Supplementary Material (ESI) for CrystEngComm


**Electronic Supplementary Information**

# Layered Crystal Structure of Bicyclic Aziridines as Revealed by Analysis of Intermolecular Interactions Energy

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**Table S1**. Selected geometrical parameters (bond lengths [Å] and torsion angles [°]) for structures **1-3** obtained from X-ray diffraction data and quantum-chemical calculations of isolated molecules by MP2/6-311G(d,p) and M05-2X/6-311G(d,p) methods.

| | **1** | | | **2** | | | **3** | | |
|---|---|---|---|---|---|---|---|---|---|
| | Exp. | Isolated | | Exp. | Isolated | | Exp. | Isolated | |
| | | M05-2X | MP2 | | M05-2X | MP2 | | M05-2X | MP2 |
| N(1)-C(2) | 1.284(3) | 1.273 | 1.296 | 1.273(4) | 1.272 | 1.296 | 1.283(7) | 1.272 | 1.296 |
| N(1)-C(3) | 1.478(3) | 1.471 | 1.474 | 1.490(4) | 1.471 | 1.474 | 1.481(6) | 1.472 | 1.474 |
| N(2)-C(1) | 1.473(3) | 1.459 | 1.477 | 1.465(4) | 1.457 | 1.476 | 1.479(6) | 1.458 | 1.474 |
| N(2)-C(12) | 1.473(2) | 1.453 | 1.467 | 1.470(4) | 1.453 | 1.467 | 1.482(6) | 1.453 | 1.467 |
| N(2)-C(3) | 1.497(3) | 1.488 | 1.490 | 1.487(4) | 1.488 | 1.491 | 1.496(6) | 1.487 | 1.491 |
| C(1)-C(2) | 1.495(3) | 1.500 | 1.494 | 1.495(4) | 1.498 | 1.493 | 1.494(6) | 1.497 | 1.493 |
| C(1)-C(12) | 1.504(3) | 1.500 | 1.501 | 1.503(4) | 1.500 | 1.501 | 1.502(7) | 1.501 | 1.507 |
| C(2)-C(6) | 1.477(2) | 1.471 | 1.469 | 1.476(4) | 1.471 | 1.468 | 1.473(7) | 1.471 | 1.468 |
| C(3)-C(5) | 1.523(2) | 1.520 | 1.522 | 1.512(5) | 1.520 | 1.522 | 1.519(7) | 1.531 | 1.523 |
| C(3)-C(4) | 1.527(3) | 1.524 | 1.526 | 1.534(5) | 1.523 | 1.526 | 1.530(8) | 1.520 | 1.526 |
| C(12)-C(13) | 1.489(3) | 1.487 | 1.485 | 1.494(4) | 1.487 | 1.484 | 1.494(7) | 1.488 | 1.485 |

