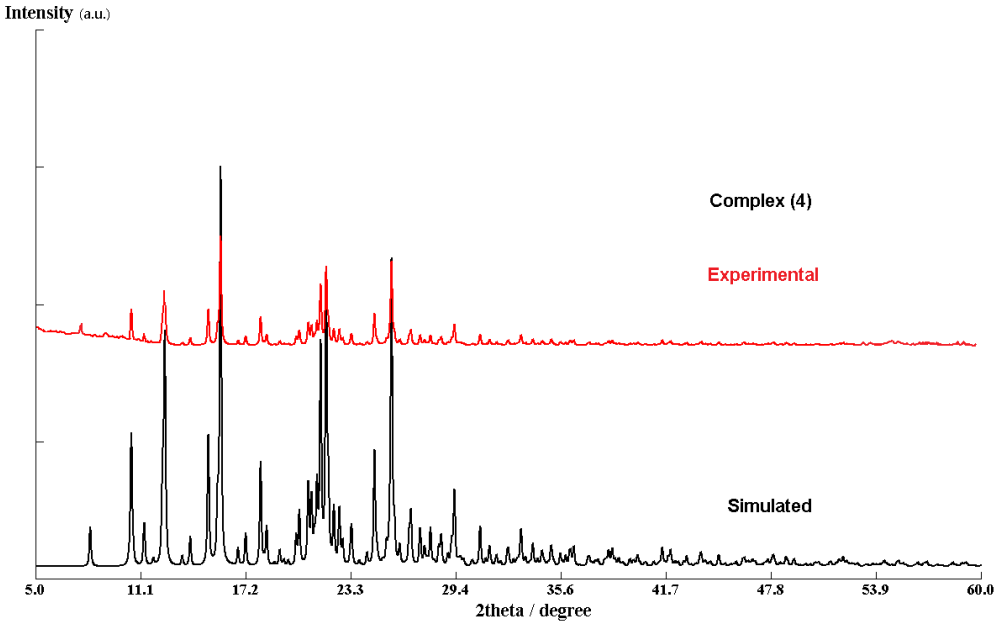


Figure S4. Experimental and simulated powder X-ray diffraction (PXRD) patterns of **4**.

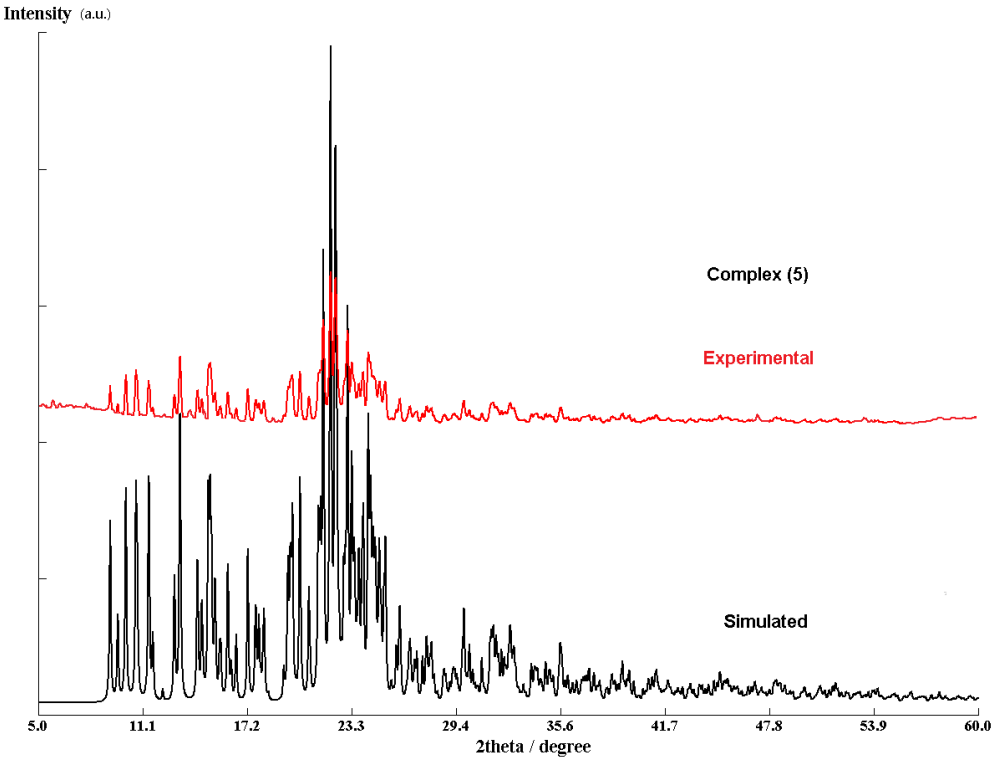


Figure S5. Experimental and simulated powder X-ray diffraction (PXRD) patterns of **5**.

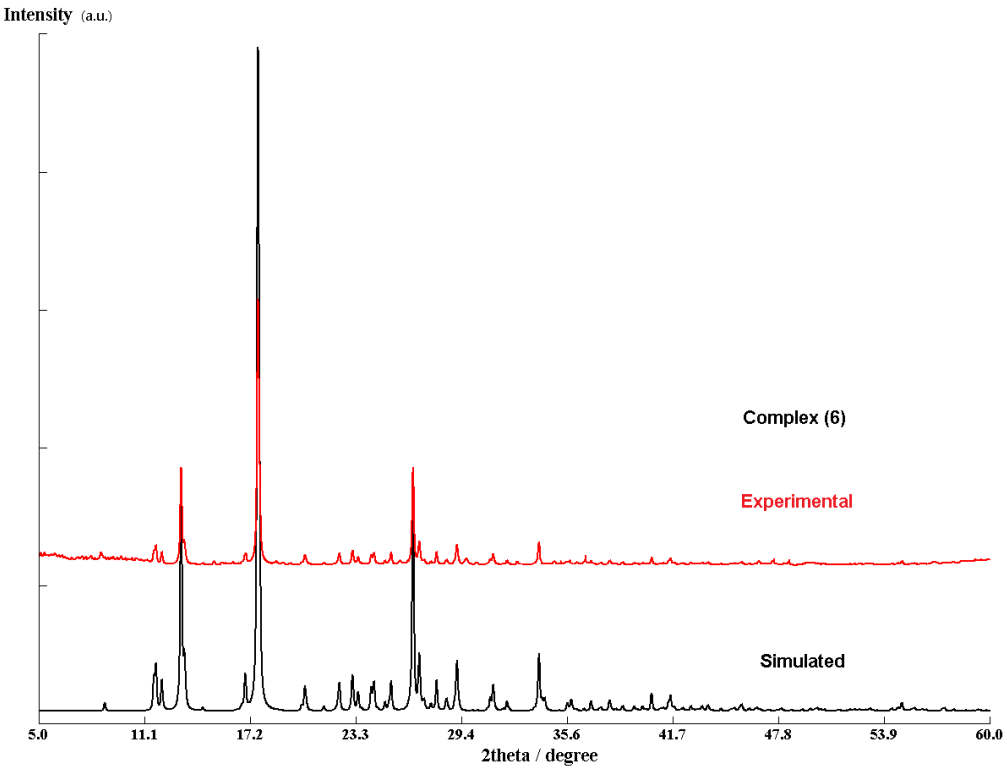


Figure S6. Experimental and simulated powder X-ray diffraction (PXRD) patterns of **6**.

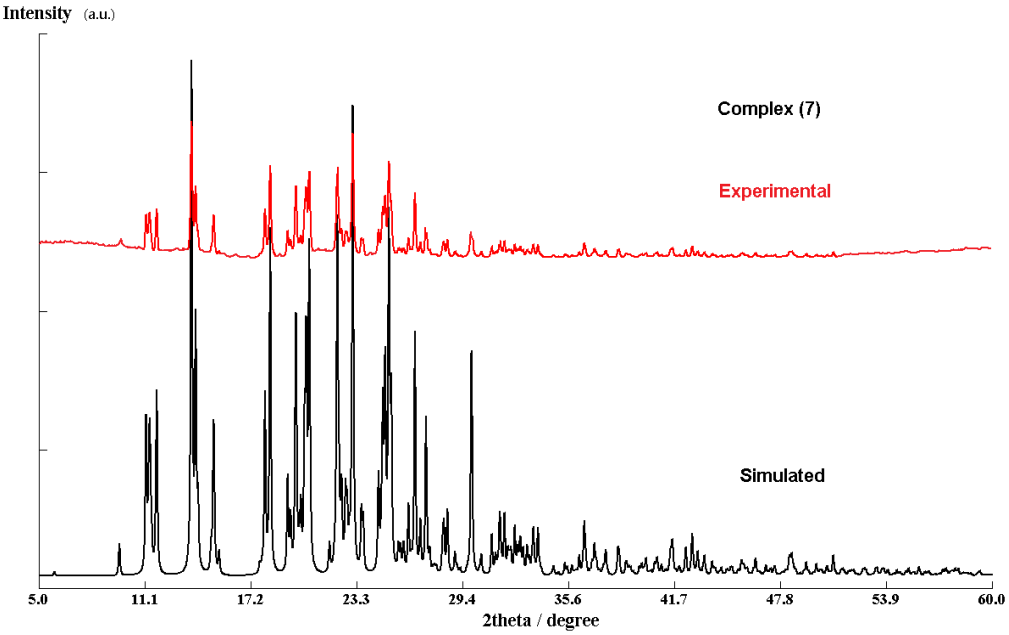


Figure S7. Experimental and simulated powder X-ray diffraction (PXRD) patterns of **7**.

3. Tables for the geometry of the hydrogen bonds in complexes (1) ~(7)

Table S1 Geometry of the Hydrogen Bonds in (**1**)

D−H···A	d(D−H)/Å	d(H···A)/Å	d(D···A)/ Å	<(D−H···A)/deg
N(1)−H(1A)···S(1)	0.86	2.41	3.266(2)	171.0
N(2)−H(2A)···O(3)#1	0.86	1.94	2.797(2)	171.7
N(4)−H(4A)···O(3)#2	0.86	2.00	2.853(2)	172.9
N(4)−H(4B)···O(1)	0.86	2.18	3.032(2)	169.2
N(5)−H(5A)···N(3)#2	0.86	2.21	3.063(2)	175.6
N(6)−H(6A)···O(3)#2	0.86	2.60	3.161(3)	124.1
N(5)−H(5B)···S(1)#3	0.86	2.72	3.455(2)	143.8
N(6)−H(6A)···O(2)#4	0.86	2.43	3.100(3)	135.0
N(6)−H(6B)···O(1W)#4	0.86	2.19	2.984(3)	153.8
N(7)−H(7A)···O(1)	0.86	2.33	3.110(3)	150.4
N(7)−H(7B)···S(3)	0.86	2.54	3.390(2)	169.1
N(8)−H(8B)···S(2)	0.86	2.67	3.502(2)	162.5
N(8)−H(8A)···O(1)#5	0.86	2.39	3.146(2)	147.0
N(9)−H(9A)···N(3)#5	0.86	2.20	3.056(3)	173.8
N(9)−H(9B)···O(1W)	0.86	2.13	2.958(3)	161.7
O(1W)−H(1WA)···S(2)#6	0.81(4)	2.51(4)	3.312(3)	171(3)
O(1W)−H(1WB)···S(3)	0.85(4)	2.82(4)	3.428(3)	130(3)

* Symmetry transformations used to generate equivalent atoms:

#1 −*x*+1, −*y*, −*z*+1 #2 −*x*+1/2, *y*+1/2, −*z*+1/2 #3 −*x*+1, −*y*+1, −*z*+1

#4 *x*−1/2, −*y*+1/2, *z*−1/2 #5 *x*+1, *y*, *z* #6 −*x*+3/2, *y*−1/2, −*z*+1/2

Table S2 Geometry of the Hydrogen Bonds in (**2**)

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)−H(1A)···O(1)#1	0.86	1.94	2.790(2)	171.5
N(2)−H(2A)···O(2)#2	0.86	1.98	2.823(2)	166.2
N(4)−H(4A)···O(1)	0.86	2.27	3.115(2)	166.2
N(4)−H(4B)···O(3)#3	0.86	2.14	2.956(2)	158.3
N(5)−H(5A)···N(3)	0.86	2.28	3.011(2)	143.6
N(5)−H(5B)···N(3)#4	0.86	2.24	3.041(2)	154.8
C(7)−H(7B)···O(3)#5	0.96	2.65	3.479(2)	144.8
C(8)−H(8A)···S(1)#6	0.96	2.92	3.856(2)	163.8
C(8)−H(8B)···O(2)#3	0.96	2.44	3.336(2)	155.2
C(8)−H(8C)···O(3)#5	0.96	2.39	3.284(2)	155.1

* Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y+1/2,-z #2 -x+1,y,-z+1/2 #3 -x+1/2,y+1/2,-z+1/2

#4 -x+1/2,y-1/2,-z+1/2 #5 -x+1/2,-y+1/2,-z+1 #6 -x,y,-z+1/2

Table S3 Geometry of Hydrogen Bonds in (**3**)

D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)−H(1A)···O(1)#1	0.86	1.98	2.830(2)	169.8
N(2)−H(2A)···S(1)#2	0.86	2.39	3.243(2)	172.2
N(4)−H(4A)···O(3)	0.86	1.93	2.788(2)	172.4
N(4)−H(4B)···S(1)#3	0.86	2.56	3.407(2)	168.2
N(5)−H(5C)···N(3)	0.86	2.21	3.069(2)	174.3
N(5)−H(5D)···O(2)#4	0.86	2.13	2.966(2)	164.6
C(5)−H(5A)···O(1)#5	0.97	2.58	3.533(4)	168.2
C(5)−H(5B)···O(2)#6	0.97	2.55	3.476(4)	160.1
C(7)−H(7B)···O(3)#4	0.97	2.56	3.497(4)	163.2
C(9)−H(9B)···O(2)#7	0.97	2.61	3.397(3)	138.3
C(11)−H(11A)···S(1)	0.97	2.96	3.829(3)	149.5
C(11)−H(11B)···O(3)#3	0.97	2.59	3.530(3)	162.3

* Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+2 #2 x,y+1,z #3 -x+1,-y+1,-z+1 #4 x,y-1,z
#5 x-1/2,-y+1/2,z-1/2 #6 x-1/2,-y+3/2,z-1/2 #7 -x+1/2,y-3/2,-z+3/2

Table S4 Geometry of the Hydrogen Bonds in (**4**)

D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)−H(1A)···O(1)#1	0.86	1.98	2.830(2)	171.1
N(2)−H(2A)···S(1)#2	0.86	2.49	3.340(2)	173.1
N(4)−H(4A)···O(1)	0.86	2.06	2.913(2)	172.0
N(4)−H(4B)···O(1W)#3	0.86	2.13	2.957(3)	160.8
N(5)−H(5C)···N(3)	0.86	2.09	2.950(2)	174.9
N(5)−H(5D)···O(2)#4	0.86	2.16	3.020(2)	174.3
O(1W)−H(11)···O(3)	0.98	1.94	2.834(3)	150.3
O(1W)−H(12)···O(2)#4	0.98	2.12	2.886(2)	133.7
C(5)−H(5B)···O(3)#3	0.97	2.39	3.347(3)	170.6
C(9)−H(9A)···S(1)#5	0.97	2.68	3.581(3)	155.3

* Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x+1/2,y+1/2,-z+1/2 #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+1

Table S5 Geometry of the Hydrogen Bonds in (**5**)

D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)−H(1A)··S(2)#1	0.86	2.49	3.346(3)	171.2
N(2)−H(2A)···S(5)#2	0.86	2.55	3.400(3)	171.1
N(4)−H(4A)···S(1)	0.86	2.60	3.427(4)	160.8

N(5)−H(5A)...S(3)	0.86	2.48	3.328(3)	169.5
N(7)−H(7A)···S(4)	0.86	2.48	3.333(3)	169.1
N(8)−H(8A)···O(2W)	0.86	1.96	2.821(4)	179.5
N(10)−H(10A)···N(3)	0.86	2.25	3.077(5)	162.4
N(10)−H(10B)···O(2)#3	0.86	2.23	3.094(5)	177.5
N(11)−H(11A)···O(1)	0.86	2.05	2.879(4)	161.3
N(11)−H(11B)···S(1)	0.86	2.63	3.483(4)	170.9
N(12)−H(12A)···O(4)#3	0.86	2.07	2.915(5)	166.5
N(12)−H(12B)···S(2)	0.86	2.63	3.486(4)	172.0
N(13)−H(13A)···N(6)#3	0.86	2.29	3.147(4)	174.2
N(13)−H(13B)···O(5)	0.86	2.21	3.061(4)	168.8
N(14)−H(14A)···O(9)#1	0.86	2.14	2.895(4)	147.0
N(14)−H(14B)···O(6)	0.86	2.09	2.934(4)	165.2
N(15)−H(15C)···O(9)#1	0.86	2.08	2.855(4)	150.1
N(15)−H(15D)···O(8)	0.86	2.24	2.995(4)	146.5
N(16)−H(16C)···N(9)#1	0.86	2.27	3.084(4)	157.6
N(16)−H(16D)···O(8)	0.86	2.20	3.055(4)	174.4
N(17)−H(17C)···O(7)#1	0.86	2.07	2.852(4)	151.4
N(17)−H(17C)···N(9)#1	0.86	2.66	3.388(4)	142.8
N(17)−H(17D)···S(5)#1	0.86	2.62	3.390(3)	148.8
N(18)−H(18D)···O(3W)	0.86	2.37	3.130(5)	147.8
N(18)−H(18E)···O(2)#4	0.86	2.09	2.931(5)	164.7
N(19)−H(19C)···O(3W)	0.86	2.29	3.071(5)	150.6
N(19)−H(19D)···O(7)	0.86	2.13	2.964(5)	162.5
O(1W)−H(11)···O(6)#3	0.98	1.95	2.806(4)	144.4
O(1W)−H(12)···O(5)	0.98	2.08	3.029(4)	161.8
O(2W)−H(21)···S(3)	0.98	2.25	3.228(3)	174.2
O(2W)−H(22)···O(1W)	0.98	1.87	2.792(4)	154.9
O(3W)−H(31)···O(3)#5	0.98	1.98	2.740(4)	132.4
O(3W)−H(32)···S(4)	0.98	2.53	3.353(3)	141.4
C(23)−H(23B)···O(2W)	0.97	2.61	3.486(6)	150.6
C(28)−H(28B)···S(3)	0.97	3.02	3.881(5)	148.7
C(35)−H(35A)···O(3)#5	0.97	2.63	3.536(6)	156.5
C(35)−H(35B)···S(4)	0.97	2.97	3.850(5)	151.4
C(39)−H(39A)···S(5)#6	0.97	3.02	3.814(5)	139.8
C(39)−H(39B)···O(3W)#7	0.97	2.45	3.362(6)	156.1
C(43)−H(43A)···S(4)	0.97	3.00	3.894(5)	153.5
C(43)−H(43B)···S(5)#1	0.97	3.01	3.830(5)	142.4
C(59)−H(59A)···O(4)#5	0.97	2.57	3.503(5)	161.1

* Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 x,y+1,z-1 #3 x,y-1,z #4 x,y-1,z+1

#5 x,y,z+1 #6 x+1,y+1,z #7 x+1,y,z

Table S6 Geometry of the Hydrogen Bonds in (**6**)

D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)−H(1A)···O(4)#1	0.86	2.06	2.920(2)	174.8
N(2)−H(2A)···O(3)#2	0.86	1.94	2.802(2)	174.2
N(4)−H(4A)···O(4)#3	0.86	2.10	2.944(2)	168.9
N(4)−H(4B)···O(1)	0.86	2.12	2.973(2)	173.9
N(5)−H(5C)···O(2)#4	0.86	2.01	2.866(2)	175.4
N(5)−H(5D)···N(3)	0.86	2.09	2.951(3)	174.0
C(5)−H(5A)···O(1)	0.97	2.55	3.445(4)	152.8
C(7)−H(7A)···O(3)#5	0.97	2.42	3.369(4)	167.5
C(7)−H(7B)···O(2)#6	0.97	2.58	3.477(4)	154.5
C(9)−H(9B)···O(1)#7	0.97	2.35	3.288(4)	161.5
C(11)−H(11B)···O(2)#8	0.97	2.43	3.304(4)	149.5

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

Table S7 Geometry of the Hydrogen Bonds in (**7**)

D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(2)−H(2A)···O(5)	0.86	1.87	2.722(3)	173.0
N(1)−H(1A)···O(1W)	0.86	1.93	2.769(2)	166.2
N(4)−H(4A)···O(2)#1	0.86	2.30	3.134(3)	164.7
N(4)−H(4B)···N(3)	0.86	2.24	3.092(3)	172.9
N(5)−H(5A)···O(1)#2	0.86	2.15	2.943(3)	153.0
N(5)−H(5B)···O(1)	0.86	2.04	2.872(3)	163.0
N(6)−H(6C)···O(3)	0.86	2.27	3.113(3)	166.4
N(6)−H(6D)···O(3)#3	0.86	2.28	3.093(3)	157.6
N(7)−H(7C)···O(5)#4	0.86	2.29	3.101(4)	157.9
C(6)−H(6B)···O(1W)#1	0.97	2.50	3.470(3)	174.1
C(13)−H(13A)···O(1W)#1	0.97	2.59	3.361(4)	136.4
C(15)−H(15B)···O(1)#5	0.97	2.53	3.470(3)	164.6
O(1W)−H(1WB)···O(4)#2	0.98	1.82	2.764(2)	161.1
O(1W)−H(1WA)···O(4)#6	0.98	1.77	2.732(2)	165.2

* Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+1/2,z+1/2 #2 -x+1,-y,-z+1 #3 -x+1/2,y+1/2,-z+3/2
#4 -x,-y+1,-z+1 #5 x,y+1,z #6 x-1/2,-y+1/2,z-1/2

4. Supplementary figures for inclusion complex (7)

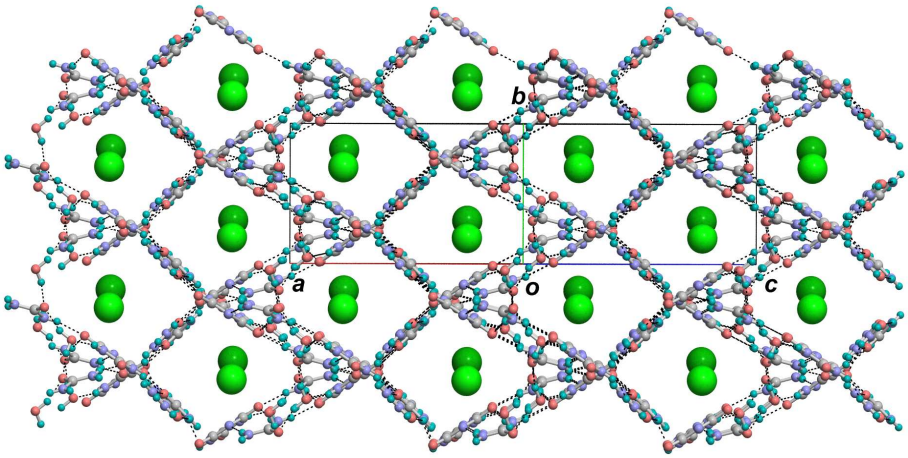


Figure S8. Perspective view of a portion of the crystal structure of $(n\text{-}C_3H_7)_4N^+C_3H_2N_3O_3^- \cdot 2(NH_2)_2CO \cdot H_2O$ (**7**) showing a channel system running along the [101] direction. Well-ordered $(n\text{-}C_3H_7)_4N^+$ cations are accommodated within each channel with cross-sectional size of about 11.2 Å x 8.9 Å.

