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# Experimental, experimental-theoretical and theoretical estimates of intermolecular interaction energies in $\eta^6$-[(5-methyl-1,3-oxazolidin-3-yl)benzene]tricarbonylchromium(0)

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## Content

## 1. Periodical DFT calculation

The DFT calculation of periodical 3D structure of **1**$_{\mathbf{theor}}$ was performed within the PBE0 exchange-correlation functional [1, 2] using *CRYSTAL17* [3]. Atomic cores were described using all electron DZP basis set [4, 5]. Atomic coordinates were optimized (experimentally observed ones has been used as the starting geometry), and cell parameters were fixed at their experimental values. The level of accuracy in evaluating the Coulomb and exchange series was controlled by five parameters for which the values of $10^{-6}$, $10^{-6}$, $10^{-6}$, $10^{-6}$ and $10^{-20}$ were used. The shrinking factor of the reciprocal space was set to four, corresponding to 30 k points in the irreducible Brillouin zone at which the Hamiltonian matrix was diagonalized.

The electron density function suitable for analysis in terms of QTAIM theory was obtained by single-point calculation of the optimized structure using modified DZP basis set (f functions has been omitted). Topological analysis of electron density was carried out with *TOPOND* [6, 7] program (a part of *CRYSTAL17* code).

The index generation scheme proposed by Le Page & Gabe [8] was applied to generate 13780 unique Miller indices up to s = 1.15 Å$^{-1}$ reciprocal resolutions. The option *XFAC* of the *CRYSTAL17* program was used to generate a set of theoretical structure factors from the electron density function, obtained by separate single-point calculation of the non-optimized experimental geometry.

## 2. Molecular and crystal invariom

To obtain a molecular invariom **1**$_{\mathbf{mol}}$, the single point calculation was performed using DFT (PBE0/dzp [1, 2, 4, 5] via Gaussian 09 program [9]. Then we have placed **1**$_{\mathbf{mol}}$ molecule in a pseudocubic cell (a = 30 Å, space group P–1) and calculated the theoretical structural amplitudes (sin θ/λ = 1.155 Å$^{-1}$) using the Tonto program [10]. Based on the calculated structural amplitudes, using the MoPro program [11] , the populations of the spherically symmetric valence shell ($P_{val}$) and the multipole parameters ($P_{lm}$) describing its deformation were obtained together with the corresponding expansion – contraction coefficients (k, k') for each of the complex atoms. The obtained values of $P_{val}$, $P_{lm}$, k, and k' were used (but they were not refined themselves) to refine the coordinates and thermal parameters of atoms by experimental reflections (sin θ/λ = 0.7 Å$^{-1}$) in real symmetry of complex. The expansion – contraction coefficients (k, k') for hydrogen atoms were equal 1.2.

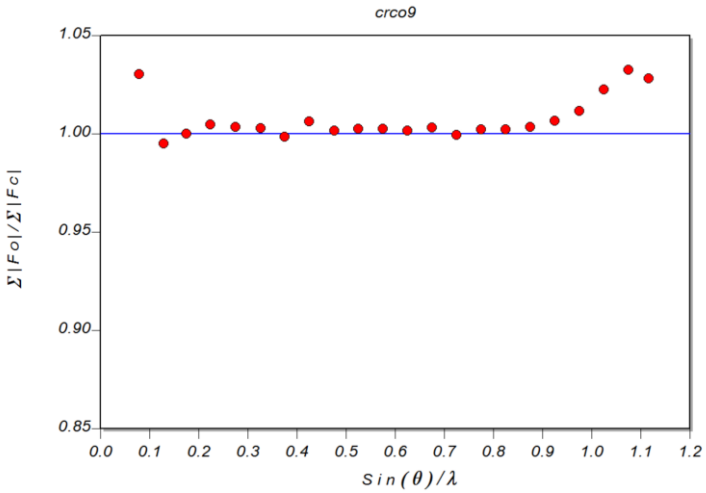
To obtain a molecular invariom **1**$_{\mathbf{cryst}}$, the single point calculation with experimental cell parameters was performed using DFT (PBE0/dzp [1-5]) via *CRYSTAL17* [3] program. The remainder of the methodology is fully consistent with obtaining a molecular invariom.