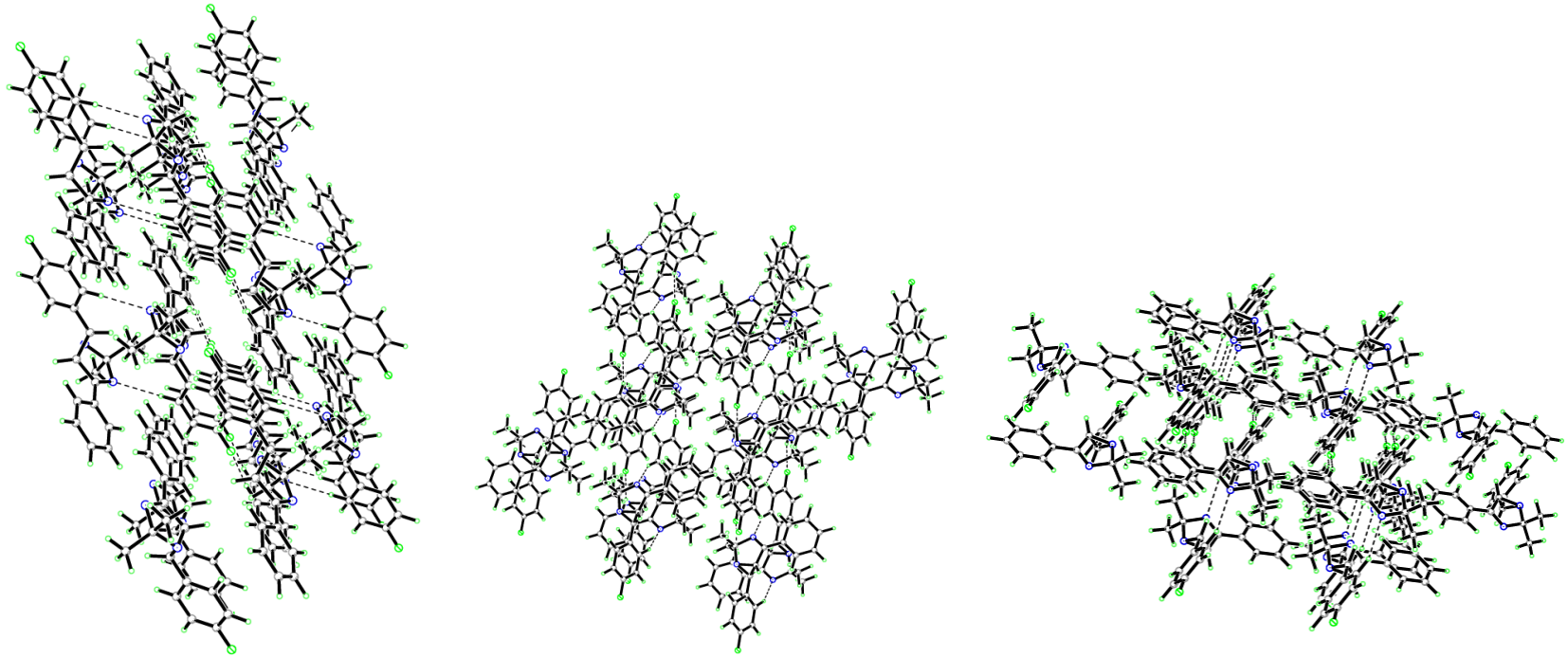
| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Hal(1)-C(16)[a] | 1.370(3) | 1.349 | 1.348 | 1.739(4) | 1.744 | 1.737 | | | |
| Hal(1)-C(9)[b] | | | | 2.102(3) | 2.112 | 2.113 | 1.905(5) | 1.902 | 1.895 |
| C1-C2-N1-C3 | 5.7(2) | 5.2 | 6.3 | 6.4(4) | 5.1 | 6.3 | 4.8(6) | 5.2 | 6.3 |
| N1-C2-C6-C11 | 12.7(2) | 12.3 | 15.7 | -6.0(5) | 11.7 | 14.5 | 7.1(8) | 11.7 | 14.9 |
| N2-C12-C13-C14 | -17.3(3) | -8.0 | -9.5 | -9.1(4) | -9.0 | -10.7 | -40.3(7) | -10.0 | -11.6 |

[a] this is the F(1)-C(16) bond in structure **1** and the Cl(1)-C(16) bond in structure **2**. [b] this is the I(1)-C(9) bond in structure **2** and the Br(1)-C(9) bond in structure **3**.

**Table S2** Symmetry codes of neighboring molecules and squares of boundary surface (BS, Å$^2$) of the Dirichlet polyhedra for basic molecule located in asymmetric of unit cell of crystal structures **1-3.**

