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Supporting information for article:

N-Oxide–*N*-oxide interactions and Cl···Cl halogen bonds in penta-chloropyridine *N*-oxide: the many-body approach to interactions in the crystal state

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Supporting Information associated with the article:

Cooperative *N*-oxide...*N*-oxide interactions and Cl…Cl halogen bonds in the crystal structure of pentachloropyridine *N*-oxide

by

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S1. Details of energy parameters estimated for model systems discussed in the paper.

All calculations done at ωB97XD/6-311+G* level of theory.

S1.1 Total energy of a single molecule of I:

HF=-2621.4087955

S1.2 Energy of trimer and its dimeric fragment.

dimer in trimer:

```
 Counterpoise corrected energy =   -5242.818377714102
                     BSSE energy =       0.001448583478
                 sum of monomers =   -5242.817767572912
              complexation energy =      -1.29 kcal/mole (raw)
              complexation energy =      -0.38 kcal/mole (corrected)
```

trimer:

```
 Counterpoise corrected energy =   -7864.228407881881
                     BSSE energy =       0.004146788596
```

```
            sum of monomers =   -7864.226392027406
         complexation energy =      -3.87 kcal/mole (raw)
         complexation energy =      -1.26 kcal/mole (corrected)
```

S1.3 Energy of dimers present in chain long of 6 molecules:

dimer 1 – 2

```
 Counterpoise corrected energy =   -5242.827086669048
                 BSSE energy =       0.004948521476
             sum of monomers =   -5242.817661583818
          complexation energy =      -9.02 kcal/mole (raw)
          complexation energy =      -5.91 kcal/mole (corrected)
```

dimer 1 – 3

```
 Counterpoise corrected energy =   -5242.825394019042
                 BSSE energy =       0.003561320127
             sum of monomers =   -5242.817788238575
          complexation energy =      -7.01 kcal/mole (raw)
          complexation energy =      -4.77 kcal/mole (corrected)
```

dimer 1 – 4

```
 Counterpoise corrected energy =   -5242.818332781834
                 BSSE energy =       0.000281631566
             sum of monomers =   -5242.817763388710
          complexation energy =      -0.53 kcal/mole (raw)
          complexation energy =      -0.36 kcal/mole (corrected)
```

dimer 1 – 5

```
 Counterpoise corrected energy =   -5242.817869657732
                 BSSE energy =       0.000027670196
             sum of monomers =   -5242.817686382152
          complexation energy =      -0.13 kcal/mole (raw)
          complexation energy =      -0.12 kcal/mole (corrected)
```

dimer 1 – 6

```
 Counterpoise corrected energy =   -5242.817788365475
                     BSSE energy =       0.000000007390
                 sum of monomers =   -5242.817688705054
              complexation energy =      -0.06 kcal/mole (raw)
              complexation energy =      -0.06 kcal/mole (corrected)
```

S1.4 Energy of complex in form of chain pattern

Chain – 2 molecules

```
                     BSSE energy =       0.004948521476
                 sum of monomers =   -5242.817661583818
              complexation energy =      -9.02 kcal/mole (raw)
              complexation energy =      -5.91 kcal/mole (corrected)
```

Chain – 3 molecules

```
 Counterpoise corrected energy =   -7864.253192151658
                     BSSE energy =       0.013242206127
                 sum of monomers =   -7864.226552967961
              complexation energy =     -25.03 kcal/mole (raw)
              complexation energy =     -16.72 kcal/mole (corrected)
```

Chain – 4 molecules

```
 Counterpoise corrected energy =  -10485.679461345870
                     BSSE energy =       0.022194443140
                 sum of monomers =  -10485.635292383040
              complexation energy =     -41.64 kcal/mole (raw)
              complexation energy =     -27.72 kcal/mole (corrected)
```

Chain – 5 molecules

```
 Counterpoise corrected energy =  -13107.106201874690
                     BSSE energy =       0.031105909584
```

```
            sum of monomers =  -13107.044242030470
         complexation energy =     -58.40 kcal/mole (raw)
         complexation energy =     -38.88 kcal/mole (corrected)
```

Chain – 6 molecules

```
 Counterpoise corrected energy =  -15728.532960883640
                 BSSE energy =       0.039960853614
            sum of monomers =  -15728.453074690640
         complexation energy =     -75.21 kcal/mole (raw)
         complexation energy =     -50.13 kcal/mole (corrected)
```