Supplementary Material (ESI) for CrystEngComm


**Electronic Supplementary Information**

# Columnar Supramolecular Architecture of Crystals of 2-(4-Iodophenyl)-1,10-Phenanthroline Derived from Values of Intermolecular Interaction Energy

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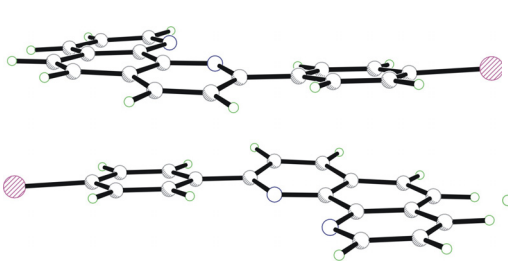
**Table S1** Symmetry codes of neighboring molecules and squares of boundary surfaces (BS, $Å^2$) of the Dirichlet polyhedra for basic molecule located in asymmetric of unit cell**.**

| Neighbor | Symmetry | BS |
|---|---|---|
| 1 | 1-x, 1-y, 1-z | 79.701 |
| 2 | 1-x, 1-y, -z | 47.999 |
| 3 | 2-x, 1-y, 1-z | 36.872 |
| 4 | 1.5-x, -0.5+y, 0.5-z | 20.645 |
| 5 | 1.5-x, 0.5+y, 0.5-z | 20.645 |
| 6 | 0.5-x, -0.5+y, 0.5-z | 19.604 |
| 7 | 0.5-x, 0.5+y, 0.5-z | 19.604 |
| 8 | -0.5+x, 0.5-y, -0.5+z | 18.668 |
| 9 | 0.5+x, 0.5-y, 0.5+z | 18.668 |
| 10 | -1+x, y, z | 15.411 |
| 11 | 1+x, y, z | 15.411 |
| 12 | -0.5+x, 0.5-y, 0.5+z | 14.125 |
| 13 | 0.5+x, 0.5-y, -0.5+z | 14.125 |
| | Total square | 367.3 |



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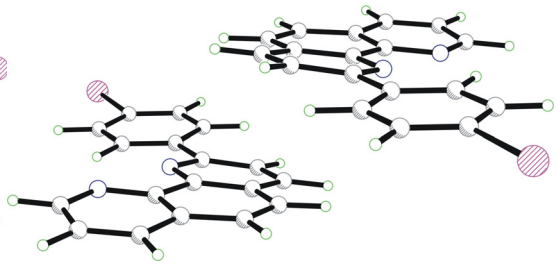

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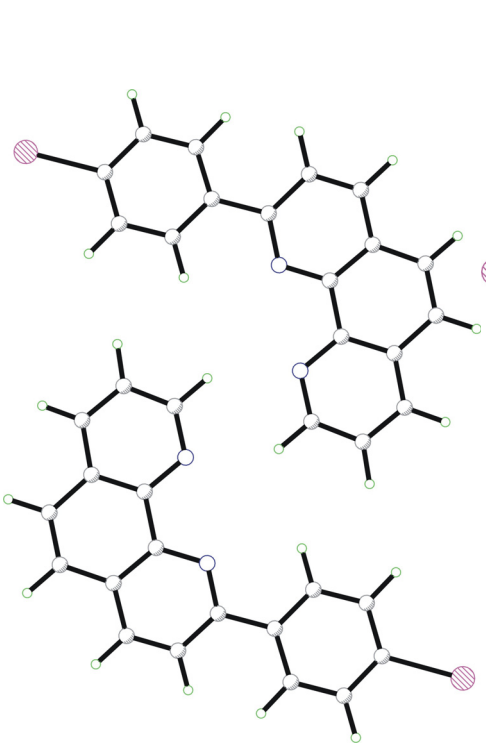

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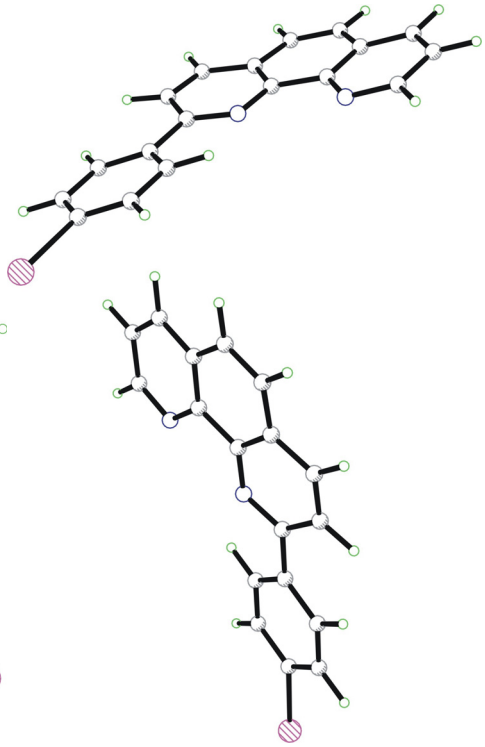