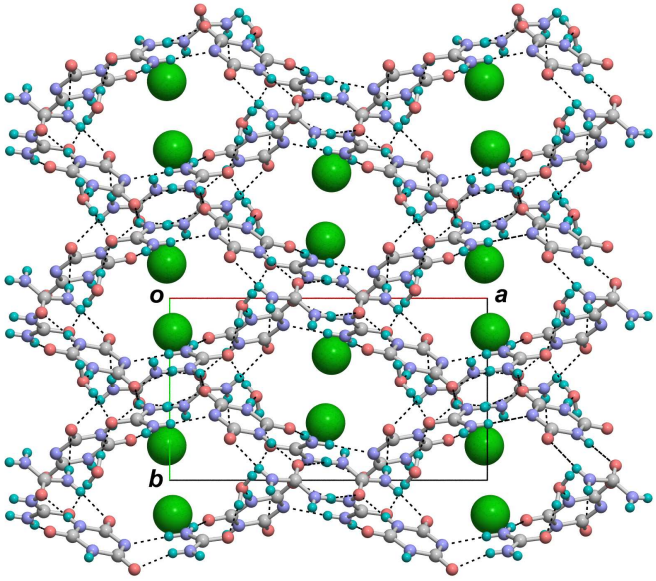


Figure S9. Perspective view of the crystal structure of $(n\text{-}C_3H_9)_4N^+C_3H_2N_3O_3^- \cdot 2(NH_2)_2CO \cdot H_2O$ (**7**) showing its channel system with cross-sectional size of about 9.4 Å x 8.9 Å. Well-ordered $(n\text{-}C_3H_7)_4N^+$ cations represented by green spheres are arranged in a zigzag fashion in each channel.

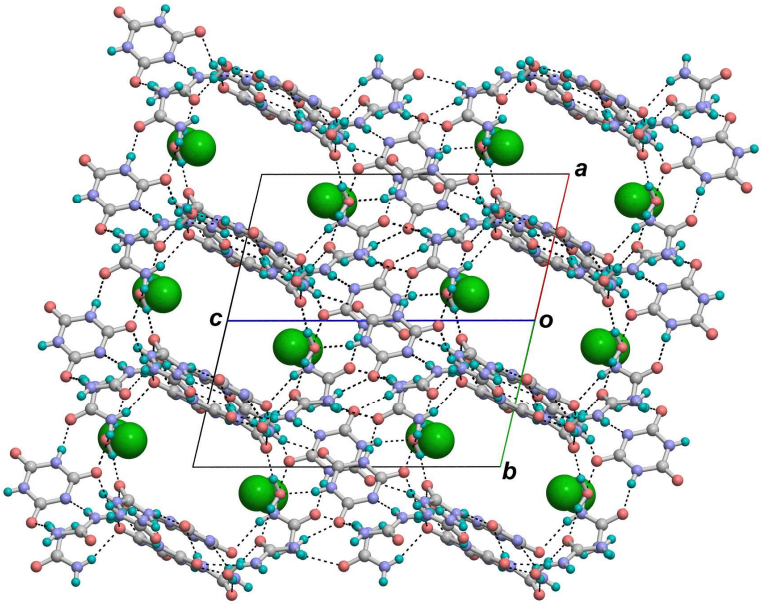


Figure S10. Perspective view of a portion of the crystal structure of (n-$C_3H_9)_4N^+C_3H_2N_3O_3^-$ · $2(NH_2)_2CO$ · H_2O (**7**) showing a channel system running along the [110] direction. Two columns of well-ordered (n-$C_3H_7)_4N^+$ cations are accommodated in each channel with size of about 7.1 Å x 9.3 Å.

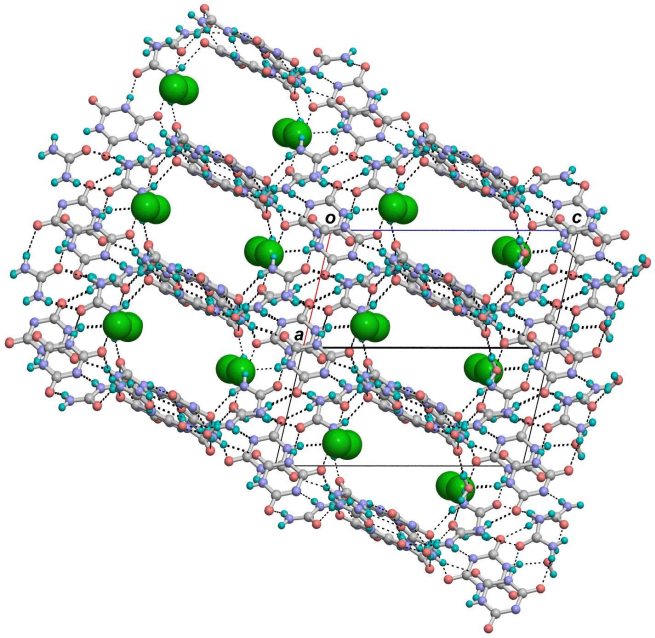
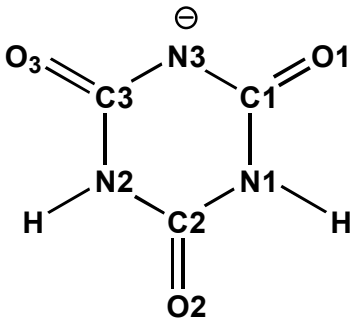
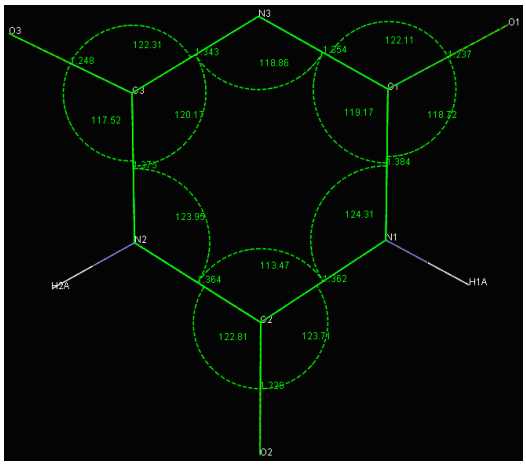


Figure S11. Perspective view of a portion of the crystal structure of (n-$C_3H_7)_4N^+C_3H_2N_3O_3^-$ · $2(NH_2)_2CO$ · H_2O (**7**) showing a channel system running along the [1 −1 0] direction. Two columns of well-ordered (n-$C_3H_7)_4N^+$ cations are accommodated within each channel with size of about 10.1 Å x 8.9 Å.

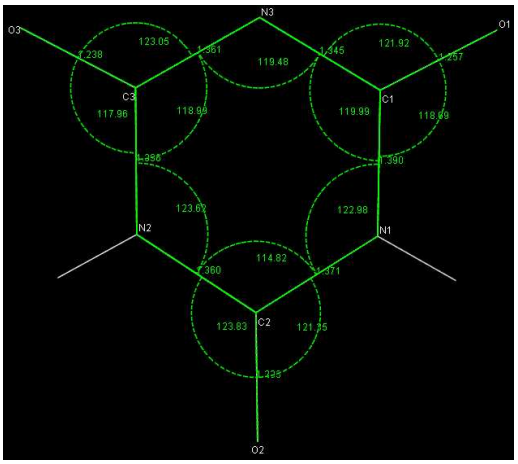
5. Comparison of the bond lengths and bond angles of isocyanurate ions in the seven new inclusion complexes:

Table S8. Selected Geometric Parameters of the Isocyanurate ion in **1-7**

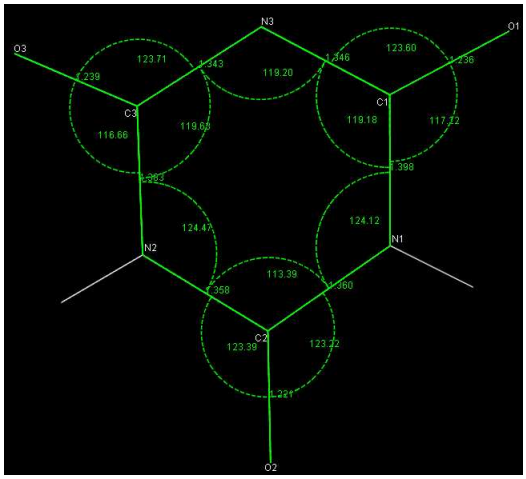




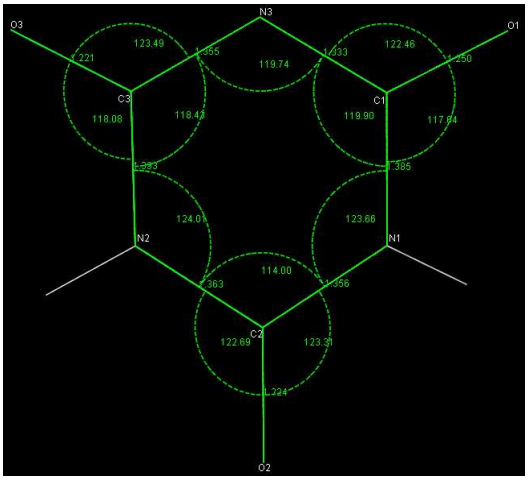
Complex (1)



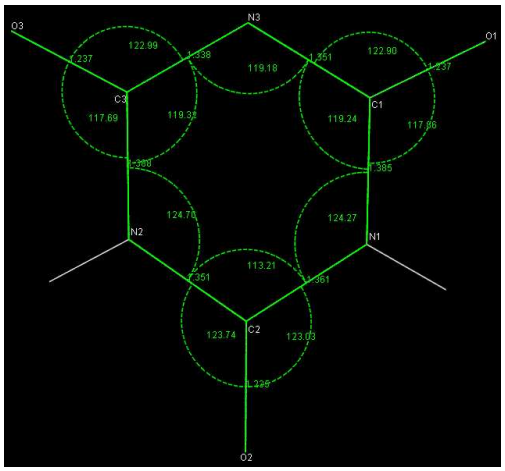
Complex (2)



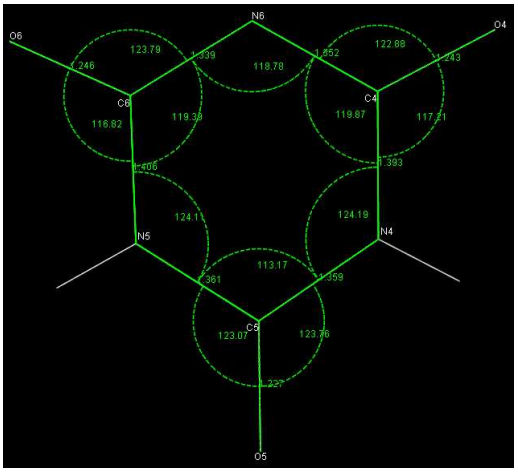
Complex (3)



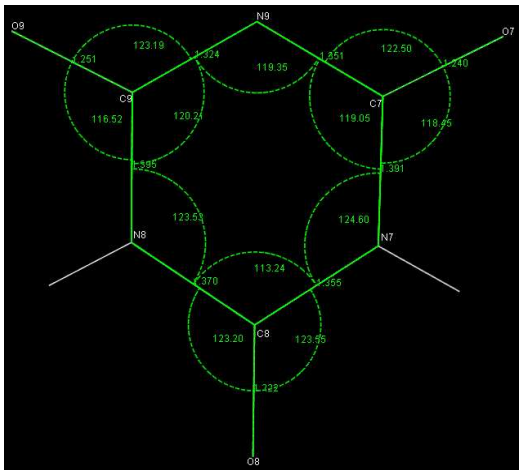
Complex (4)



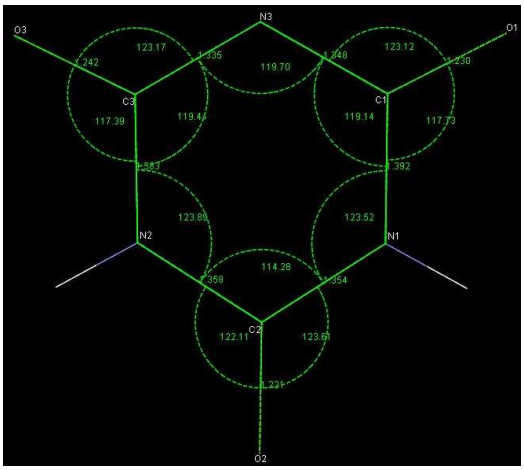
Complex (5) a



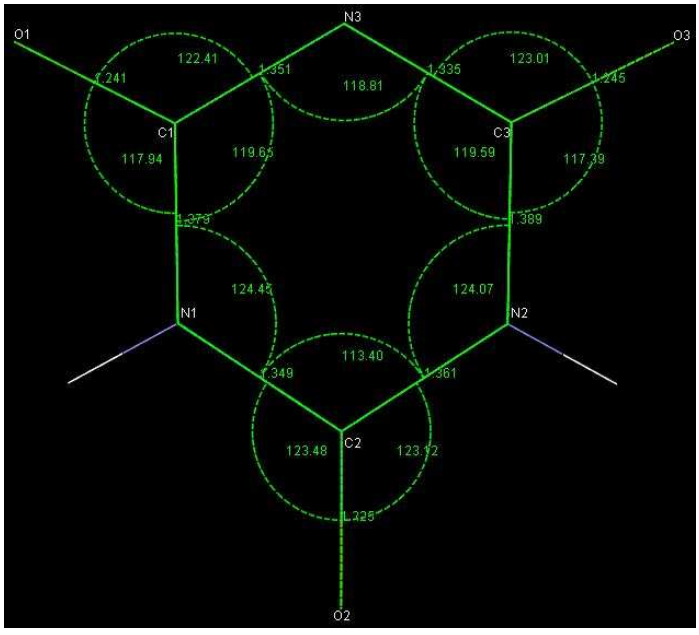
Complex (5) b



Complex (5) c



Complex (6)