Analysis of topology of experimentally–theoretical ρ(r) function was carried out using the WINXPRO program package [12].

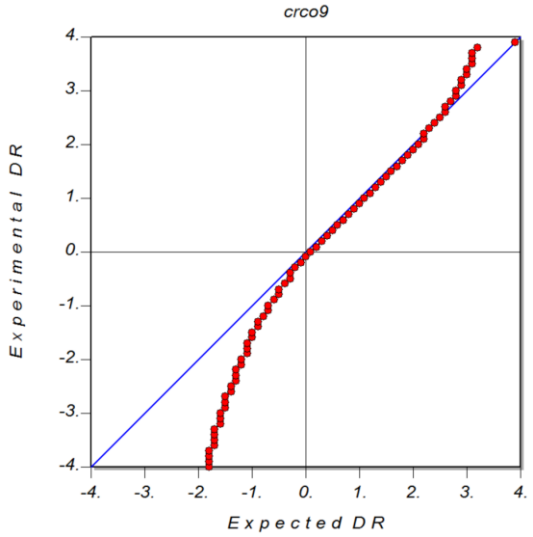
### 3. Theoretical calculation of lattice energy.

Geometry **1**$_{exp}$ has been optimized ( see  Periodical DFT calculation). Then, recalculated the total energy value per molecule. Then only one molecule was left in pseudocubic cell (a = 30 Å, space group P1) geometry was optimised and its geometry was optimised. The lattice energy is the difference of the values obtained.

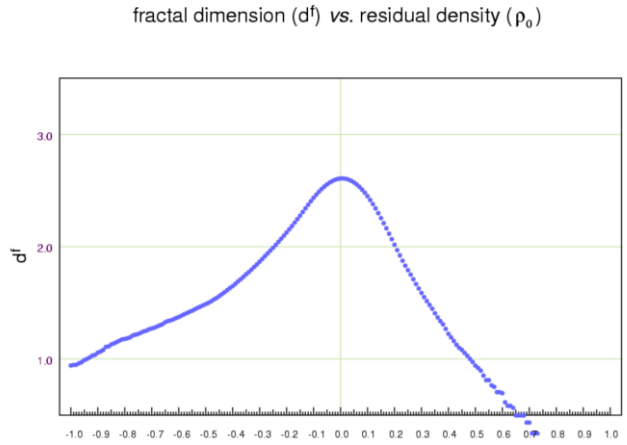
### 4. Fo/Fc vs resolution




### 5. Normal probability



## 6. Fractal dimension vs residual density




7. **Table S1.** The main distances and topological parameters of electron density in coordination sphere of the Cr atom obtained experimentally (**1**$_{exp}$), experimentally–theoretically (**1**$_{mol}$, **1**$_{cryst}$) and theoretically (**1**$_{theor}$, **1**$_{thmul}$).

