



STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 78 (2022)

Supporting information for article:

**Structure of the high-temperature phase of caesium nitrate –
importance of high-resolution data**

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Material for deposit / Table 3**Experimental details****Crystal data**

Chemical formula	CsNO ₃
M_r	194.9
Crystl colour	colourless
Crystal system, space group	Cubic, $Pm\bar{3}m$
Temperature (K)	440(5)
a (Å)	4.5226(6)
V (Å ³)	92.50(2)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	9.83
Crystal size (mm)/habitus	0.39 × 0.93 × 0.78/prism

Data collection

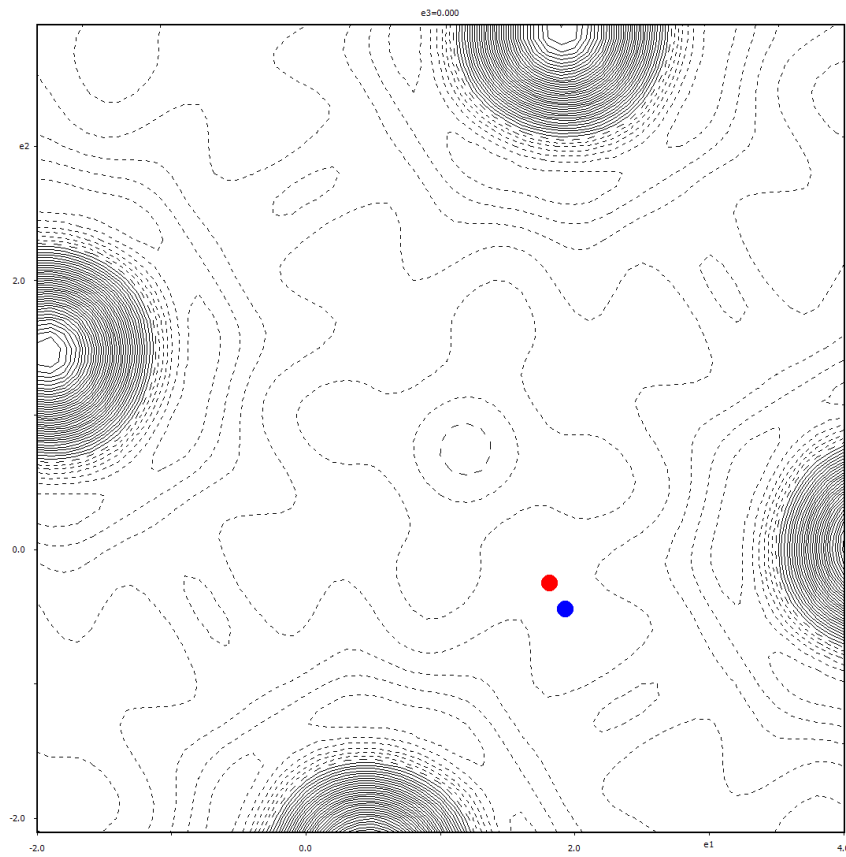
Diffractometer	Xcalibur
Absorption correction	Multi-scan <i>CrysAlis PRO</i> 1.171.40.67a (Rigaku Oxford Diffraction, 2018)
T_{\min} , T_{\max}	0.347, 0.464
Measurement method	ω scans
No. of measured, independent and observed [$I > 3\sigma(I)$] independent reflections	4035, 109, 74
R_{int}	0.0372
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.995000

