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Supporting information for article:

A heuristic approach to evaluate peri interactions vs. intermolecular interactions in an overcrowded naphthalene

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A heuristic approach to evaluate peri interactions vs. intermolecular interactions in overcrowded naphthalene

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Supporting information

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Figure S12: Molecular conformations showing the angular geometries of the type II Cl•••Cl interactions in the geometry of trimer T1

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Figure S17: Molecular packing diagram of Octachloronaphthalene (OCN) viewed along b axis. The right arrow indicates the direction of dipole moment vector. Blue indicates the c axis, red indicates the a axis, and green indicates the b axis.
Figure S18: (a) Comparison of $\rho$ values for all covalent bonds obtained from experiment and theory. (b) Comparison of $\nabla^2 \rho$ values for all covalent bonds obtained from experiment and theory.

**Table S1: Monopole Populations, Radial Parameters and Net Atomic Charges**

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**Table S3: Quadrupole Population Parameters**

**Table S4: Octupole Population Parameters.**

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**Table S6: Aim charge of the individual atoms derived from the experimental multipole modeled electron density.**

**Table S7: Electrostatic Potential calculated at the nuclear sites of each atom.**

**Table S8: Topological features obtained for all covalent bonds in OCN.** $r_1$ and $r_2$ are the distances from the BCP to the first atom (A) and second atom (B), respectively. The interaction length, $R_{ij} = (r_1 + r_2)$. The values obtained from periodic calculations using the M062X/TZVP method are given in italics.

### S1. Quality of multipole modeling

The topological features of the intra and intermolecular interactions have been explored on the basis of multipole modeling on experimental structure factors using the Hansen–Coppens formalism. The Hirshfeld rigid bond (Hirshfeld, 1976) test applied to all covalent bonds validates the quality of the multipole model after the final cycle of refinement. The C(9)-Cl(8) single bond is found to have the largest difference of mean square displacement amplitude (DMSDA) value of $4 \times 10^{-4}$ Å$^2$. The residual electron density peaks are -0.44 and 0.47e Å$^{-3}$ with an RMS value of 0.09 eÅ$^{-3}$ for minimum and maximum values, respectively at full resolution (1.08 Å$^{-1}$, Fig. S4). The fractal dimension plot (Meindl & Henn, 2008) (Fig S5) which provides the overall distribution of residual electron density in the unit cell is symmetric in nature and parabolic in shape ($\sin\theta/\lambda \leq 0.8$Å$^{-1}$).

### S2. Computational details

#### S2.1. Periodic DFT calculation

Positional parameters obtained from the experimental charge density model have been used for density functional calculations using the hybrid exchange correlational functional M062X (Zhao & Truhlar, 2008) with TZVP (Schäfer et al., 1992; Peintinger et al., 2013) basis set included in CRystal14 package (Dovesi et al., 2013). The shrinking factors (IS1, IS2, and IS3) and the reciprocal lattice vectors were set to 4 (with 30 k-points in irreducible Brillouin zone). The
bielectronic Coulomb and exchange series values for the truncation parameter were set as ITOL1-ITOL4 = 7 and ITOL5 = 14, respectively, for the calculations. The level shifter was set to 0.3 Hartree/cycle as 30% mixing of Fock/KS matrices (FMIXING) given in the input. An SCF convergence limit of the order of $10^{-6}$ Hartree was used. In the static model, atomic thermal displacement parameters for all atoms were set to zero. Structure factors were calculated for a resolution of 1.11Å$^{-1}$, which were used for the theoretical multipolar model. Refinements and analysis for the theoretical charge density model were performed using the XD software package following the same methodology used for the experimental charge density modeling.

**S2.2. NCI Analysis**

NCImilano (Saleh et al., 2013) has been performed with the rho (electron density) and gradrho (gradient of electron density) grid files obtained from experimentally modeled electron density. It generated RDG and $\rho^*\text{sign}(\lambda_2)$ cube files with rho (r) cutoff value 0 to 0.05 au. Reduced density gradient (RDG) isosurface value was generated at 0.6 au and plotted in MoleCoolQt software (Hübschle & Dittrich, 2011). The color scale of RDG surfaces is $-0.02 < r < 0.015$ au.