| | | | | | |
|---|---|---|---|---|---|
| **1**$_{exp}$ | | | | | |
| | $d$, Å | $v$(**r**), a.u. | $\rho$(**r**), a.u. | $\nabla^2\rho$(**r**), a.u. | $h_e$(**r**), a.u. |
| Cr(1)–C(1) | 1.8407(8) | -0.248 | 0.137 | 0.464 | -0.066 |
| Cr(1)–C(2) | 1.8241(7) | -0.271 | 0.144 | 0.527 | -0.069 |
| Cr(1)–C(3) | 1.8420(7) | -0.287 | 0.150 | 0.503 | -0.080 |
| Cr(1)–C(4) | 2.2559(7) | -0.064 | 0.056 | 0.202 | -0.007 |
| Cr(1)–C(6) | 2.2225(7) | -0.076 | 0.062 | 0.245 | -0.007 |
| O(1)–C(1) | 1.1610(12) | -1.553 | 0.471 | -1.058 | -0.909 |
| O(2)–C(2) | 1.1625(9) | -1.688 | 0.500 | -1.458 | -1.026 |
| O(3)–C(3) | 1.1599(10) | -1.689 | 0.493 | -0.948 | -0.963 |
| **1**$_{mol}$ | | | | | |
| Cr(1)–C(1) | 1.8400(18) | -0.239 | 0.133 | 0.489 | -0.058 |
| Cr(1)–C(2) | 1.824(2) | -0.249 | 0.136 | 0.502 | -0.062 |
| Cr(1)–C(3) | 1.846(2) | -0.232 | 0.130 | 0.477 | -0.056 |
| Cr(1)–C(5) | 2.2060(17) | -0.078 | 0.064 | 0.229 | -0.104 |
| Cr(1)–C(7) | 2.2069(17) | -0.079 | 0.065 | 0.232 | -0.105 |
| O(1)–C(1) | 1.154(2) | -1.509 | 0.453 | -0.306 | -0.793 |
| O(2)–C(2) | 1.158(2) | -1.487 | 0.450 | -0.370 | -0.790 |
| O(3)–C(3) | 1.150(3) | -1.534 | 0.456 | -0.227 | -0.796 |
| **1**$_{cryst}$ | | | | | |
| Cr(1)–C(1) | 1.8391(16) | -0.229 | 0.128 | 0.505 | -0.051 |
| Cr(1)–C(2) | 1.8266(18) | -0.252 | 0.136 | 0.527 | -0.060 |
| Cr(1)–C(3) | 1.8445(19) | -0.216 | 0.123 | 0.495 | -0.046 |
| Cr(1)–C(5) | 2.2063(15) | -0.078 | 0.064 | 0.225 | -0.010 |
| Cr(1)–C(7) | 2.2089(15) | -0.079 | 0.065 | 0.223 | -0.011 |
| O(1)–C(1) | 1.1543(19) | -1.506 | 0.454 | -0.414 | -0.805 |
| O(2)–C(2) | 1.158(2) | -1.495 | 0.449 | -0.198 | -0.772 |
| O(3)–C(3) | 1.150(2) | -1.543 | 0.457 | -0.223 | -0.799 |
| **1**$_{theor}$ | | | | | |

| | | | | | |
|---|---|---|---|---|---|
| Cr(1)–C(1) | 1.8073 | -0.261 | 0.144 | 0.565 | -0.060 |
| Cr(1)–C(2) | 1.7960 | -0.273 | 0.146 | 0.602 | -0.061 |
| Cr(1)–C(3) | 1.8022 | -0.268 | 0.145 | 0.589 | -0.060 |
| Cr(1)–C(5) | 2.2007 | -0.079 | 0.064 | 0.216 | -0.012 |
| Cr(1)–C(7) | 2.1943 | -0.080 | 0.065 | 0.217 | -0.013 |
| O(1)–C(1) | 1.1682 | -1.581 | 0.426 | 0.826 | -0.687 |
| O(2)–C(2) | 1.1716 | -1.555 | 0.423 | 0.775 | -0.681 |
| O(3)–C(3) | 1.1685 | -1.577 | 0.426 | 0.805 | -0.680 |
| **$\mathbf{1}_{\mathbf{thmul}}$** | | | | | |
| Cr(1)–C(1) | 1.8388(14) | -0.244 | 0.133 | 0.531 | -0.055 |
| Cr(1)–C(2) | 1.8235(15) | -0.258 | 0.138 | 0.546 | -0.061 |
| Cr(1)–C(3) | 1.8440(16) | -0.229 | 0.127 | 0.524 | -0.049 |
| Cr(1)–C(5) | 2.2068(13) | -0.077 | 0.063 | 0.236 | -0.009 |
| Cr(1)–C(7) | 2.2062(13) | -0.074 | 0.061 | 0.225 | -0.008 |
| O(1)–C(1) | 1.1573(19) | -1.521 | 0.453 | -0.176 | -0.782 |
| O(2)–C(2) | 1.1617(19) | -1.488 | 0.445 | -0.073 | -0.753 |
| O(3)–C(3) | 1.154(2) | -1.520 | 0.452 | -0.102 | -0.773 |

