

Supplementary Information

Using Bar Infrared Spectra and Coincidence Indexes to Study the Diversity of Solid Cyanuric Acid Structures

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											I001504A	3
										15.04	I001504B	2
											I001504S	2
15.00	4.50	0.050	3.88	0.017	NH ₄ Br	9.79	0.100	r.t./ca. 28+	NH ₄ OH _{aq} /acetone		I001506A	3
										15.06	I001506B	3
											I001506C	3
											I001506S	3
											I001602A	4
16.00	4.50	0.050	3.88	0.017	NH ₄ Br	9.79	0.100	r.t./ca. 28+	NH ₄ OH/acetone	16.02	I001602B	4
											I001602C	4
											I001602S	4
											I001705A	2
										17.05	I001705B	2
											I001705C	2
											I001705S	2
											I001706A	3
17.00	4.50	0.050	3.88	0.017	NH ₄ Br	9.79	0.100	0	H ₂ O/acetone	17.06	I001706B	3
											I001706C	2
											I001706S	2
										17.10	I001710S	2
										17.18	I001718A	2
											I001718S	2
											I001804A	3
										18.04	I001804B	3
18.00	4.50	0.050	3.88	0.017	NH ₄ Br	9.79	0.100	0	NH ₄ OH/acetone		I001804C	3
											I001804S	3
										18.06	I001806S	3
										18.09	I001809S	4
											I001906A	4
19.00	4.50	0.050	3.88	0.017	NH ₄ Br	9.79	0.100	0	NH ₄ OH _{aq} /acetone	19.06	I001906B	4
											I001906C	4
											I001906S	4
										20.04	I002004S	4
20.00	4.50	0.050	3.88	0.017	KBr	13.80	0.012	0	H ₂ O/acetone	20.06	I002006A	4
											I002006B	4
											I002006S	4
											I002104A	4
										21.04	I002104B	4
21.00	4.50	0.050	3.88	0.017	KBr	13.80	0.116	0	NH ₄ OH _{aq} /acetone		I002104C	4
											I002104S	4
										21.06	I002106S	4

22.00	4.50	0.050	3.88	0.017	NH ₄ Br	9.79	0.100	0	H ₂ O/acetone	22.04	I002204S	3	
										22.06	I002206S	3	
23.00	4.50	0.050	3.88	0.017	NH ₄ Br	9.79	0.100	0	NH ₄ OH _{aq} /acetone	23.04	I002304A	3	
											I002304B	3	
											I002304C	3	
											I002304S	3	
24.00	0.00	0.000	3.88	0.017	0	0.00	0.000	-10	NH ₄ OH _{aq} /acetone	24.04	I002404S	3	
										24.06	I002406S	3	
25.00	0.00	0.000	3.88	0.017	0	0.00	0.000	r.t./ca. 28+	NH ₄ OH _{aq} /acetone	25.04	I002504S	3	
											26.04	I002604S	4
												I002606A	4
												I002606B	4
26.00	4.50	0.050	3.88	0.017	KBr	13.80	0.116	25	H ₂ O/acetone	26.06	I002606C	4	
												I002606S	4
												I002704S	3
												I002718S	3
27.00	4.50	0.050	3.88	0.017	KCl	7.50	0.100	25	H ₂ O/acetone	27.04	I002704S	3	
										27.18	I002718S	3	
28.00	10.00	0.111	8.62	0.371	NH ₄ Br	21.76	0.222	25	H ₂ O/acetone	28.04	I002804A	2	
												I002804B	2
												I002804C	2
												I002804S	2
28.06											I002806S	2	
												I002904S	2
29.00	10.00	0.111	8.62	0.371	NH ₄ Cl	11.88	0.222	25	H ₂ O/acetone	29.04	I002904S	2	
										29.15	I002915S	2	
31.00	0.00	0.000	3.88	0.017	0	0.00	0.000	-15	NH ₄ OH	31.02	I003102S	4	
											33.04	I003304S	3
												I003309A	2
												I003309B	2
												I003309C	2
												I003309D	2
												I003309E	2
												I003309S	2
												I003311A	2
												I003311B	2
33.00	100.00	1.110	86.40	0.372	NH ₄ Br	217.62	2.222	25	H ₂ O/acetone	33.09	I003311C	2	
												I003311S	2
												I004718A	2
												I004718B	2
47.00	0.00	0.000	86.40	0.372	0	0.00	0.000	25	NH ₄ OH/acetone	47.18	I004718C	2	
												I004718S	3

205.00	4.50	0.050	3.88	0.017	KBr	11.90	0.100	r.t./ca. 28+	H ₂ O/acetone	205.10	I020510A	1	
											I020510B	1	
											I020510C	1	
											I020510D	1	
											I020510S	1	
210.00	4.50	0.050	3.88	0.017	0	0.00	0.000	r.t./ca. 28+	HCl/H ₂ O/acetone	210.04	I021004A	2	
											I021004B	2	
											I021004S	2	
										210.23	I021023A	2	
											I021023B	2	
											I021023C	2	
212.00	0.00	0.000	3.88	0.017	KCl	7.50	0.100	r.t./ca. 28+	AcrNit/H ₂ O/ acetone	212.04	I021204A	2	
											I021204B	2	
											I021204S	2	
										212.18	I021218A	2	
											I021218B	2	
											I021218S	2	
214.00	4.50	0.050	3.88	0.017	KCl	7.50	0.100	r.t./ca. 28+	H ₂ O/acetone	214.05	I021405S	2	
215.00	0.00	0.000	3.88	0.017	KCl	7.50	0.100	r.t./ca. 28+	AcrNit/H ₂ O/ acetone	215.09	I021509S	2	
ACN	Sigma-Aldrich reagent No. 185809										ACN3	IPACN3A	ACN
												IPACN3B	ACN
												IPACN3C	ACN
												IPACN3S	ACN
											ACN4	IPACN4A	ACN
												IPACN4B	ACN
												IPACN4C	ACN
												IPACN4S	ACN
											ACN5	IPACN5A	ACN
												IPACN5B	ACN
												IPACN5C	ACN
												IPACN5S	ACN
											ACN	IPACNA	ACN
												IPACNB	ACN
												IPACNC	ACN
												IPACNS	ACN

r.t.: room temperature; AcrNit: acrylonitrile; ACN: cyanuric acid.