SUPPLEMENTARY MATERIAL

1. In Table 1, the results of computer simulations of slow MAS ^{13}C and ^{2}H spectra are given. The parameters $\Delta\delta$ and η denote the anisotropy and asymmetry of ^{13}C chemical shielding, while e^2Qq/h and η in the case of ^{2}H denote the quadrupole coupling constant and asymmetry parameter of electric field gradient tensor, respectively.
2. The crystal structure data for Cyanuric Acid (neutron diffraction), Melamine (neutron diffraction) and 1:1 Cyanuric Acid : Melamine complex (X-ray diffraction) are given in Table 2. The ^{13}C, ^{15}N and ^{2}H resonance assignments for Cyanuric Acid and Melamine are based on the crystal structure data. For the 1:1 Cyanuric Acid:Melamine complex, the ambiguity in identifying the stacked rings of Cyanuric Acid and Melamine leads to the number of inequivalent ^{13}C and ^{15}N atoms in the ring to be two each. NMR results correctly determine them to be four each (two for Cyanuric Acid and two for Melamine) as discussed in the main paper.
3. In Figure 1, the experimental and theoretically simulated ^{2}H slow MAS spectra are shown for Cyanuric Acid, Melamine and 1:1 Cyanuric Acid:Melamine complex. The spinning speed employed is indicated.
4. Figure 2 shows ^{1}H-^{13}C cross-polarization dynamics for the different ring carbons in Cyanuric Acid, Melamine and the 1:1 Cyanuric Acid:Melamine complex. Experimental data are fit to the equation $I = I(0) / (1- T_{IS} / T_{1\rho}) * (\exp (- \tau/ T_{1\rho}) – \exp (- \tau/ T_{IS}))$ and the "best fit" curves are shown in Figure 2. The CP dynamics for undoped and Cu^{2+} doped samples are shown and the cross-polarization time (T_{IS}) and proton rotating frame spin-lattice relaxation time ($T_{1\rho}{}^{H}$), determined from the fit, are also indicated.
5. In Figures 3A, 3B and 3C, the experimental and theoretically simulated ^{13}C slow MAS spectra are shown for Cyanuric Acid (1A), Melamine (1B) and 1:1 Cyanuric Acid:Melamine complex (1C). The spinning speeds employed are indicated.

Table - 1

RESULTS OF COMPUTER SIMULATION OF ^{13}C AND ^{2}H SLOW MAS SPECTRA

System	**^{13}C Simulation results**			**^{2}H Simulation results**	
	$\delta\Delta$ ***(ppm)***	**δ_{iso} (ppm)**	□	**e^2Qq/h** ***(kHz)***	□
CYANURIC ACID	134.3 135.8	149.0 151.3	0.56 0.61	180.5	0.19
MELAMINE	146.2 151.3 153.0	167.8 166.2 166.2	2.56 2.38 2.37	200.1 200.1 213.5	0.23 0.14 0.21
1:1 CYANURIC ACID:MELAMINE	144.6 152.7	153.6 165.2	0.53 2.32	140.0 207.0	0.26 0.16

^{13}C isotropic shifts (δ_{iso}) are with reference to tetramethyl silane

Table – 2

Structural Data

System	Molecular symmetry	Crystal symmetry	No. of inequivalent sites			Hydrogen bond distances
			^{13}C	^{15}N	^{2}H	
CA (*ND)* (Ref. 1)	6m2	C2/n a= 7.90 Å □=90.0^0 b= 6.73 Å □=130.67^0 c=11.95 Å □=90.0^0	2	2	2	H_1—O_1=1.758 H_2—O_2=1.774
MA *(ND)* (Ref. 2)	---	$P2_1/a$ a=10.61 Å □=90.0^0 b= 7.49 Å □=112.26^0 c= 7.29 Å □=90.0^0	3	6	6	H_1—N_9=2.052 H_2—N_8=2.110 H_4—N_7=2.001 H_6—N_8=2.080
CA:MA *(XD)* (Ref. 3)	---	**C2/m** a=14.85 Å □=90.0^0 b= 9.64 Å □=92.26^0 c= 3.58 Å □=90.0^0	2	4	Nd	------

ND: Neutron Diffraction XD: X-ray Diffraction

References: 1. Coppens, P.; Vos, A. *Acta. Crysallogr.*. 1971, *B27*, 146.
2. Vargheese, J.N.; O'Connell,M.; Maslen, E.N. *Acta. Crystallogr.* 1977, *B33*, 2102.
3. Ranganathan, A.; Pedireddi,V.R.; Rao, C.N.R. *J. Am. Chem. Soc.*, 1999, *121*, 1752.