Complex (7)

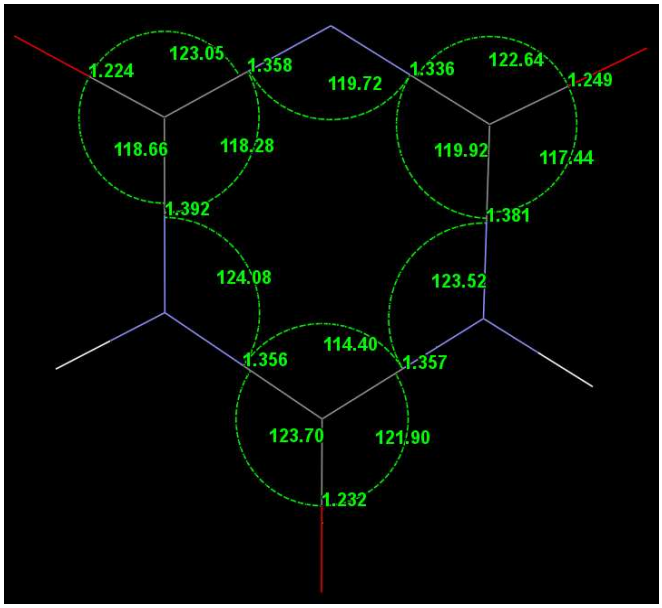
Complex	C1−O1/Å	C2−O2/Å	C3−O3/Å	C1−N1/Å	N1−C2/Å	C2−N2/Å
1	1.237(2)	1.220(2)	1.248(2)	1.384(2)	1.362	1.364
2	1.257	1.233	1.238	1.345	1.390	1.371
3	1.236	1.221	1.239	1.346	1.360	1.358
4	1.250	1.224	1.221	1.385	1.356	1.363
5	1.237	1.235	1.237	1.385	1.361	1.351
	1.243	1.227	1.246	1.393	1.359	1.361
	1.240	1.222	1.251	1.391	1.355	1.370
6	1.230	1.221	1.242	1.348	1.354	1.359
7	1.241	1.225	1.245	1.379	1.349	1.361
Complex	**N2−C3/Å**	**C3−N3/Å**	**N3−C1/Å**	**N1−C1−N3/ °**	**C1−N1−C2/ °**	**N1−C2−N2/ °**
1	1.357	1.343	1.354	119.17	124.31	113.47
2	1.360	1.361	1.345	119.99	122.98	114.82
3	1.383	1.343	1.346	119.18	124.12	113.39
4	1.393	1.355	1.333	119.90	123.66	114.00
5	1.388	1.338	1.351	119.24	124.27	113.21
	1.406	1.339	1.352	119.87	124.19	113.17
	1.395	1.324	1.351	119.05	124.60	113.24
6	1.383	1.335	1.348	119.14	123.52	114.28
7	1.389	1.335	1.351	119.65	124.45	113.40
Complex	**C2−N2−C3/ °**	**N2−C3−N3/ °**	**C3−N3−C1/ °**	**N3−C1−O1/ °**	**N1−C1−O1/ °**	**N1−C2−O2/ °**
1	123.95	120.17	118.86	122.11	118.72	123.71
2	123.62	118.99	119.48	121.92	118.09	121.35
3	124.47	119.63	119.20	123.60	117.22	123.22
4	124.0	118.43	119.74	122.46	117.64	123.31
5	124.70	119.32	119.18	122.90	117.86	123.03
	124.11	119.39	118.78	122.88	117.21	123.76
	123.53	120.21	119.35	122.50	118.45	123.55
6	123.89	119.44	119.70	123.12	117.73	123.61
7	124.07	119.59	118.81	122.41	117.94	123.48
Complex	**N2−C2−O2/ °**	**N2−C3−O3/ °**	**N3−C3−O3/ °**			
1	122.81	117.52	122.31			
2	123.83	117.96	123.05			
3	123.39	116.66	123.71			
4	122.69	118.08	123.49			
5	123.74	117.69	122.99			
	123.07	116.82	123.79			
	123.20	116.52	123.19			
6	122.11	117.39	123.17			
7	123.12	117.39	123.01			

6. The geometries of isocyanurate ions (without disorder or coordinating with metal ion) retrieved from CSD Version 5.36 (May 2015 update).

Refcode:

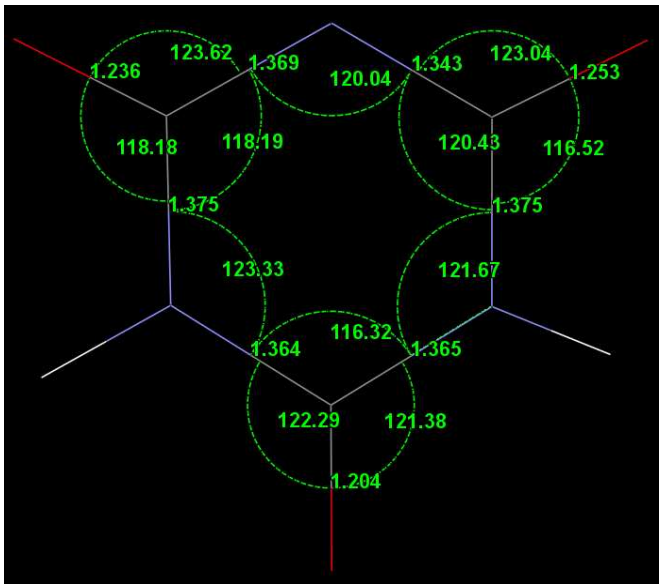
CIHHUX
Bis(Ethylenedioxy)tetrathiafulvalenium radical hemikis(isocyanurate)
Barszcz, B; Lapinski, A.; Graja, A.; Flakina, A. M.; Chekhlov, A. N.; Lyubovskaya, R.N. *Chem. Phys.* **2006**, *330*, 486−494.
Comment: The isocyanurate ion is disordered and no atomic coordinates are provided.

DIRNUP
N-Benzyl-2-hydroxyethanaminium isocyanurate
Comment: There is only one independent isocyanurate ion in the asymmetric unit.



Contreras-Espejel, C.A.; Garcia-Eleno, M. A.; Santacruz-Juarez, E.; Reyes-Martinez, R.; Morales-Morales, D. *Acta Crystallogr., Sect.E: Struct. Rep. Online*, **2013**, *69*, o1741−o1742.

DUCJOA
Penta-aqua-(isocyanurato-*N*)-cobalt(II) isocyanurate dihydrate
Comment: One of the two isocyanurate ion is coordinated to Co^{2+} ion. Another isocyanurate ion is hydrogen-bonded to the isocyanurato ligand.

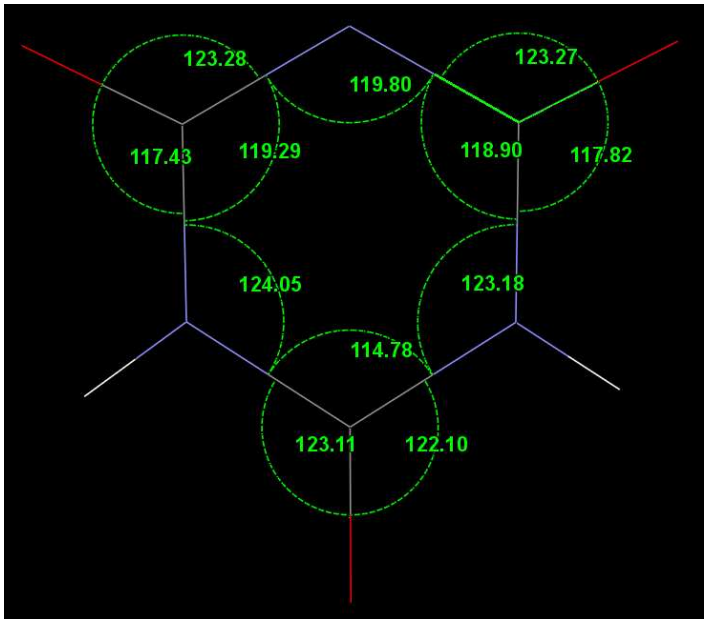


Agre, V. M.; Sisoeva, T. F.; Trunov, V. K.; Gurevich, M. Z.; Branzburg, M. Z. *Koord. Khim. (Russ.) (Coord. Chem.)* **1986**, *12*, 122−127.

DUCJOA01

Penta-aqua-(isocyanurato-*N*)-cobalt(II) isocyanurate dihydrate

Comment: One of the two isocyanurate ion is coordinated to Co^{2+} ion. Another isocyanurate ion is hydrogen-bonded to the isocyanurato ligand.



Falvello, L.R.; Pascual, I.; Tomas, M. *Inorg. Chim. Acta* **1995**, *229*, 135−142.

KAYSOT

Tetraphenylphosphonium isocyanurate

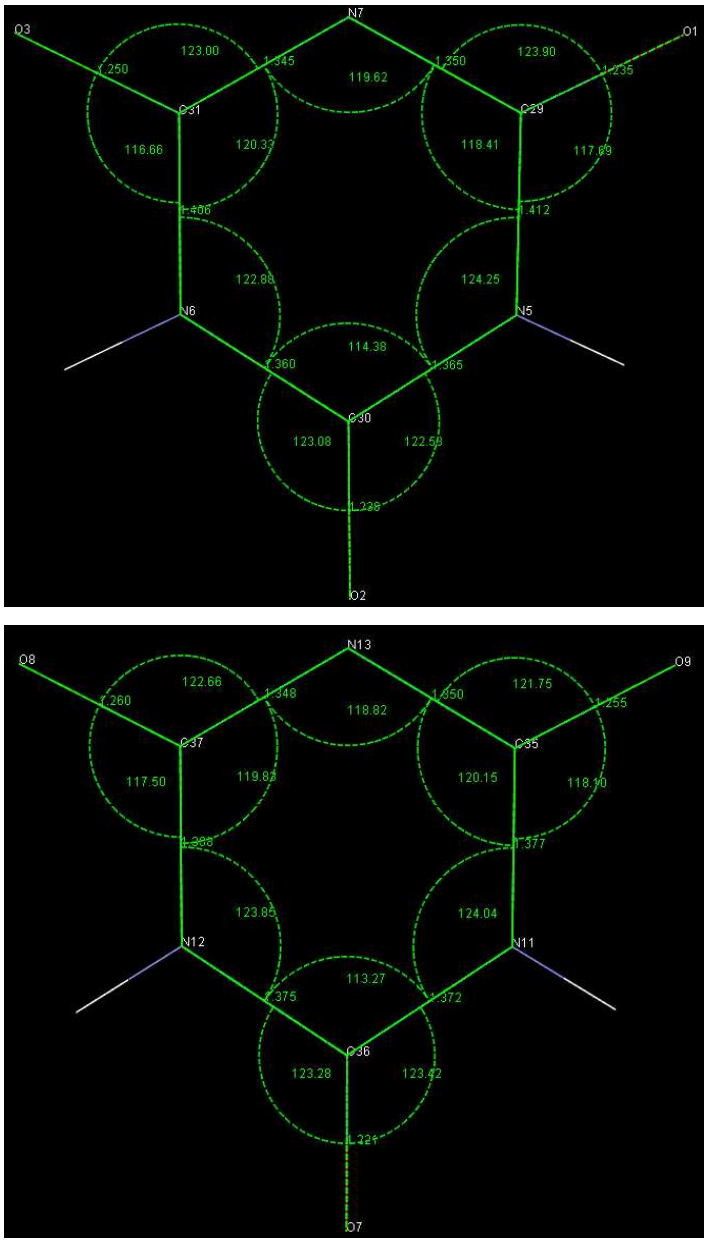
Comment: The isocyanurate ion is disordered.