**S2.3. NICS**

The nucleus independent chemical shift (NICS) has been calculated using the GAUSSIAN09 (Frisch et al., 2009) package by the GIAO (London, 1937; Cheeseman et al., 1996) method at the M062X/6-311+g* level of density functional theory.

**S2.4. Geometry optimization**

Energy optimization (taking the initial geometry from crystalline phase minima) was performed using the integral equation formalism (IEF) version of the polarizable continuum solvation model (PCM) (Tomasi et al., 2005) at wB97XD (Chai & Head-Gordon, 2008)/6-311+g* level to examine the dielectric field effect of crystallizing solvent (benzene) on the optimized conformation of OCN.

**S2.5. Energy vs. dihedral angle scans**

The $\phi_1$(Cl(4)-C(4)-C(6)-Cl(5)) dihedral angle was varied, and energy was estimated at the interval of $-0.0524^\circ$ in 25 steps, allowing the geometry to be relaxed at each point of $f_1$. In case of $\phi_2$(Cl(1)-C(1)-C(9)-Cl(8)), energy was estimated at the interval of $-0.5444^\circ$ in 25 steps. Calculations were performed using PCM at wB97XD/6-311+g* level.
Figure S1  (a) Scatter plot depicting the variation of $F_{\text{obs}}$ with $F_{\text{cal}}$. (b) Variation of $F_{\text{obs}}^2/F_{\text{cal}}^2$ with $(\sin \theta)/\lambda$.

Figure S2  3D residual density plot at $\pm 0.2 \text{ eÅ}^{-3}$ contour intervals

Figure S3  Fractal dimension plot for data $(\sin \theta/\lambda \leq 0.8 \text{Å}^{-1})$
Figure S4  Cl⋯Cl Interaction motifs of top half of OCN

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Figure S8  3D deformation density; (b) 3D Laplacian plot of the Cl(1)•••Cl(8) interaction region; (c) 3D deformation density and (d) 3D Laplacian plot of the Cl(4)•••Cl(5) interaction region. Blue represents charge concentration (CC) and red represents charge depletion (CD) in deformation maps drawn at the intervals of ±0.08 eÅ⁻³. 3D Laplacian isosurfaces is plotted at -17.5eÅ⁻⁵.
**Figure S9**  (a) Potential energy scan for dihedral angle $\phi_2$ (b) Potential energy scan for dihedral angle $\phi_1$

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**Figure S11** (a) 2D deformation density; (b) 2D Laplacian plot of the intermolecular Cl(5)⋯Cl(3) interaction region. Blue (solid lines) and red (broken lines) colors represent positive, negative contours respectively (reversed in case of Laplacian). Contours are drawn at the intervals of $\pm 0.05$ e\ Å$^3$. Laplacian is plotted on logarithmic contours.
**Figure S12** Molecular conformations showing the angular geometries of the type II Cl•••Cl interactions in the geometry of trimer T1

![Figure S12](image1)

**Figure S13** Molecular conformations showing the angular geometries of the type II Cl•••Cl interactions in the crystal geometry of trimer T1°

![Figure S13](image2)

**Figure S14** Molecular conformations showing the angular geometries of the type II Cl•••Cl interactions in the optimized geometry of trimer T1'.

![Figure S14](image3)

**Figure S15** (a) Plot of RDG (reduced density gradient) vs. electron density (ρ). (b) Plot of RDG (reduced density gradient) vs. electron density electron density multiplied by the sign of the second Hessian eigen value (ρ*sign(λ₂)) for peri interaction between Cl(1)•••Cl(8).

![Figure S15](image4)
Figure S16 (a) Plot of RDG (reduced density gradient) vs. electron density ($\rho$). (b) Plot of RDG (reduced density gradient) vs. electron density multiplied by the sign of the second Hessian eigen value ($\rho \cdot \text{sign}(\lambda_2)$) for peri interaction between Cl(4)⋅⋅⋅Cl(5).

