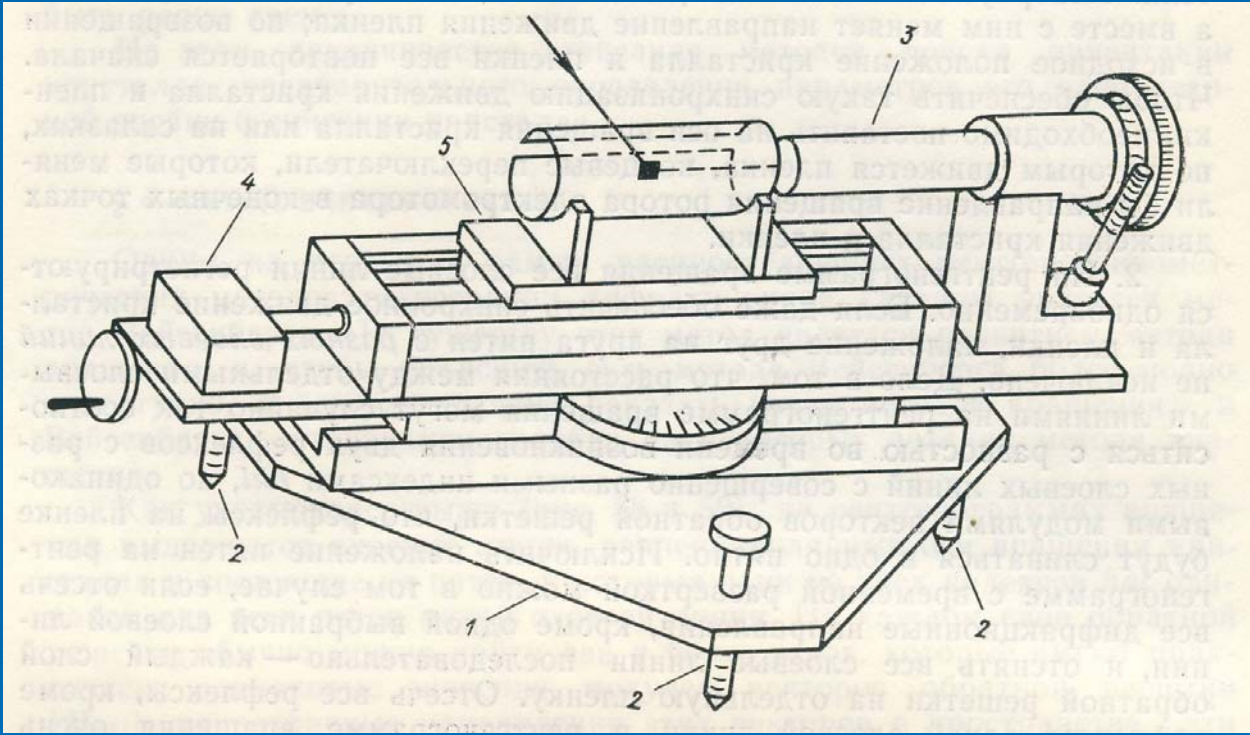
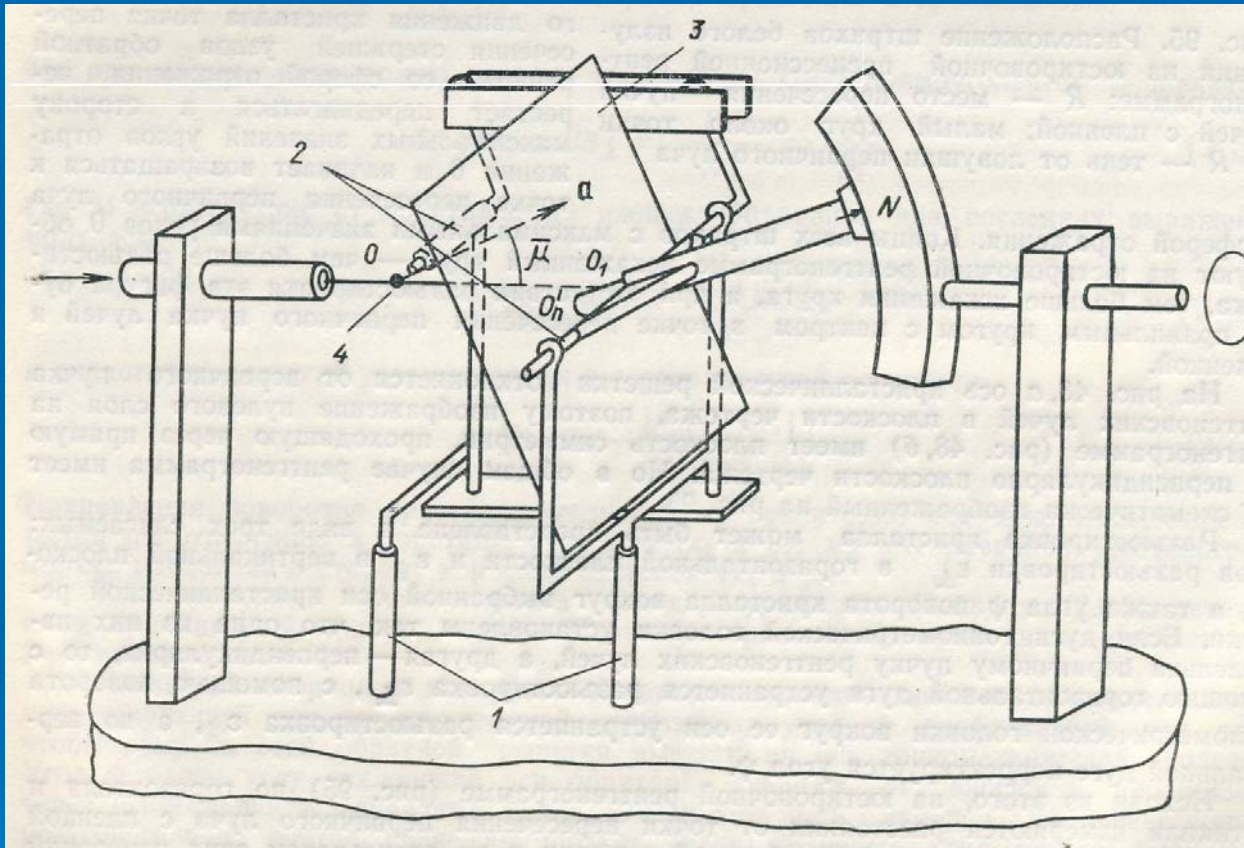
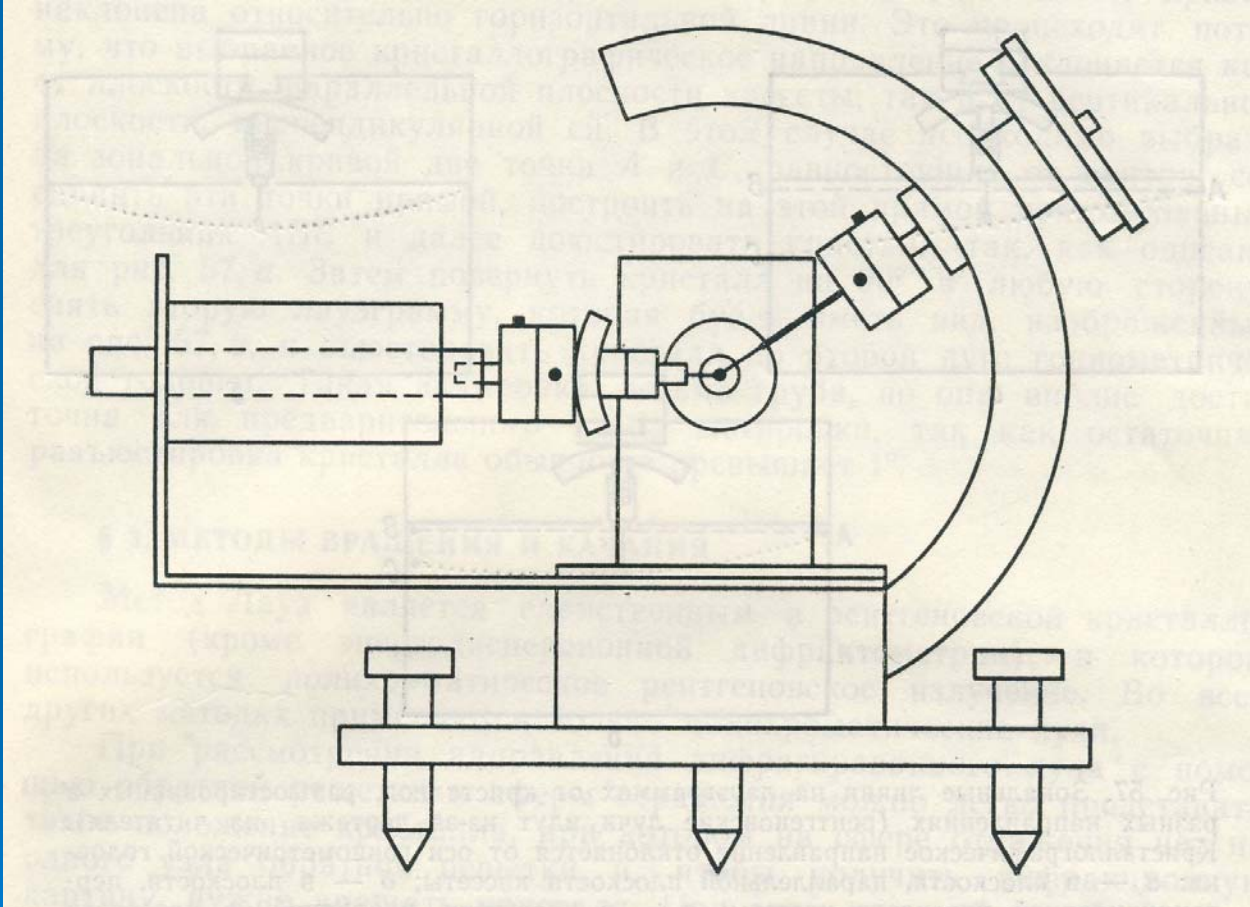