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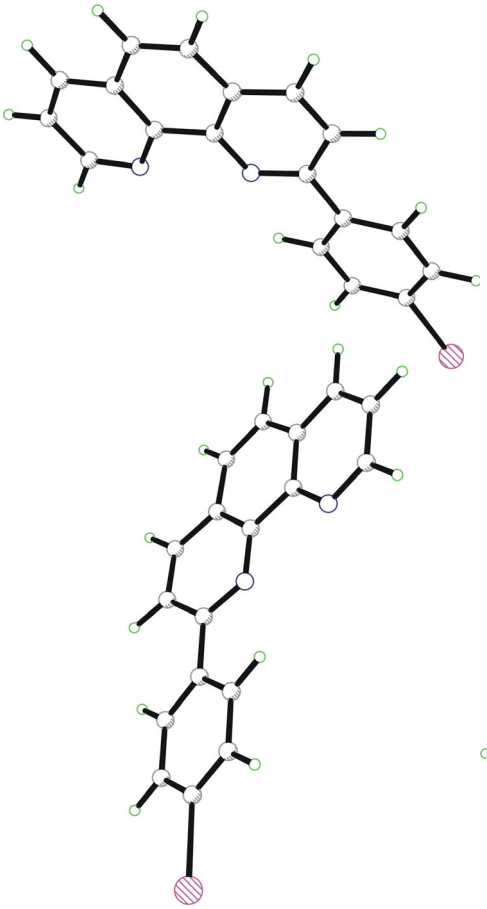

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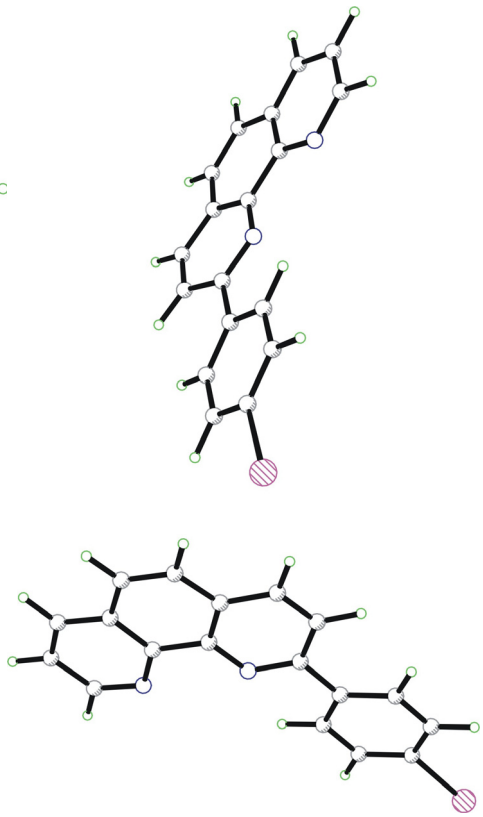

