Electronic Supplementary Material (ESI) for CrystEngComm.


SUPPORTING INFORMATION

# Geometrical and energetic characteristics of Se···Se interactions in crystal structures of organoselenium molecules

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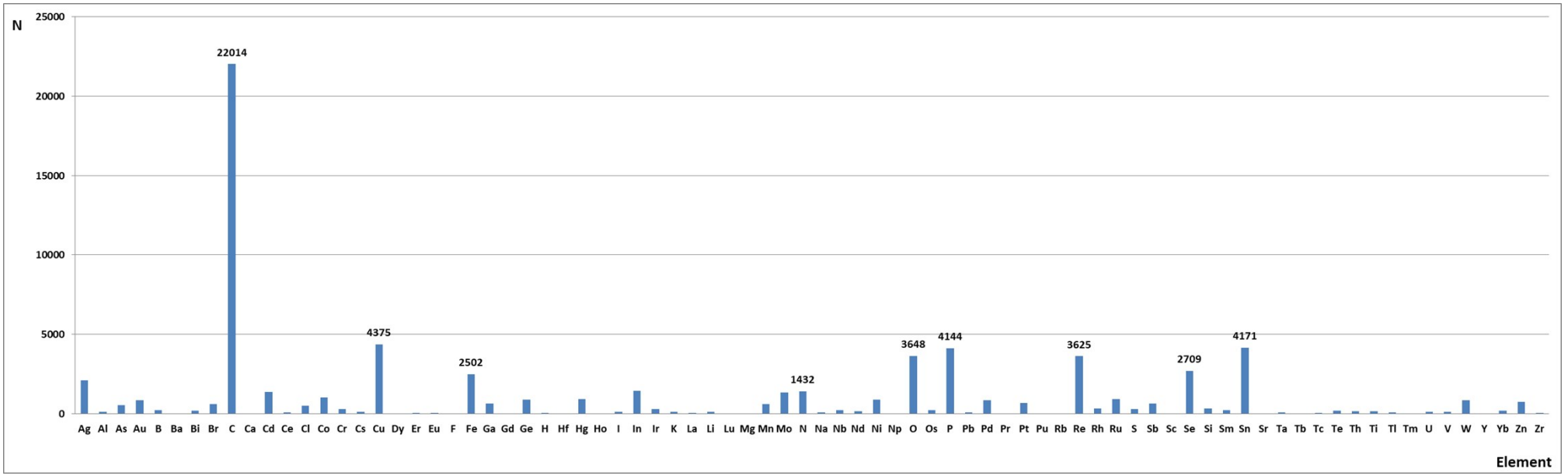


**Figure S1.** Distribution of elements at X position in Se-X fragments extracted from CSD.

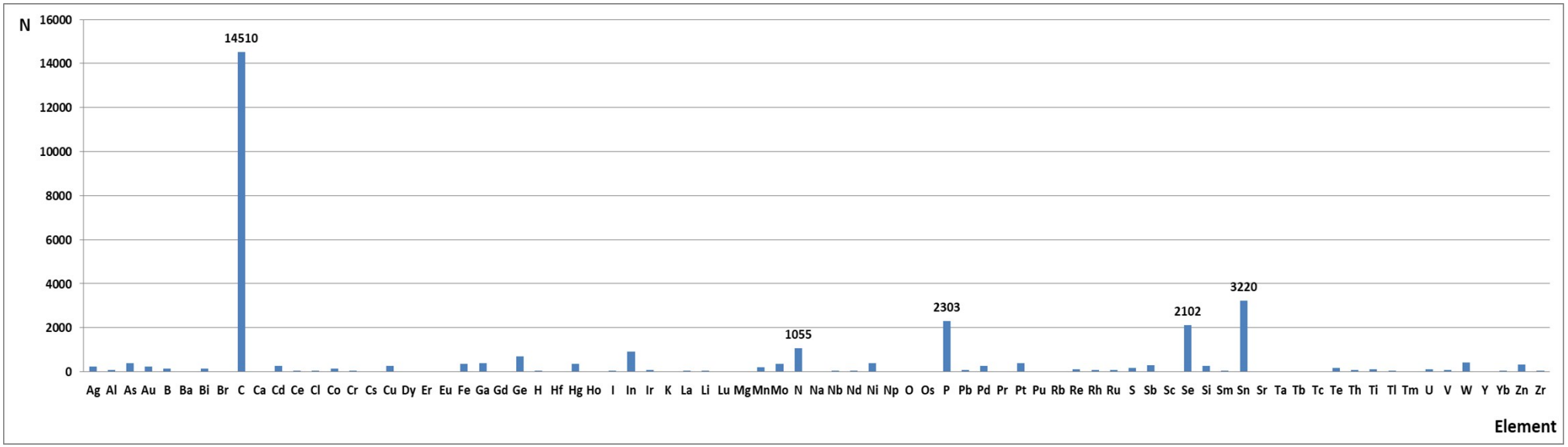


**Figure S2.** Distribution of elements at X position in Se-X fragments in structures in which Se atom is connected to two other atoms.