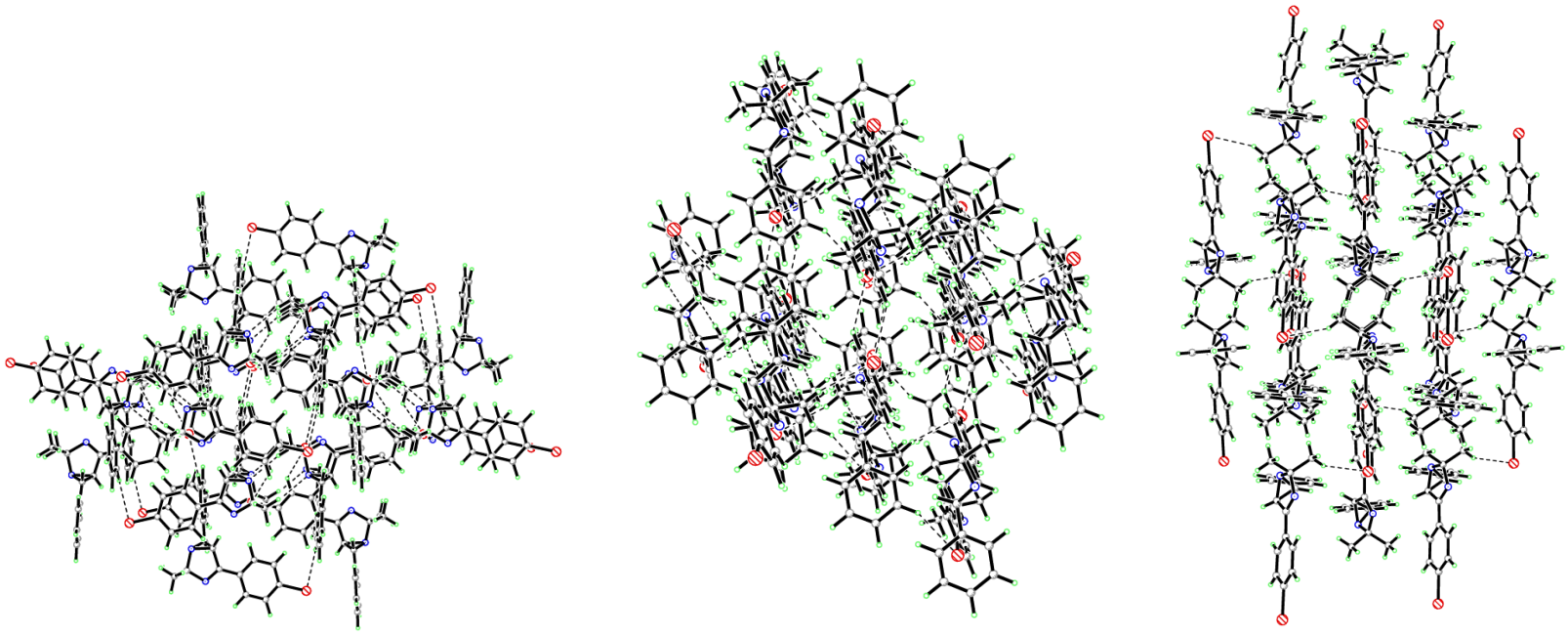
| | Structure 1 | | Structure 2 | | Structure 3 | |
|---|---|---|---|---|---|---|
| Neighbor | Symmetry | BS | Symmetry | BS | Symmetry | BS |
| 1 | (-x, -y, 1-z) | 61.1 | (-1-x, -y, -z) | 70.2 | (1-x, 1-y, -z) | 59.8 |
| 2 | (-x, 1-y, 1-z) | 60.0 | (-x, -y, -z) | 59.6 | (x-0.5, 0.5-y, -0.5+z) | 59.4 |
| 3 | (-x, 1-y, -z) | 44.5 | (-1-x, -1-y, -z) | 52.6 | (0.5+x, 0.5-y, 0.5+z) | 59.4 |
| 4 | (1-x, 1-y, -z) | 29.9 | (-x, 1-y, 1-z) | 50.6 | (1-x, -y, -z) | 36.2 |
| 5 | (x-1, y, z+1) | 25.0 | (-x, 1-y, -z) | 40.6 | (x, y, z-1) | 22.2 |
| 6 | (1+x, y, z-1) | 25.0 | (x, y-1, z) | 20.3 | (x, y, z+1) | 22.2 |
| 7 | (x, y, z-1) | 22.6 | (x, 1+y, z) | 20.3 | (-0.5+x, 0.5-y, 0.5+z) | 19.4 |
| 8 | (x, y, z+1) | 22.6 | (x, y, z-1) | 18.8 | (0.5+x, 0.5-y, -0.5+z) | 19.4 |
| 9 | (-x, -y, 2-z) | 22.2 | (x, y, 1+z) | 18.8 | (1-x, -y, -1-z) | 18.8 |
| 10 | (-1-x, -y, 2-z) | 18.1 | (x-1, y-1, z) | 17.3 | (0.5-x, -0.5+y, -0.5-z) | 18.0 |
| 11 | (1-x, -y, 1-z) | 17.4 | (1+x, 1+y, z) | 17.3 | (0.5-x, 0.5+y, -0.5-z) | 18.0 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 12 | (x-1, y, z) | 9.8 | (x, y-1, z-1) | 12.5 | (1.5-x, -0.5+y, 0.5-z) | 12.5 |
| 13 | (x+1, y, z) | 9.8 | (x, 1+y, 1+z) | 12.5 | (1.5-x, 0.5+y, 0.5-z) | 12.5 |
| 14 | (x, y-1, z+1) | 4.4 | (1+x, 1+y, 1+z) | 8.6 | (1.5-x, -0.5+y, -0.5-z) | 8.9 |
| 15 | (x, y+1, z-1) | 4.4 | (x-1, y-1, z-1) | 8.6 | (1.5-x, 0.5+y, -0.5-z) | 8.9 |
| 16 | (1-x, 1-y, 1-z) | 1.0 | (-1-x, -y, 1-z) | 3.9 | (1-x, 1-y, -1-z) | 2.6 |
| 17 | | | (-x, 2-y, 1-z) | 2.2 | | |
| | Total square | 377.9 | | 437.1 | | 397.9 |