8. **Table S2.** The geometrical and topological parameters of the selected intermolecular interactions in the unit cell of **$\mathbf{1}_{\mathbf{exp}}$**.

| Contact | *d*, Å | $v(\mathbf{r})$, a.u. | $\rho(\mathbf{r})$, a.u. | $\nabla^2\rho(\mathbf{r})$, a.u. | $h_e(\mathbf{r})$, a.u. |
|---|---|---|---|---|---|
| **O(1)…O(4)** | 3.396 | -0.0011 | 0.0023 | 0.0105 | 0.0008 |
| **O(1)…C(6)** | 3.348 | -0.0023 | 0.0045 | 0.0196 | 0.0013 |
| **O(1)…H(13C)** | 2.807 | -0.0014 | 0.0025 | 0.0130 | 0.0009 |
| **O(2)…H(7A)** | 2.412 | -0.0042 | 0.0071 | 0.0323 | 0.0019 |
| **O(2)…H(10B)** | 2.438 | -0.0036 | 0.0058 | 0.0298 | 0.0019 |
| **O(2)…H(12A)** | 2.823 | -0.0019 | 0.0040 | 0.0162 | 0.0011 |
| **O(2)…H(13A)** | 2.862 | -0.0012 | 0.0025 | 0.0114 | 0.0008 |
| **O(2)…H(13B)** | 2.715 | -0.0022 | 0.0039 | 0.0192 | 0.0013 |
| **O(3)…N(1)** | 3.388 | -0.0022 | 0.0047 | 0.0180 | 0.0011 |
| **O(3)…C(8)** | 3.365 | -0.0023 | 0.0049 | 0.0180 | 0.0011 |
| **O(3)…H(5A)** | 2.489 | -0.0017 | 0.0021 | 0.0179 | 0.0014 |
| **C(6)…H(13C)** | 2.821 | -0.0025 | 0.0053 | 0.0189 | 0.0011 |
| **C(13)…H(4A)** | 3.058 | -0.0017 | 0.0037 | 0.0140 | 0.0009 |
| **H(5A)…H(13B)** | 2.552 | -0.0008 | 0.0015 | 0.0085 | 0.0006 |
| **H(6A)…H(11A)** | 2.144 | -0.0007 | 0.0014 | 0.0072 | 0.0005 |

9. **Table S3**[a]. The geometrical and topological parameters of the selected intermolecular interactions in the unit cell of **1**$_{mol}$.

| Contact | *d*, Å | $v(\mathbf{r})$, a.u. | $\rho(\mathbf{r})$, a.u. | $\nabla^2\rho(\mathbf{r})$, a.u. | $h_e(\mathbf{r})$, a.u. |
|---|---|---|---|---|---|
| **O(1)…O(4)** | 3.391 | -0.0013 | 0.0026 | 0.0121 | 0.0009 |
| **O(1)…H(13C)** | 2.883 | -0.0015 | 0.0029 | 0.0138 | 0.0010 |
| O(1)…H(6A) | 2.780 | -0.0026 | 0.0050 | 0.0212 | 0.0013 |
| O(1)…H(8A) | 3.117 | -0.0007 | 0.0015 | 0.0075 | 0.0006 |
| O(2)…H(6A) | 2.665 | -0.0035 | 0.0062 | 0.0270 | 0.0016 |
| **O(2)…H(7A)** | 2.476 | -0.0051 | 0.0083 | 0.0374 | 0.0021 |
| **O(2)…H(10B)** | 2.526 | -0.0038 | 0.0061 | 0.0311 | 0.0020 |
| **O(2)…H(12A)** | 2.875 | -0.0020 | 0.0040 | 0.0168 | 0.0011 |
| **O(2)…H(13A)** | 2.954 | -0.0013 | 0.0028 | 0.0117 | 0.0008 |
| **O(2)…H(13B)** | 2.784 | -0.0024 | 0.0044 | 0.0200 | 0.0013 |
| **O(3)…N(1)** | 3.392 | -0.0020 | 0.0041 | 0.0169 | 0.0011 |
| **O(3)…C(8)** | 3.370 | -0.0019 | 0.0041 | 0.0159 | 0.0010 |
| **O(3)…H(5A)** | 2.586 | -0.0026 | 0.0038 | 0.0249 | 0.0018 |
| O(3)…H(12B) | 2.888 | -0.0020 | 0.0041 | 0.0171 | 0.0011 |
| O(3)…H(13B) | 2.993 | -0.0016 | 0.0036 | 0.0140 | 0.0009 |
| **C(6)…H(13C)** | 2.868 | -0.0029 | 0.0062 | 0.0202 | 0.0011 |
| **C(13)…H(4A)** | 3.121 | -0.0017 | 0.0037 | 0.0144 | 0.0009 |
| **H(6A)…H(11A)** | 2.301 | -0.0020 | 0.0033 | 0.0186 | 0.0013 |