Figure 1

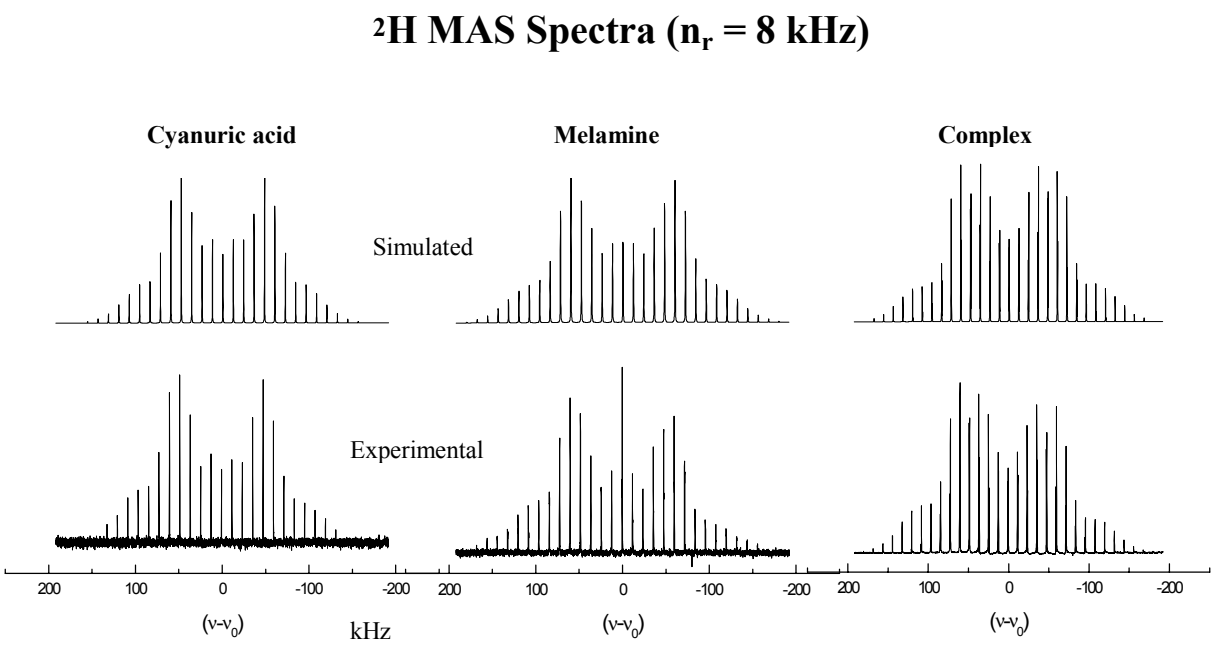
^{2}H MAS Spectra (n_r = 8 kHz)
Cyanuric acid
Melamine
Complex
Simulated
Experimental
200
100
0
-100
-200
(ν-ν$_0$)
kHz