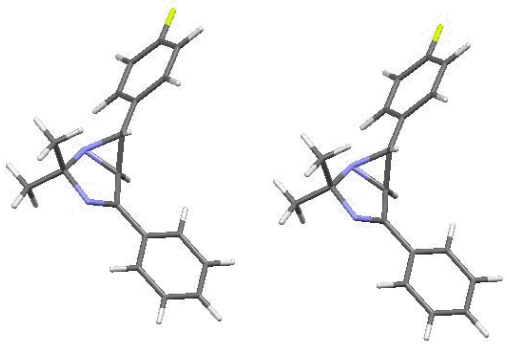
1 2 3

Fig. S1. The crystal packing of 1 as seen along 1) [100]; 2) [010]; 3) [001] directions.



1 2 3

Fig. S2. The crystal packing 3 as seen along 1) [100]; 2) [010]; 3) [001] directions.



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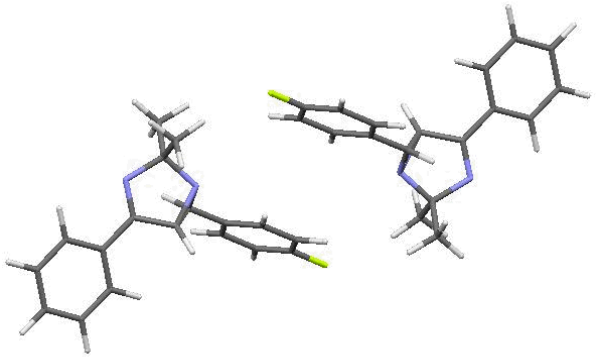

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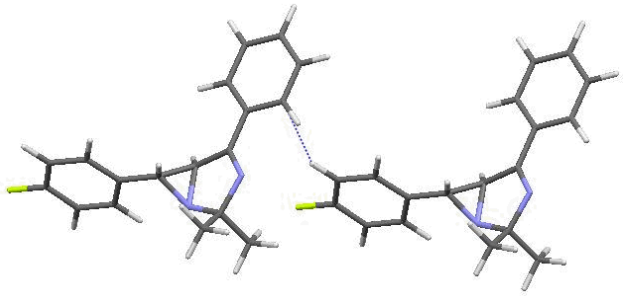

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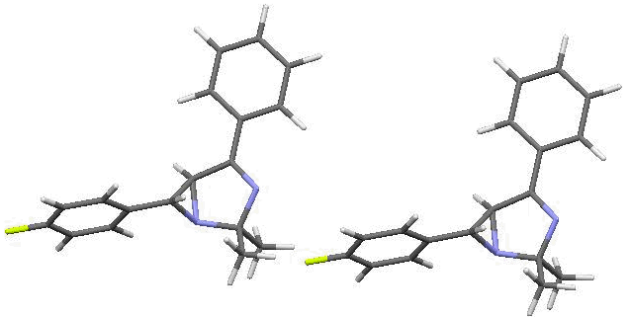