Refinement

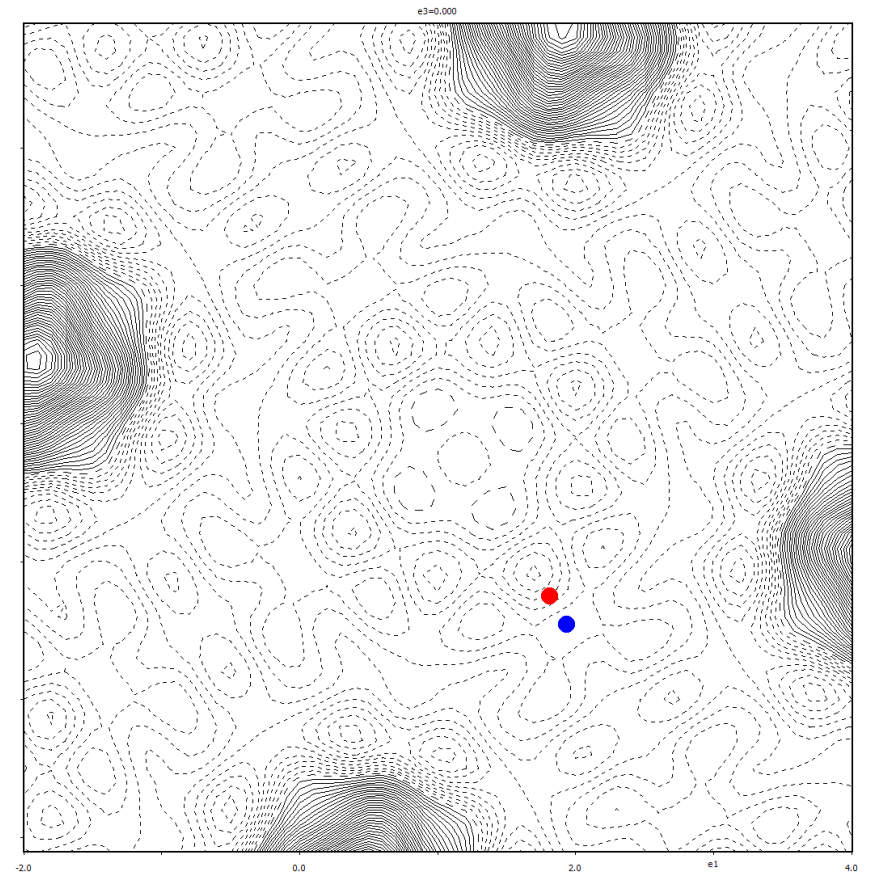
Refinement was carried out on intensities

$R[I > 3\sigma(I)]$, $wR(I)$, S	0.0144, 0.0589, 1.87
No. of reflections all/observed	109/74
No. of parameters	14
No. of restraints	2
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ ($e \text{ \AA}^{-3}$)	0.64, -0.38

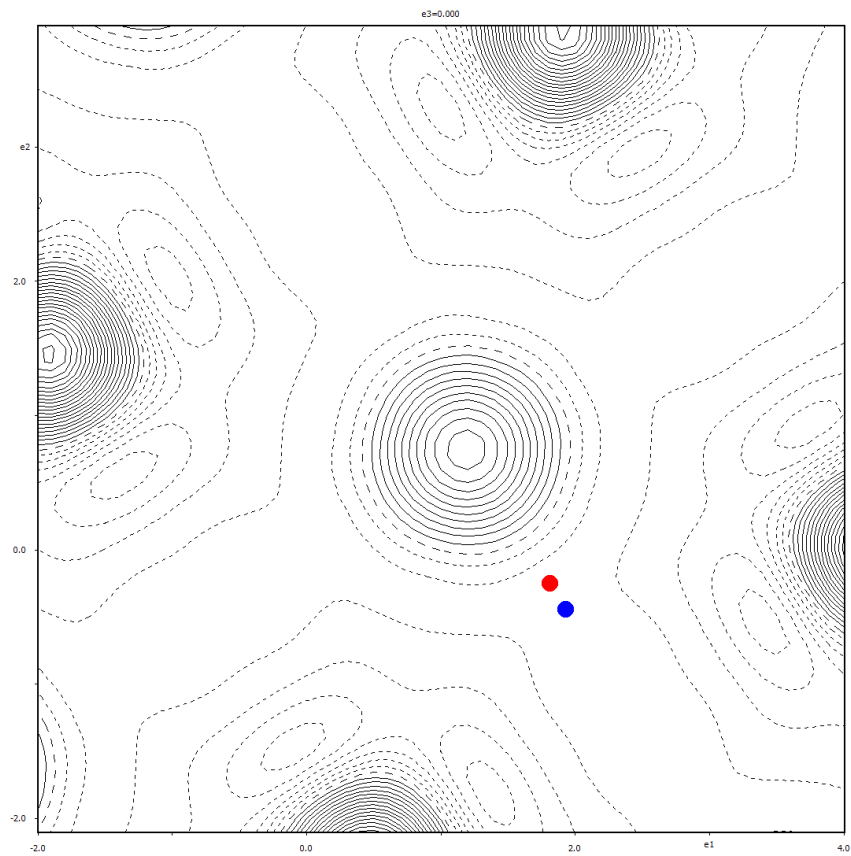
Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SUPERFLIP* (Palatinus & Chapuis, 2007), *JANA2006* (Petříček *et al.*, 2014), *Diamond 3.2e* (Brandenburg, 2015).