Figure 2

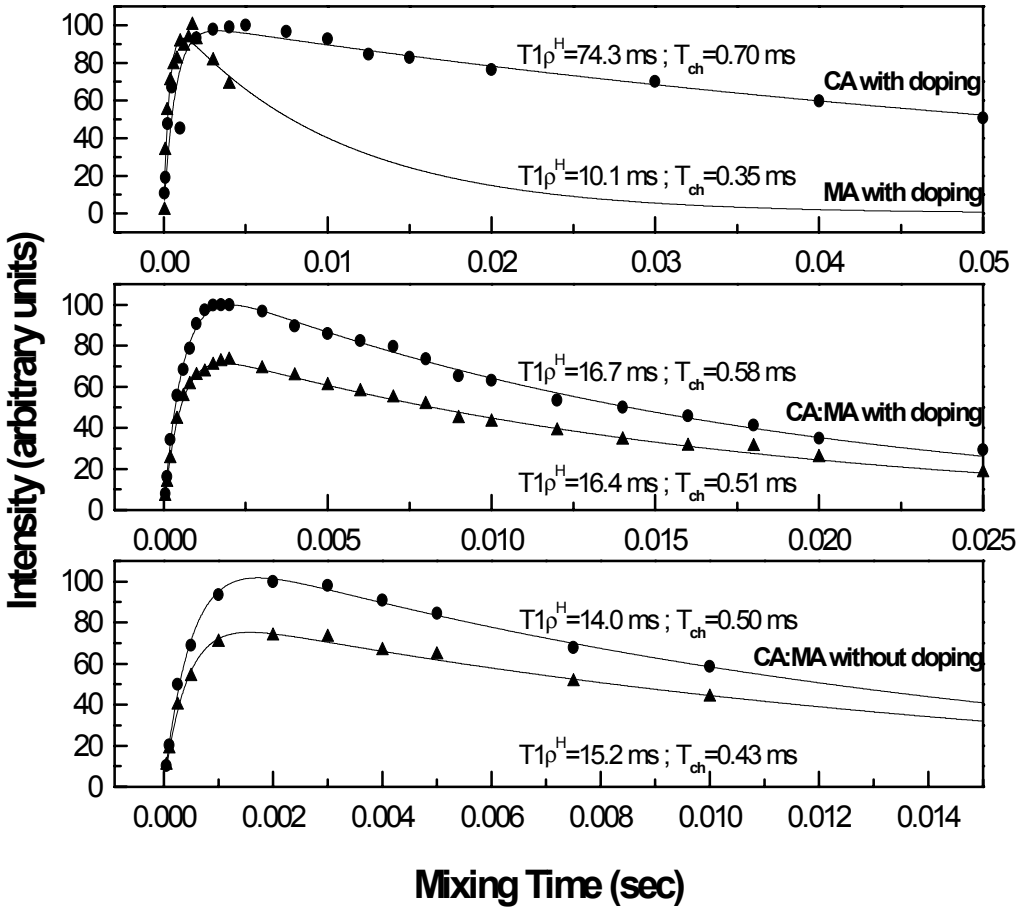
Intensity (arbitrary units)
Mixing Time (sec)
T1ρ^H=74.3 ms ; T_ch=0.70 ms
CA with doping
T1ρ^H=10.1 ms ; T_ch=0.35 ms
MA with doping
T1ρ^H=16.7 ms ; T_ch=0.58 ms
CA:MA with doping
T1ρ^H=16.4 ms ; T_ch=0.51 ms
T1ρ^H=14.0 ms ; T_ch=0.50 ms
CA:MA without doping
T1ρ^H=15.2 ms ; T_ch=0.43 ms

Figure 3C

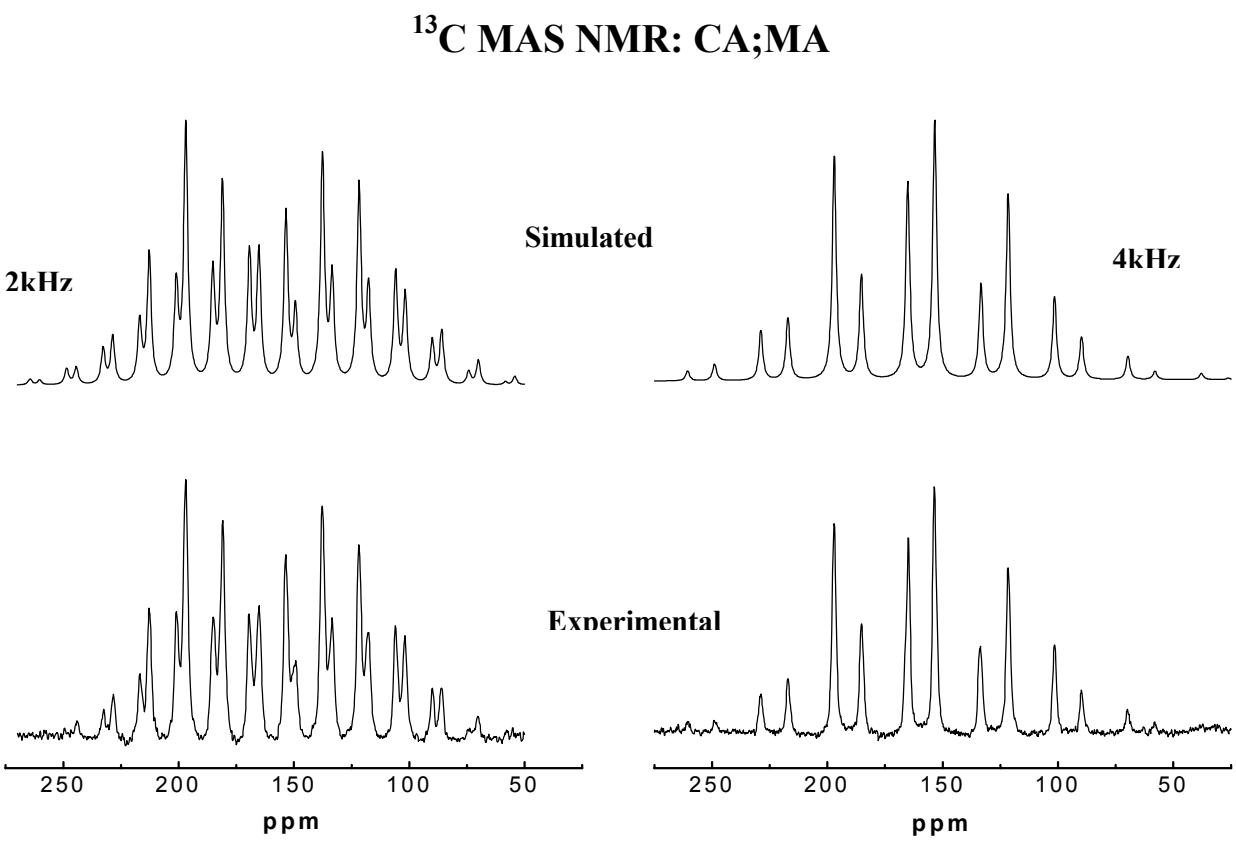
^{13}C MAS NMR: CA;MA
2kHz
Simulated
4kHz
Experimental
250
200
150
100
50
ppm
250
200
150
100
50
ppm