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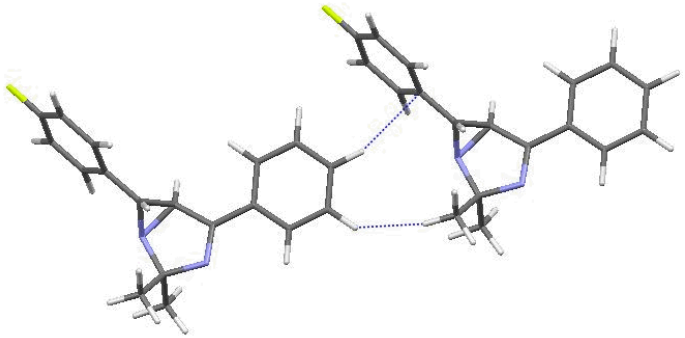

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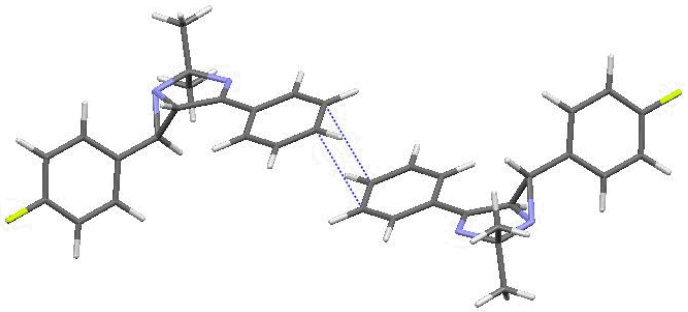

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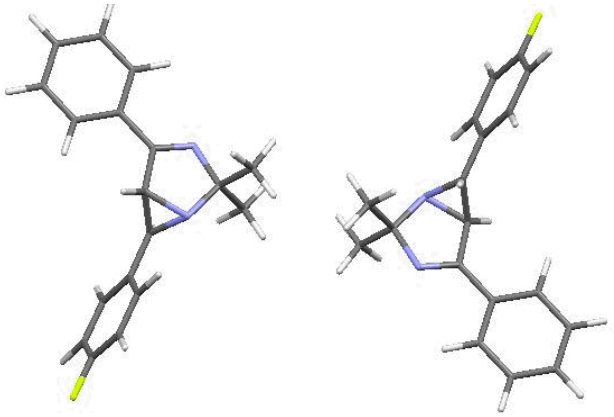

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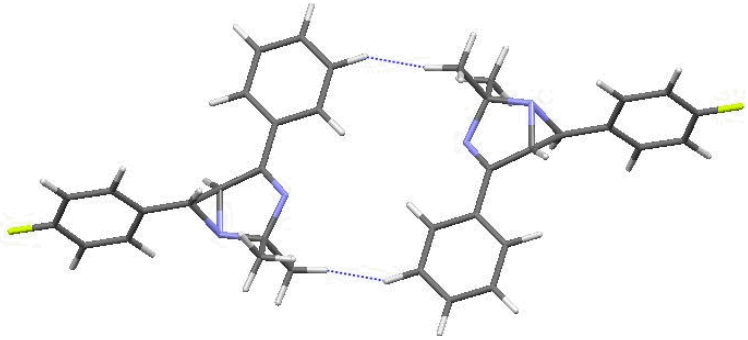