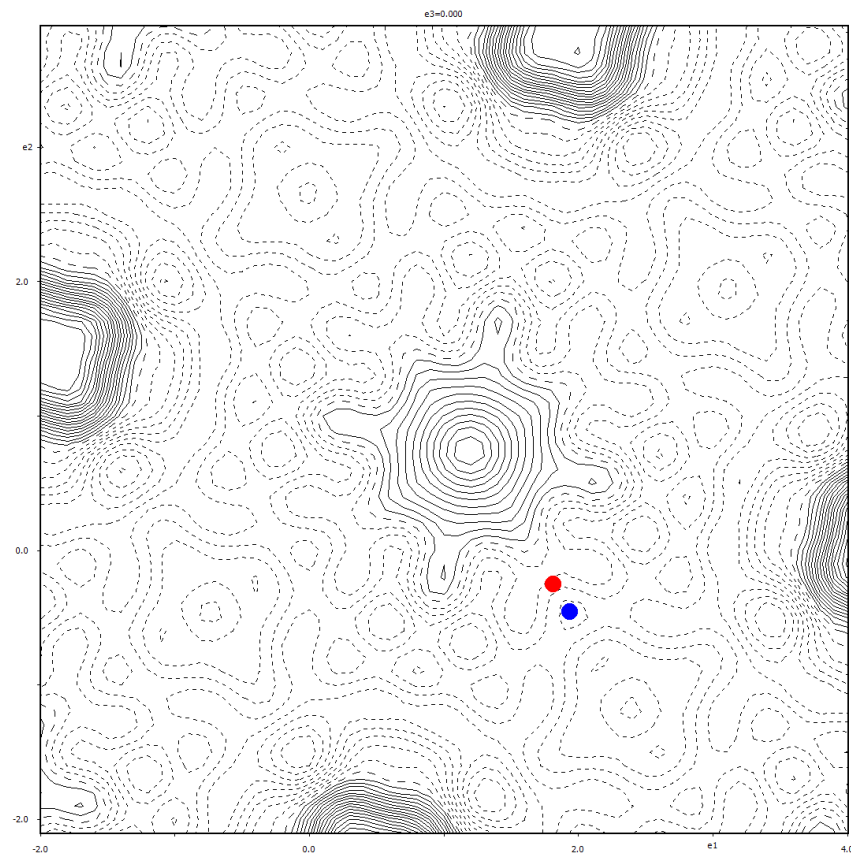
a)



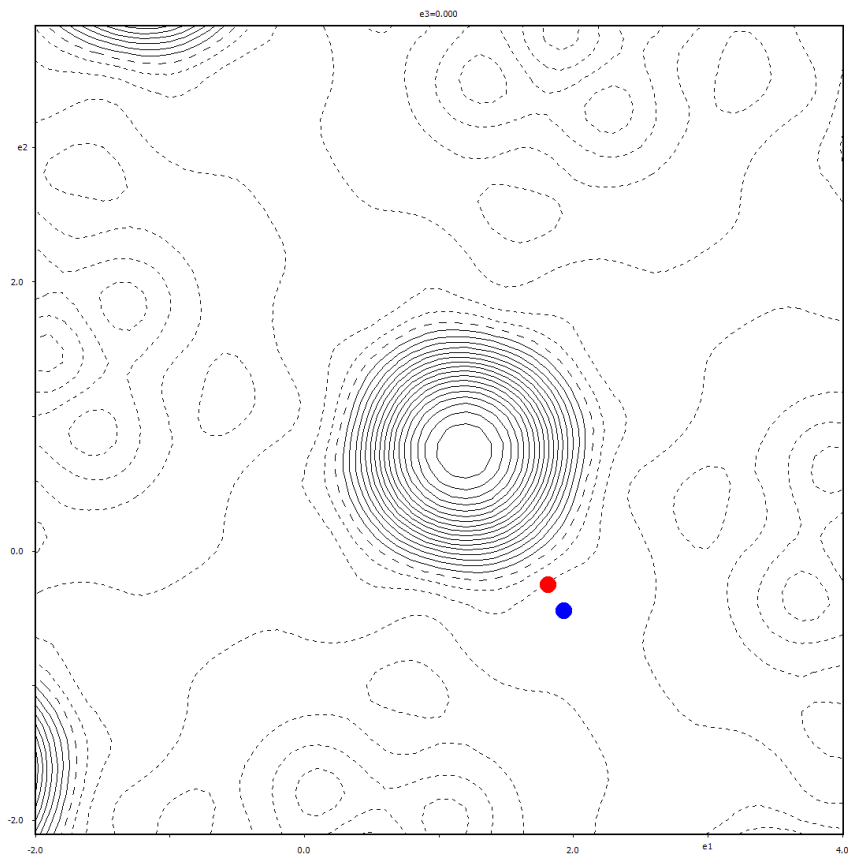
b)