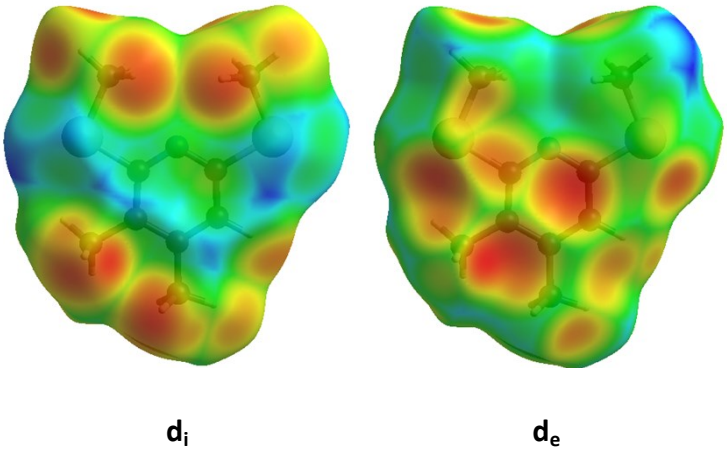


**Figure S3.** The Hirshfeld surface for DEHTER crystal structure mapped with $d_i$ and $d_e$, respectively.

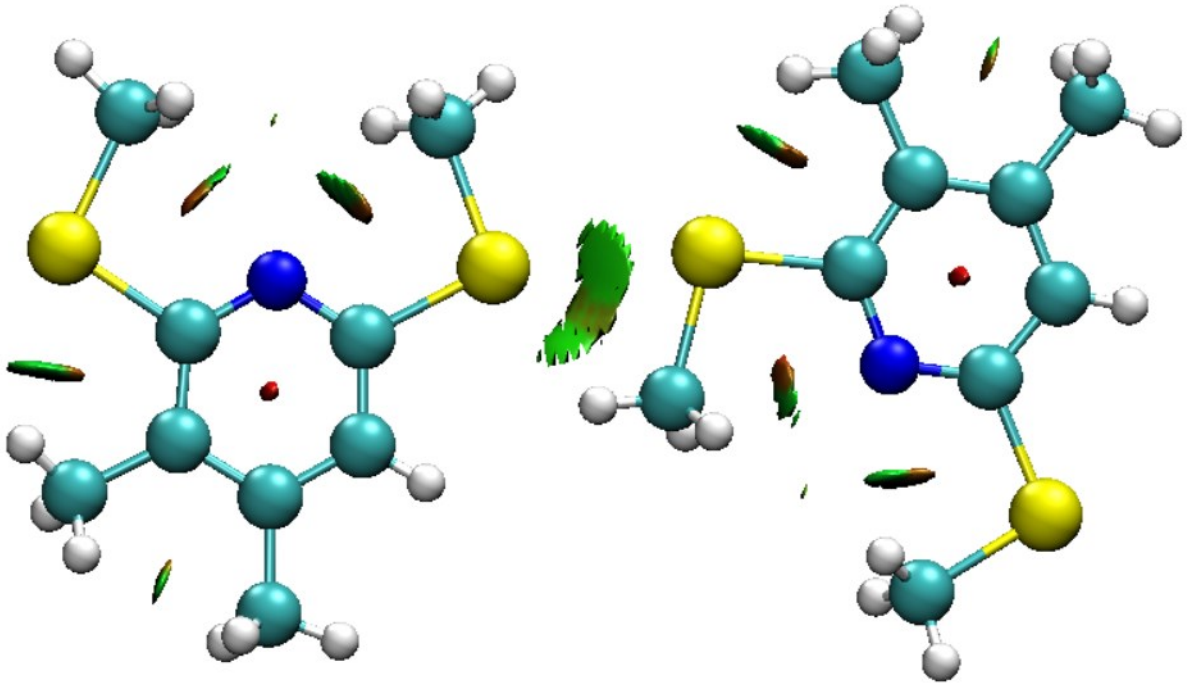

**Figure S4.** Calculated plots of non-covalent interaction isosurfaces for fragment of DEHTER crystal structure (MP2/cc-PVDZ level of theory). Isosurface value used to plot RDG surfaces was 0.5. Green isosurface represents area where attractive non-covalent interactions occur, while brown area corresponds to the repulsive interactions (colour range -0.035 to 0.02) .

## Geometries of model systems used for quantum chemical calculations

**Model system A**

| | | | |
|---|---|---|---|
| H | 2.140525 | 0.644779 | 1.391478 |
| Se | 2.14925 | 0.467681 | -0.044617 |
| C | 2.561906 | -1.422827 | 0.016942 |
| H | 3.520531 | -1.590311 | 0.492207 |
| H | 2.61256 | -1.754059 | -1.015019 |
| H | 1.779195 | -1.969224 | 0.528512 |
| Se | -2.149254 | -0.467682 | 0.044617 |
| H | -2.140529 | -0.64478 | -1.391478 |
| C | -2.56191 | 1.422827 | -0.016942 |
| H | -3.520454 | 1.590323 | -0.492364 |
| H | -1.779115 | 1.969247 | -0.528358 |
| H | -2.612564 | 1.754059 | 1.01502 |