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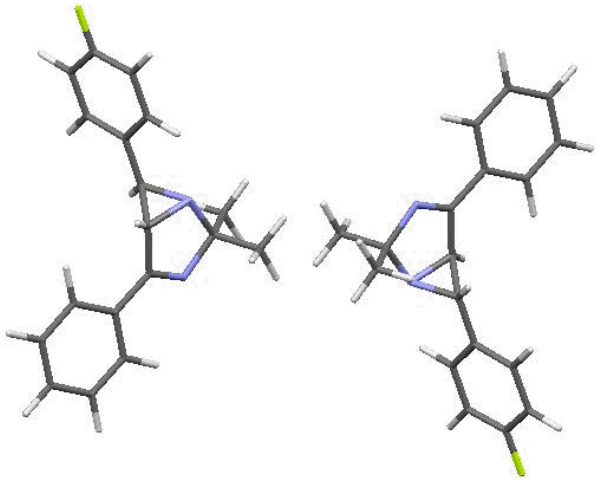
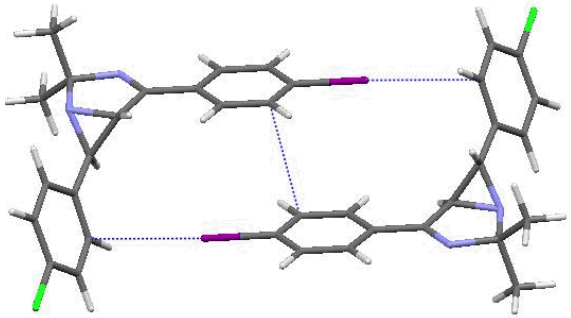
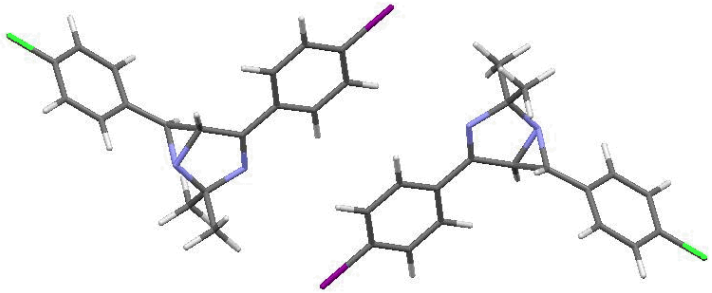


1_16

Fig. S3. Dimers formed by the basic molecule and molecules of its first coordination sphere in crystal structures **1**. Numbering of dimers corresponds to Table 3.



2_3



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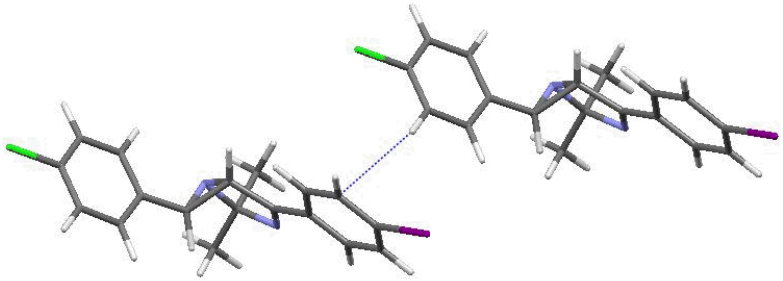

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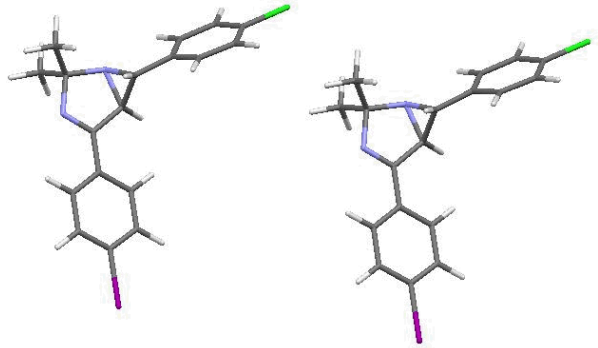

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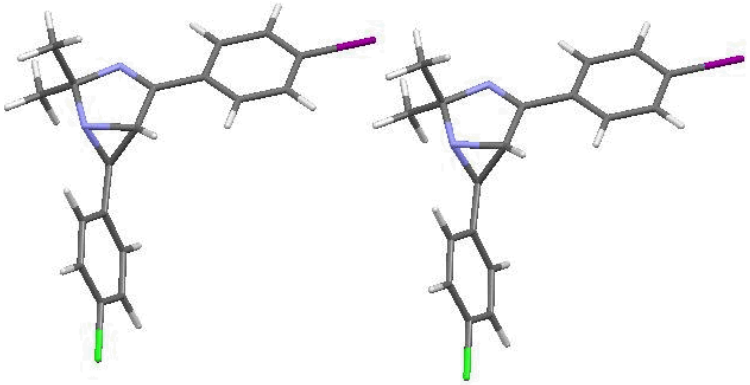