Figure S17 Molecular packing diagram of Octachloronaphthalene (OCN) viewed along b axis. The right arrow indicates the direction of dipole moment vector. Blue indicates the c axis, red indicates the a axis, green indicates the b axis.
Figure S18 (a) Comparison of \( \rho \) values for all covalent bonds obtained from experiment and theory. (b) Comparison of \( \nabla^2 \rho \) values for all covalent bonds obtained from experiment and theory.

Table S1  Monopole Populations, Radial Parameters and Net Atomic Charges.

| Atom  | \( P_{\text{val}} \) | Kappa | \( P_{00} \) | Kappa' | Atomic charge |
|-------|------------------|-------|-------------|--------|---------------|
| CL(1) | 6.939            | 1.023 | 0           | 0.994  | 0.061         |
| CL(2) | 6.797            | 1.024 | 0           | 0.985  | 0.203         |
| CL(3) | 7.166            | 1.017 | 0           | 1.022  | -0.166        |
| CL(4) | 7.213            | 1.018 | 0           | 0.981  | -0.214        |
| CL(5) | 7.104            | 1.022 | 0           | 0.989  | -0.104        |
| CL(6) | 7.105            | 1.021 | 0           | 0.976  | -0.105        |
| CL(7) | 6.873            | 1.023 | 0           | 1.009  | 0.127         |
| CL(8) | 6.940            | 1.020 | 0           | 0.990  | 0.060         |
| C(1)  | 3.860            | 1.024 | 0           | 0.976  | 0.140         |
| C(2)  | 4.018            | 1.020 | 0           | 0.974  | -0.018        |
| C(3)  | 3.981            | 1.015 | 0           | 0.994  | 0.019         |
| C(4)  | 4.195            | 1.007 | 0           | 1.014  | -0.195        |
| C(10) | 3.811            | 1.038 | 0           | 0.988  | 0.190         |
| C(5)  | 4.215            | 1.003 | 0           | 1.038  | -0.215        |
| C(6)  | 4.016            | 1.020 | 0           | 0.994  | -0.016        |
| C(7)  | 4.069            | 1.007 | 0           | 0.980  | -0.069        |
| C(8)  | 3.792            | 1.034 | 0           | 0.992  | 0.208         |
Table S2  Dipole Population Parameters.

| Atom | D11⁺   | D11⁻   | D10    | Kappa' |
|------|--------|--------|--------|--------|
| CL(1)| 0.077  | -0.024 | -0.014 | 0.994  |
| CL(2)| -0.006 | 0.016  | -0.004 | 0.985  |
| CL(3)| -0.075 | -0.052 | 0.007  | 1.022  |
| CL(4)| 0.068  | 0.002  | 0.042  | 0.981  |
| CL(5)| 0.049  | 0.034  | 0.007  | 0.989  |
| CL(6)| -0.036 | -0.038 | -0.034 | 0.976  |
| CL(7)| -0.010 | 0.011  | 0.025  | 1.009  |
| CL(8)| 0.033  | -0.024 | -0.003 | 0.990  |
| C(1) | -0.013 | 0.012  | 0.027  | 0.976  |
| C(2) | -0.003 | 0.059  | 0.023  | 0.974  |
| C(3) | -0.015 | 0.018  | 0.021  | 0.994  |
| C(4) | -0.021 | 0.010  | 0.027  | 1.014  |
| C(10)| -0.013 | 0.008  | -0.002 | 0.988  |
| C(5) | -0.018 | 0.020  | 0.022  | 1.038  |
| C(6) | -0.009 | 0.022  | 0.036  | 0.994  |
| C(7) | -0.019 | 0.022  | 0.040  | 0.980  |
| C(8) | 0.012  | 0.054  | -0.021 | 0.992  |
| C(9) | -0.014 | -0.038 | -0.027 | 0.967  |

Table S3  Quadrupole Population Parameters.

