



FOUNDATIONS  
ADVANCES

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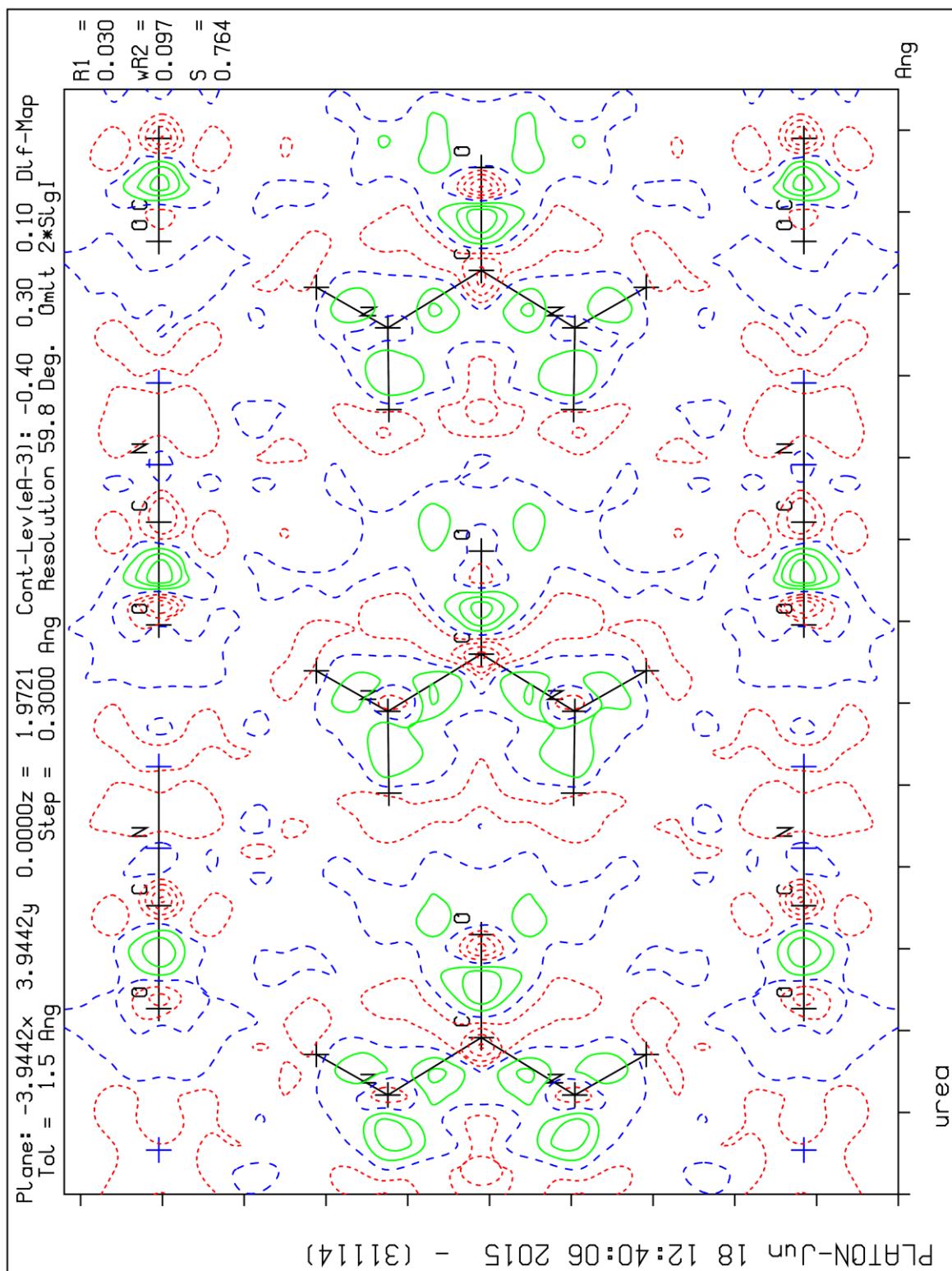
**Supporting information for article:**

**Dynamic quantum crystallography: lattice-dynamical models refined against diffraction data. I. Theory**

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**Table S1.** Refinement statistics and indicators for all IAM (first left column) and normal mode models for tested datasets.  $NrRefUij$  stands for number of refined  $U_{ij}$  parameters in IAM refinement, for *NoMoRe* it equals number of refined frequencies. For urea values in bracket shows number of symmetry independent parameters, which were refined. In case of all statistics after *NoMoRe* refinements first value is a results of a refinement, for which frequencies from 6-31G(d,p) were used, whereas second, in italic were TZP.

IAM ( <i>SHELX</i> )		<i>NoMoRe</i>				
Refined frequencies	Maximum level of convergence	wR2	$\bar{S}_{nH}$	$\bar{S}_H$	OS	
<b>Urea 123K X-ray data</b>						
<i>wR2=0.081</i>	<b>0 - 3(3)</b>	$5.5 \cdot 10^{-2} / 5 \cdot 10^{-2}$	0.1581/ <i>0.1297</i>	0.13/ <i>0.10</i>	0.57/ <i>0.67</i>	0.776/ <i>0.721</i>
<i>NrRefUij=18(11)</i>	<b>0 - 7(5)</b>	$5.5 \cdot 10^{-2} / 5 \cdot 10^{-2}$	0.1248/ <i>0.1000</i>	0.04/ <i>0.03</i>	1.03/ <i>0.84</i>	0.702/ <i>0.746</i>
	<b>0 - 11(7)</b>	$5.5 \cdot 10^{-2} / 5.5 \cdot 10^{-2}$	0.1043/ <i>0.0964</i>	0.04/ <i>0.02</i>	1.00/ <i>0.85</i>	0.994/ <i>0.992</i>



