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Supporting information for article:

Synthesis, structural elucidation, characterization and theoretical DFT study of 1-(*o*-tolyl)biguanidium chloride

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Supplementary Materials

3.5. IR spectroscopy

FT-IR spectroscopy was used to verify the functional groups present in the crystal, and to investigate their vibrational behavior in the solid state. The IR spectrum of the title crystalline compound is shown in Fig. S3. The characteristic vibrational modes of the compound can be compared to those of similar materials (Belhouchet *et al.*, 2005; Shanmuga *et al.*, 2000; Calve *et al.*, 1989). In the high-frequency region, the bands spreading between 3600 and 2800 cm^{-1} corresponds to the valence vibrations of N-H and C-H groups interconnected by a system of hydrogen bonds in the crystal (Smirani *et al.*, 2004). Bands in the 1660 - 1150 cm^{-1} region correspond to the N-H and C-H bending vibrations and to the valence vibrations of C=C, C-C, C=N and C-N groups (Kaabi *et al.*, 2003; Oueslati et *al.*, 2005). The observed bands in the range 1000 – 400 cm^{-1} can be attributed to the out of plane bending modes of C-H, C=C and C-C groups (Oueslati *et al.*, 2005).

References

Belhouchet, M., Bahri, M., Savariault, J. M. & Mhiri, T. (2005). *Spectrochimica. Acta* Part. **A61**, 387-393.

Calve, N. L., Romain, F., Limage, M. H. & Novak. A. (1989). *J. Mol. Struct.* **200**, 131-147.

Kaabi, K., Rayes, A., Ben Nasr, C., Rzaigui, M. & Lefebvre, F. (2003). *Mat. Res. Bull.* **38**, 741-747.

Oueslati, A., Rayes, A., Ben Nasr, C. & Lefebvre, F. (2005). *Mat. Res. Bull.* **40**, 1680-1698.

Oueslati, A., Ben Nasr, C., Durif, A. & Lefebvre, F. (2005). *Mat. Res. Bull.* **40**, 970-980.

Shanmuga, S. R., Fun, H. K., Zhao, P. S., Jian, F. F., Lu, L. D., Yang, X. J. & Wang, X. (2000). *Acta Cryst.* **C56**, 742-743.

Smirani, W., Ben Nasr, C. & Rzaigui, M. (2004). *Mat. Res. Bull.* **39**, 1103-1111.