| Atom | Q20    | Q21⁺   | Q21⁻   | Q22⁺   | Q22⁻   | Kappa' |
|------|--------|--------|--------|--------|--------|--------|
| CL(1)| -0.222 | 0.075  | 0.135  | 0.180  | -0.010 | 0.994  |
| CL(2)| -0.325 | 0.019  | -0.029 | 0.121  | 0.059  | 0.985  |
| CL(3)| -0.197 | -0.116 | -0.081 | 0.199  | 0.062  | 1.022  |
| CL(4)| -0.229 | 0.113  | -0.083 | 0.221  | -0.070 | 0.981  |
### Table S4  Octupole Population Parameters.

| Atom | O30  | O31+ | O31- | O32+ | O32- | O33+ | O33- | Kappa' |
|------|------|------|------|------|------|------|------|--------|
| CL(1)| 0.069 | 0.010 | 0.007 | -0.044 | 0.005 | -0.020 | 0.018 | 0.994 |
| CL(2)| 0.033 | 0.018 | -0.038 | 0.010 | -0.009 | 0.022 | 0.008 | 0.985 |
| CL(3)| 0.031 | 0.011 | 0.023 | 0.012 | 0.034 | 0.085 | -0.015 | 1.022 |
| CL(4)| 0.025 | 0.040 | -0.001 | 0.034 | 0.055 | -0.001 | 0.028 | 0.981 |
| CL(5)| 0.041 | 0.038 | 0.005 | -0.025 | 0.056 | -0.036 | 0.024 | 0.989 |
| CL(6)| 0.048 | -0.023 | 0.029 | 0.044 | 0.045 | 0.077 | 0.005 | 0.976 |
| CL(7)| 0.041 | 0.000 | 0.055 | 0.038 | -0.013 | 0.002 | 0.016 | 1.009 |
| CL(8)| 0.054 | 0.008 | 0.033 | -0.019 | 0.030 | -0.012 | -0.011 | 0.990 |
| C(1) | 0.215 | -0.001 | -0.020 | 0.205 | 0.047 | 0.026 | 0.032 | 0.976 |
| C(2) | 0.244 | -0.013 | 0.020 | 0.189 | 0.036 | -0.017 | 0.000 | 0.974 |
| C(3) | 0.170 | -0.025 | 0.016 | 0.184 | -0.019 | 0.006 | 0.024 | 0.994 |
| C(4) | 0.211 | -0.010 | -0.006 | 0.163 | 0.035 | 0.006 | -0.001 | 1.014 |
| Atom | H40 | H41+ | H41- | H42+ | H42- | H43+ | H43- | H44+ | H44- | Kappa' |
|------|-----|------|------|------|------|------|------|------|------|-------|
| C(5) | 0.219 | 0.018 | 0.030 | 0.145 | -0.014 | 0.016 | 0.016 | 0.988 |
| C(6) | 0.205 | -0.020 | 0.011 | 0.147 | 0.015 | -0.038 | 0.007 | 1.038 |
| C(7) | 0.216 | 0.003 | 0.009 | 0.194 | -0.035 | 0.005 | 0.004 | 0.994 |
| C(8) | 0.230 | -0.013 | 0.002 | 0.208 | 0.028 | 0.022 | 0.023 | 0.980 |
| C(9) | 0.213 | -0.005 | 0.008 | 0.178 | 0.038 | -0.039 | 0.006 | 0.992 |
| C(10) | 0.251 | -0.066 | 0.020 | 0.195 | 0.001 | 0.008 | 0.037 | 0.967 |