**Model system B**

| | | | |
|---|---|---|---|
| H | -1.853686 | 0.590548 | -1.381283 |
| Se | -2.10211 | 0.475633 | 0.039594 |
| C | -2.558434 | -1.404988 | -0.016338 |
| H | -3.431482 | -1.56899 | -0.635838 |
| H | -2.78713 | -1.690186 | 1.005223 |
| H | -1.720334 | -1.992068 | -0.371038 |
| Se | 2.102114 | -0.475634 | -0.039593 |
| H | 1.85369 | -0.590549 | 1.381283 |
| C | 2.558438 | 1.404987 | 0.016338 |
| H | 3.431381 | 1.56901 | 0.63598 |
| H | 1.72028 | 1.992086 | 0.370873 |
| H | 2.787134 | 1.690185 | -1.005222 |

**Model system C**

| | | | |
|---|---|---|---|
| H | -1.948422 | -0.574018 | 1.391839 |
| Se | -1.91878 | -0.400697 | -0.044438 |
| C | -1.835566 | 1.532554 | 0.01651 |
| H | -2.717474 | 1.93893 | 0.496079 |
| H | -1.805187 | 1.865647 | -1.015649 |
| H | -0.936919 | 1.86142 | 0.523629 |
| Se | 1.918784 | 0.400697 | 0.044438 |
| C | 1.83557 | -1.532554 | -0.01651 |
| H | 1.948426 | 0.574018 | -1.391839 |
| H | 2.717396 | -1.938921 | -0.496235 |
| H | 0.936837 | -1.861421 | -0.523474 |
| H | 1.805191 | -1.865647 | 1.015649 |

**Model system D**

| | | | |
|---|---|---|---|
| H | 1.9761770 | -1.8536650 | -1.0283380 |
| Se | 0.8493260 | -1.5870250 | -0.1606290 |
| C | 0.8493260 | -3.3379040 | 0.6655190 |
| H | 0.6701460 | -4.1097410 | -0.0727560 |
| H | 0.0343930 | -3.3332220 | 1.3818200 |
| H | 1.7815240 | -3.5150730 | 1.1875410 |
| Se | -0.9436950 | 1.7633600 | -0.1606290 |
| H | -2.0705460 | 2.0300000 | -1.0283380 |
| C | -0.9436950 | 3.5142390 | 0.6655190 |
| H | -1.8758930 | 3.6914080 | 1.1875410 |
| H | -0.7645150 | 4.2860760 | -0.0727560 |
| H | -0.1287620 | 3.5095570 | 1.3818200 |

**Model system E**

| | | | |
|---|---|---|---|
| H | 1.0564220 | 0.0371990 | 1.0036630 |
| Se | 1.7861080 | -0.0467680 | -0.2430590 |
| C | 3.5258910 | 0.2432580 | 0.5551480 |
| H | 3.5709610 | 1.2140410 | 1.0331020 |
| H | 4.2405550 | 0.2137000 | -0.2606990 |
| H | 3.7590660 | -0.5436500 | 1.2617570 |
| Se | -1.8811140 | -0.3941790 | 0.1044910 |
| C | -2.6228110 | 1.3940670 | 0.0918540 |
| H | -1.9975650 | -0.5923770 | -1.3241330 |
| H | -3.6417610 | 1.3834870 | -0.2749120 |
| H | -2.0081230 | 2.0594570 | -0.5016980 |
| H | -2.6182980 | 1.7295690 | 1.1236690 |

**Table S1.** Distribution of angle formed between two C-Se-X planes (P1/P2 angle) in CSD crystal containing Se···Se contacts.

| P1/P2(°) | N |
|---|---|
| 0-10 | 1483 |
| 10-20 | 234 |
| 20-30 | 228 |
| 30-40 | 230 |
| 40-50 | 324 |
| 50-60 | 403 |
| 60-70 | 620 |
| 70-80 | 803 |
| 80-90 | 674 |

**Table S2.** Interaction energies for model systems A-E calculated at CCSD(T)/CBS level of theory.

| **model system A** | | **model system B** | | **model system C** | | **model system D** | | **model system E** | |
|---|---|---|---|---|---|---|---|---|---|
| d[a] | ΔE[b] | d | ΔE | d | ΔE | d | ΔE | d | ΔE |
| 4.20 | -0.48 | 4.00 | -0.63 | 3.70 | -2.19 | 3.70 | -0.91 | 3.60 | -1.99 |
| 4.30 | -0.52 | 4.10 | -0.69 | 3.75 | -2.27 | 3.80 | -0.94 | 3.70 | -2.13 |
| 4.40 | -0.54 | 4.20 | -0.71 | 3.80 | -2.31 | 3.90 | -0.93 | 3.80 | -2.11 |
| 4.50 | -0.53 | 4.25 | -0.72 | 3.90 | -2.30 | 4.00 | -0.89 | 3.85 | -2.07 |
| 4.60 | -0.52 | 4.30 | -0.71 | 4.00 | -2.22 | 4.10 | -0.83 | 3.90 | -2.01 |

a distances are given in Å

b Interaction energies are given in kcal/mol