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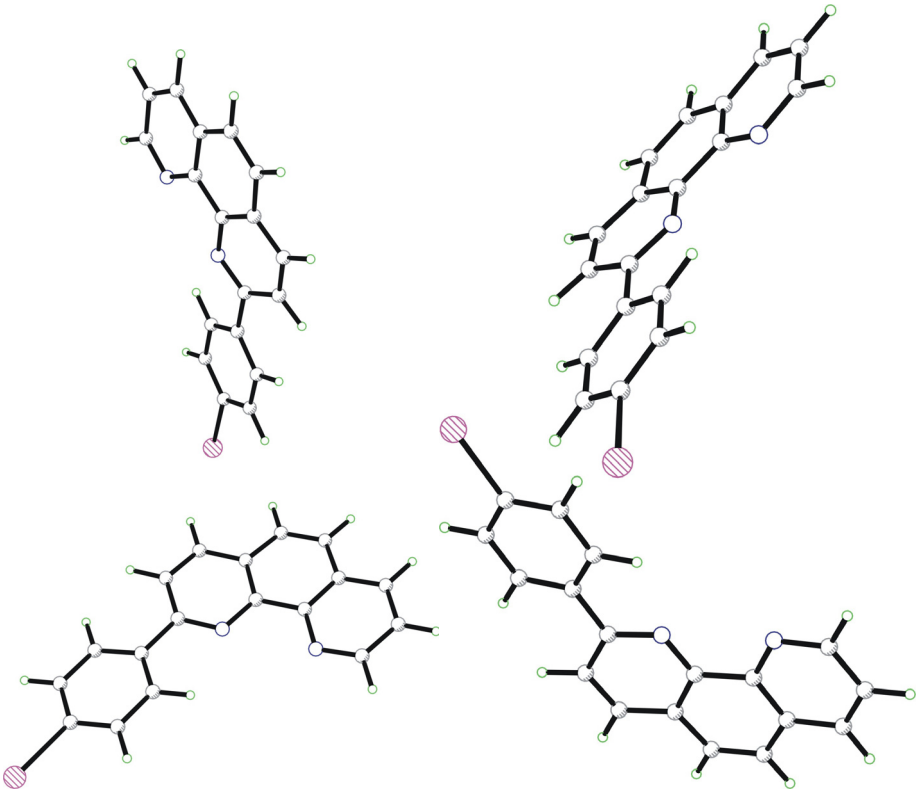
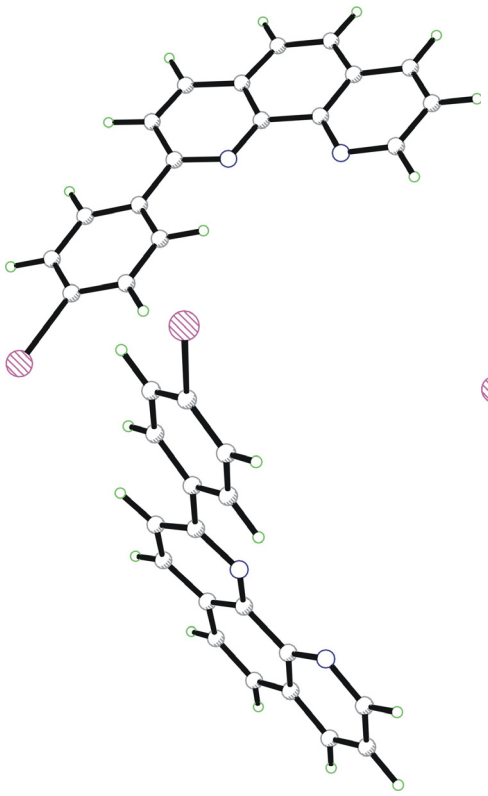


Dimer 7 Dimer 8



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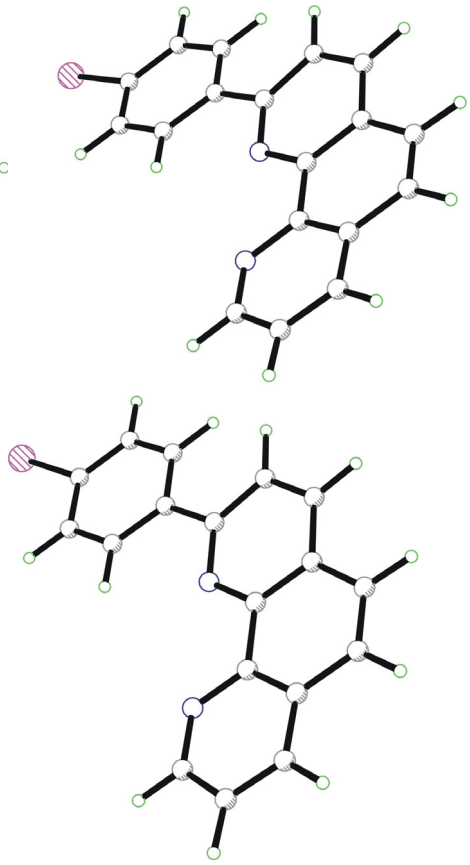