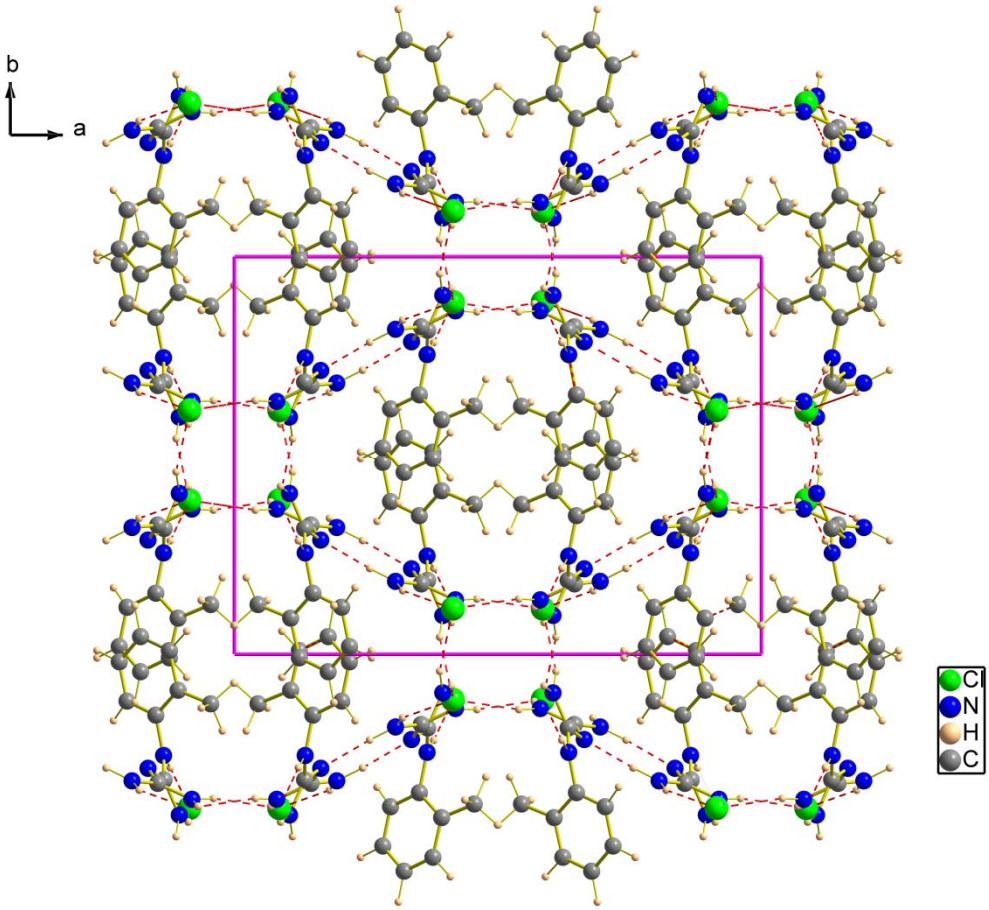

Figure S1. Crystal packing arrangement viewed along *c*-axis. Dotted lines indicate hydrogen bonds.

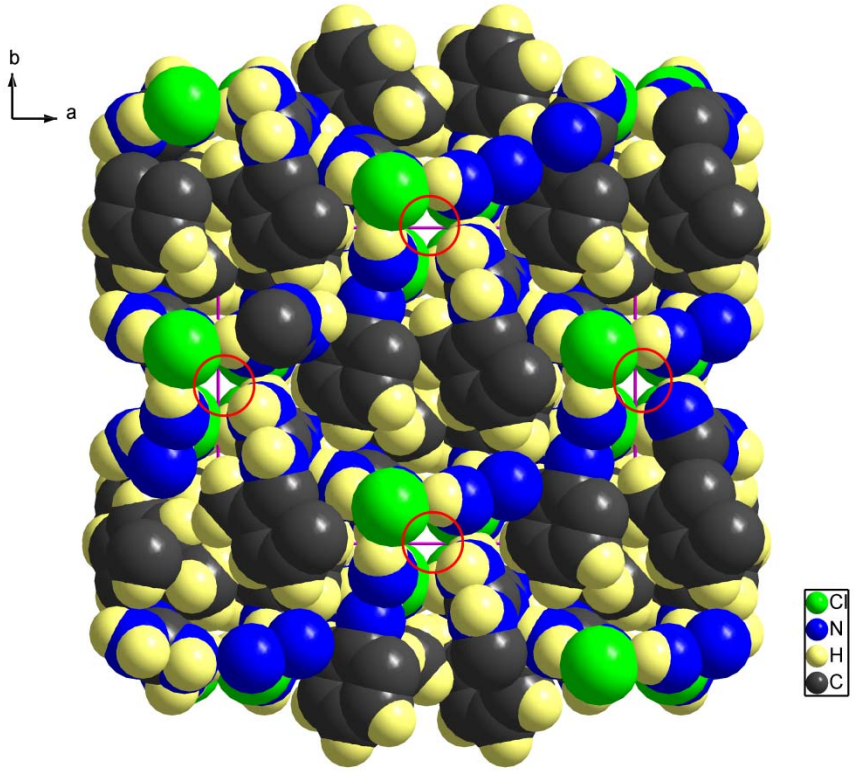

Figure S2. Crystal packing arrangement viewed along *c*-axis with space filling model.