Flakina, A.M.; Chekhlov, A.N.; Kushch, P.P.; Lyubovskaya, R.N. *Zh. Obshch. Khim. (Russ.) (Russ. J. Gen. Chem.)*, **2005**, *75*, 381−385.

KEDYUO

8-Dimethylaminonaphthalene-1-dimethylammonium isocyanurate isocyanuric acid dihydrate

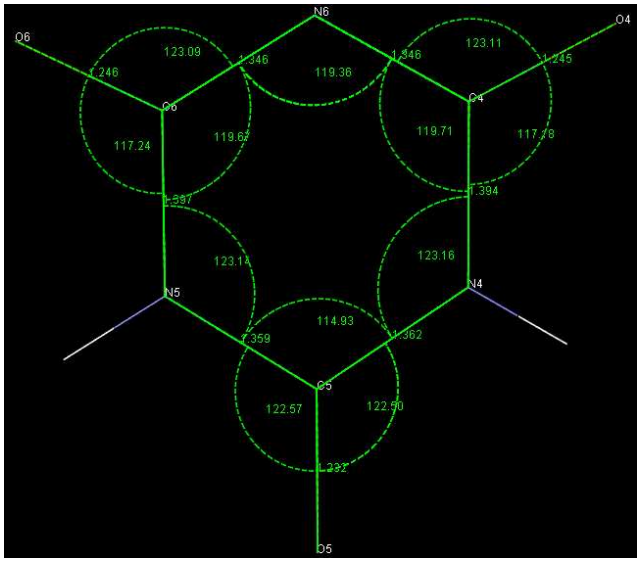
Comment: There are two independent isocyanurate ions in the asymmetric unit.

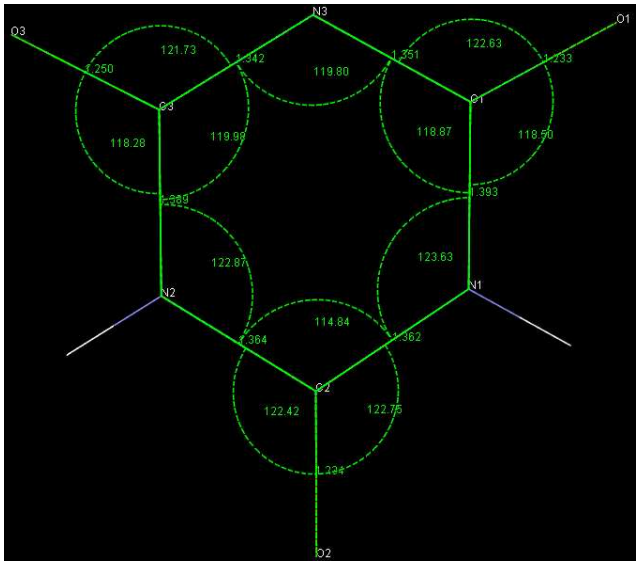


Nichol, G. S.; Clegg, W. *Cryst. Growth Des.*, **2006**, *6*, 451−460.

LAFLOV
Tetraphenylphosphonium isocyanurate pentahydrate
Comment: The isocyanurate ion is disordered.
Chekhlov, A.N.; *Zh. Neorg. Khim. (Russ.) (Russ. J. Inorg. Chem.)*, **2009**, *54*, 2068−2072.

MOHCUI
Guanidinium isocyanurate hemihydrate
Comment: There are two independent isocyanurate ions in the asymmetric unit.



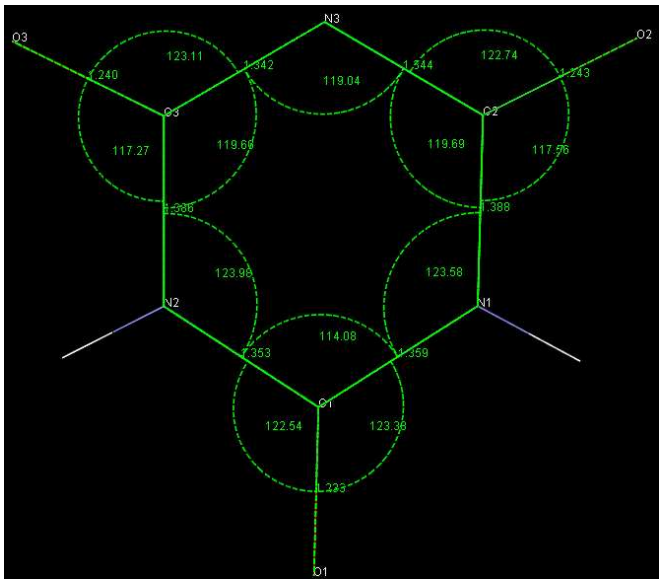


El-Gamel, N.E.A.; Wagler, J.; Kroke, E. *J. Mol. Struct.*, **2008**, *888*, 204−213

MOPYEV

Guanidinium isocyanurate

Comment: There is only one independent isocyanurate ion in the asymmetric unit.

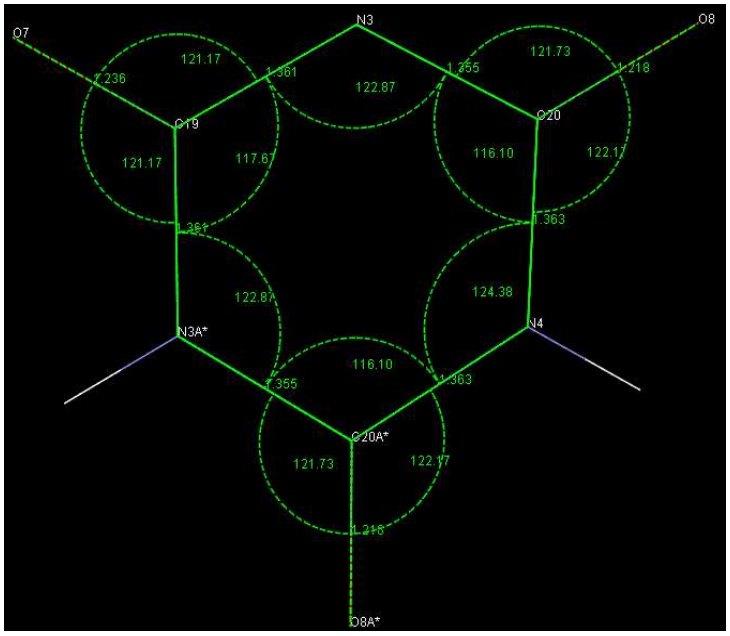


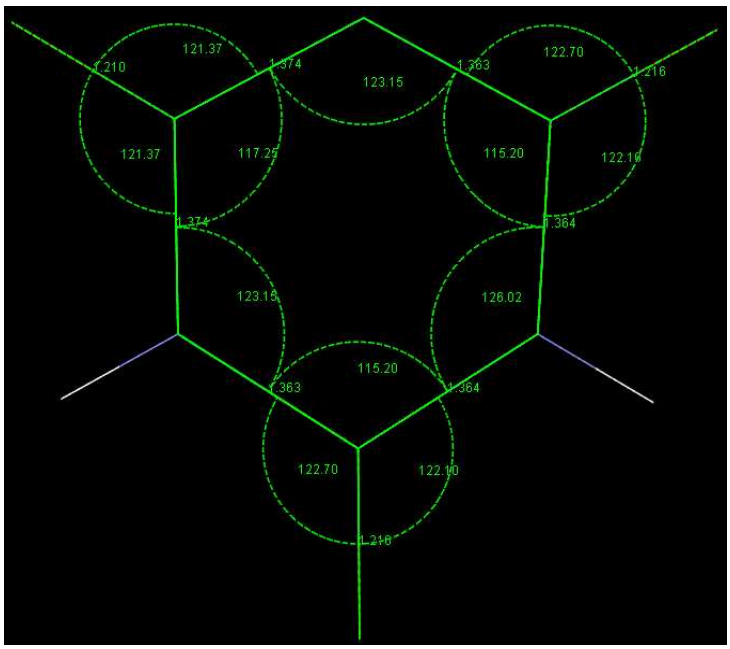
Sivashankar, K. *Proc. Indian Acad. Sci., Chem. Sci.*, **2000**, *112*, 607−614.

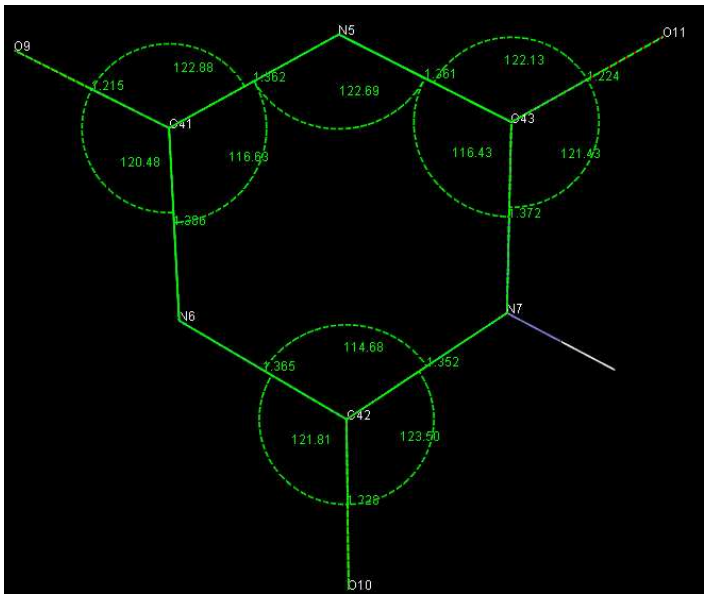
QELXEL

4,7,13,16,21,24-Hexaoxa-1-aza-10-azoniabicyclo(8.8.8.)hexacosane isocyanurate

Comment: The H(N) atoms of both independent molecules are disordered with occupancies 0.7:0.3 and 0.5:0.5.





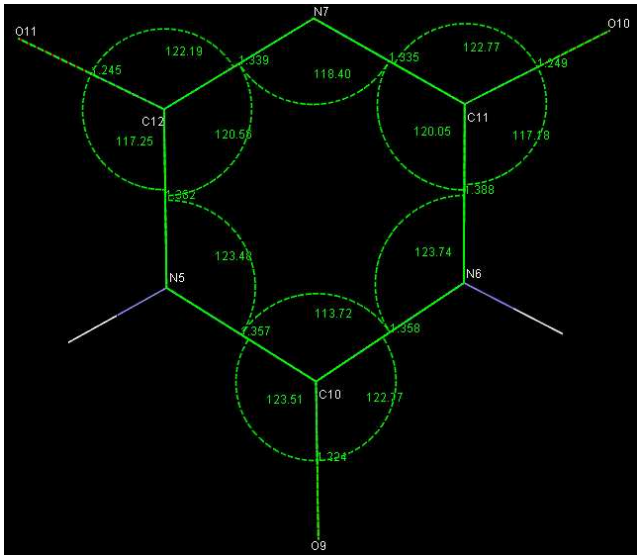


Chekhlov, A. N. *Zh. Strukt. Khim. (Russ.)(J. Struct. Chem.)*, **2006**, *47*, 71−77.

WEGTAE

(1,10-diazonia-18-crown-6) isocyanurate isocyanuric acid tetrahydrate

Comment: The (1,10-diazonia-18-crown-6) cation resides on an inversion centre and there is only one independent isocyanurate ions in the asymmetric unit.

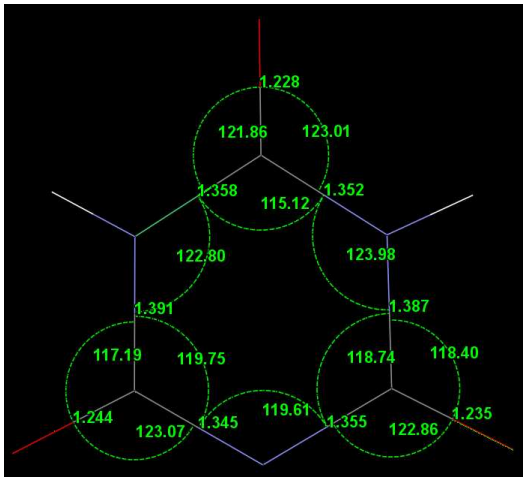


Chekhlov, A. N. *Zh. Obshch. Khim. (Russ.) (Russ. J. Gen. Chem.)*, **2005**, *75*, 1803−1807.