[a] The interactions coinciding with the experiment are highlighted in bold.

10. **Table S4**[a]. The geometrical and topological parameters of the selected intermolecular interactions in crystal packing of **1**$_{cryst}$.

| Contact | $d$, Å | $v(\mathbf{r})$, a.u. | $\rho(\mathbf{r})$, a.u. | $\nabla^2\rho(\mathbf{r})$, a.u. | $h_e(\mathbf{r})$, a.u. |
|---|---|---|---|---|---|
| **O(1)…O(4)** | 3.387 | -0.0014 | 0.0028 | 0.0126 | 0.0009 |
| **O(1)….H(13C)** | 2.809 | -0.0017 | 0.0031 | 0.0154 | 0.0011 |
| O(1)…H(6A) | 2.742 | -0.0027 | 0.0052 | 0.0221 | 0.0014 |
| O(1)…H(8A) | 3.041 | -0.0007 | 0.0015 | 0.0076 | 0.0006 |
| O(2)…H(6A) | 2.612 | -0.0036 | 0.0064 | 0.0281 | 0.0017 |
| **O(2)…H(7A)** | 2.421 | -0.0055 | 0.0090 | 0.0399 | 0.0022 |
| **O(2)…H(10B)** | 2.434 | -0.0047 | 0.0073 | 0.0370 | 0.0023 |
| **O(2)…H(12A)** | 2.816 | -0.0020 | 0.0038 | 0.0173 | 0.0012 |
| **O(2)…H(13A)** | 2.891 | -0.0016 | 0.0032 | 0.0144 | 0.0010 |
| **O(2)…H(13B)** | 2.690 | -0.0027 | 0.0047 | 0.0229 | 0.0015 |
| **O(3)…N(1)** | 3.391 | -0.0020 | 0.0041 | 0.0168 | 0.0011 |
| **O(3)…H(5A)** | 2.495 | -0.0031 | 0.0042 | 0.0299 | 0.0022 |
| O(3)…H(12B) | 2.833 | -0.0020 | 0.0039 | 0.0168 | 0.0011 |
| O(3)…H(13B) | 2.931 | -0.0017 | 0.0037 | 0.0145 | 0.0010 |
| **C(6)…H(13C)** | 2.816 | -0.0029 | 0.0061 | 0.0204 | 0.0011 |
| **C(13A)…H(4A)** | 3.040 | -0.0018 | 0.0038 | 0.0153 | 0.0010 |

[a] The interactions coinciding with the experiment are highlighted in bold.

11. **Table S5**[a]. The geometrical and topological parameters of the selected intermolecular interactions in the unit cell of **1**$_{\mathbf{theor}}$.