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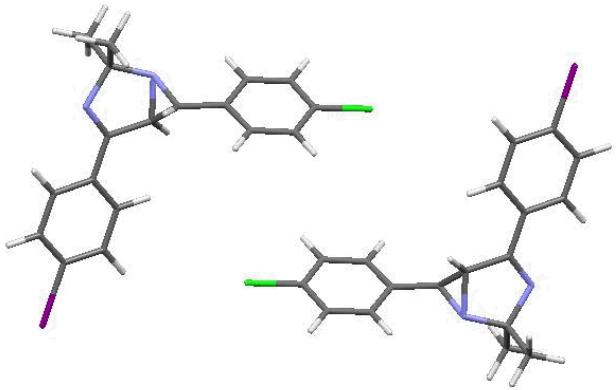

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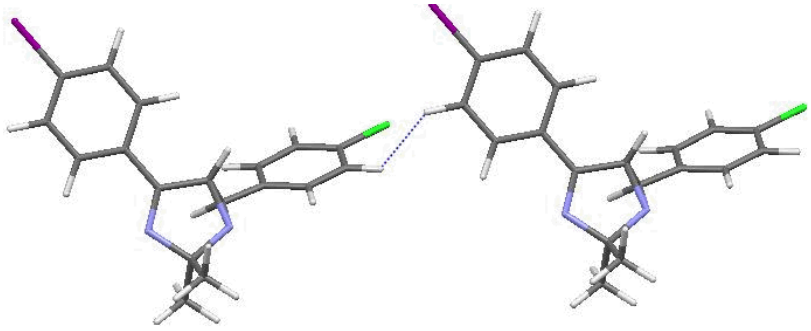

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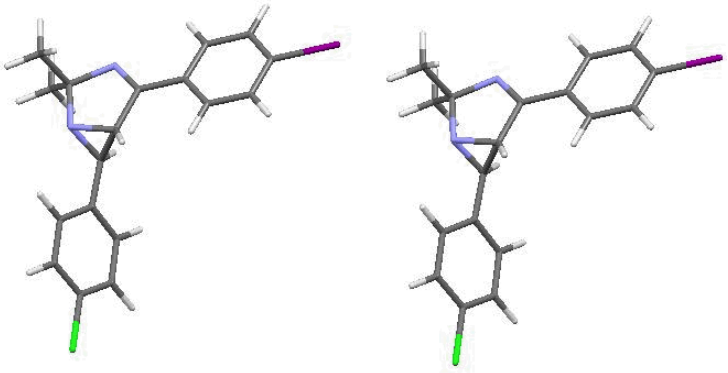

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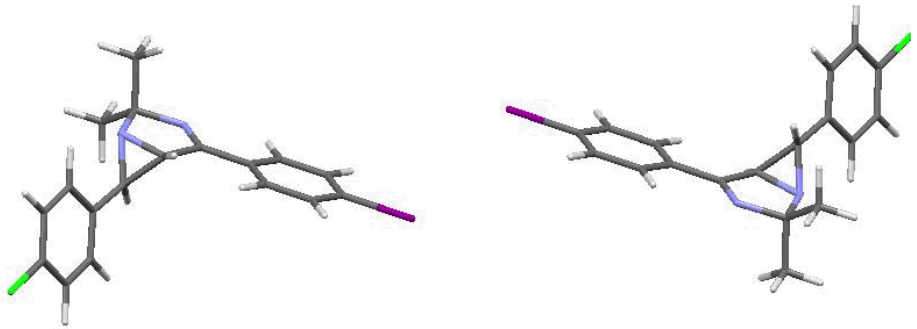
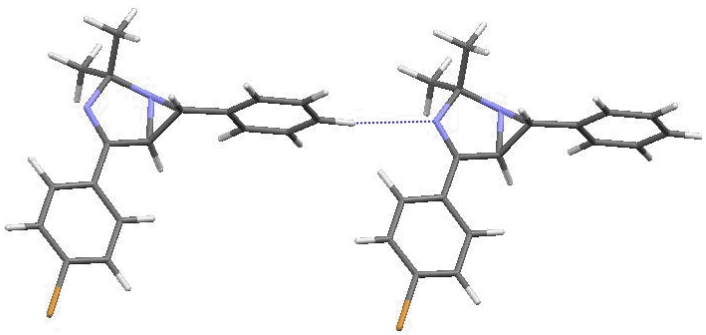
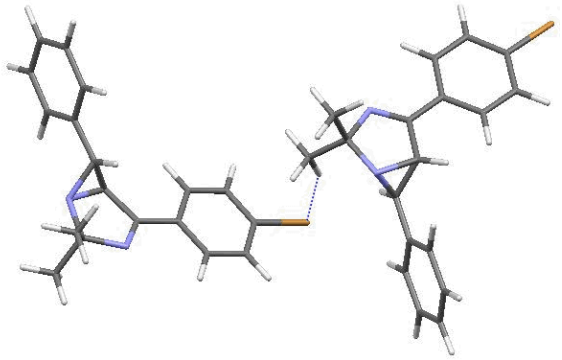