XILLEK

Pentaaqua(isocyanurato)iron(II) isocyanurate dehydrate

Comment: One of the two isocyanurate ion is coordinated to Fe^{2+} ion. Another isocyanurate ion is hydrogen-bonded to the isocyanurato ligand.



Liu, M. –S.; Zhou, Z. –Y.; Zhu, L. –C.; Zhou, X. –X.; Cai, Y. −P. *Acta Crystallogr., Sect. E: Struct. Rep. Online* **2007**, *63*, m2578.

XORMOH

Bis(bis(Ethylenedithio)tetrathiafulvalenium) isocyanurate

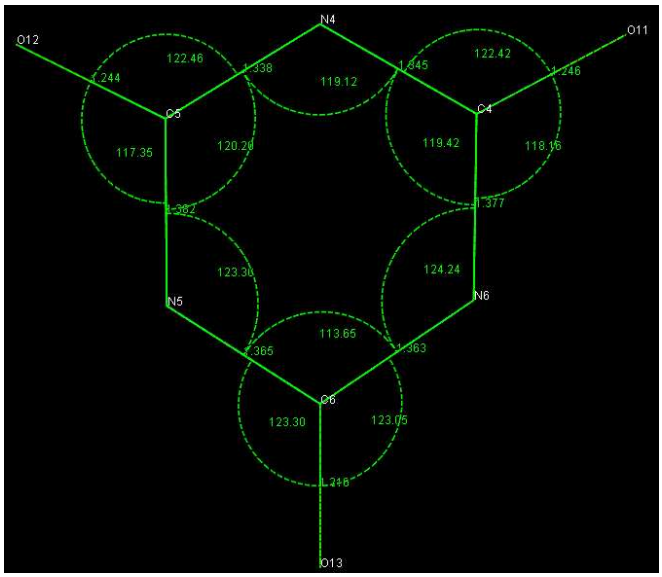
Comment: The isocyanurate ion is disordered.

Flakina, A. M.; Chekhlov, A. N.; Kaplunov, M. G.; Van, K. V.; Lyubovskaya, R.N. *Izv. Akad. Nauk SSSR, Ser. Khim.(Russ.) (Russ. Chem. Bull.)*, **2008**, *57*, 99−104.

YIWBOV

Hexa-aqua-(cyanuric acid-O)-calcium hydroxide isocyanurate

Comment: One of the two isocyanurate ion is coordinated to Ca^{2+} ion. Another isocyanurate ion is hydrogen-bonded to the isocyanurato ligand.

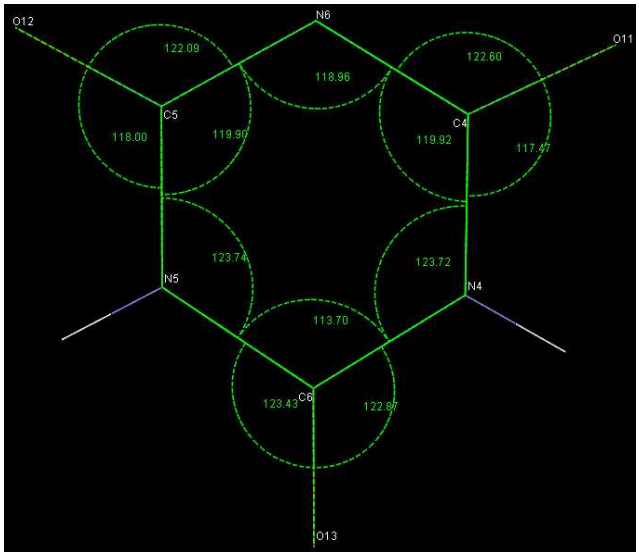


Lin, Z. -B.; Chen, C.-Z.; Gao, D. -S.; Huang, X. -Y., Li, D. *Jiegou Huaxue (Chin. J. Struct. Chem.)* **1995**, *14*, 61−64.

YIWBOV01

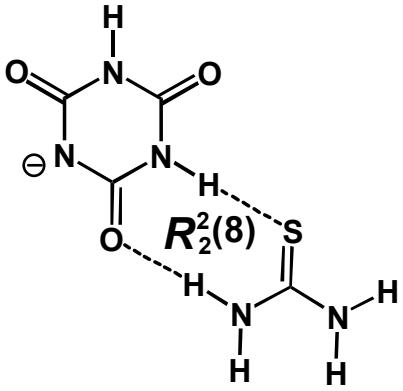
Hexa-aqua-(isocyanurato-*O*)-calcium isocyanurate monohydrate

Comment: Hydrogen atoms were located and a better refinement of **YIWBOV** has been done.

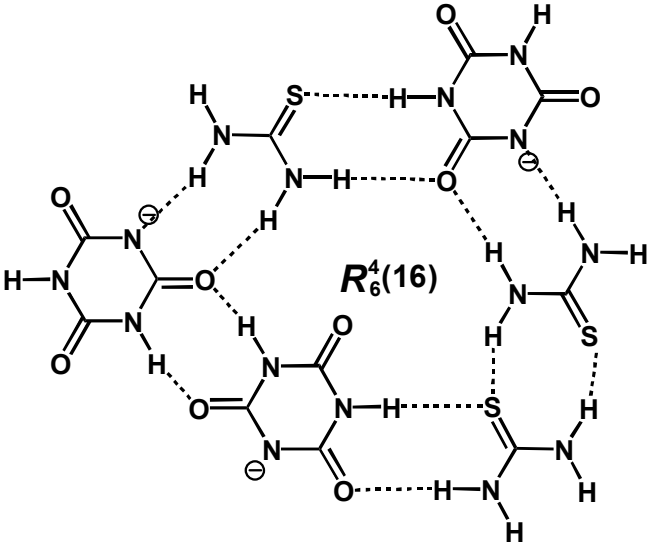


Chekhlov, A. N. *Zh. Neorg. Khim. (Russ.) (Russ. J. Inorg. Chem.)*, **2006**, *51*, 799−803.

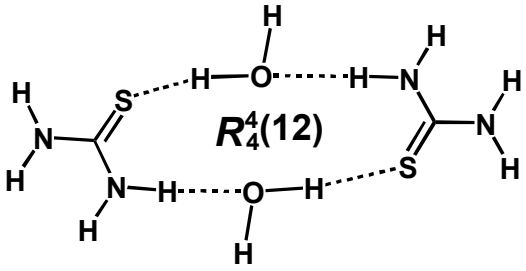
7. The representative linkage modes and hydrogen-bonding motifs in the seven new inclusion complexes.



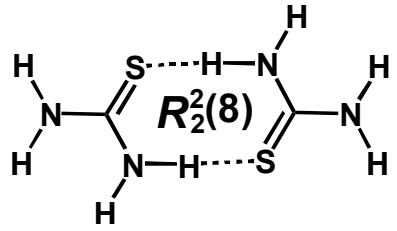
in complex (**1**)



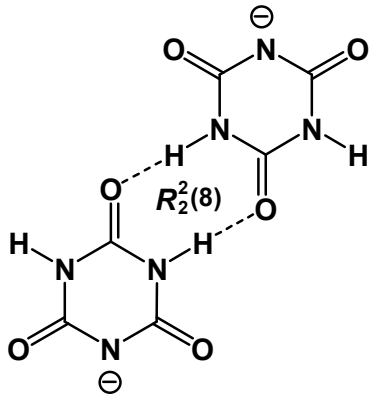
in complex (**1**)



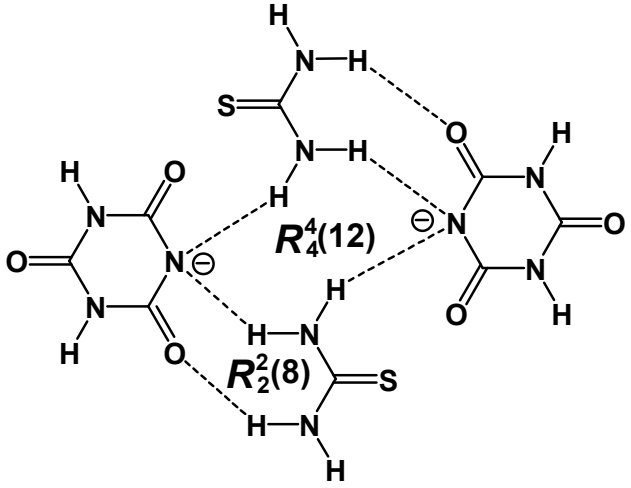
in complex (**1**)



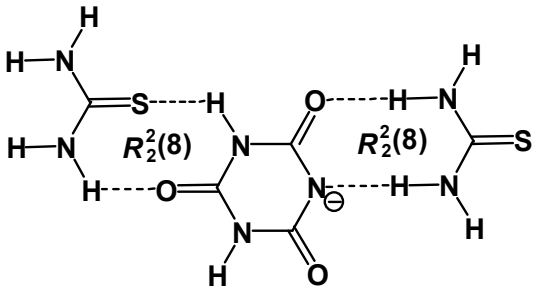
in complex (**1**)



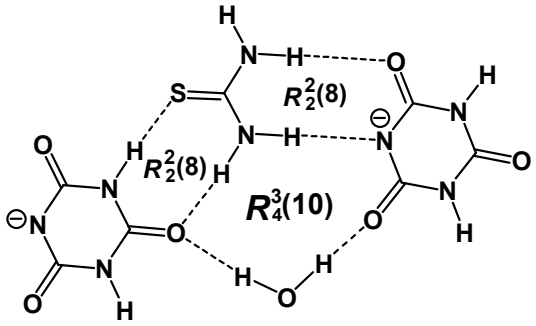
in complex (**2**)



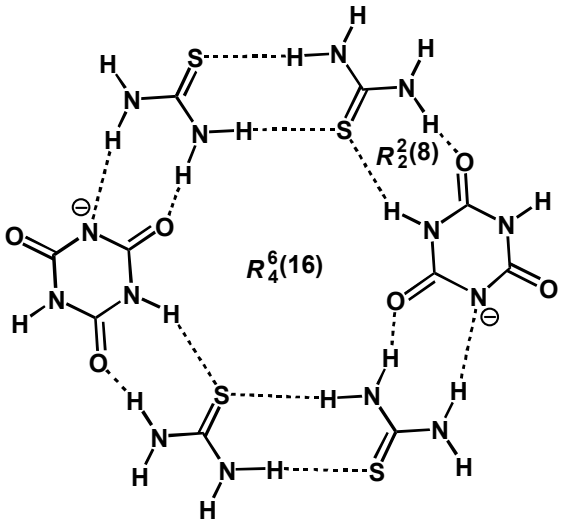
in complex (**2**)



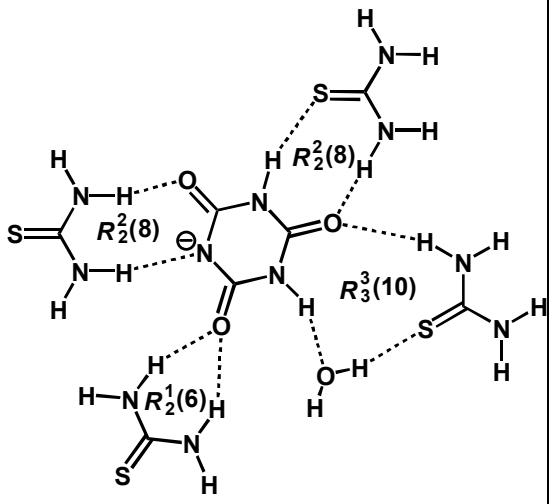
in complex (**3**)