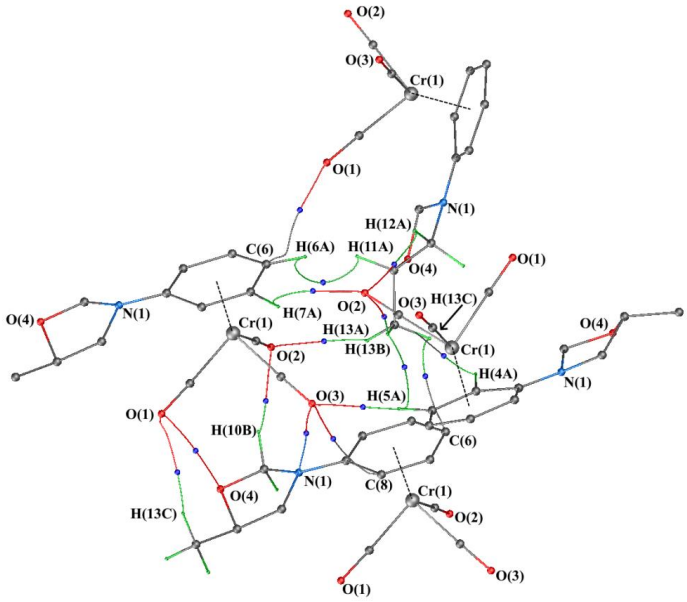
| Contact | *d*, Å | $v(\mathbf{r})$, a.u. | $\rho(\mathbf{r})$, a.u. | $\nabla^2\rho(\mathbf{r})$, a.u. | $h_e(\mathbf{r})$, a.u. |
|---|---|---|---|---|---|
| O(1)...H(6A) | 2.5827 | -0.0039 | 0.0065 | 0.0303 | 0.0018 |
| O(1)...H(8A) | 3.2226 | -0.0007 | 0.0015 | 0.0061 | 0.0004 |
| O(1)...H(10B) | 3.0659 | -0.0013 | 0.0028 | 0.0120 | 0.0009 |
| O(1)...H(11A) | 3.0115 | -0.0014 | 0.0030 | 0.0118 | 0.0008 |
| **O(1)...H(13C)** | 2.5791 | -0.0038 | 0.0064 | 0.0260 | 0.0014 |
| O(2)...H(6A) | 2.6499 | -0.0034 | 0.0056 | 0.0283 | 0.0018 |
| **O(2)...H(7A)** | 2.4492 | -0.0058 | 0.0089 | 0.0391 | 0.0020 |
| **O(2)...H(10B)** | 2.3976 | -0.0064 | 0.0099 | 0.0380 | 0.0016 |
| **O(2)...H(12A)** | 2.7686 | -0.0026 | 0.0049 | 0.0194 | 0.0011 |
| **O(2)...H(13A)** | 2.9113 | -0.0018 | 0.0036 | 0.0140 | 0.0008 |
| **O(2)...H(13B)** | 2.7512 | -0.0027 | 0.0051 | 0.0205 | 0.0012 |
| **O(3)...C(8)** | 3.3872 | -0.0017 | 0.0036 | 0.0137 | 0.0086 |
| O(3)...H(5A) | 2.3265 | -0.0068 | 0.0103 | 0.0409 | 0.0017 |
| O(3)...H(12B) | 2.8985 | -0.0019 | 0.0036 | 0.0148 | 0.0009 |
| O(3)...H(13B) | 2.8300 | -0.0022 | 0.0043 | 0.0178 | 0.0011 |
| C(5)...H(13A) | 3.1399 | -0.0014 | 0.0036 | 0.0139 | 0.0010 |
| **C(6)...H(13C)** | 2.8489 | -0.0025 | 0.0054 | 0.0195 | 0.0012 |
| H(4A)...H(13C) | 2.4340 | -0.0022 | 0.0046 | 0.0186 | 0.0012 |
| **H(5A)...H(13B)** | 2.5660 | -0.0015 | 0.0033 | 0.0150 | 0.0011 |
| **H(6A)...H(11A)** | 2.1754 | -0.0041 | 0.0070 | 0.0250 | 0.0011 |
| H(10A)…H(12B) | 2.5536 | -0.0014 | 0.0032 | 0.0109 | 0.0007 |

[a] The interactions coinciding with the experiment are highlighted in bold.