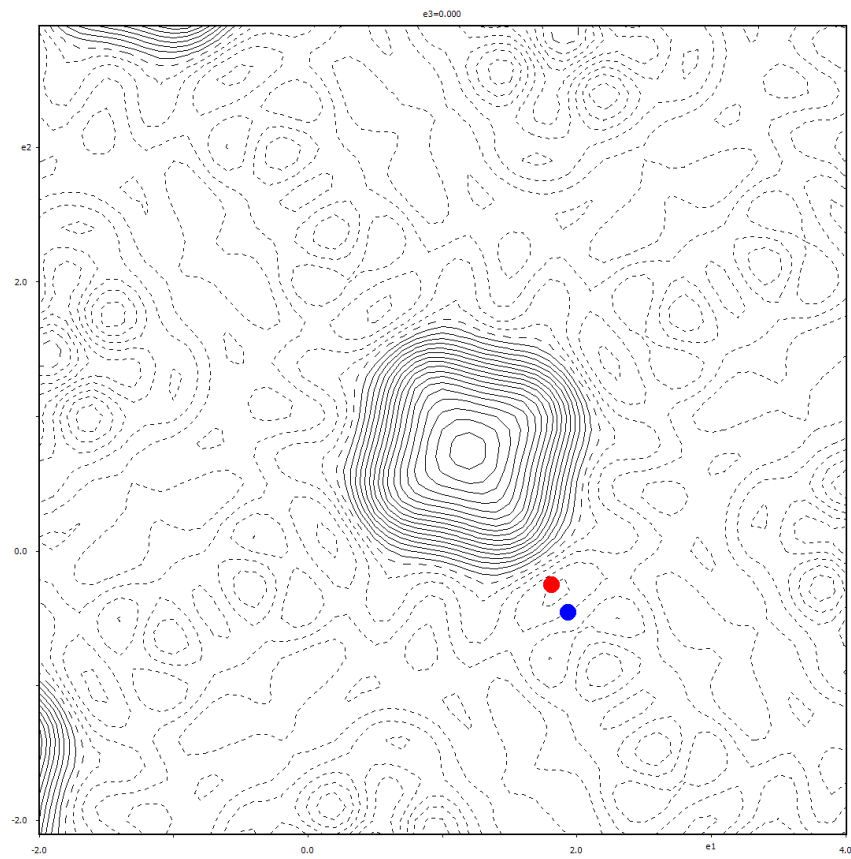
c)



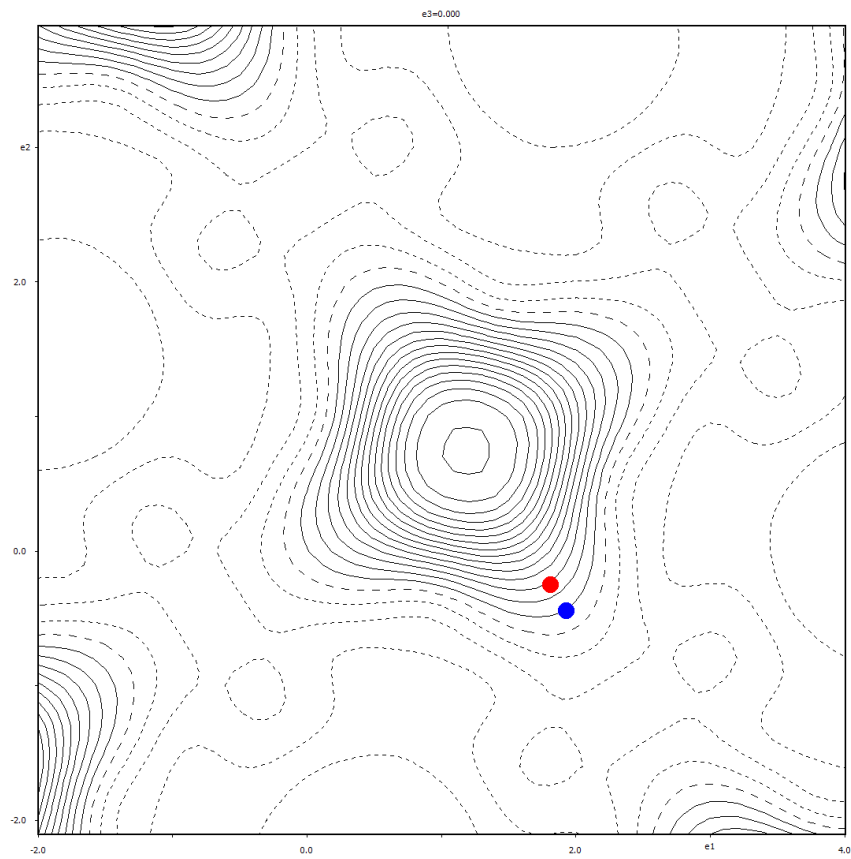
d)