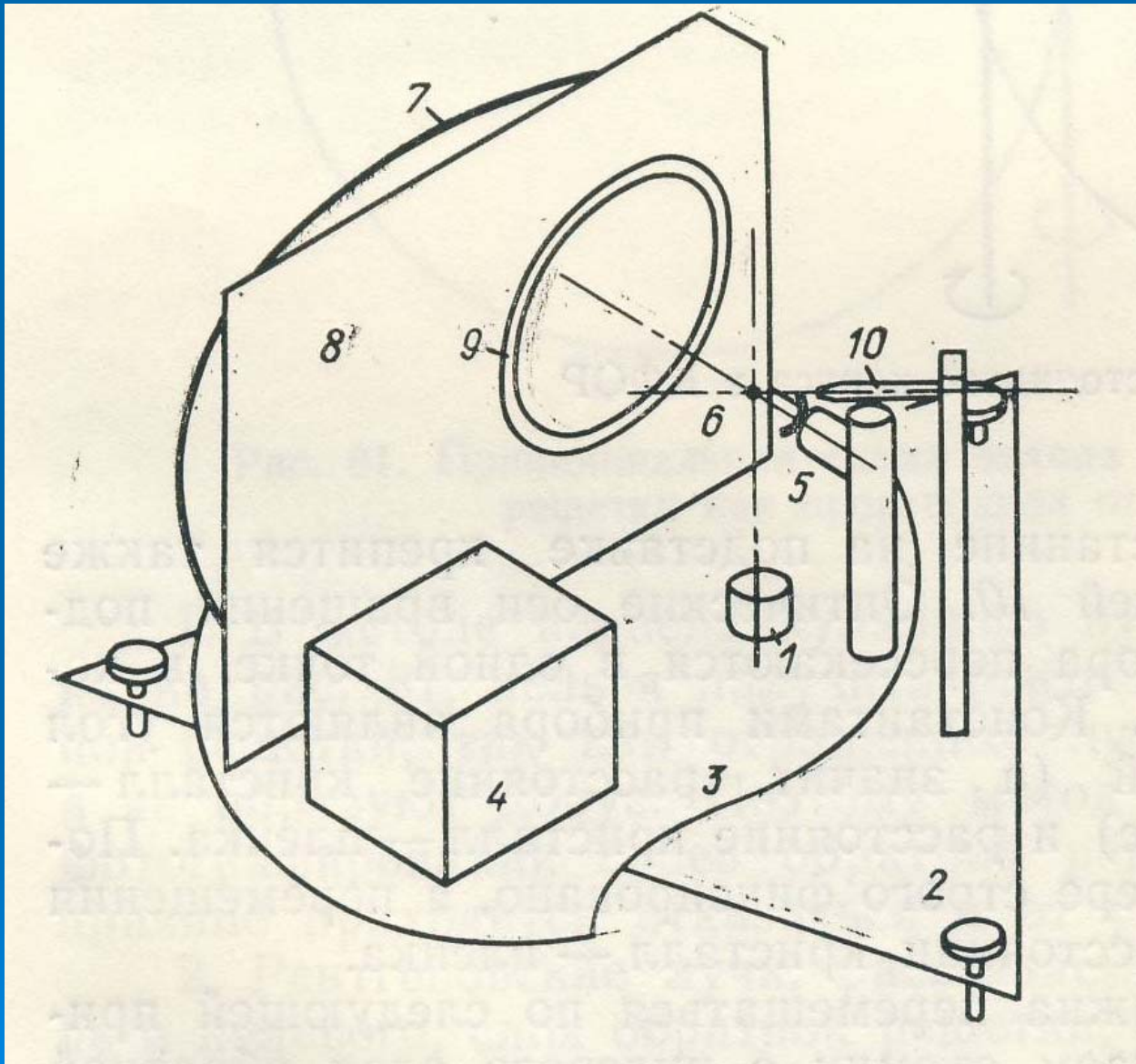
Л.А.Асланов

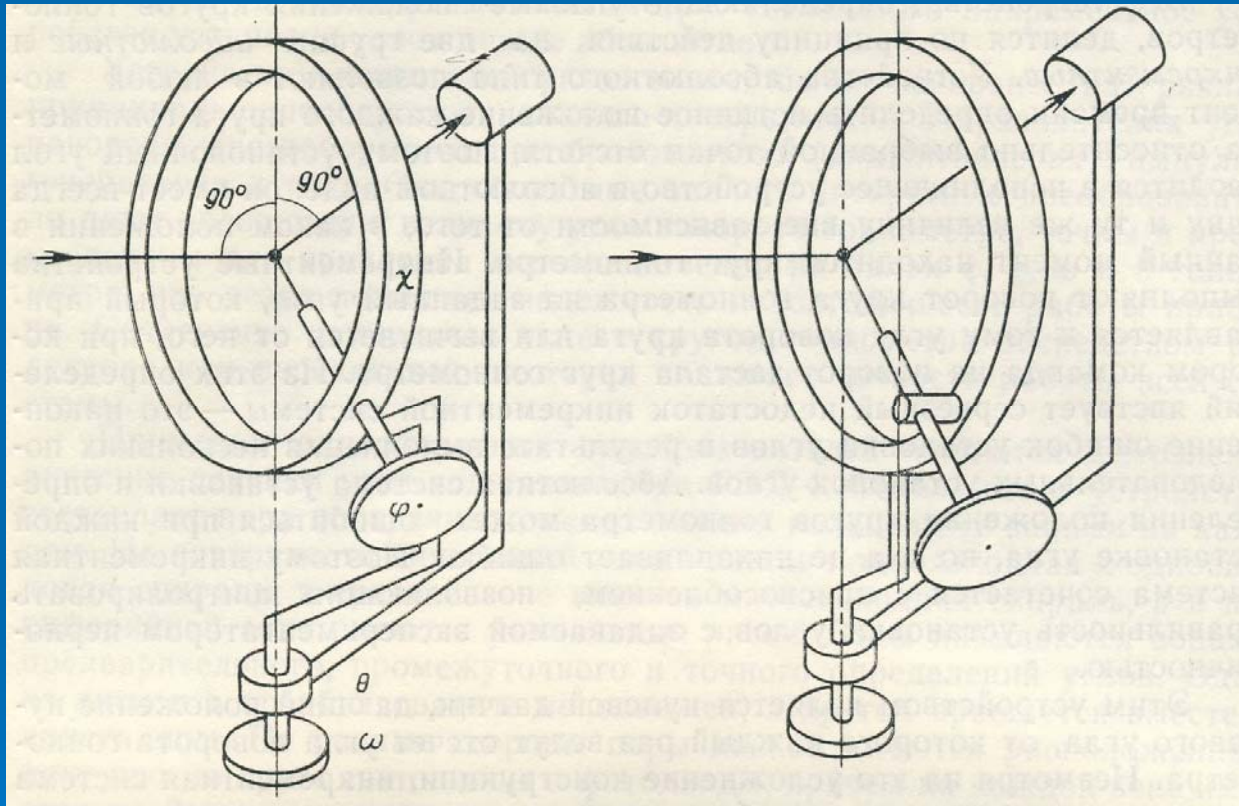
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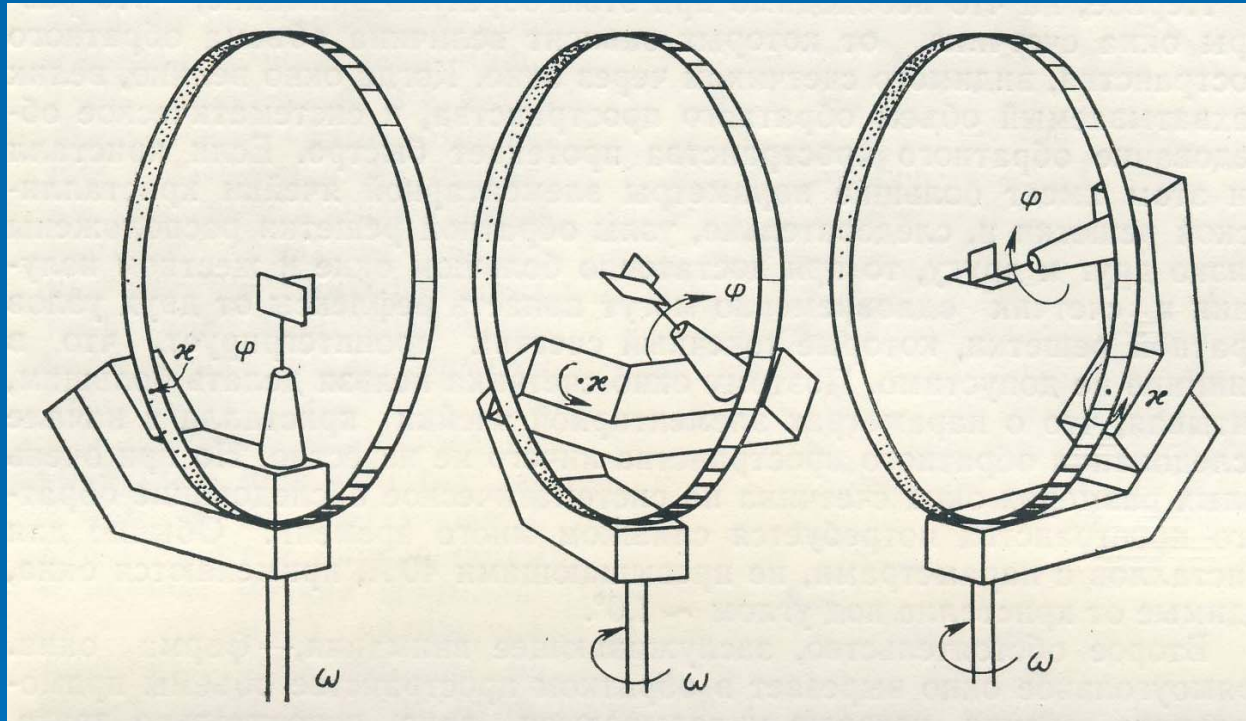




