Electronic Supplementary Material (ESI) for Chemical Communications

Supplementary Information

The Crystal Structure of L-Arginine

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Solid-State ^{13}C NMR Spectroscopy

Solid-state ^{13}C NMR data was acquired on a Chemagnetics Infinity Plus spectrometer, operating at a ^{13}C Larmor frequency of 75.48 MHz and with magic-angle spinning at 12 kHz. The spectra were acquired with ramped ^{1}H→^{13}C cross-polarization[1] using a contact time of 2 ms, TPPM ^{1}H decoupling[2] during acquisition, and a recycle delay of 3 s. The FID was acquired over 17.2 hours with 20480 acquisitions co-added.

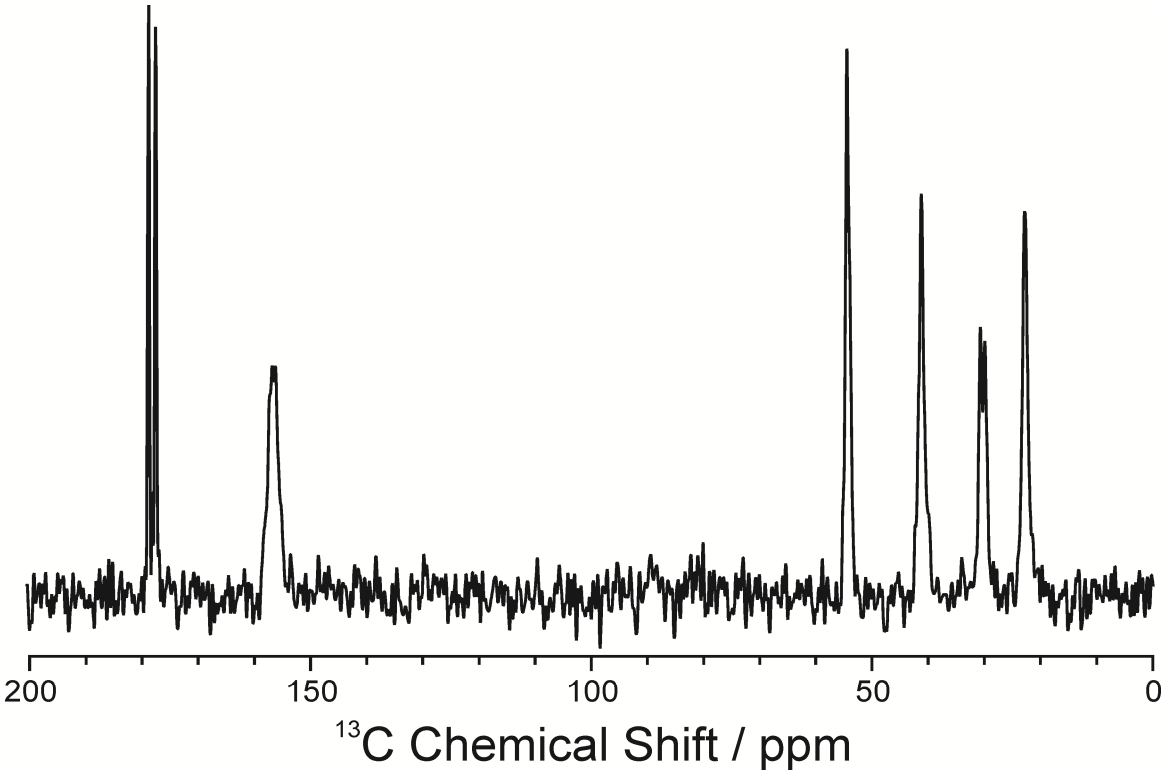

Figure S1 High-resolution solid-state ^{13}C NMR spectrum of L-arginine. For the carboxylate (~178 ppm) and C_β (~30 ppm) environments, two peaks (in approximately 1:1 intensity ratio) are observed, suggesting that there are two crystallographically independent molecules in the asymmetric unit.

Comparison of Crystal Structures of L-Arginine and L-Arginine Dihydrate

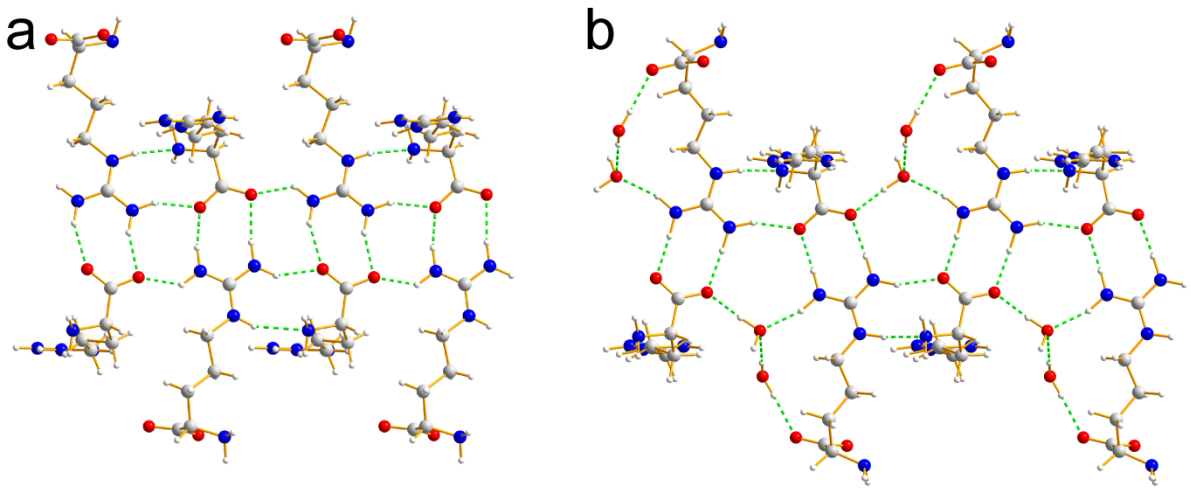

Figure S2 The hydrogen-bonded ribbons in (a) L-arginine viewed perpendicular to the (041) plane and (b) L-arginine dihydrate[3] viewed perpendicular to the (301) plane.

References

1. G. Metz, X. L. Wu and S. O. Smith, *J. Magn. Reson. A*, 1994, **110**, 219-227.

2. A. E. Bennett, C. M. Rienstra, M. Auger, K. V. Lakshmi and R. G. Griffin, 1995, **103**, 6951-6958.

3. M. S. Lehmann, J. J. Verbist, W. C. Hamilton and T. F. Koetzle, *J. Chem. Soc. Perk. Trans. 2*, 1973, 133-137.