

*Supporting Information for*

**A Magic-Angle Spinning NMR Method for the Site-Specific  
Measurement of Proton Chemical-Shift Anisotropy in  
Biological and Organic Solids**

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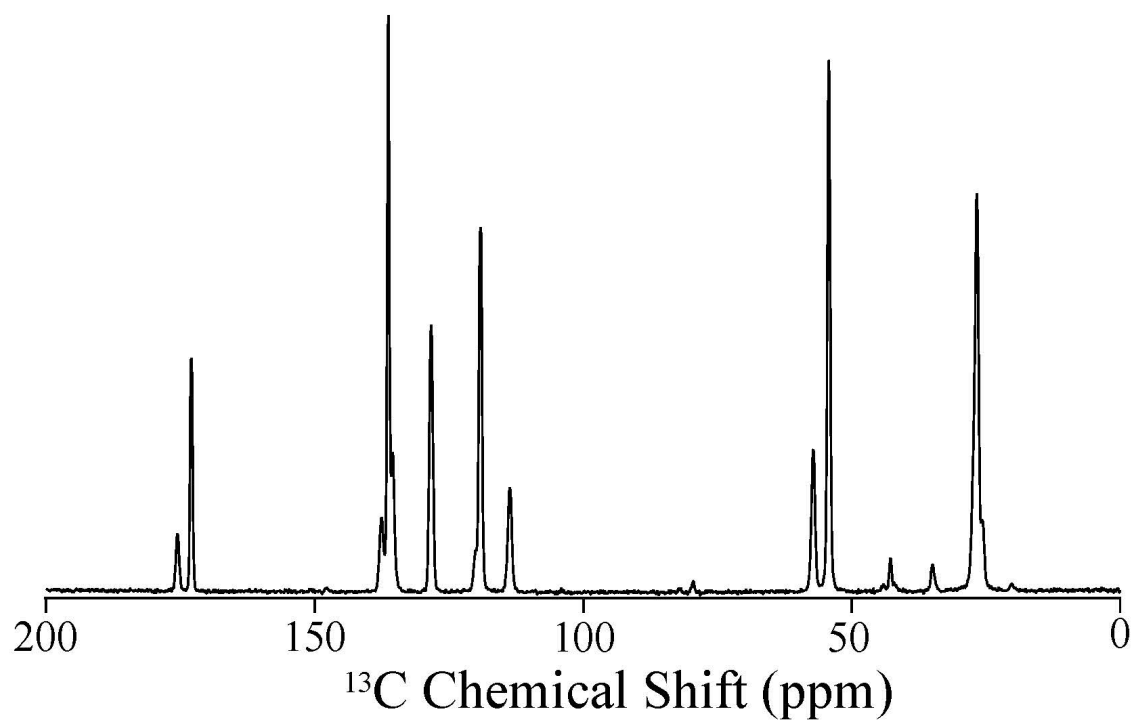
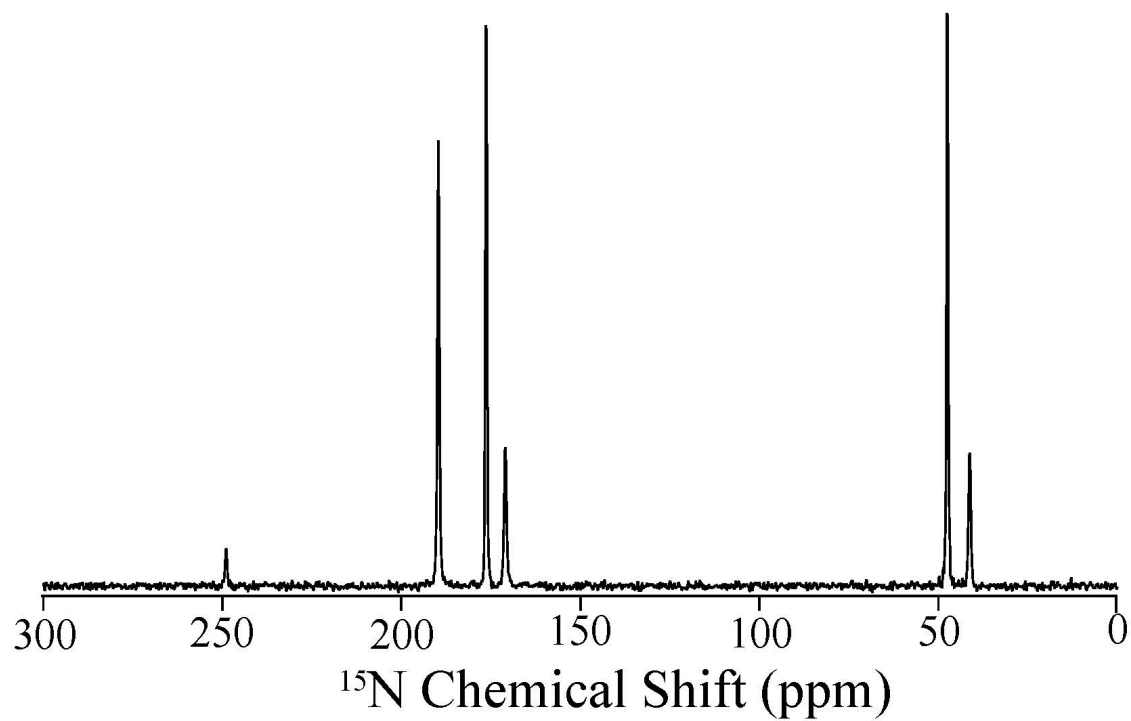
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Dedicated to the 70th birthday of Professor Dr. Shimon Vega



**Figure S1.**  $^{13}\text{C}$  and  $^{14}\text{N}$  spectra of the mixture of cationic and neutral histidine crystallites.

**Table S1.**  $^{15}\text{N}$  and  $^{13}\text{C}$  chemical shifts (ppm) of cationic and neutral histidine as reported by Li and Hong<sup>[1]</sup> and as measured in the present work.

	cationic histidine		neutral histidine	
	Li&Hong	present work	Li&Hong	present work
$^{15}\text{NH}_4$	47.6	47.5	41.5	41.3
$^{15}\text{N}\delta 1$	190.0	189.7	249.4	249.0
$^{15}\text{N}\epsilon 2$	176.3	176.3	171.1	171.0
$^{13}\text{C}'$	173.2	173	175.6	175.5
$^{13}\text{C}\alpha$	54.1	54.2	57.0	57.1
$^{13}\text{C}\beta$	26.0	25.5	27.0	26.7
$^{13}\text{C}\gamma$	128.7	128.4	137.7	137.6
$^{13}\text{C}\epsilon 1$	136.3	136.3	135.3	135.4
$^{13}\text{C}\delta 2$	119.4	119.3	113.6	113.7

**Table S2.**  $^1\text{H}$  isotropic chemical shifts (ppm) of cationic histidine as reported by Li and Hong<sup>[1]</sup> and as presently calculated by DFT.

	Li&Hong	DFT
$^1\text{H-N}\delta 1$	16.8	15.8
$^1\text{H-N}\epsilon 2$	12.6	11.7
$^1\text{H-C}\epsilon 1$	9.3	7.8
$^1\text{H-C}\delta 2$	8.0	7.4
$^1\text{H-C}\alpha$	3.5	3.4

#### Reference

[1] S. Li, M. Hong, *J. Am. Chem. Soc.* **2011**, 133, 1534–1544.