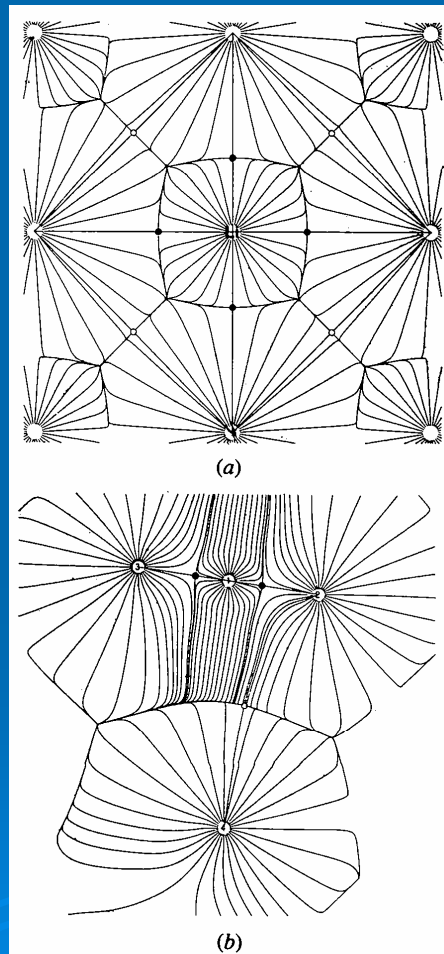




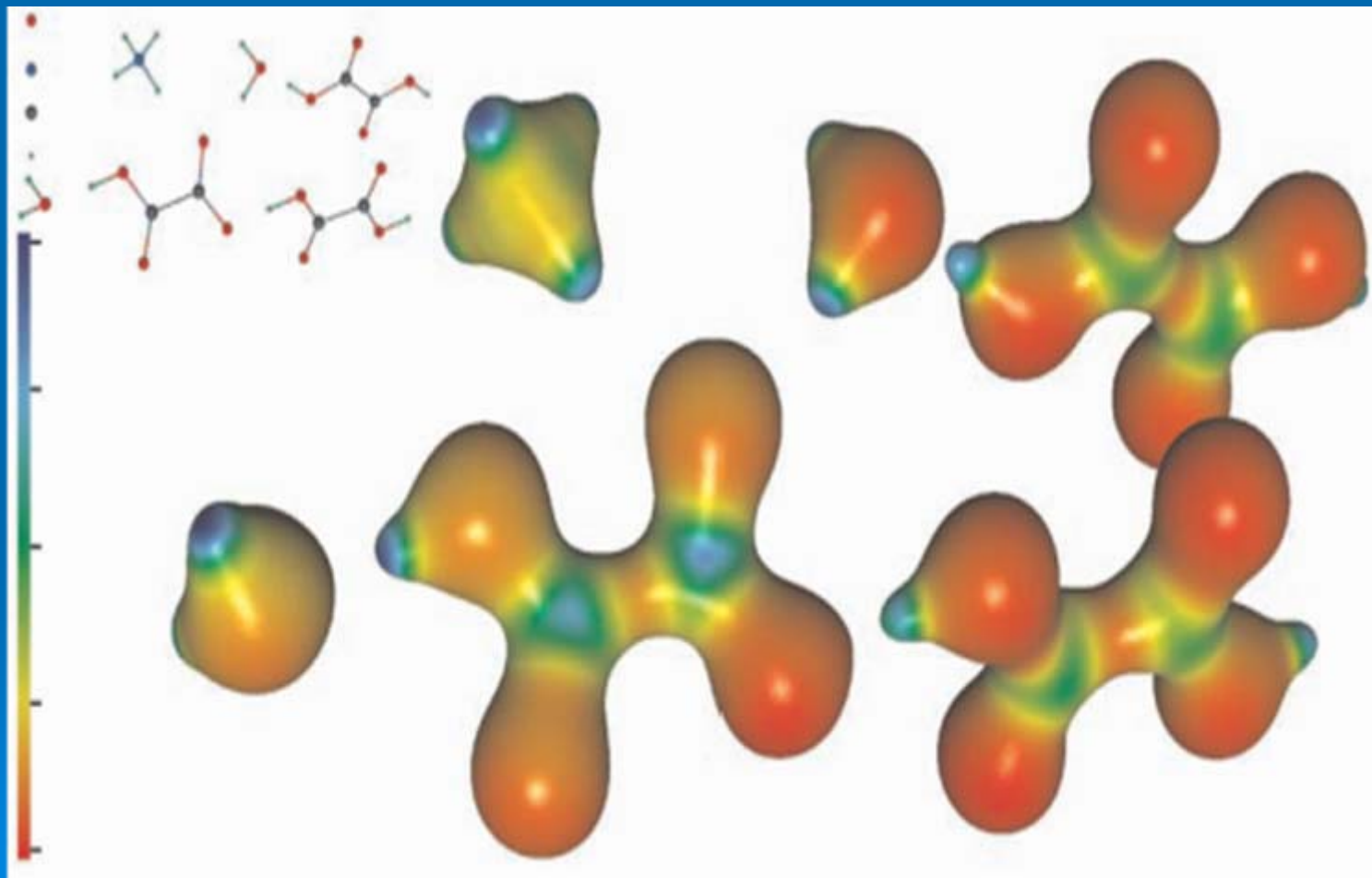




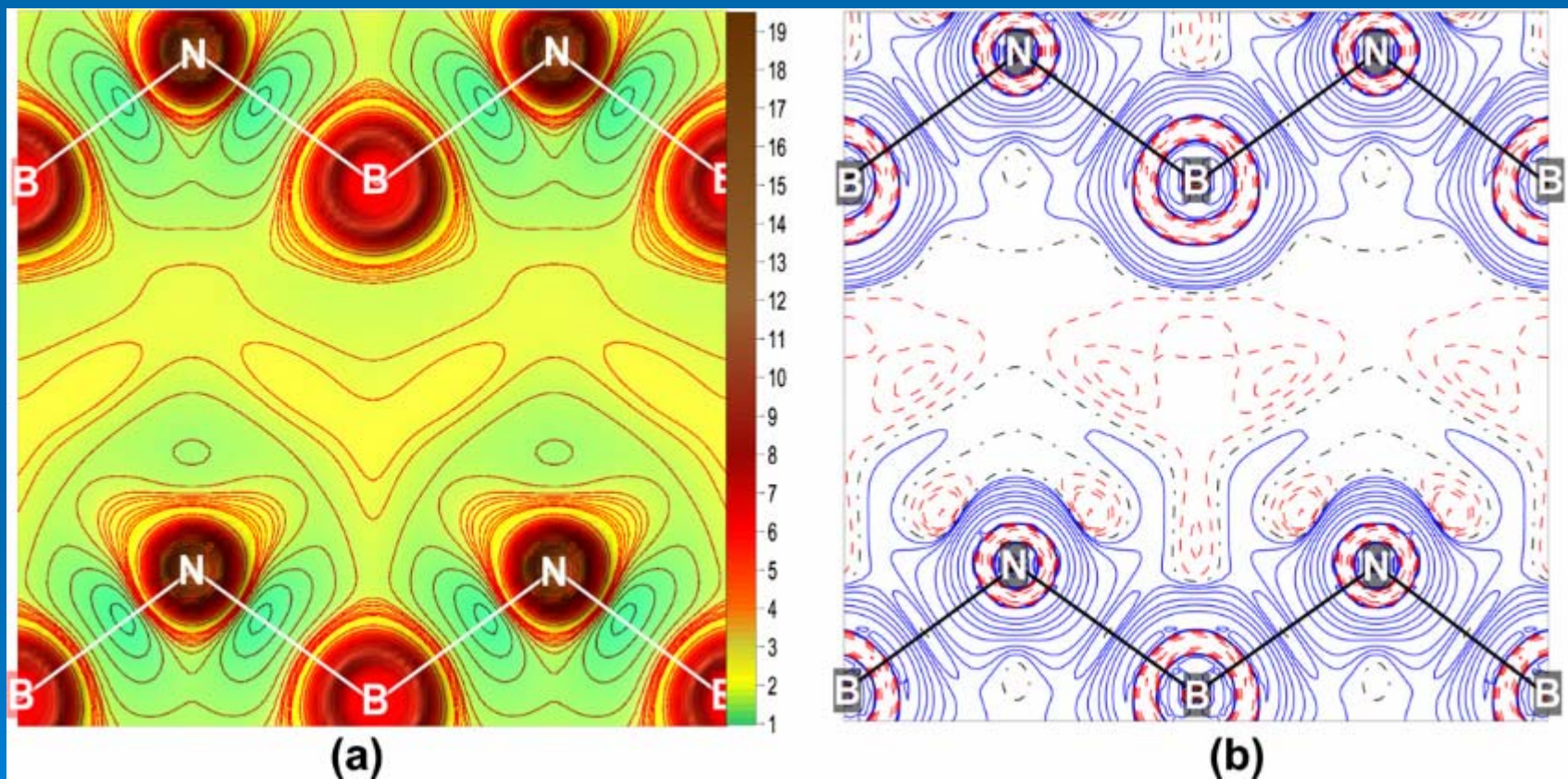
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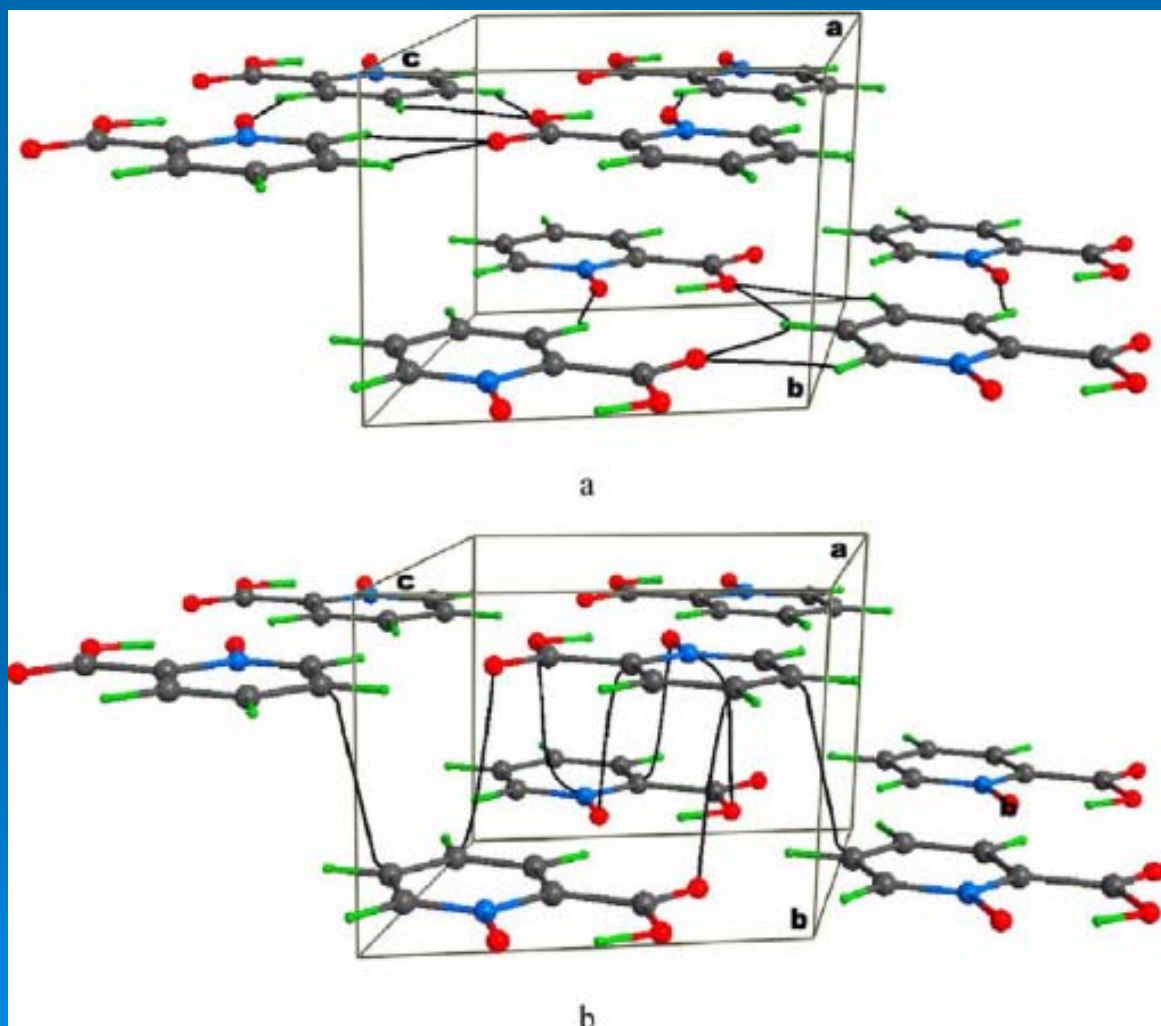
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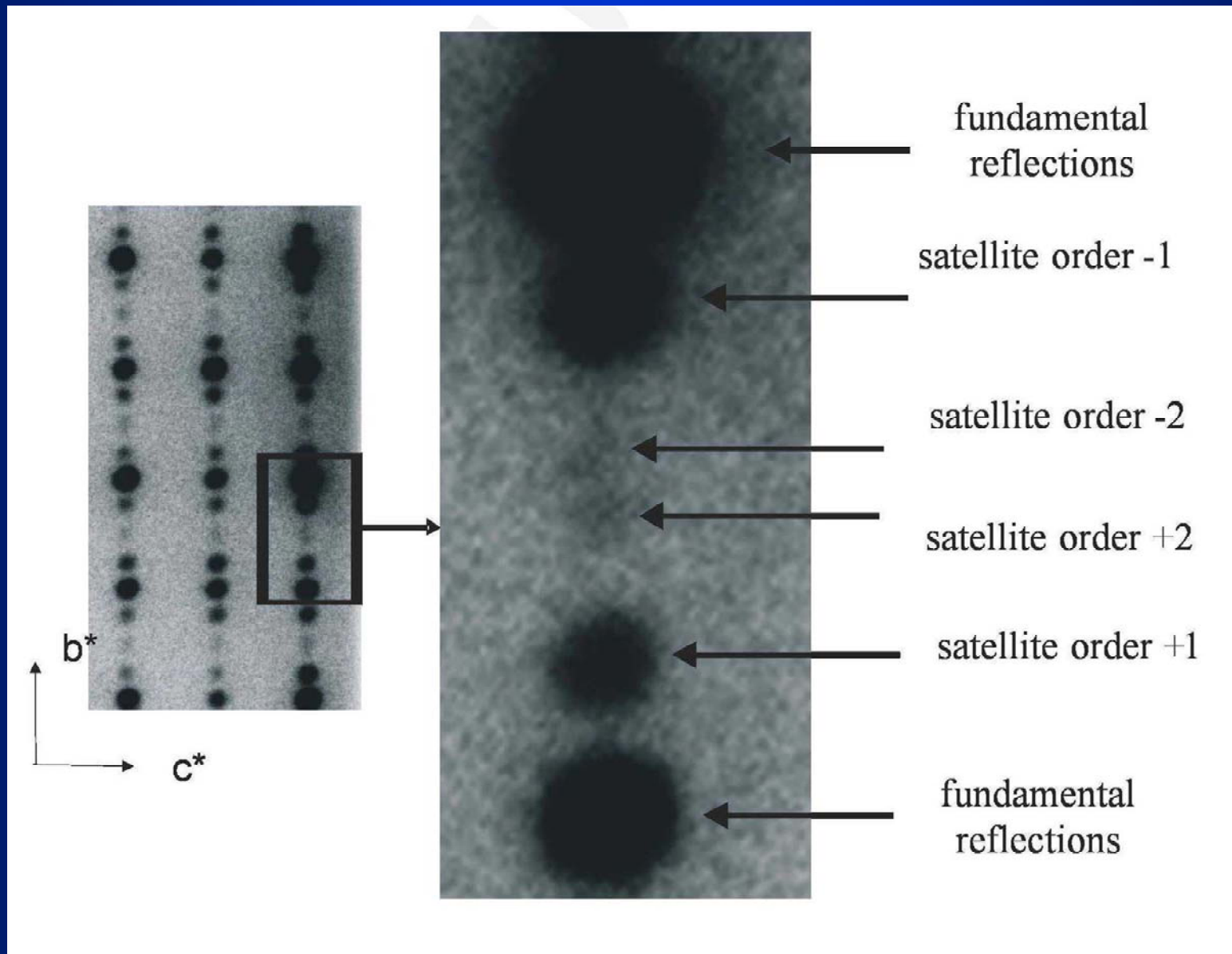


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The incommensurately modulated crystal structure of $\beta\text{-Pb}_2\text{BiVO}_6$
P. Roussels et al. // Acta Cryst. (2009) B65, 416.

Diffraction pattern of a modulated single crystal contains satellite reflections in the interstitials of the reciprocal lattice

$$\mathbf{H}(hkl) = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \quad \leftarrow \text{a main reflection}$$

$$\mathbf{q}(\alpha\beta\gamma) = \alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^* \quad \leftarrow \text{a modulation vector}$$

$$\mathbf{S}(hklm) = \mathbf{H}(hkl) + m\mathbf{q} \quad \leftarrow \text{a satellite}$$

$$= (h \pm m\alpha)\mathbf{a}^* + (k \pm m\beta)\mathbf{b}^* + (l \pm m\gamma)\mathbf{c}^*$$

There are different kinds of the structure modulation:

Displacive modulation:

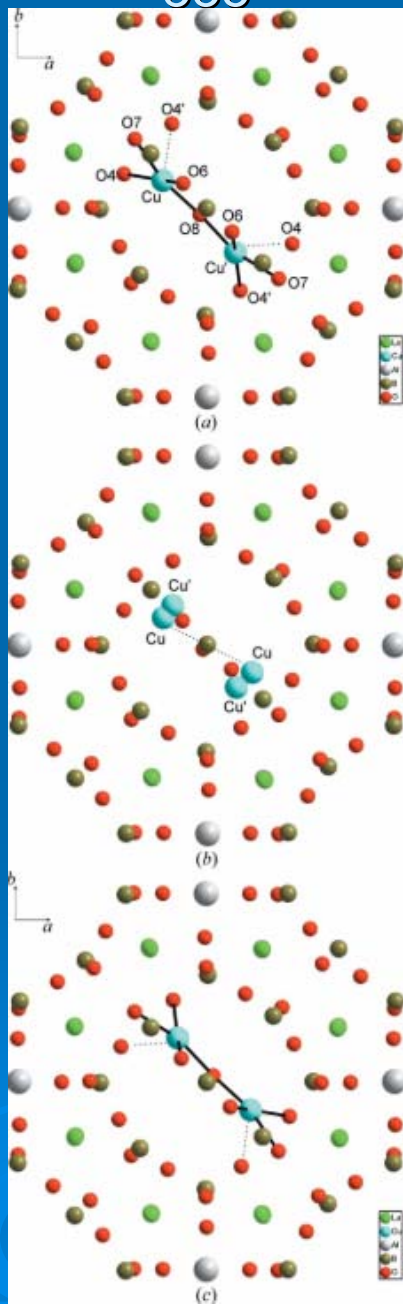
$$\mathbf{r} = \mathbf{r}^0 + \mathbf{n} + \sum_k \{ \mathbf{s}_k \sin[2\pi k\mathbf{q} \cdot (\mathbf{r}^0 + \mathbf{n})] + \mathbf{c}_k \cos[2\pi k\mathbf{q} \cdot (\mathbf{r}^0 + \mathbf{n})] \}$$

Occupation modulation:

$$\rho = \rho^0 + \sum_k \{ s\rho_k \sin[2\pi k\mathbf{q} \cdot (\mathbf{r}^0 + \mathbf{n})] + c\rho_k \cos[(2\pi k\mathbf{q} \cdot (\mathbf{r}^0 + \mathbf{n}))] \}$$

Since translational symmetry is broken, atomic coordinates depend on the lattice position. We should select a unit cell of the periodic lattice as an origin; \mathbf{n} is a translation between the origin and the cell under consideration; $\mathbf{r}^0(x^0, y^0, z^0)$ are basic atomic coordinates and the last term defines atomic displacement.

A modulation function can be expanded into Fourier series as here. Legendre polynomials can also be used to expand the stepwise functions such as **crenels** and **saw-tooth** functions.