Figure 3B

^{13}C MAS NMR: Melamine

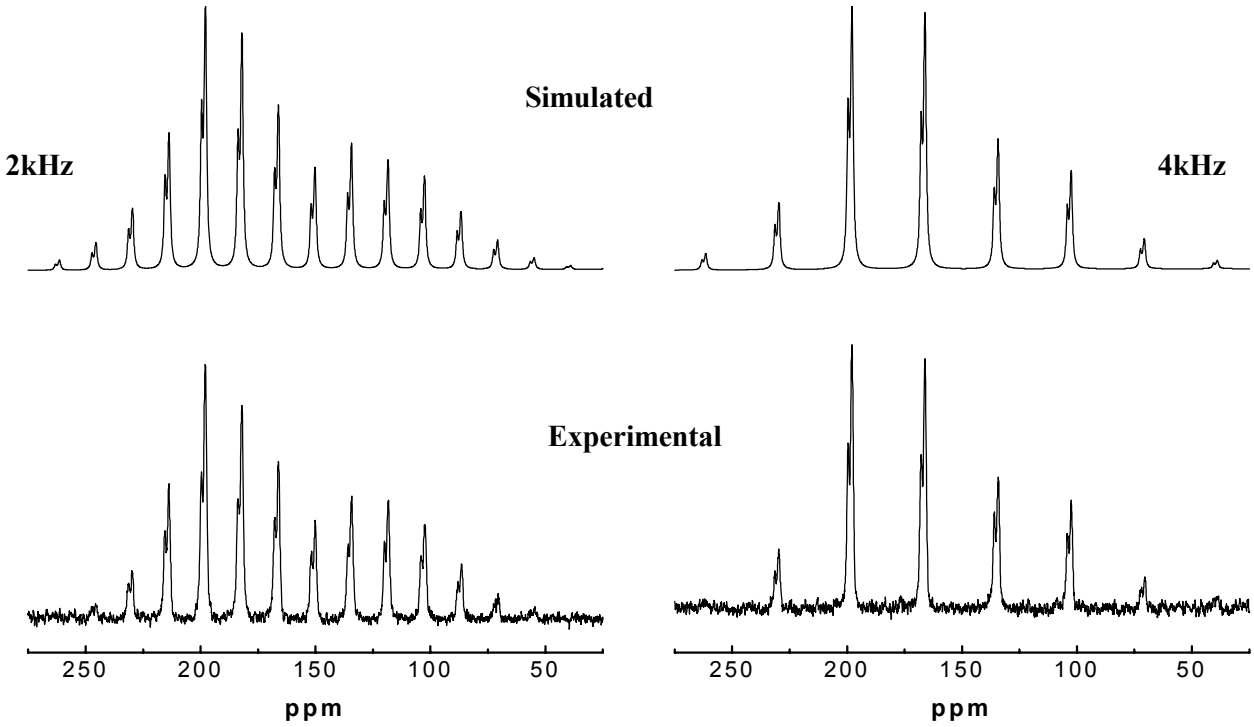

Figure 3A

^{13}C MAS NMR: Cyanuric acid