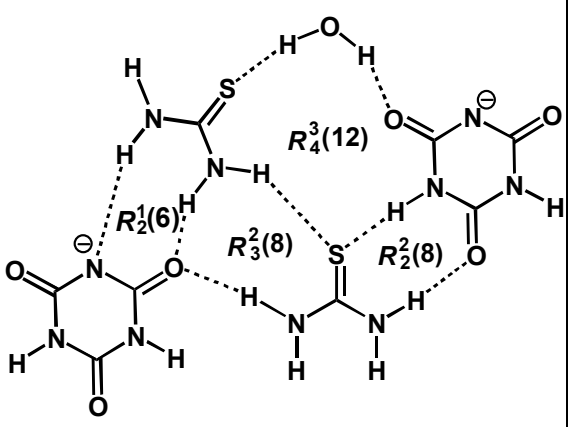
in complex (**4**)



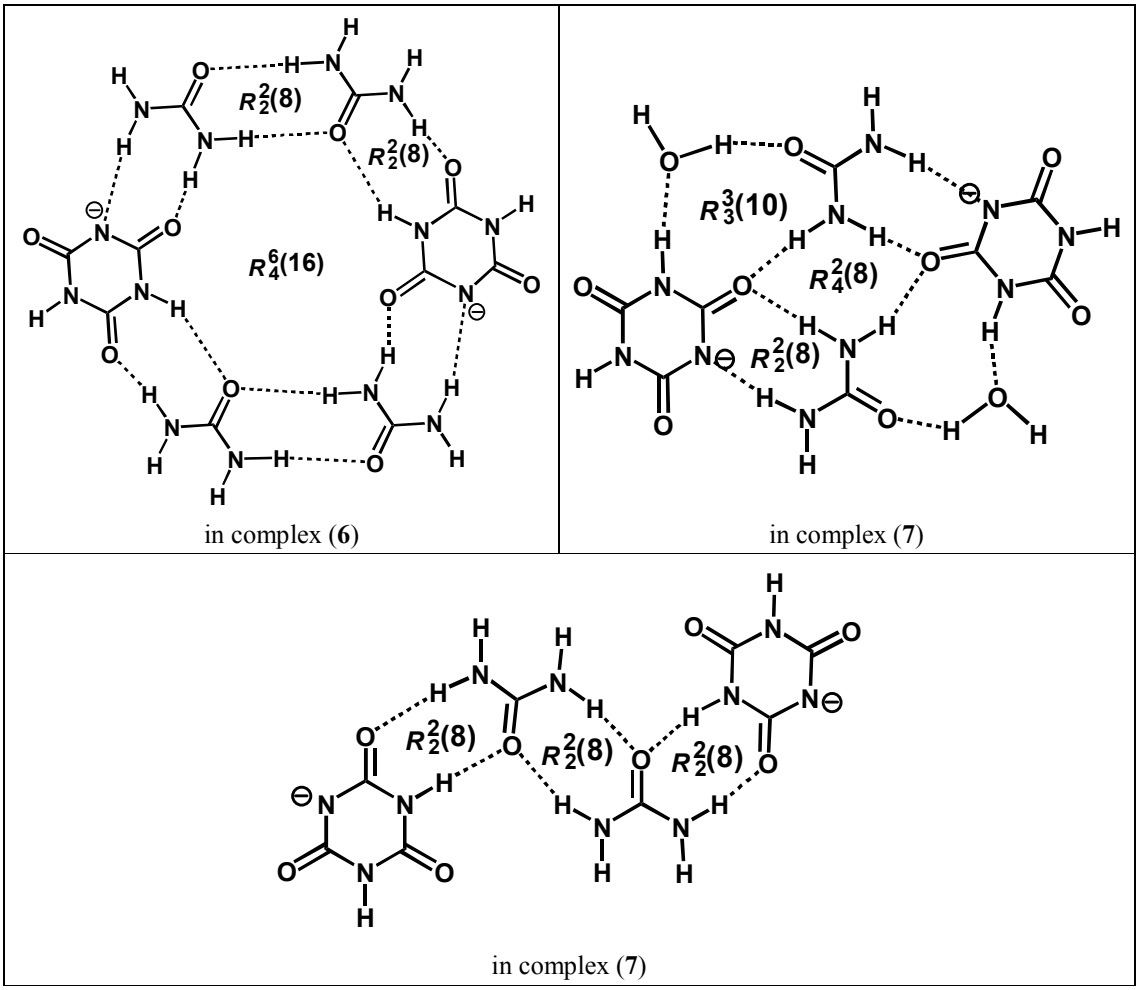
in complex (**5**)



in complex (**5**)



in complex (**5**)



8. Hydrogen-bonding interactions between isocyanurate ion and its neighboring chemical species in each inclusion complex.

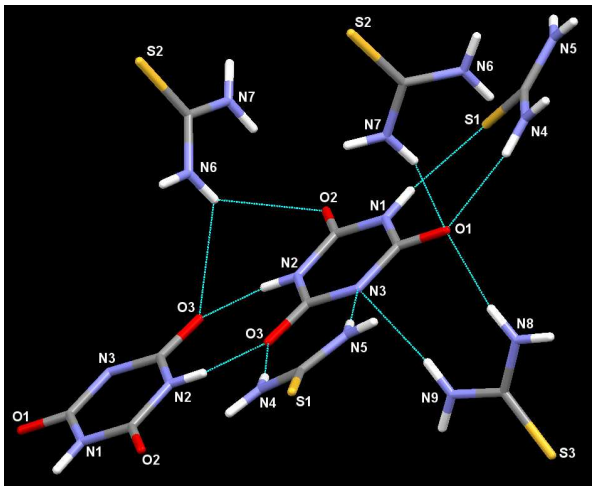


Figure S12. Isocyanurate ion in complex (**1**)

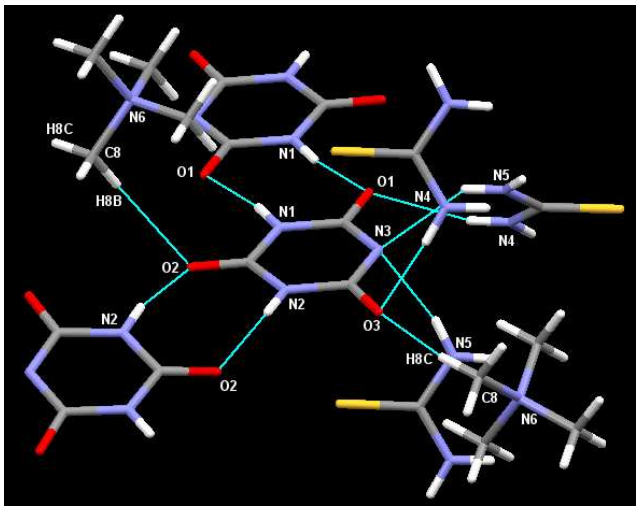


Figure S13. Isocyanurate ion in complex (**2**)

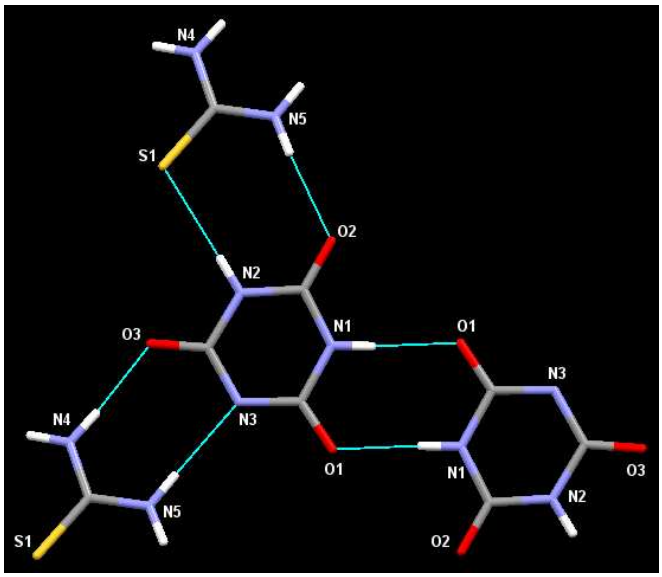


Figure S14. Isocyanurate ion in complex (**3**)

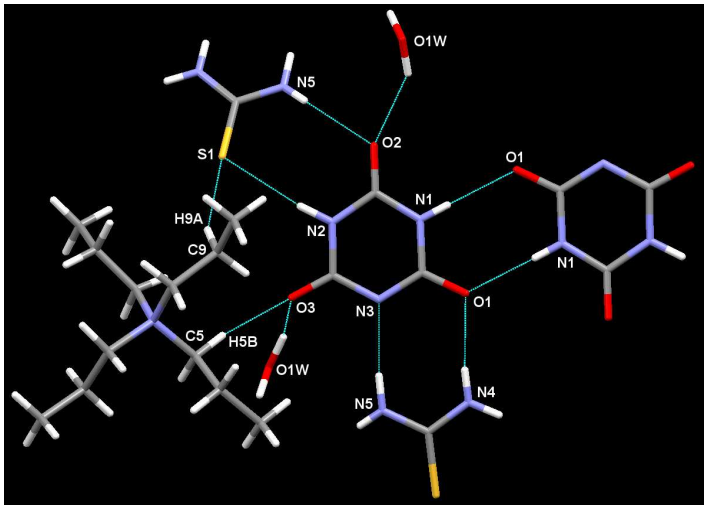


Figure S15. Isocyanurate ion in complex (**4**)

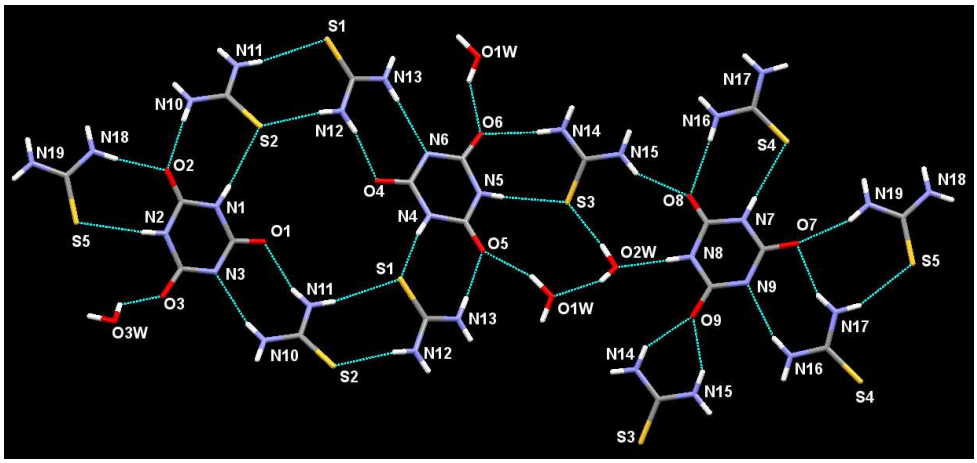


Figure S16. Isocyanurate ion in complex (**5**)

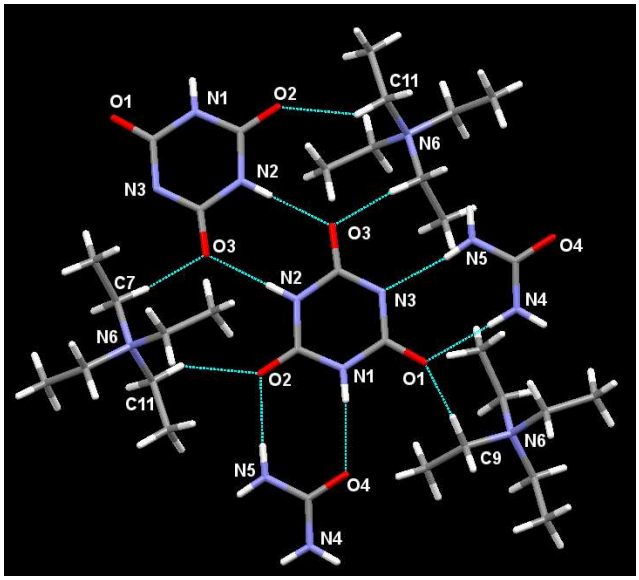


Figure S17. Isocyanurate ion in complex (**6**)