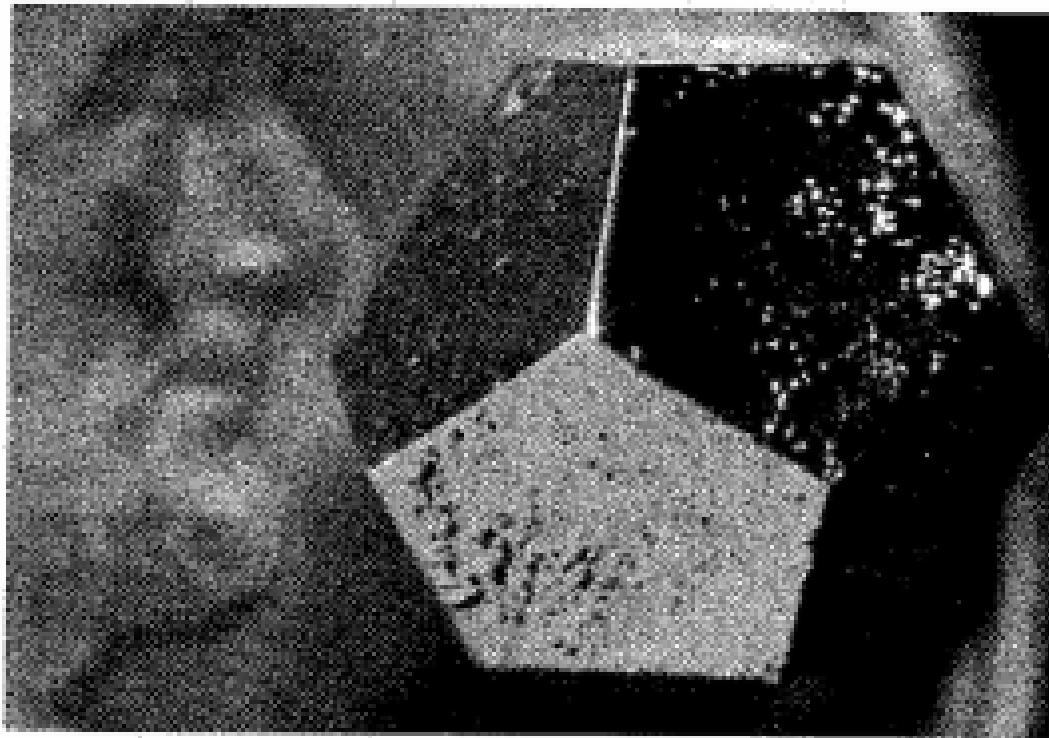
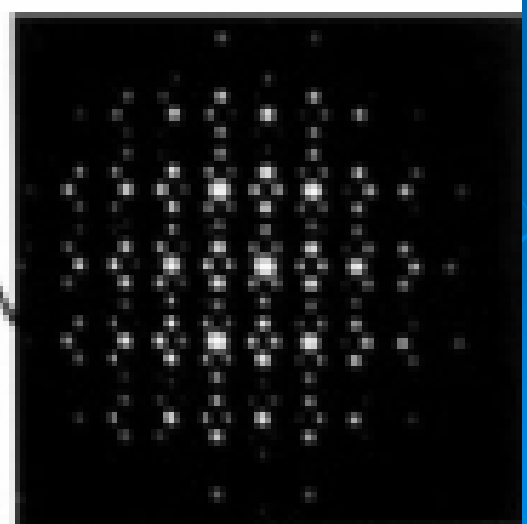
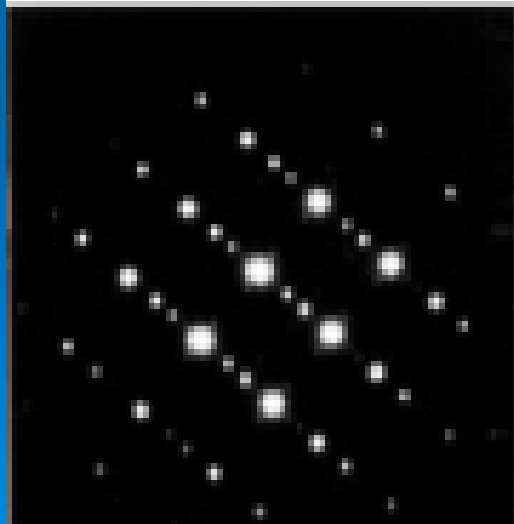
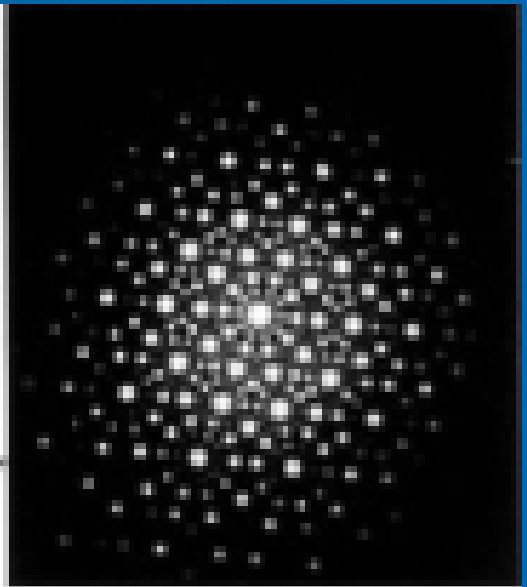
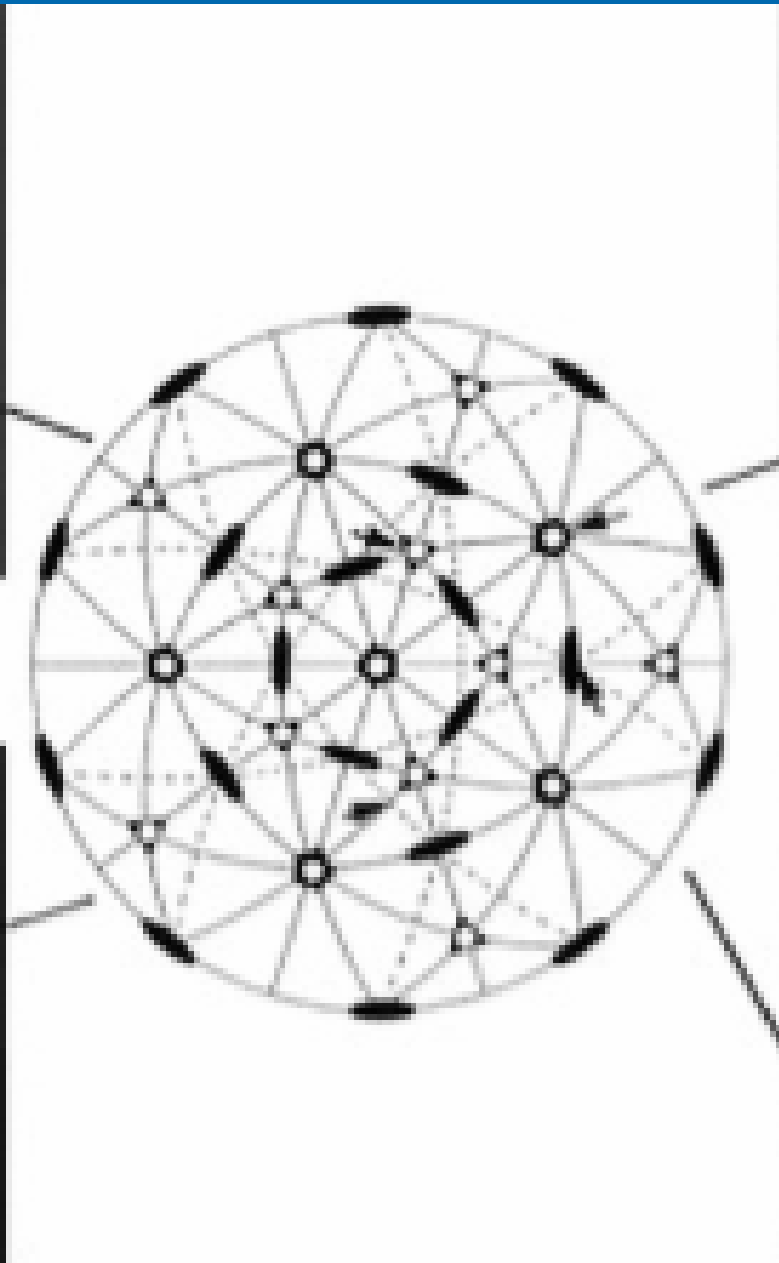
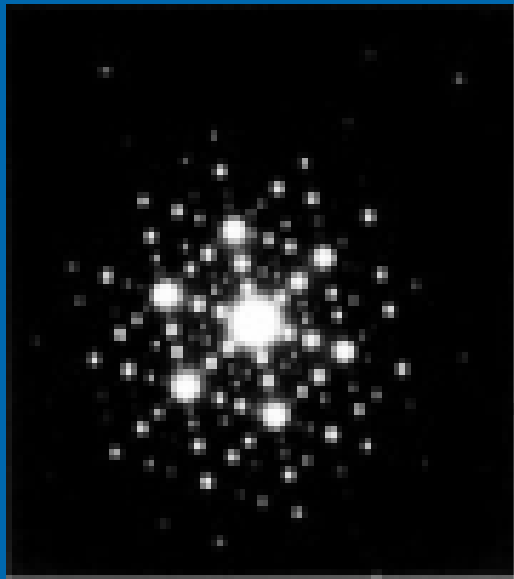
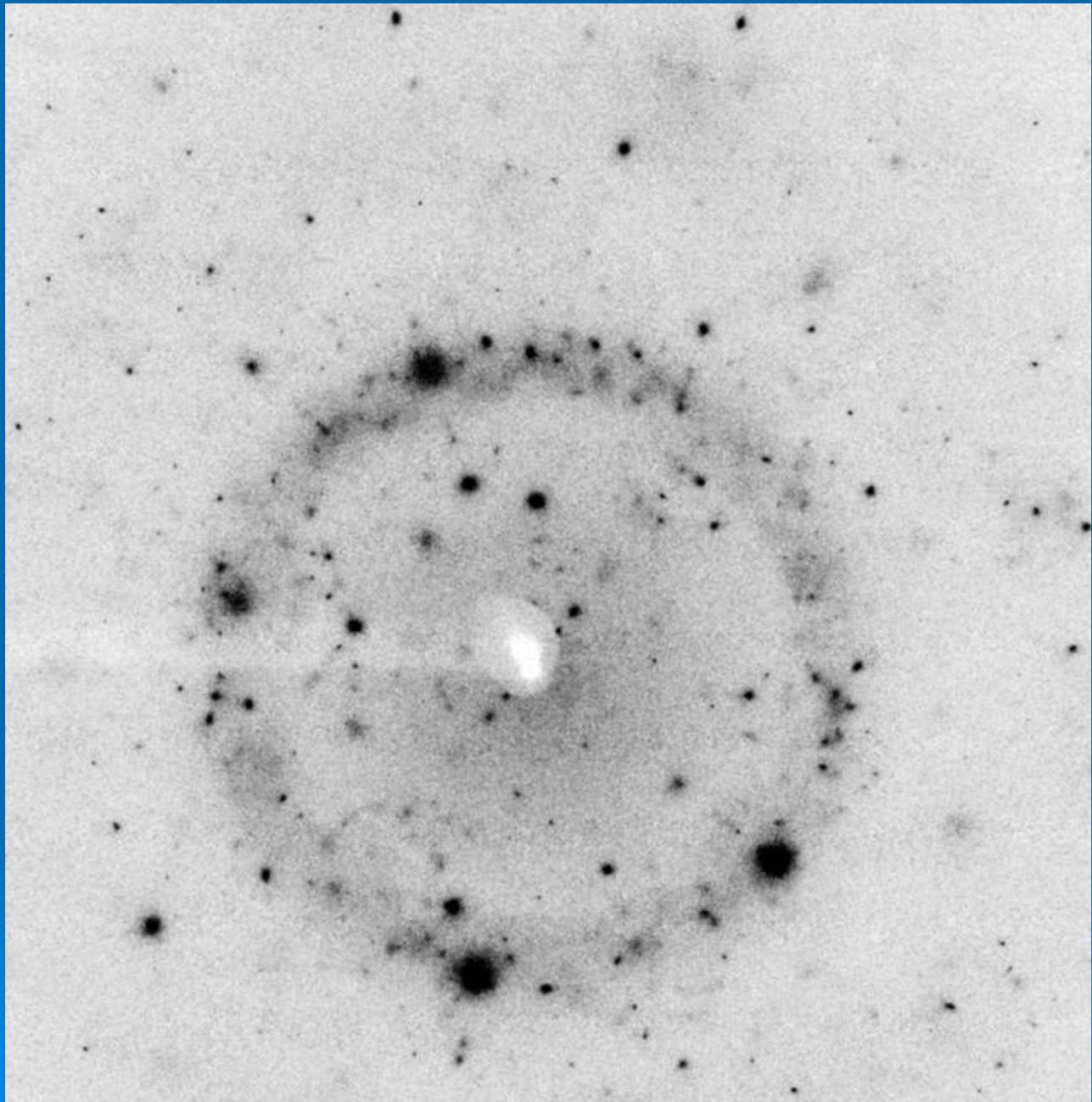
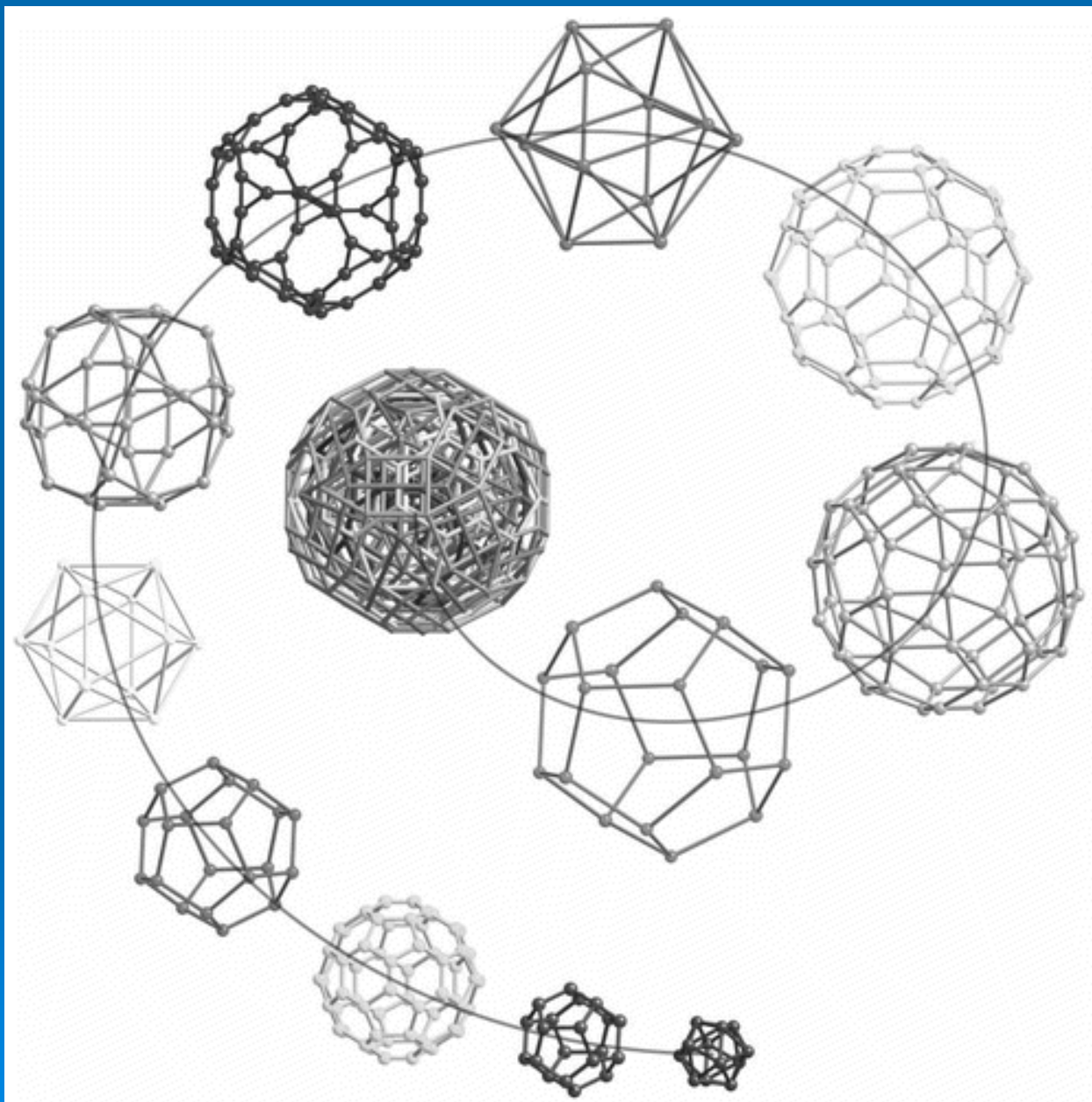
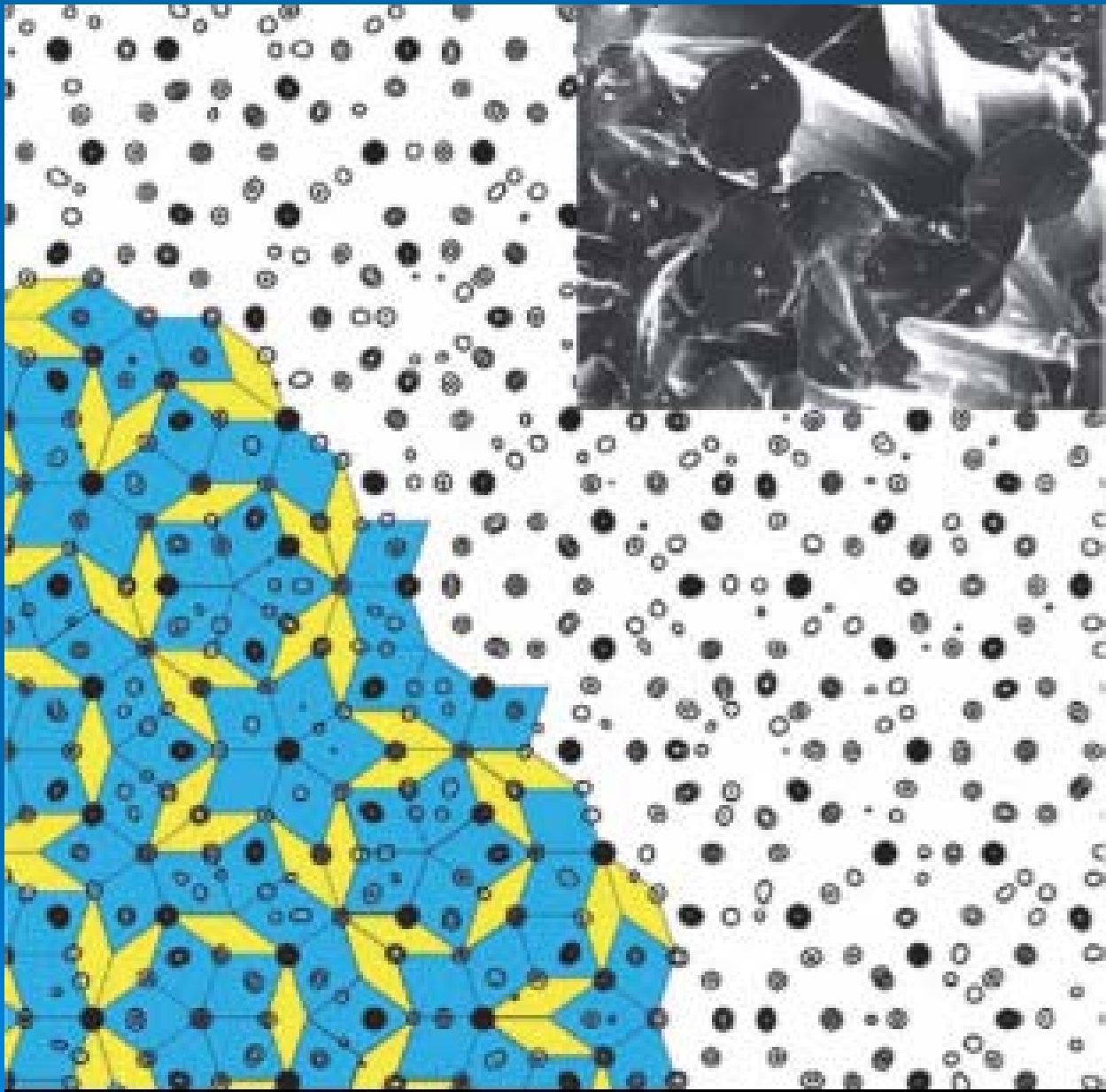