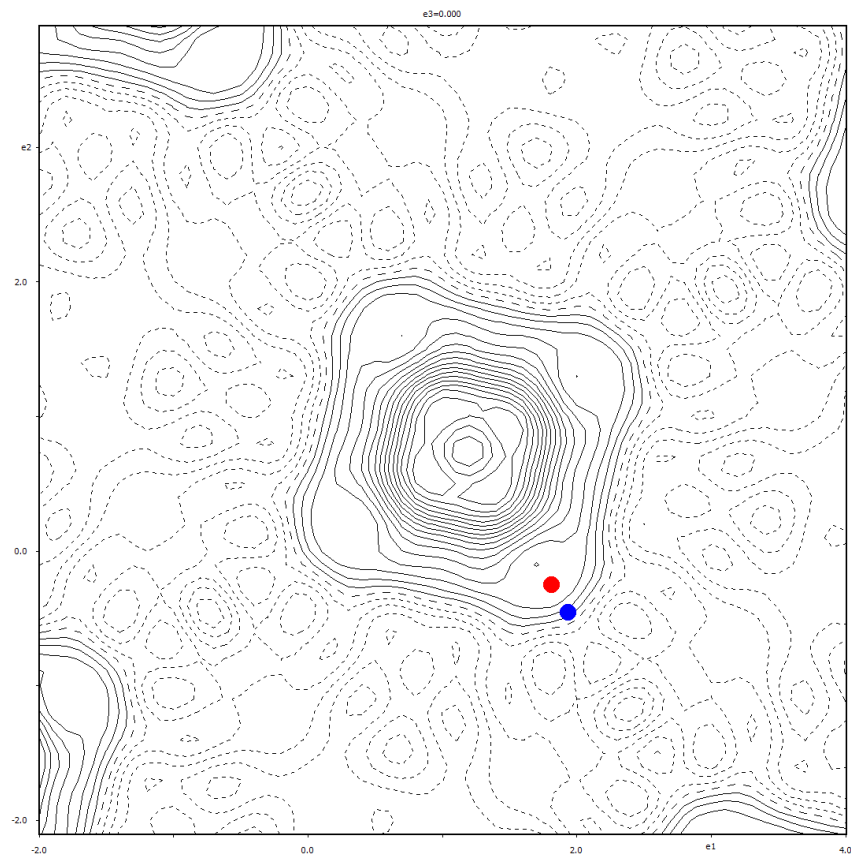
e)