**Table S5** Hexadecapole Population Parameters

| Atom | H40 | H41+ | H41- | H42+ | H42- | H43+ | H43- | H44+ | H44- | Kappa' |
|------|-----|------|------|------|------|------|------|------|------|-------|
| CL(1) | -0.008 | 0.009 | 0.03 | -0.077 | 0.01 | 0.044 | 0.03 | 0.01 | 0.013 | 0.994 |
| CL(2) | 0.129 | -0.011 | 0.059 | -0.039 | 0.01 | 0.029 | -0.026 | 0.032 | 0.054 | 0.985 |
| CL(3) | 0.02 | 0.004 | -0.025 | -0.011 | -0.033 | -0.006 | -0.048 | 0.006 | -0.042 | 1.022 |
| CL(4) | -0.033 | 0.007 | -0.036 | -0.022 | 0.032 | 0.026 | -0.029 | 0.032 | -0.011 | 0.981 |
| CL(5) | -0.008 | -0.002 | 0.016 | -0.051 | 0.025 | 0.064 | 0.013 | 0.021 | -0.031 | 0.989 |
| CL(6) | 0.118 | 0.06 | 0 | 0.043 | -0.025 | -0.026 | -0.017 | 0.023 | -0.018 | 0.976 |
| CL(7) | 0.013 | 0.008 | -0.057 | -0.017 | -0.02 | 0.013 | -0.043 | 0.073 | 0.039 | 1.009 |
| CL(8) | -0.011 | 0.009 | -0.052 | -0.039 | 0.007 | 0.057 | -0.055 | 0.024 | 0.013 | 0.990 |
| C(1) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.976 |
| C(2) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.974 |
| C(3) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.994 |
| C(4) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1.014 |
| C(10) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.988 |
| C(5) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1.038 |
| C(6) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.994 |
| C(7) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.98 |
| C(8) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.992 |
| C(9) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.967 |
**Table S6**  Aim charge of the individual atoms derived from the experimental ($Q_{\text{exp}}$) and theoretical ($Q_{\text{theo}}$) multipole modeled electron density.

| Atom  | $Q_{\text{exp}}$ | $Q_{\text{theo}}$ |
|-------|------------------|------------------|
| CL(1) | -0.0369          | -0.1818          |
| CL(2) | 0.1108           | -0.1351          |
| CL(3) | -0.2626          | -0.1513          |
| CL(4) | -0.3238          | -0.0740          |
| CL(5) | -0.2123          | -0.0333          |
| CL(6) | -0.1954          | -0.1388          |
| CL(7) | 0.0121           | -0.0455          |
| CL(8) | -0.0258          | -0.1698          |
| C(1)  | 0.2185           | 0.0000           |
| C(2)  | 0.0715           | 0.0209           |
| C(3)  | 0.1256           | 0.0956           |
| C(4)  | -0.0633          | 0.1798           |
| C(10) | 0.1457           | 0.1916           |
| C(5)  | -0.0856          | 0.2308           |
| C(6)  | 0.0506           | 0.0881           |
| C(7)  | 0.0707           | 0.0543           |
| C(8)  | 0.2551           | -0.0240          |
| C(9)  | 0.1471           | 0.1006           |

**Table S7**  Electrostatic Potential (eÅ$^{-1}$) calculated at the nuclear sites of each atom. $V_{\text{exp}}$-Potential calculated from the experimental multipole model; $V_{\text{theory}}$-Potential calculated from the theoretical multipole model.

| Atom  | $V_{\text{exp}}$ | $V_{\text{theory}}$ |
|-------|------------------|---------------------|
| CL(1) | -121.666         | -121.853            |
| CL(2) | **-121.610**     | **-121.764**        |
| CL(3) | -122.066         | -121.710            |
Table S8  Topological features obtained for all covalent bonds in OCN. $r_1$ and $r_2$ are the distances from the BCP to the first atom (A) and second atom (B), respectively. The interaction length, $R_{ij} = (r_1 + r_2)$. The values obtained from periodic calculations using the M062X/TZVP method are given in italics.