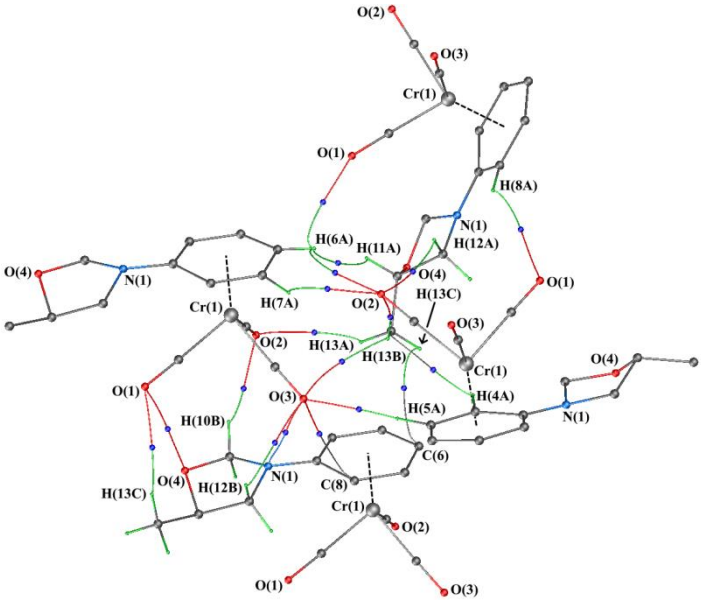
12. **Table S6**[a]. The topological parameters of the selected intermolecular interactions in the unit cell of **1**$_{\mathbf{thmul}}$.

| Contact | $v(\mathbf{r})$, a.u. | $\rho(\mathbf{r})$, a.u. | $\nabla^2\rho(\mathbf{r})$, a.u. | $h_e(\mathbf{r})$, a.u. |
|---|---|---|---|---|
| **O(1)…O(4)** | -0.001 | 0.003 | 0.012 | 0.001 |
| O(1)…H(6A) | -0.003 | 0.005 | 0.021 | 0.001 |
| O(1)…H(8A) | -0.001 | 0.002 | 0.007 | 0.001 |
| **O(1)…H(13C)** | -0.001 | 0.003 | 0.013 | 0.001 |
| O(2)…H(6A) | -0.003 | 0.005 | 0.026 | 0.002 |
| **O(2)…H(7A)** | -0.005 | 0.008 | 0.037 | 0.002 |
| **O(2)…H(10B)** | -0.004 | 0.007 | 0.031 | 0.002 |
| **O(2)…H(12A)** | -0.002 | 0.003 | 0.016 | 0.001 |
| **O(2)…H(13A)** | -0.001 | 0.003 | 0.013 | 0.001 |
| **O(2)…H(13B)** | -0.002 | 0.005 | 0.019 | 0.001 |
| **O(3)…N(1)** | -0.002 | 0.004 | 0.016 | 0.001 |
| O(3)…H(12B) | -0.002 | 0.004 | 0.015 | 0.001 |
| O(3)…H(13B) | -0.002 | 0.003 | 0.014 | 0.001 |
| **O(3)…H(5A)** | -0.002 | 0.003 | 0.024 | 0.002 |
| **C(6)…H(13C)** | -0.002 | 0.006 | 0.018 | 0.001 |
| **H(6A)…H(11A)** | -0.002 | 0.003 | 0.018 | 0.001 |
| **C(4)....H(7A)** | -0.001 | 0.004 | 0.014 | 0.0008 |