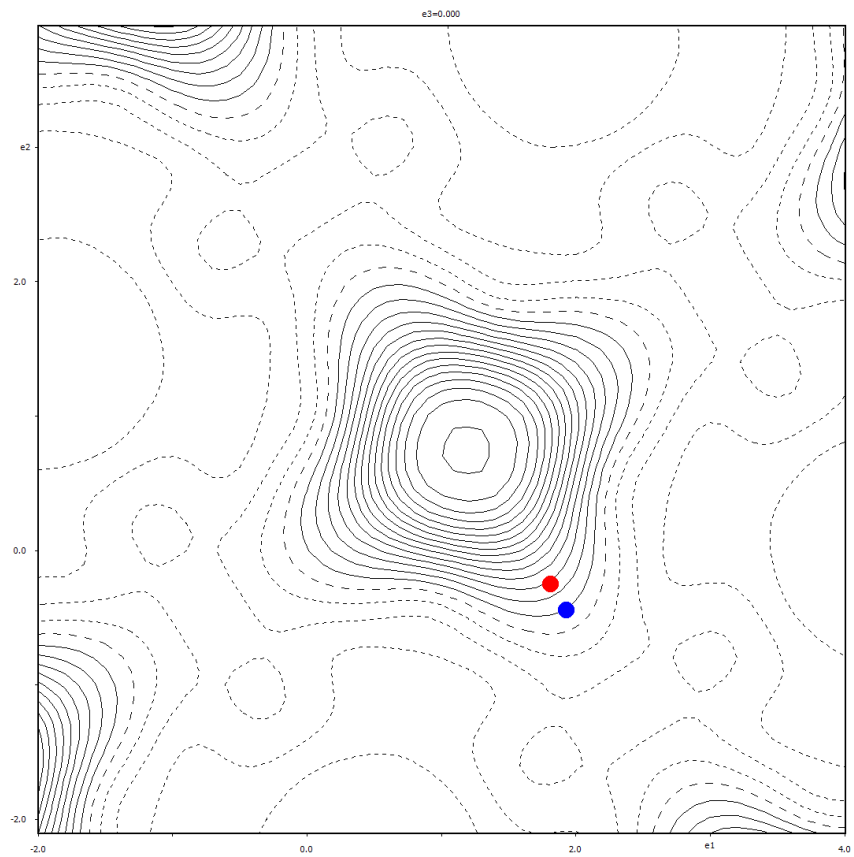
f)



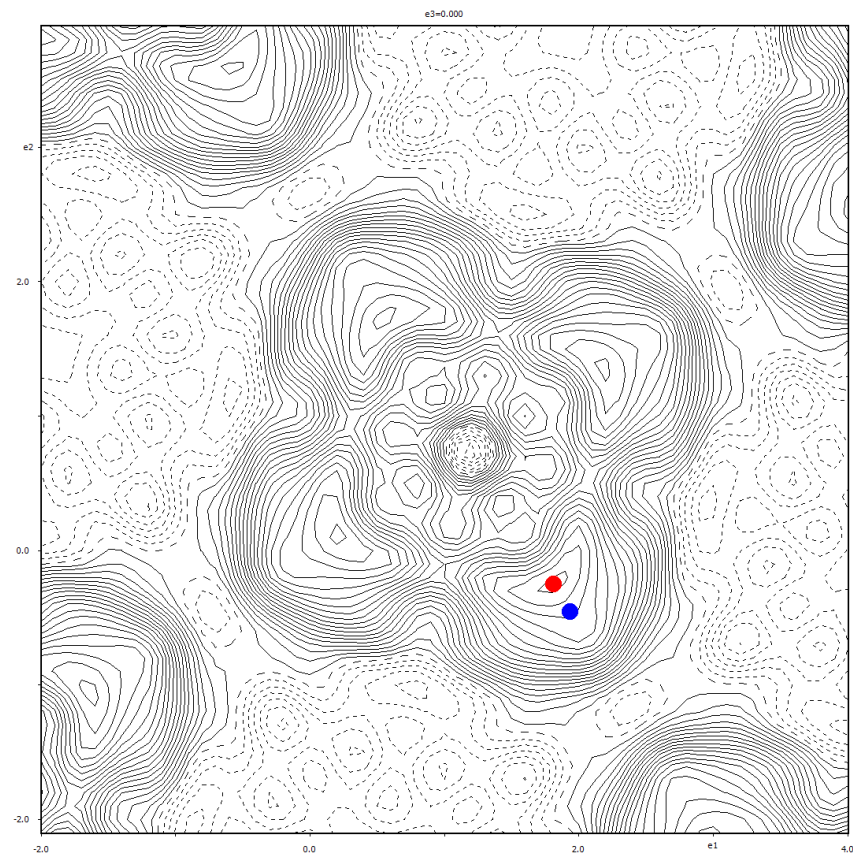
g)



h)



i)



j)

- **The difference electron density maps**

a), c), e), g), i) calculated for the low-theta angles ($\sin\Theta_{\max}/\lambda = 0.671639 \text{ \AA}^{-1}$)

b), d), f), h), j) calculated for the high-theta angle ($\sin\Theta_{\max}/\lambda = 0.995000 \text{ \AA}^{-1}$)

a), b) for $z=0.0$; c), d) for $z=0.1$; e), f) for $z=0.2$; g), h) for $z=0.3$;

i), j) for $z=0.5$.

The red point corresponds to the projection of the position of O2

from the adopted model refined on the high-theta angle data

while the blue point to the projection of O1ⁱⁱⁱ (symmetry code: (iii) z, x, y).