

Supplementary information to

Non-covalently generated 3D supramolecular crystal structure in a new family of hybrid nitrates **templated by piperazine: thermal behavior and *in vitro* antimicrobial potential**

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Table SI3: Selected bond distances and angles relative to the protonated piperazine moiety

Compound (1) Compound (2) Compound (3)

| | | | |
|------------------------|-------------|-------------|-------------|
| C1—C2 | 1.516 (2) | 1.507 (2) | 1.515 (3) |
| C3—C4 | 1.518 (2) | 1.513 (2) | 1.514 (3) |
| C5—C6 | 1.517 (2) | 1.513 (2) | 1.512 (3) |
| N5—C2 | 1.485 (2) | 1.487 (2) | 1.492 (3) |
| N5—C3 | 1.491 (2) | 1.490 (2) | 1.488 (3) |
| N6—C1 | 1.494 (2) | 1.496 (2) | 1.489 (3) |
| N6—C4 | 1.482 (2) | 1.484 (2) | 1.487 (3) |
| N7—C5 | 1.497 (2) | 1.495 (2) | 1.495 (3) |
| N7—C6 ⁱⁱ | 1.492 (2) | 1.486 (2) | 1.486 (3) |
| C2—C1—N6 | 110.56 (14) | 110.34 (13) | 110.27 (19) |
| C1—C2—N5 | 109.11 (13) | 109.83 (12) | 109.0 (2) |
| C4—C3—N5 | 110.11 (14) | 110.10 (13) | 110.34 (19) |
| C3—C4—N6 | 110.15 (13) | 109.84 (12) | 109.60 (19) |
| C2—N5—C3 | 111.70 (14) | 111.90 (14) | 111.34 (19) |
| C1—N6—C4 | 111.65 (14) | 111.66 (13) | 111.90 (19) |
| C6—C5—N7 | 110.05 (14) | 110.09 (13) | 110.11 (19) |
| C5—C6—N7 ⁱⁱ | 109.82 (14) | 109.60 (13) | 109.5 (2) |
| C5—N7—C6 ⁱⁱ | 110.72 (13) | 111.10 (13) | 110.49 (19) |

Symmetry code: (ii) -x+3, -y, -z+1.