Fig. 1.17. Specimen of icosahedral HoMgZn. Quasicrystals may have the shape of a dodecahedron. Six Miller indices are needed in this case. Photograph courtesy of I. R. Fisher (Stanford) and P. C. Canfield (Ames Laboratory)









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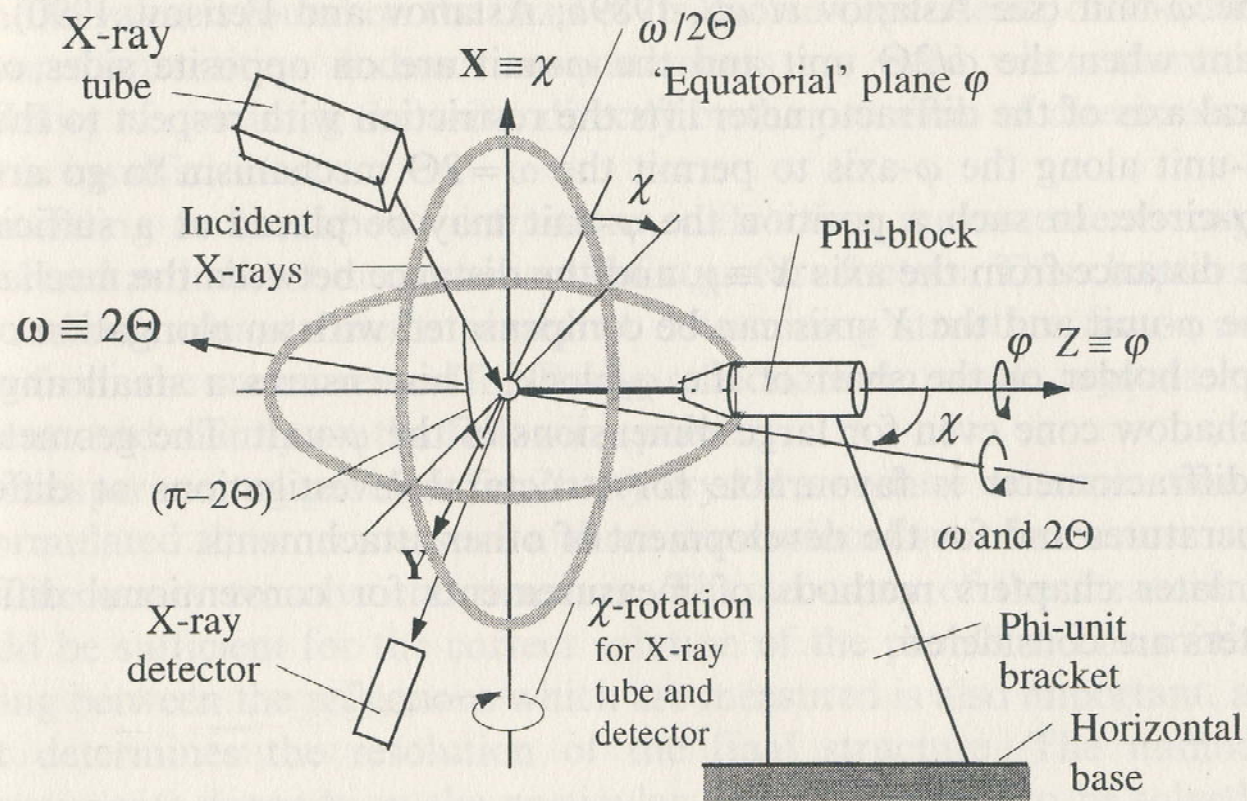
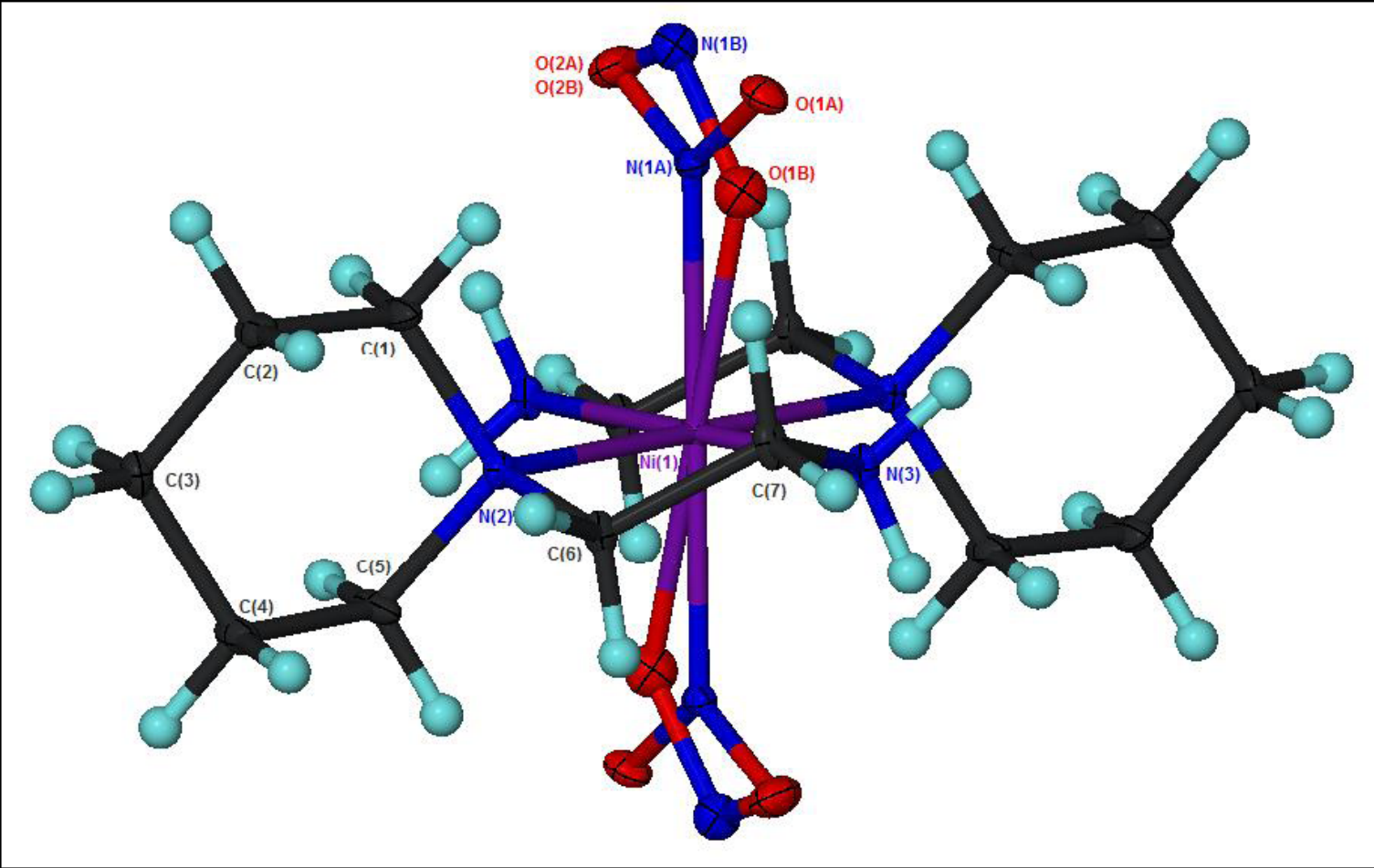
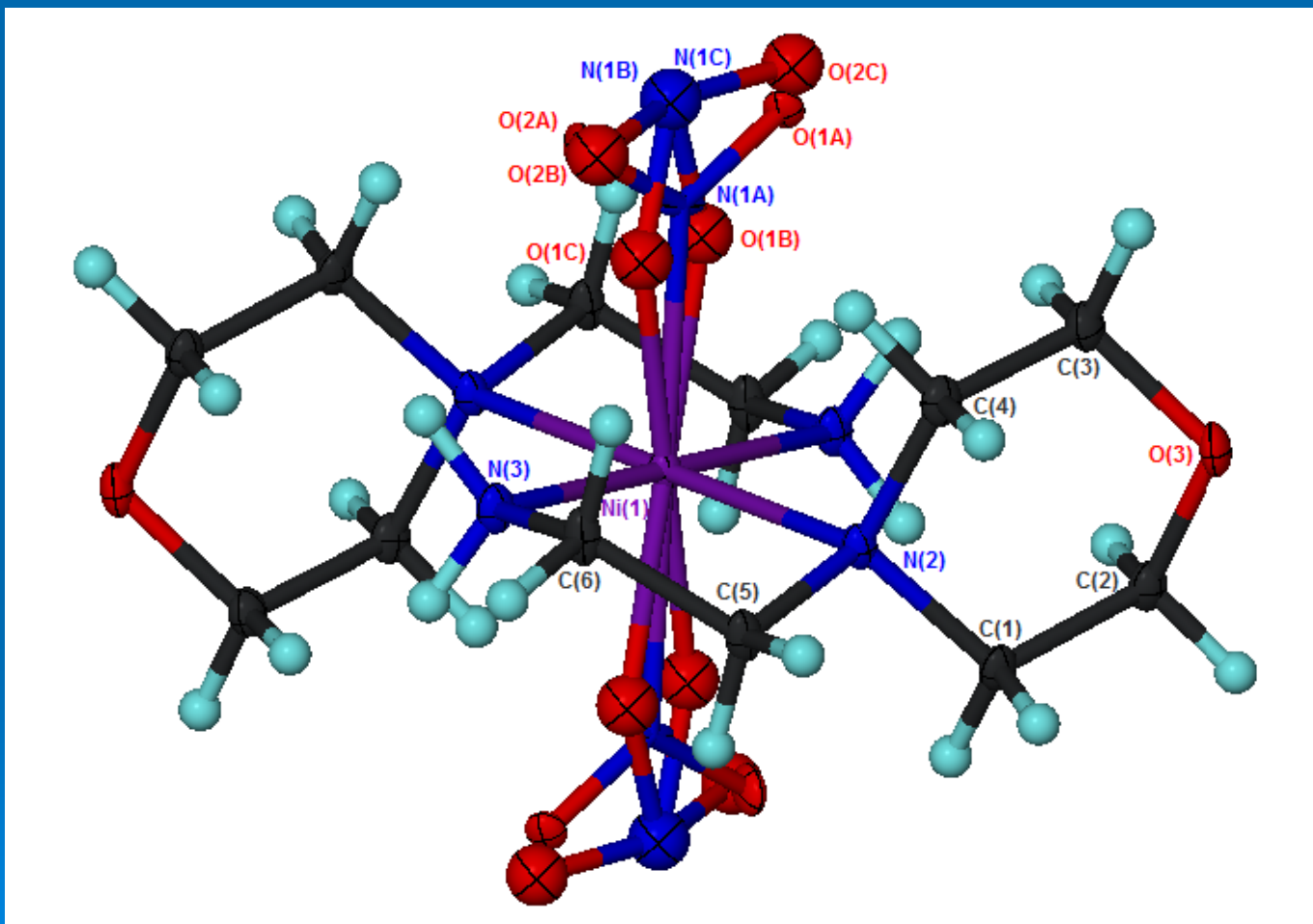
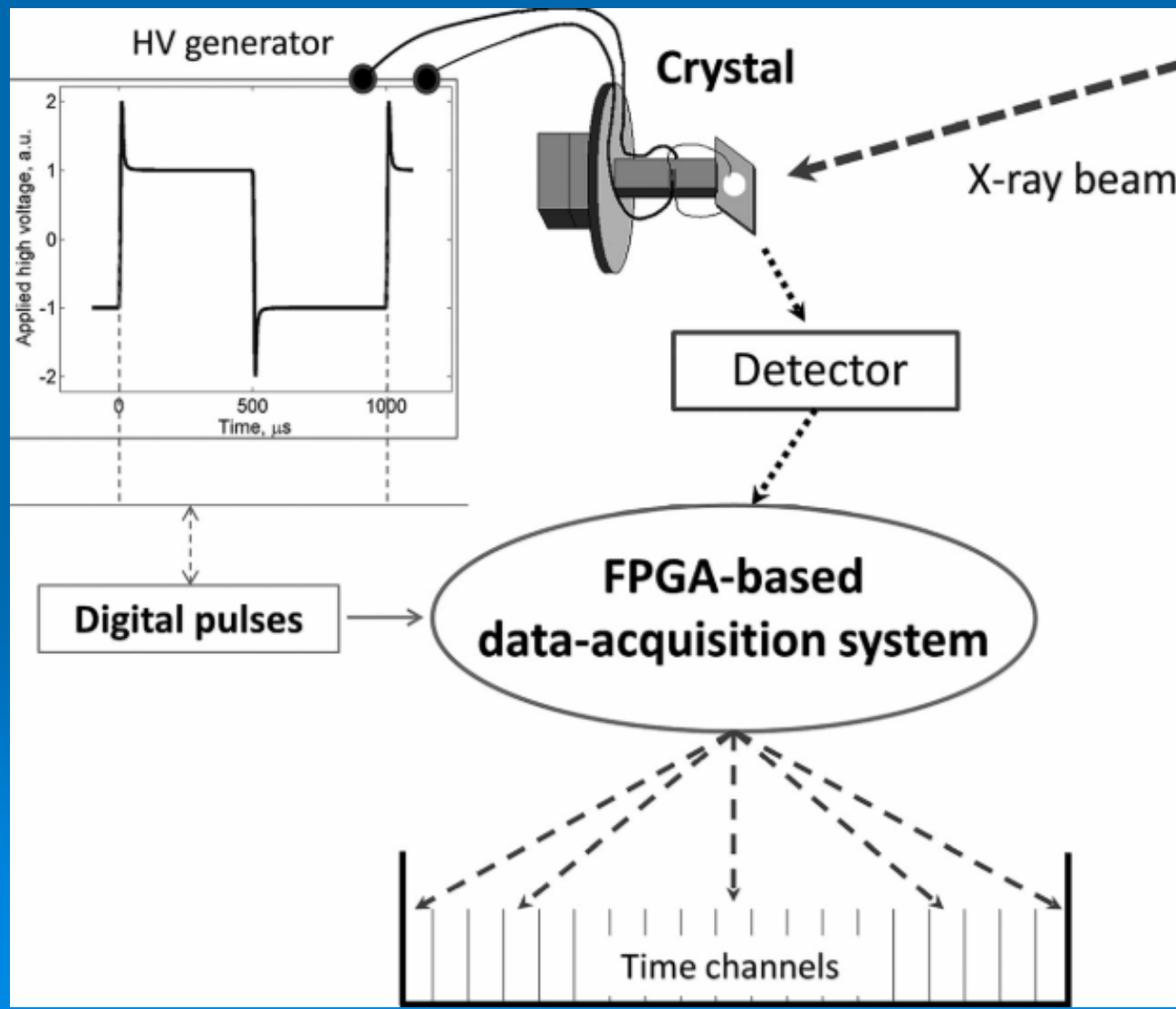