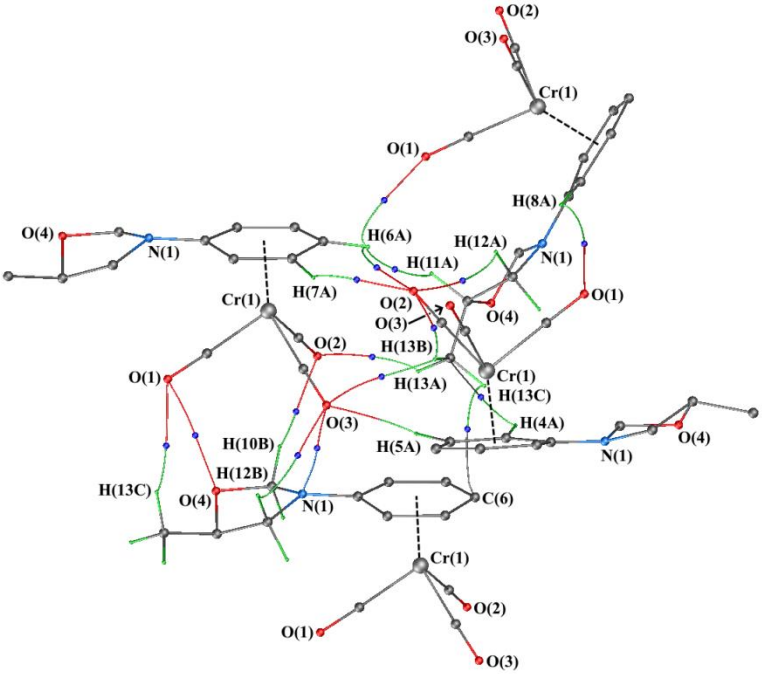
[a] The interactions coinciding with the experiment are highlighted in bold.




13. **Figure S1**. Experimental molecular graph of the intermolecular interactions in the unit cell of **1**$_{exp}$. The critical points (blue color – CP(3,-1) are presented by points.




14. **Figure S2**. Experimentally-theoretical molecular graph of the intermolecular interactions in the unit cell of **1**$_{mol}$. The critical points (blue color – CP(3,-1) are presented by points.




15**. Figure S3**. Experimentally-theoretical molecular graph of the intermolecular interactions in the unit cell of **1**$_{cryst}$. The critical points (blue color – CP(3,-1) are presented by points.

16. The multipole refinement of the disorder.

A fragment of **1**$_{exp}$ complex is disordered (0.743/0.257) (Figure 4S). Therefore, in the multipole refinement process of the atoms electronic parameters ($P_{val}$, $P_{lm}$, k, and k'), we first refined the undisordered part of the complex and then refined the disordered one.

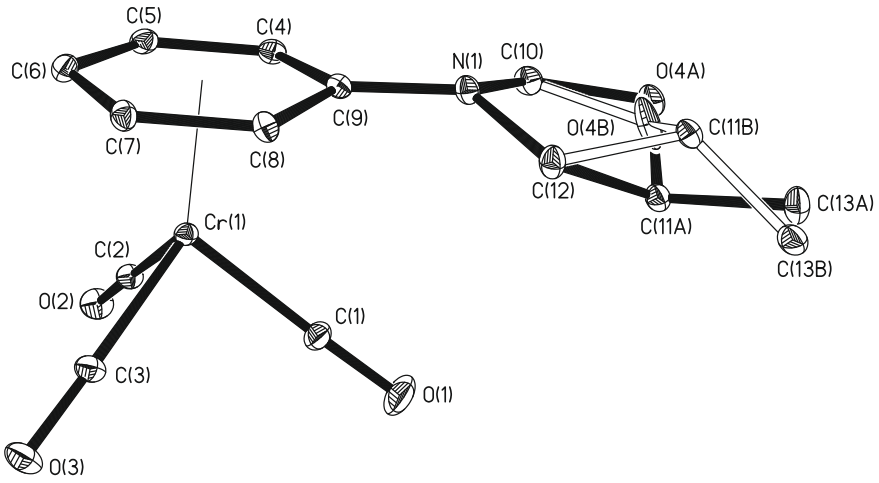



**Figure S4**. Disorder in **1**$_{exp}$.

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