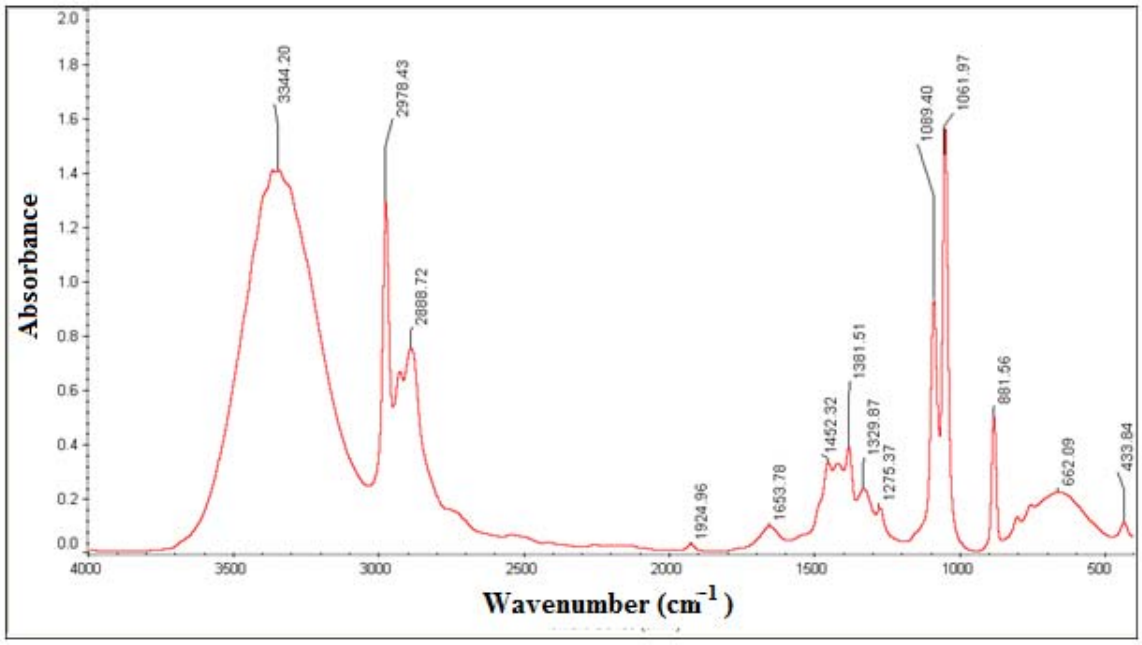

Figure S3. Infrared absorption spectrum of $(C_9H_{14}N_5)Cl$.

Table S1. Selected bond distances and angles (Å, º) in the biguanidium moiety.

N2—C8	1.3307 (13)	N6—C7	1.3334 (13)
N2—C7	1.3407 (13)	C9—C1	1.3936 (16)
N3—C7	1.3335 (13)	C9—C2	1.3989 (16)
N4—C2	1.3513(14)	C1—C4	1.4042 (17)
N4—C8	1.3516 (14)	C1—C5	1.4908 (18)
N4—C9	1.4180 (14)	C2—C3	1.3830 (17)
N5—C2	1.3382 (14)	C3—C6	1.384 (2)
N5—C8	1.3385 (13)	C4—C6	1.386 (2)
C8—N2—C7	122.45 (8)	C9—C1—C4	116.97 (10)
C8—N4—C9	125.79 (9)	C9—C1—C5	123.11 (10)
C2—C3—C6	119.17 (12)	C4—C1—C5	119.89 (11)
C1—C4—C6	121.55 (11)	C9—C2—C3	120.25 (11)
N2—C7—N6	124.80 (8)	C3—C6—C4	120.53 (12)
N2—C7—N3	117.52 (9)	N2—C8—N5	125.25 (8)
N6—C7—N3	117.62 (8)	N4—C9—C1	121.39 (9)
N4—C8—N2	118.59 (9)	N4—C9—C2	116.90 (9)
N4—C8—N5	116.04 (9)	C1—C9—C2	121.51 (10)