Fig. 3.22. Representation of angular movements and axes positioning in the diffractometer RMD with a non-movable phi-unit.

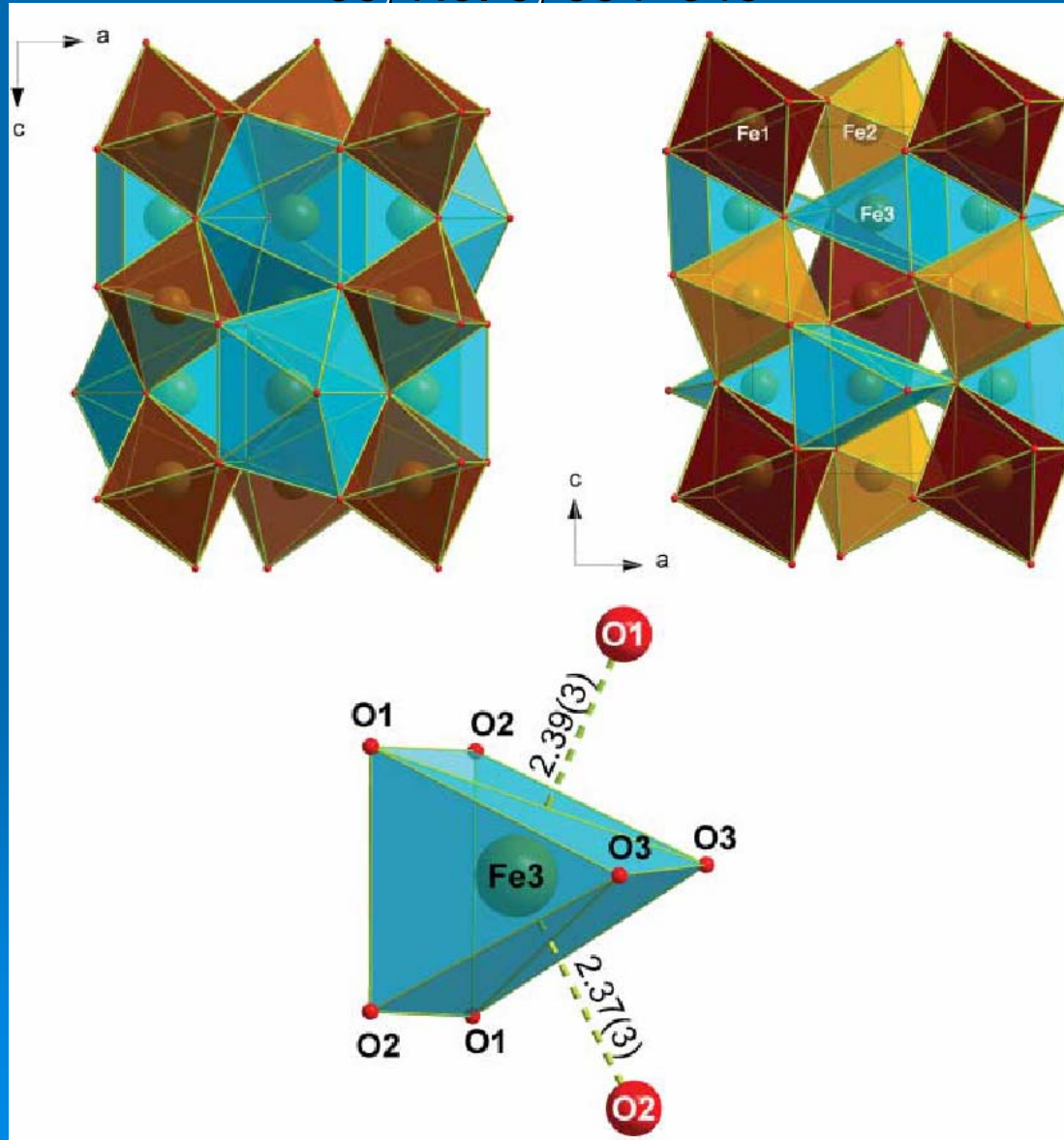


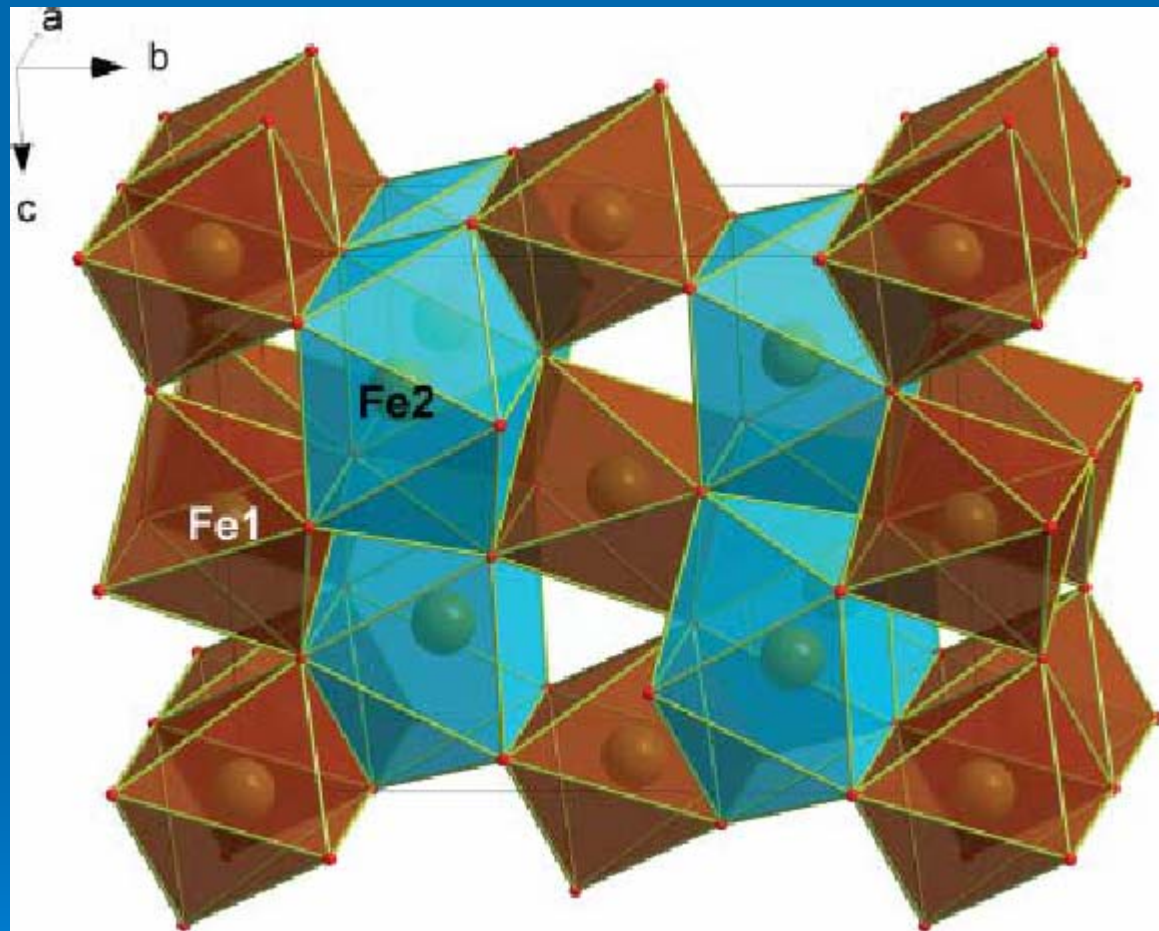


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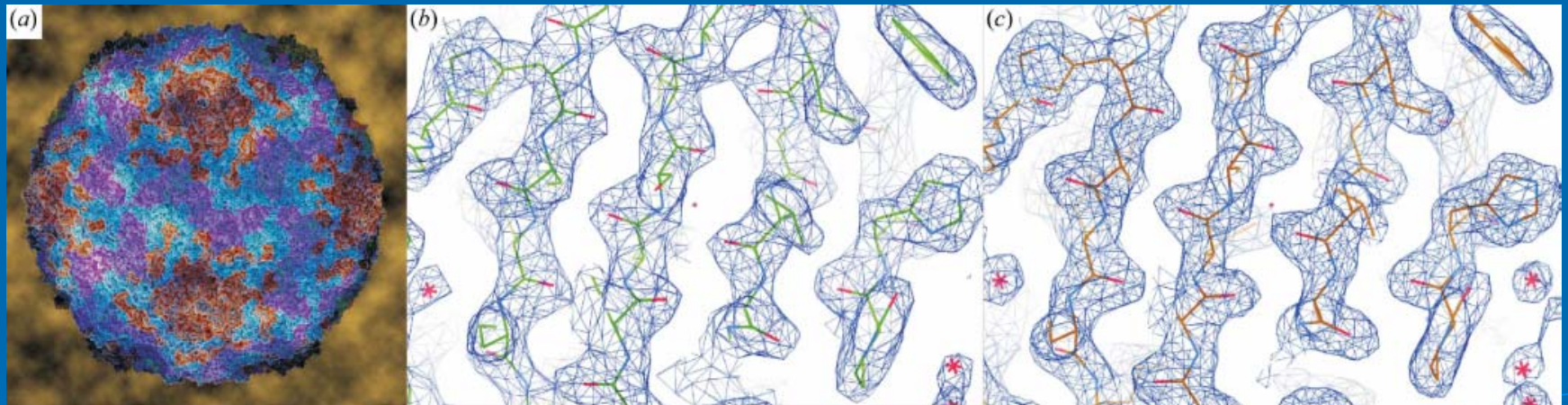


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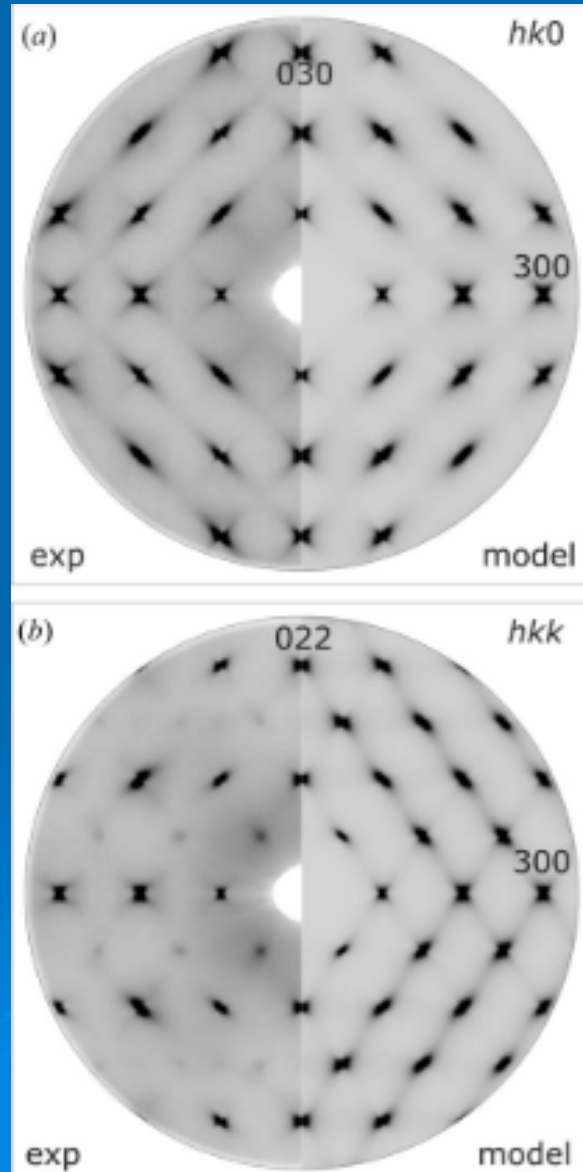