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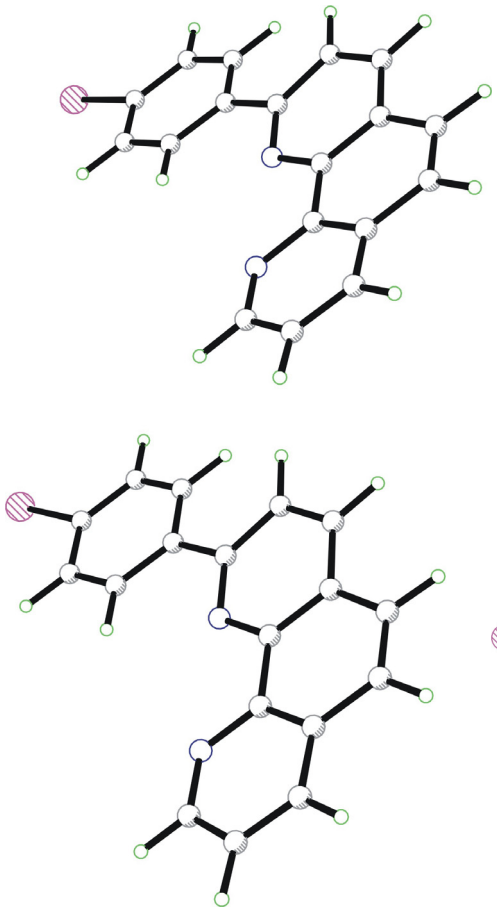

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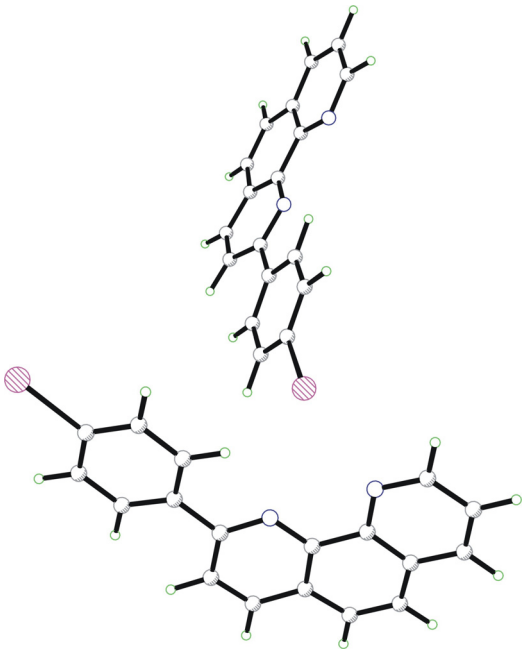

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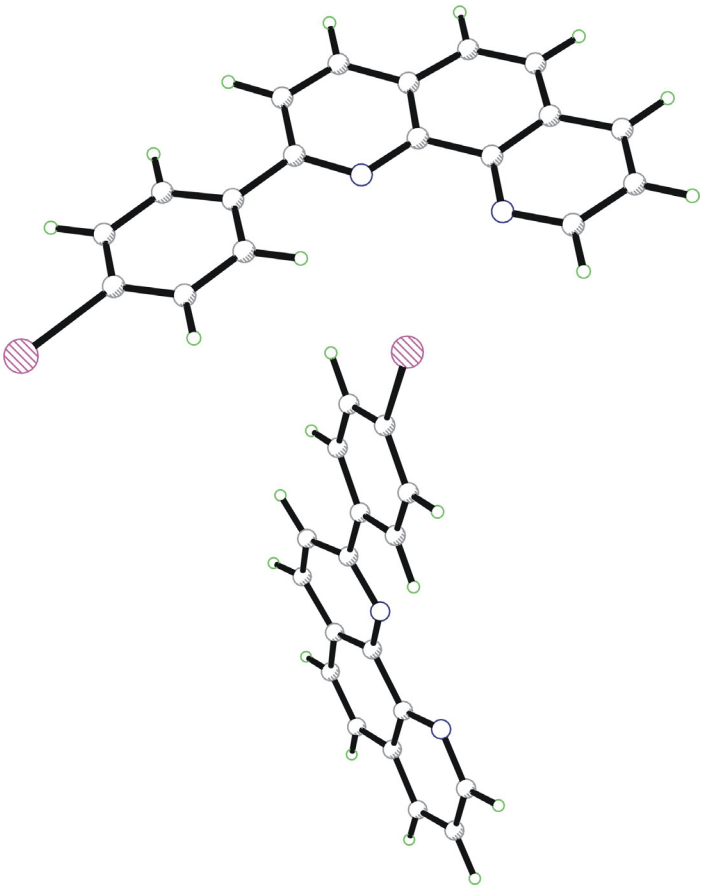

Dimer 13

Fig. S1. Dimers formed by the basic molecule and molecules of its first coordination sphere in the crystal. Numbering of dimers corresponds to Table S1.