2_17

Fig. S4. Dimers formed by the basic molecule and molecules of its first coordination sphere in crystal structures **2**. Numbering of dimers corresponds to Table 3.

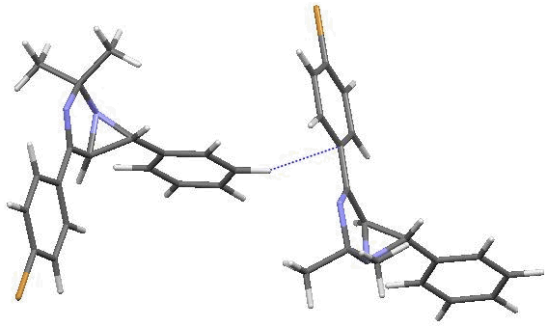


3_5



3_7

3_9



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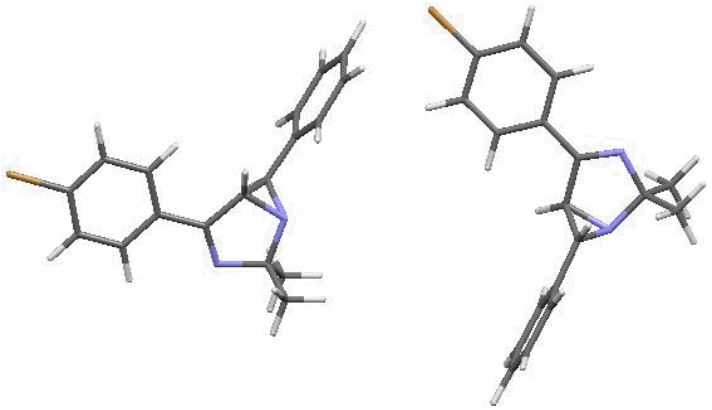

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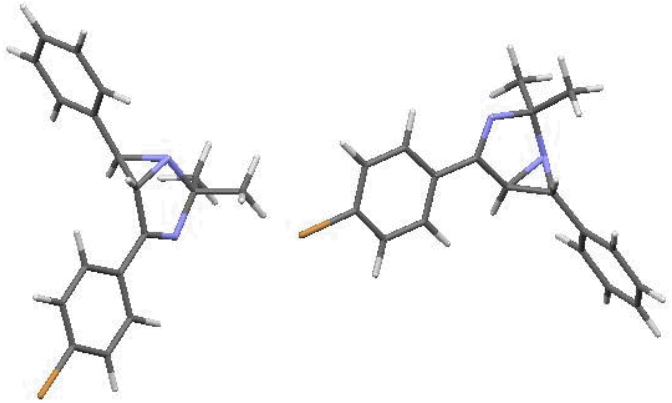
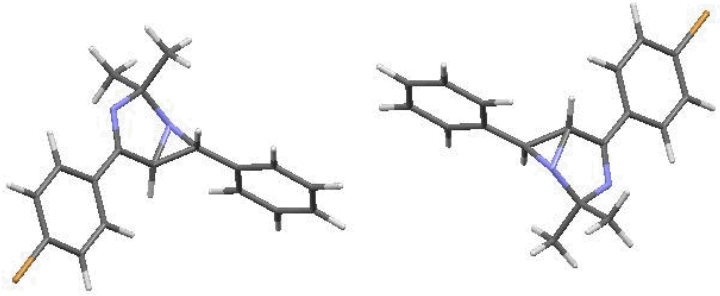


3_14



3_16

Fig. S5. Dimers formed by the basic molecule and molecules of its first coordination sphere in crystal structures **3**. Numbering of dimers corresponds to Table 3.