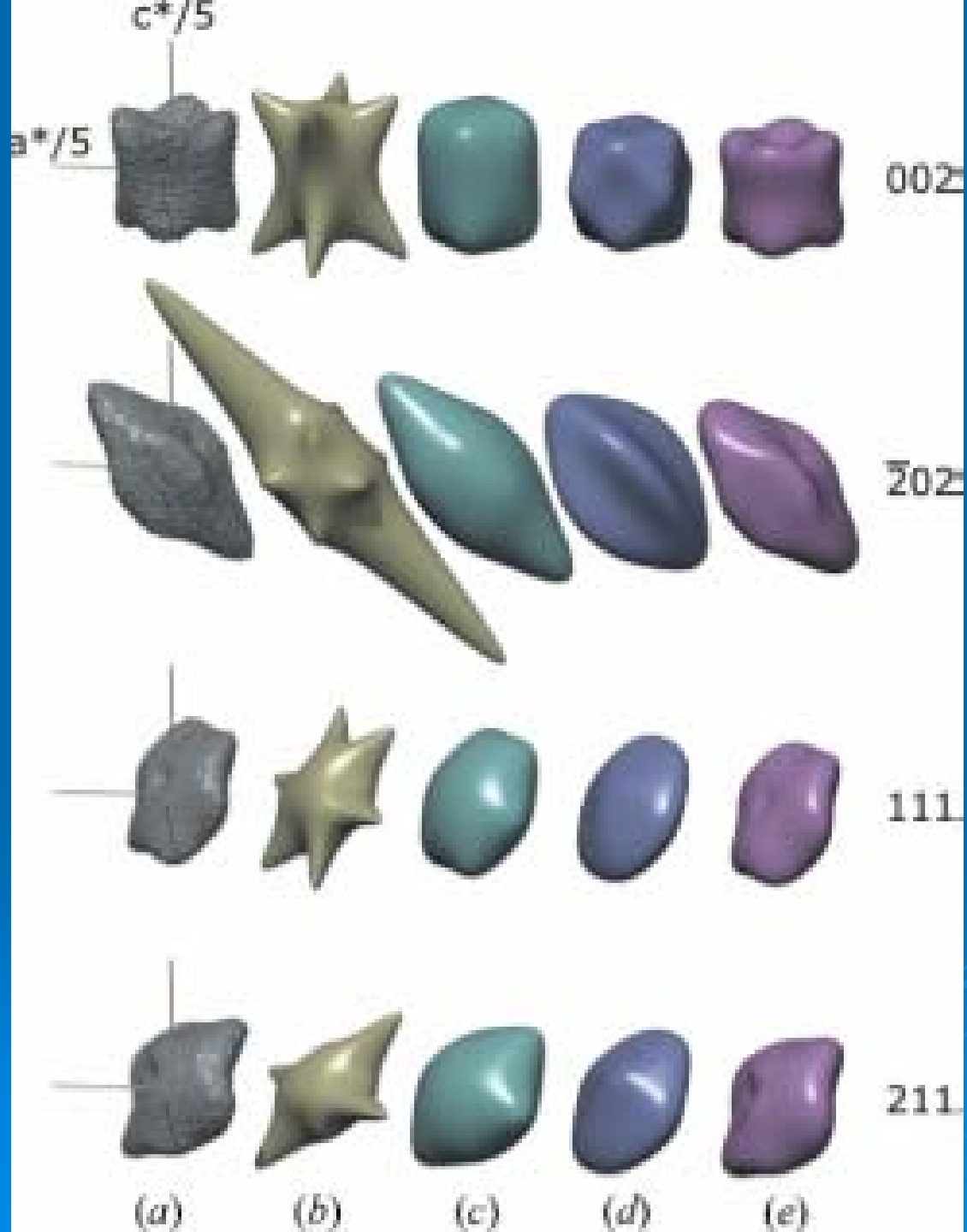


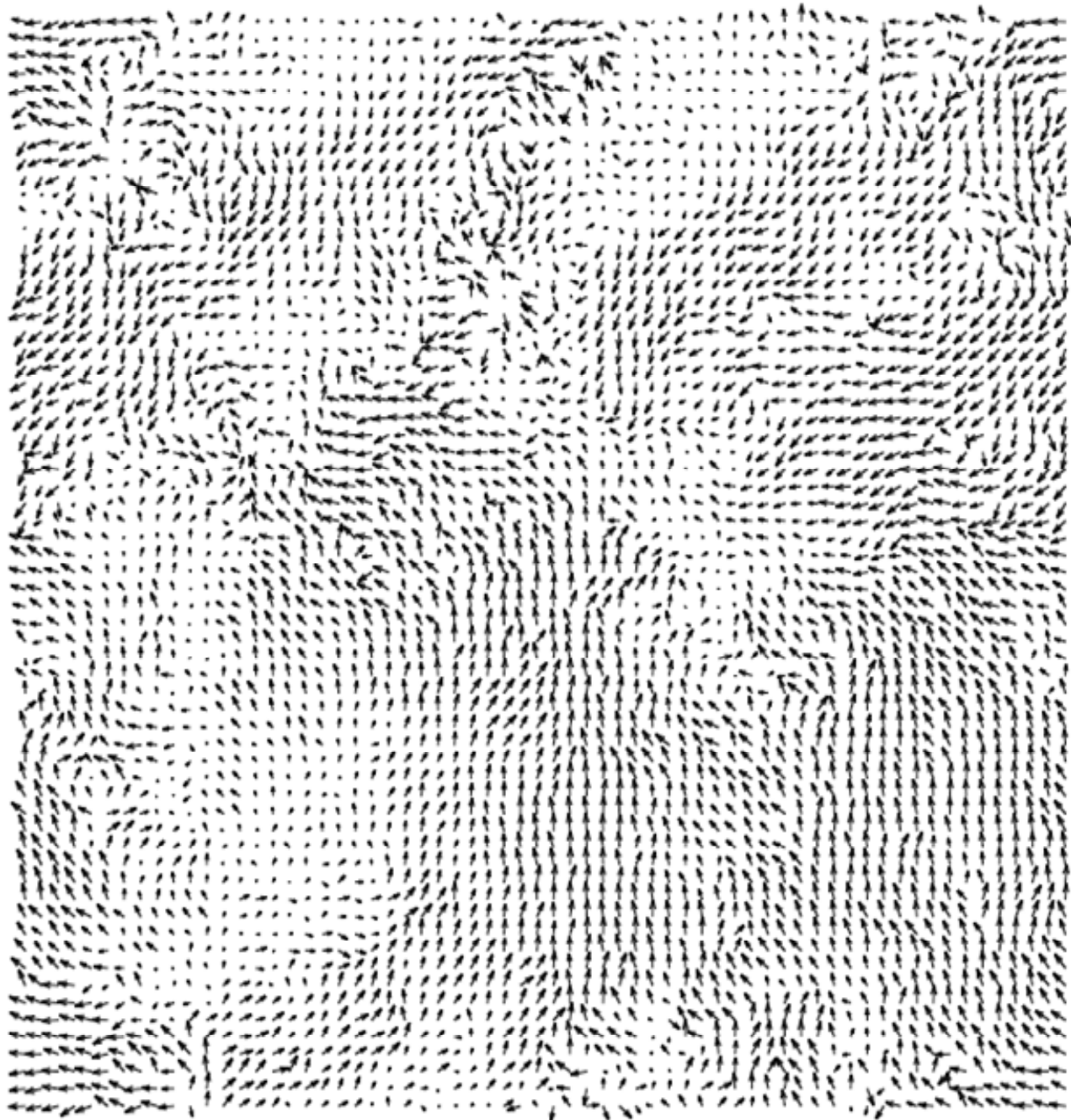
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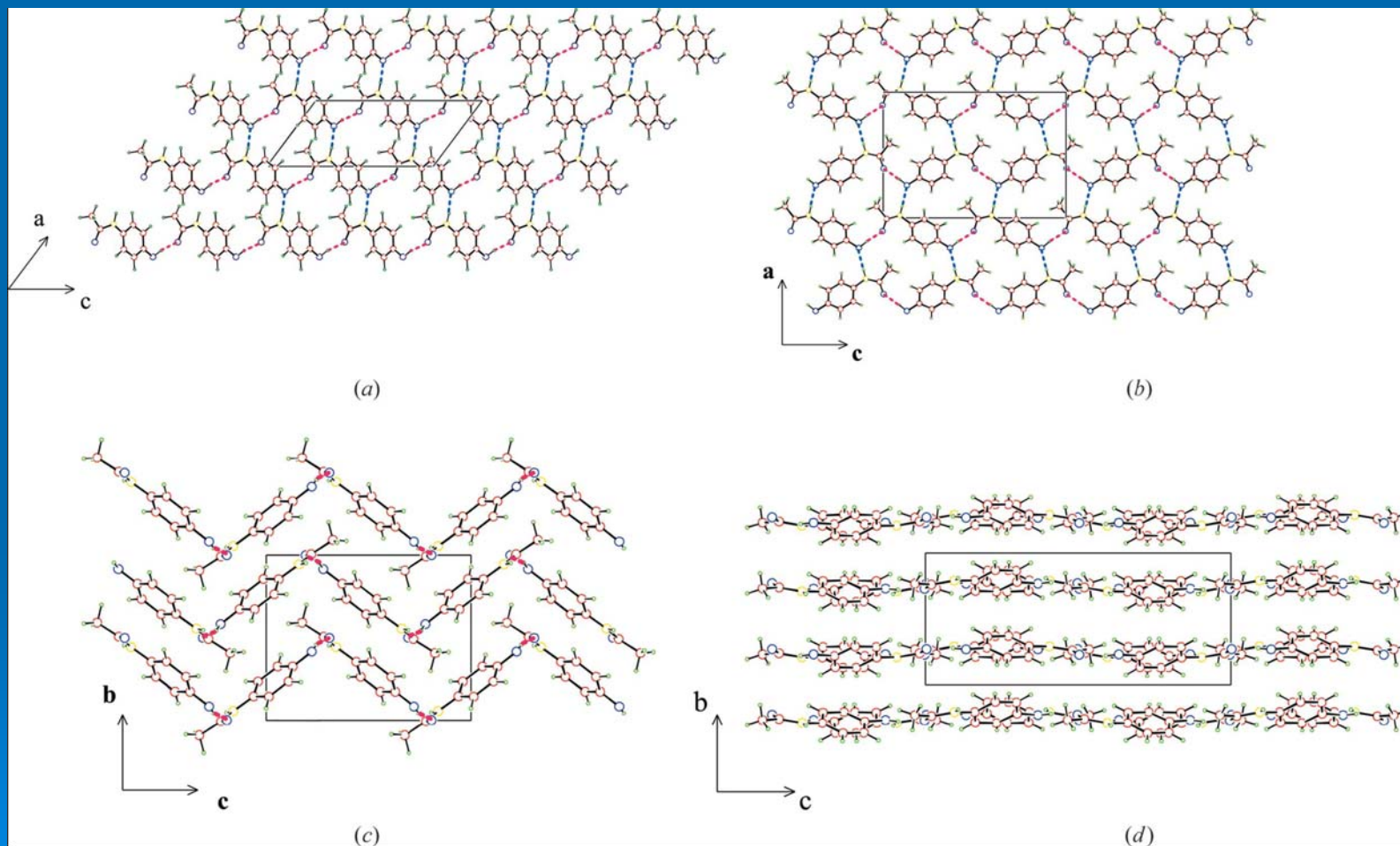
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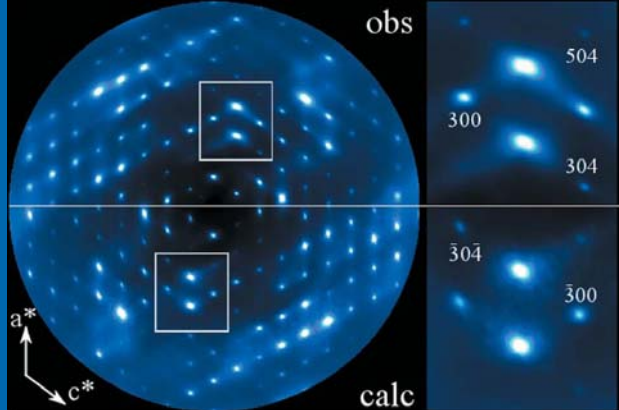




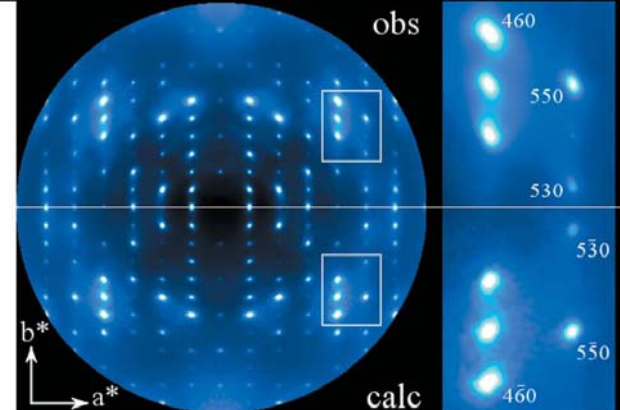


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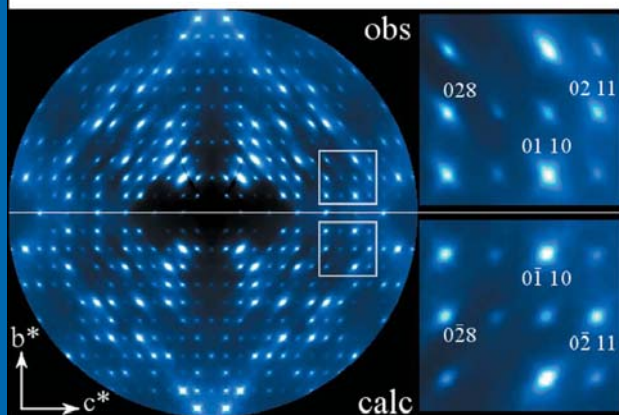