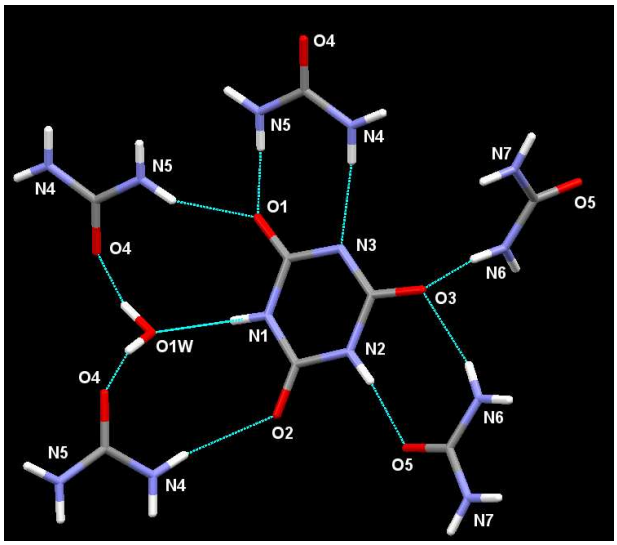
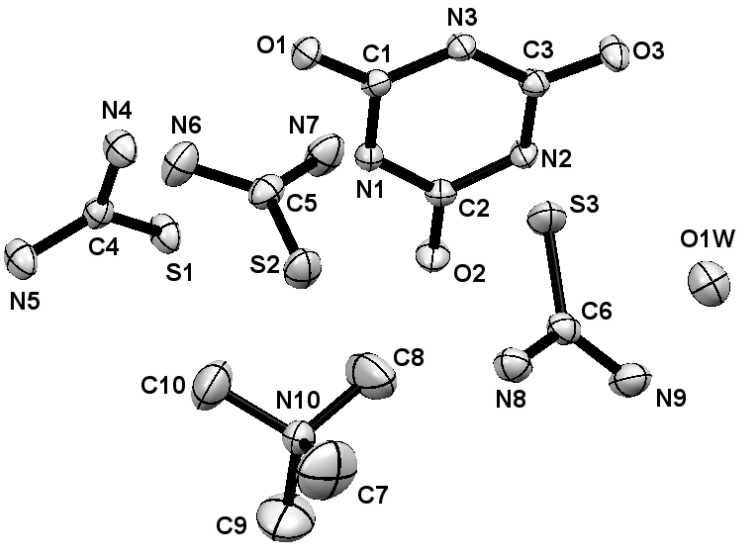
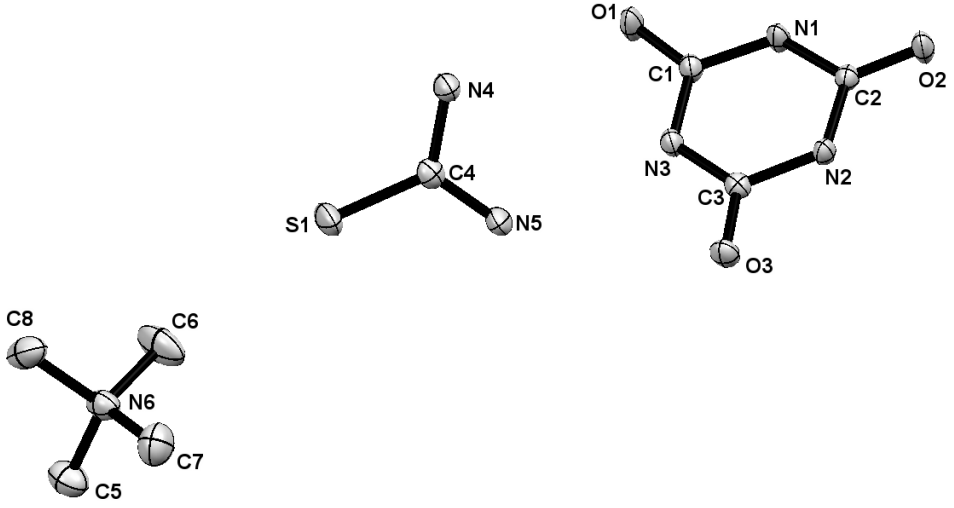


Figure S18. Isocyanurate ion in complex (**7**)

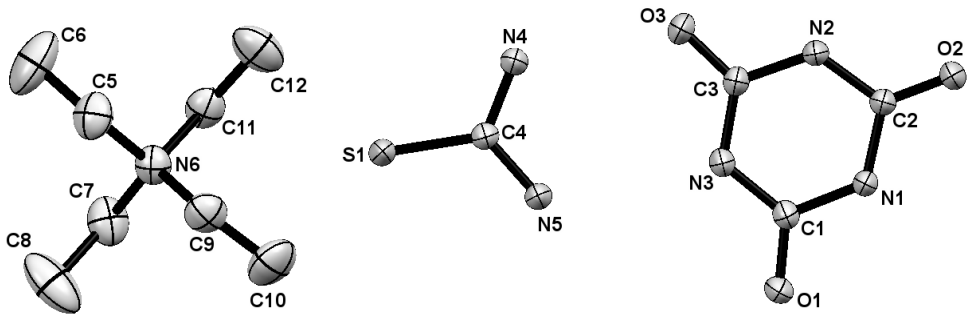
10. ORTEP drawings for complexes (1)~(7)



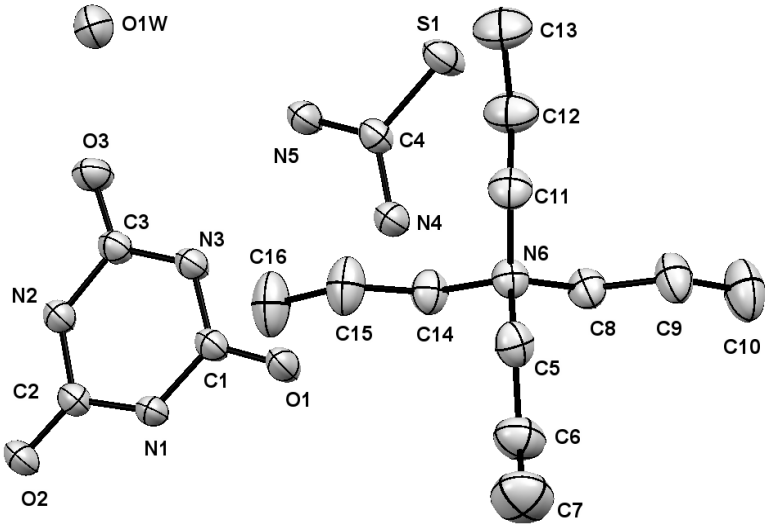
ORTEP drawings for $(CH_3)_4N^+C_3H_2N_3O_3^- \cdot 3(NH_2)_2CS \cdot H_2O$ (1). Thermal ellipsoids are drawn in 30% probability level. Hydrogen atoms are omitted for clarity.



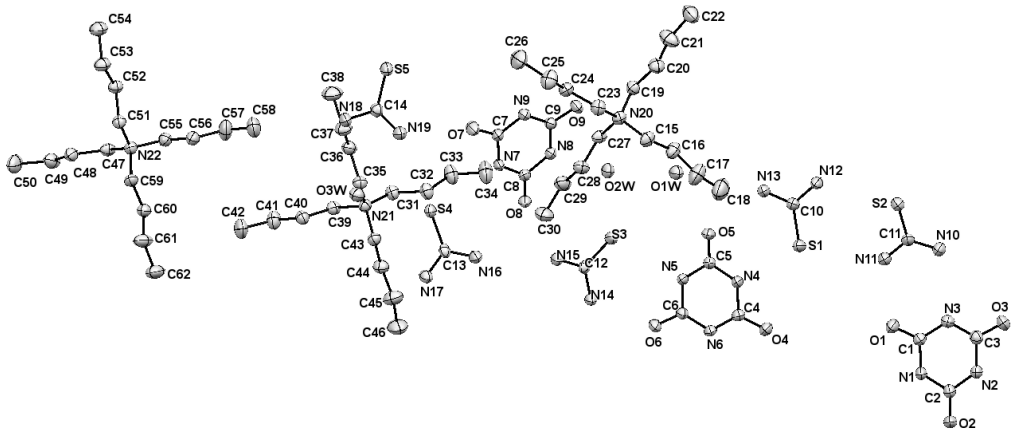
ORTEP drawings for $(CH_3)_4N^+C_3H_2N_3O_3^- \cdot (NH_2)_2CS$ (2). Thermal ellipsoids are drawn in 50% probability level. Hydrogen atoms are omitted for clarity.



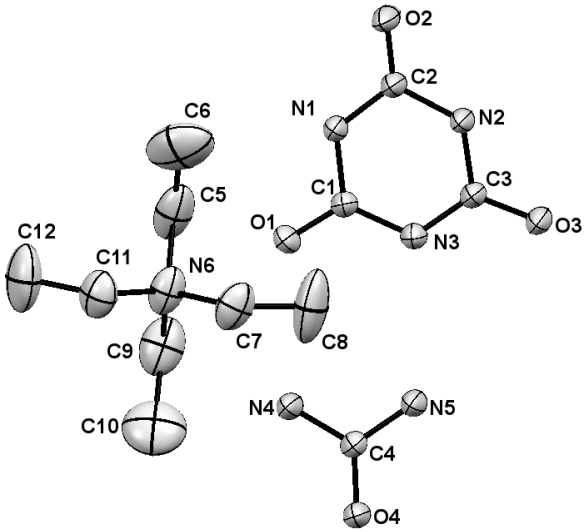
ORTEP drawings for $(C_2H_5)_4N^+C_3H_2N_3O_3^- \cdot (NH_2)_2CS$ (3). Thermal ellipsoids are drawn in 30% probability level. Hydrogen atoms are omitted for clarity.



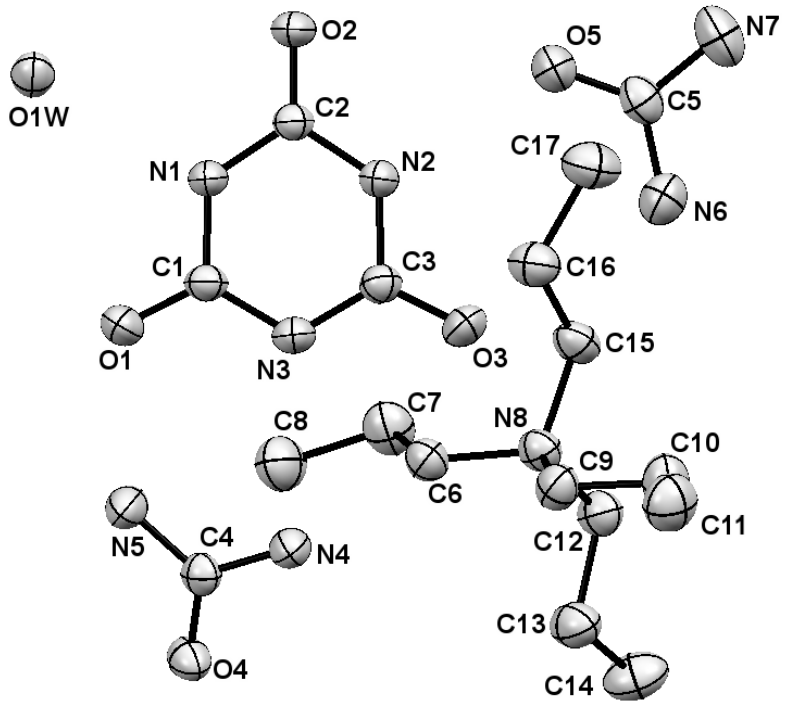
ORTEP drawings for $(n\text{-}C_3H_7)_4N^+C_3H_2N_3O_3^- \cdot (NH_2)_2CS \cdot H_2O$ (4). Thermal ellipsoids are drawn in 30% probability level. Hydrogen atoms are omitted for clarity.



ORTEP drawings for $3[(n\text{-}C_4H_9)_4N^+C_3H_2N_3O_3^-] \cdot 5(NH_2)_2CS \cdot 3H_2O$ (5). Thermal ellipsoids are drawn in 30% probability level. Hydrogen atoms are omitted for clarity.



ORTEP drawings for $(C_2H_5)_4N^+C_3H_2N_3O_3^- \cdot (NH_2)_2CO$ (6). Thermal ellipsoids are drawn in 30% probability level. Hydrogen atoms are omitted for clarity.



ORTEP drawings for $(n\text{-}C_3H_7)_4N^+C_3H_2N_3O_3^- \cdot 2(NH_2)_2CO \cdot H_2O$ (7). Thermal ellipsoids are drawn in 30% probability level. Hydrogen atoms are omitted for clarity.