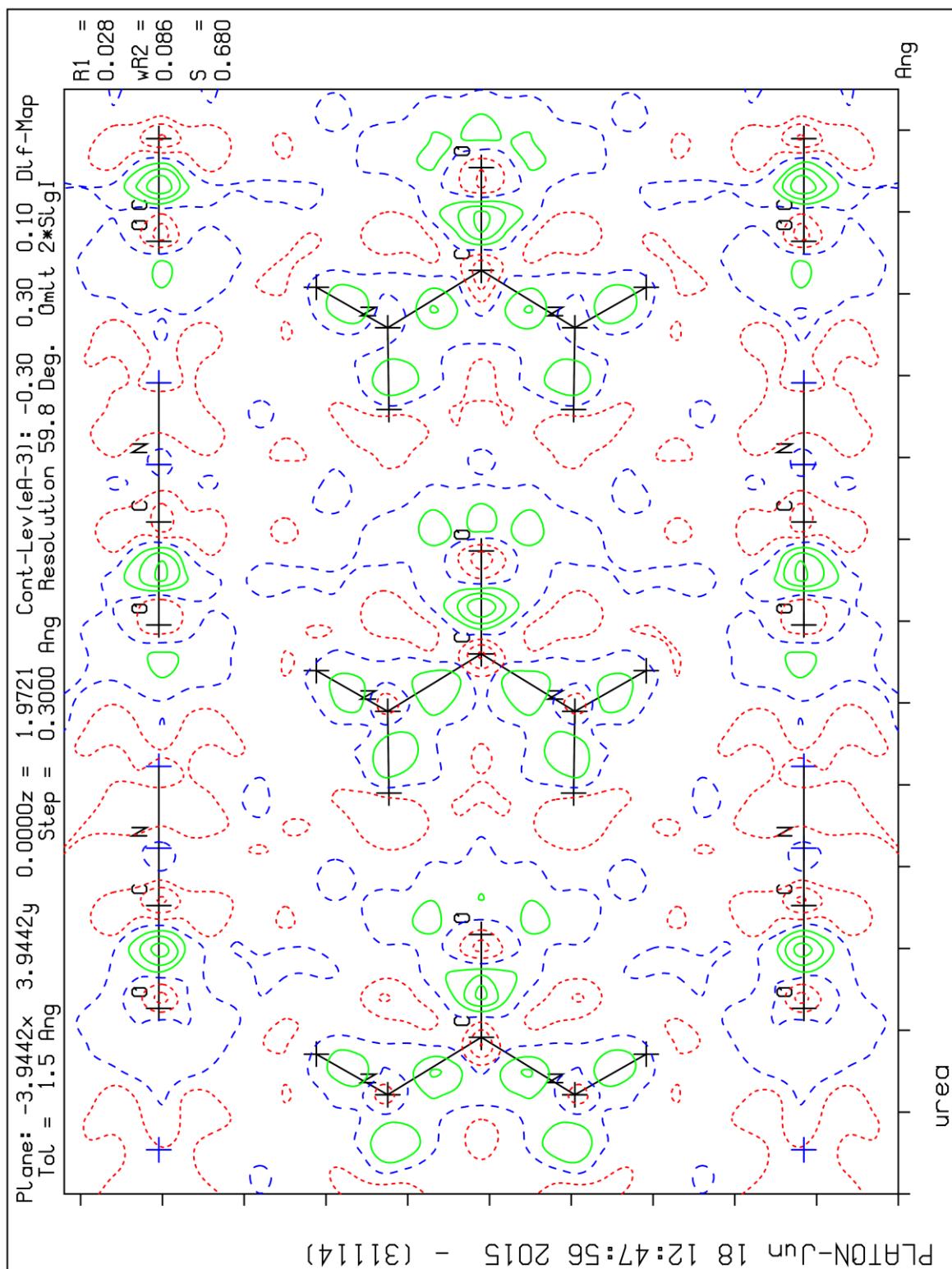


Figure S1 *Upper picture:* The residual density of urea after NoMoRe refinement of 12 frequencies (7 independent), using the TZP calculations. The residual density map was produced by the Platon program.

The contour level is 0.10 e/Å<sup>3</sup>. *Lower picture:* The residual density of urea after standard IAM refinement in SHELXL. The residual density map was produced by the Platon program. The contour level is 0.10 e/Å<sup>3</sup>.

Scaling parameters and Mean Frequency Scaling Factors (MFSF) are given for each refinement reported in the manuscript.

First column: name or number of the refined parameter.

Second column: refinement of model based on 631G(d,p) basis.

Third column: refinement of model based on TZP basis.

#### MFSF and 4 refined frequencies

6-31G(d,p) TZP

MFSF 0.7762 0.7214

1	1.7666	1.8475
2	0.9515	0.9633
3	0.9515	0.9633
4	2.5954	1.3760

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#### MFSF and 8 refined frequencies

6-31G(d,p) TZP

MFSF 0.7023 0.7465

1	1.5036	1.5126
2	1.0280	1.0864
3	1.0280	1.0864
4	1.5524	1.1593
5	1.3142	1.1982
6	0.6382	0.5190
7	0.6382	0.5190
8	1.0860	1.0852

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#### MFSF and 12 refined frequencies

6-31G(d,p) TZP

MFSF 0.9948 0.9931

1 1.4636 1.5090  
2 1.1038 1.0877  
3 1.1038 1.0877  
4 1.7673 1.2020  
5 1.4298 1.1214  
6 0.5462 0.5168  
7 0.5462 0.5168  
8 1.0837 1.0792  
9 0.6341 0.6718  
10 0.6341 0.6718  
11 1.0038 1.0995  
12 1.0038 1.0995