| Atom A | Atom B | $R_{ij}$ (Å) (A-B) | $r_1$ (Å) (A-CP) | $r_2$ (Å) (CP-B) | $\rho(\mathbf{r})_{cp}$ (eÅ$^{-3}$) | $\nabla^2 \rho$ (eÅ$^{-5}$) | $\lambda_1$ | $\lambda_2$ | $\lambda_3$ | $\varepsilon$ |
|--------|--------|-------------------|------------------|------------------|-------------------------------|-----------------|-------------|-------------|-------------|-------------|
| C(1)   | CL(1)  | 1.7211            | 0.7968           | 0.9243           | 1.27                          | -0.45            | -7.24       | -6.78       | 13.57       | 0.07        |
|        |        | 1.7207            | 0.8038           | 0.9169           | 1.25                          | -0.22            | -6.69       | -6.14       | 12.61       | 0.09        |
| C(2)   | CL(2)  | 1.7119            | 0.7868           | 0.9251           | 1.29                          | -2.03            | -8.43       | -6.99       | 13.40       | 0.21        |
|        |        | 1.7110            | 0.7956           | 0.9160           | 1.30                          | -1.29            | -7.32       | -6.32       | 12.36       | 0.16        |
| C(3)   | CL(3)  | 1.7131            | 0.7875           | 0.9256           | 1.34                          | -0.74            | -7.93       | -6.53       | 13.72       | 0.21        |
|        |        | 1.7130            | 0.7931           | 0.9199           | 1.3                           | -1.15            | -7.07       | -6.61       | 12.52       | 0.07        |
| C(4)   | CL(4)  | 1.7220            | 0.7981           | 0.9239           | 1.29                          | -0.90            | -7.46       | -6.47       | 13.84       | 0.15        |
|        |        | 1.7193            | 0.8007           | 0.9186           | 1.27                          | -0.58            | -7.30       | -5.59       | 12.31       | 0.31        |
| C(5)   | CL(5)  | 1.7203            | 0.7927           | 0.9276           | 1.31                          | -1.95            | -7.34       | -6.48       | 11.87       | 0.13        |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|   |   |   |   |   |   |   |
| C(7) | CL(6) | 1.7201 | 0.8027 | 0.9174 | 1.26 | -0.43 | -7.14 | -6.31 | 13.02 | 0.13 |
| C(8) | CL(7) | 1.7112 | 0.7911 | 0.9201 | 1.31 | -1.78 | -8.96 | -6.53 | 13.71 | 0.37 |
| C(9) | CL(8) | 1.7132 | 0.7912 | 0.922 | 1.30 | -1.1 | -7.93 | -6.26 | 13.09 | 0.27 |
| C(1) | C(2) | 1.3841 | 0.6831 | 0.701 | 2.09 | -18.44 | -18.14 | -12.1 | 11.79 | 0.50 |
| C(1) | C(10) | 1.4352 | 0.7156 | 0.7196 | 1.81 | -13.88 | -15.24 | -10.59 | 11.95 | 0.44 |
| C(3) | C(2) | 1.4188 | 0.6903 | 0.7285 | 1.97 | -15.77 | -16.07 | -11.75 | 12.05 | 0.37 |
| C(3) | C(4) | 1.3797 | 0.6707 | 0.709 | 2.04 | -16.63 | -16.86 | -11.4 | 11.63 | 0.48 |
| C(5) | C(4) | 1.4330 | 0.7001 | 0.7329 | 1.9 | -13.76 | -15.59 | -11.17 | 13.00 | 0.40 |
| C(5) | C(6) | 1.4332 | 0.7018 | 0.7314 | 1.85 | -13.14 | -14.73 | -11.03 | 12.62 | 0.34 |
| C(5) | C(10) | 1.4383 | 0.7062 | 0.7321 | 1.89 | -14.3 | -15.34 | -11.61 | 12.65 | 0.32 |
| C(7) | C(6) | 1.3804 | 0.6894 | 0.691 | 2.15 | -18.86 | -18.23 | -12.62 | 11.99 | 0.44 |
| C(7) | C(8) | 1.4176 | 0.7085 | 0.7091 | 2.01 | -17.2 | -16.84 | -12.27 | 11.91 | 0.37 |
| C(9) | C(8) | 1.3840 | 0.6586 | 0.7254 | 2.03 | -17.7 | -17.59 | -11.63 | 11.51 | 0.51 |
| C(10) | C(9) | 1.4369 | 0.7033 | 0.7336 | 1.86 | -14.01 | -15.58 | -10.93 | 12.49 | 0.42 |
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