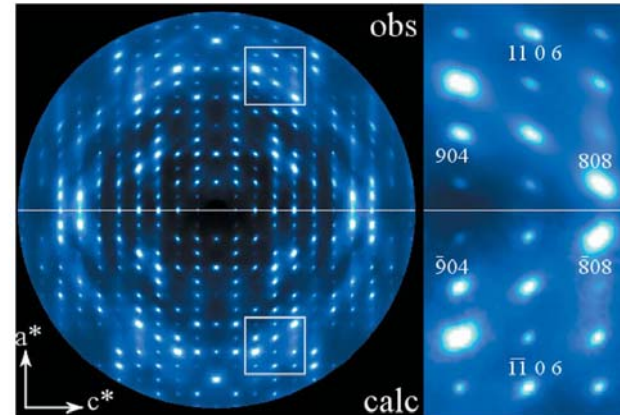
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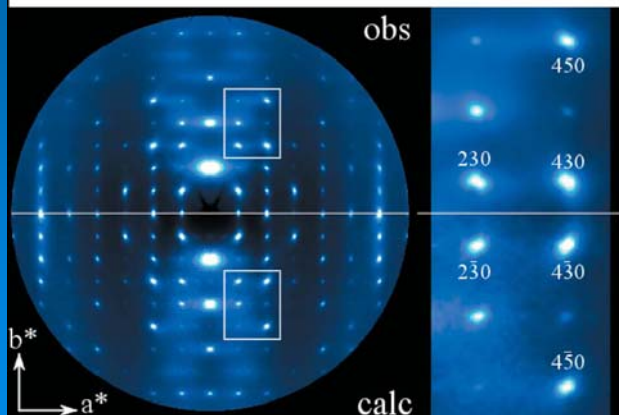
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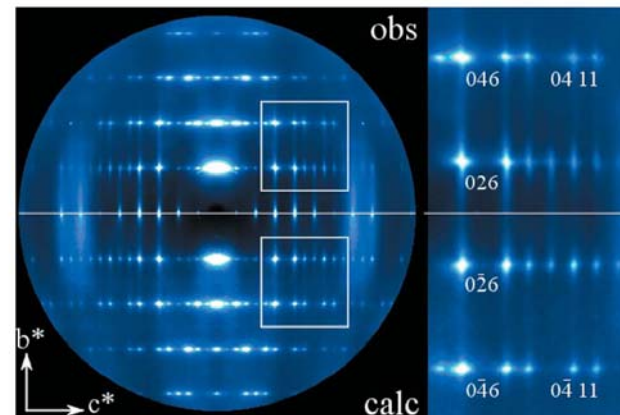
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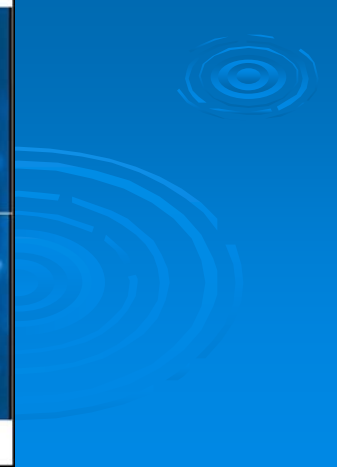
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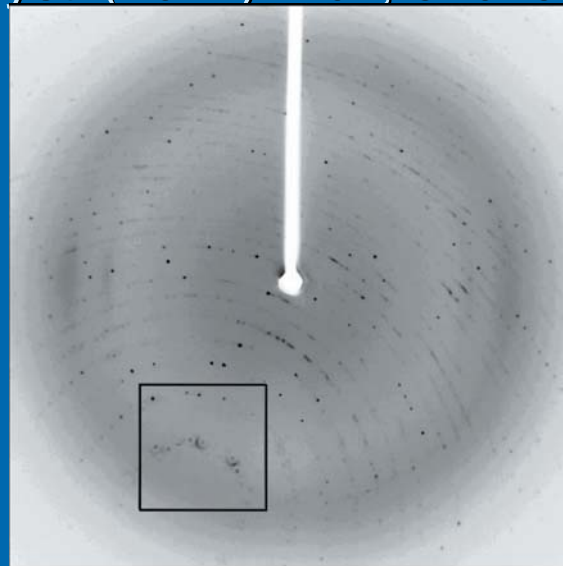
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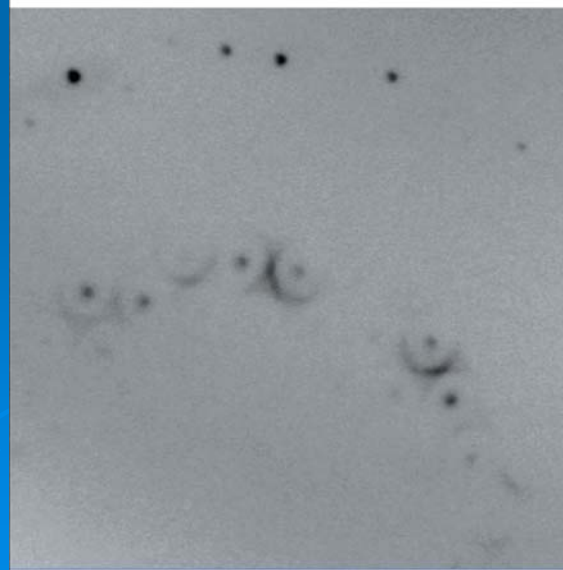
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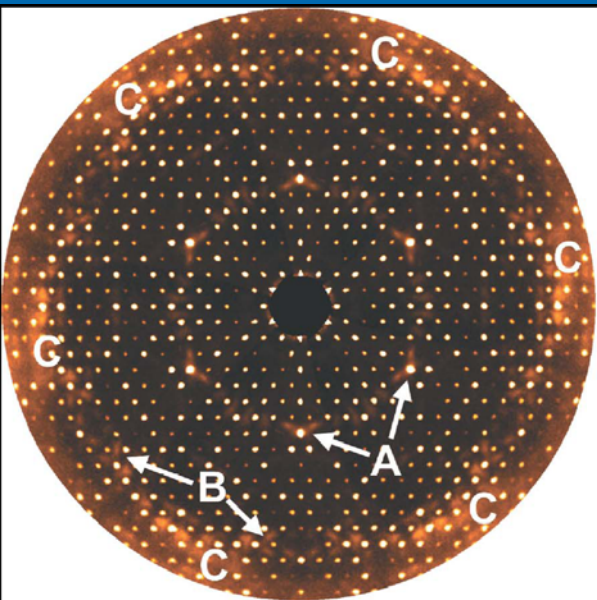
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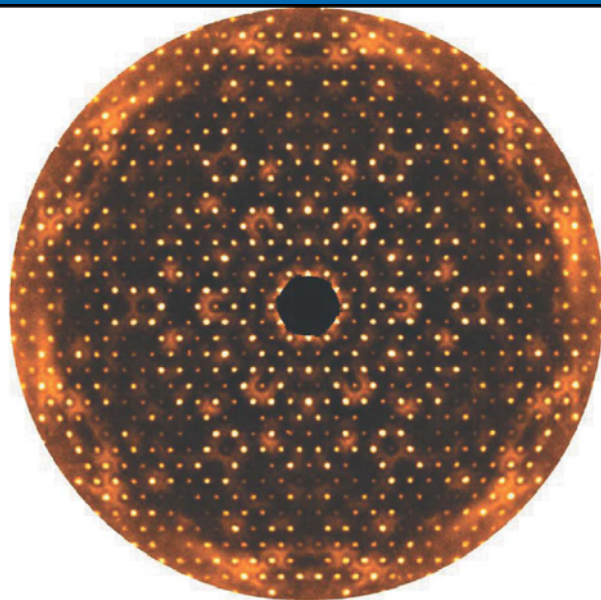
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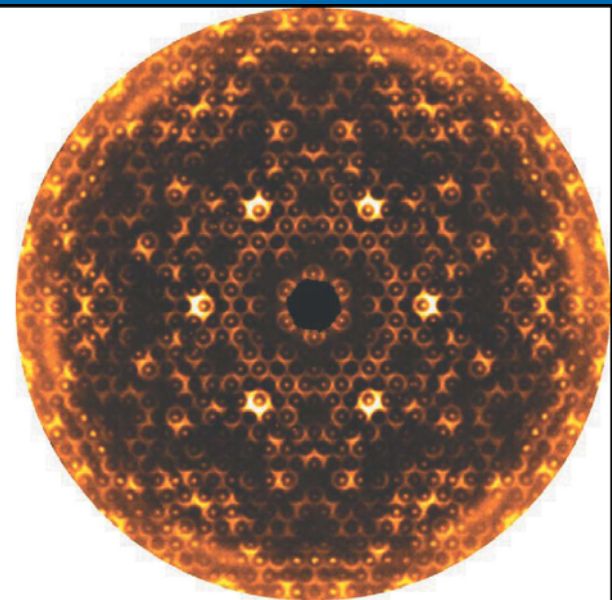
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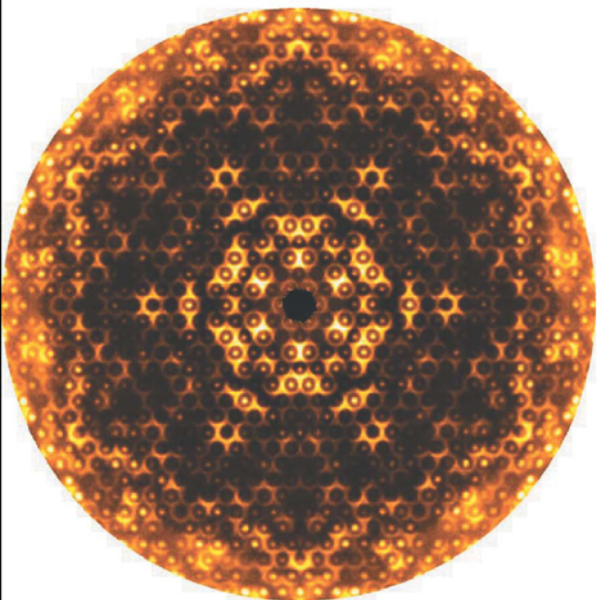
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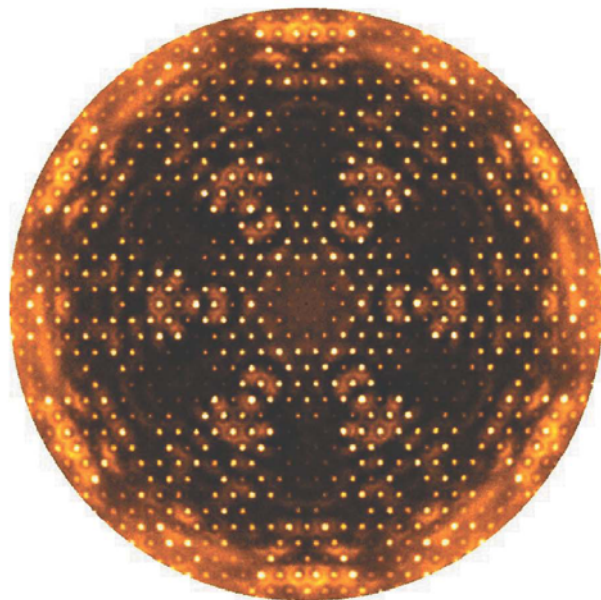
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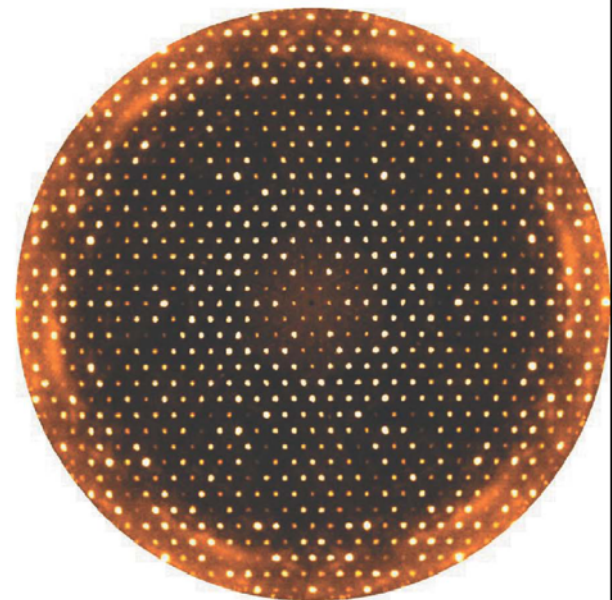
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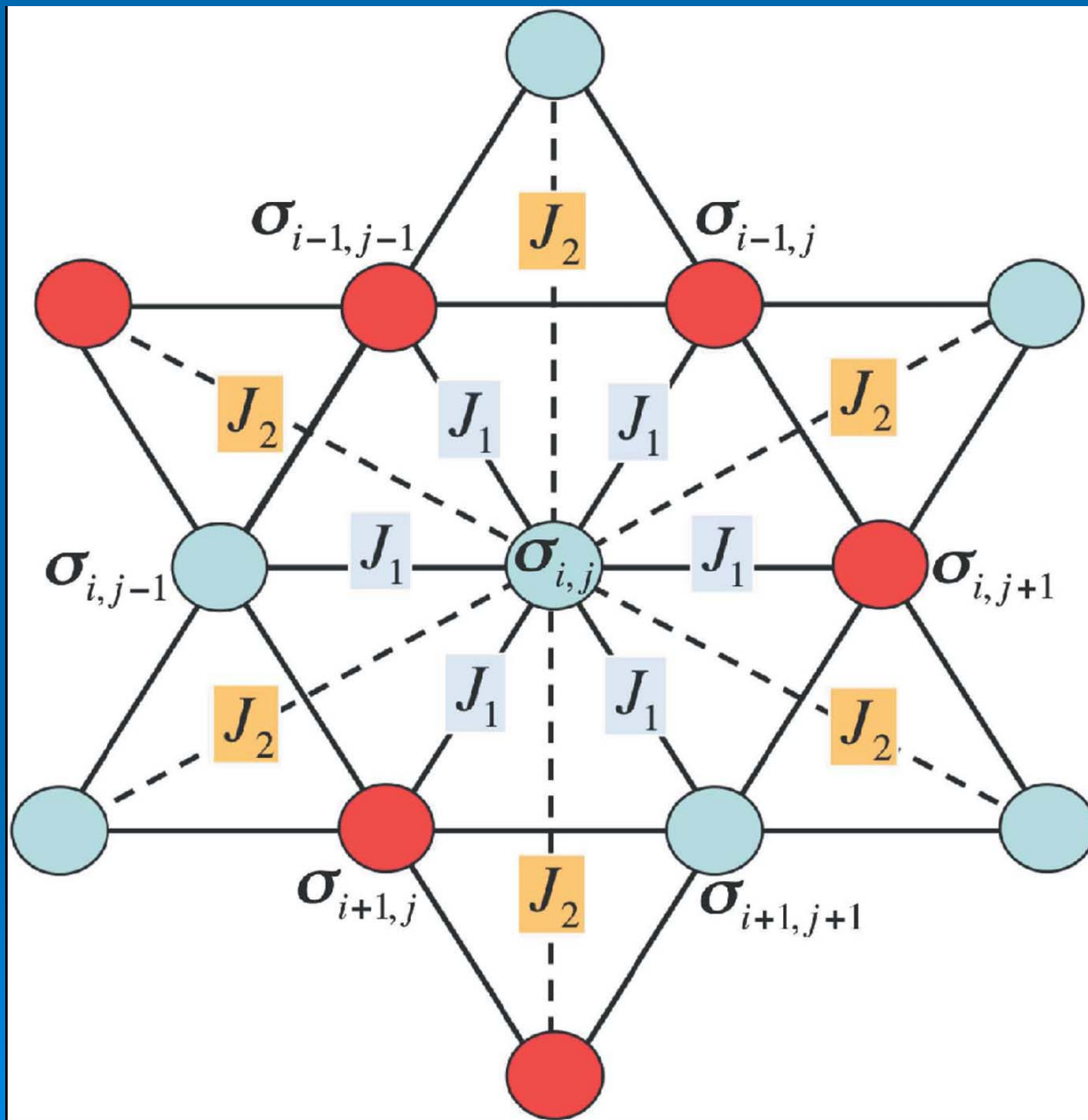
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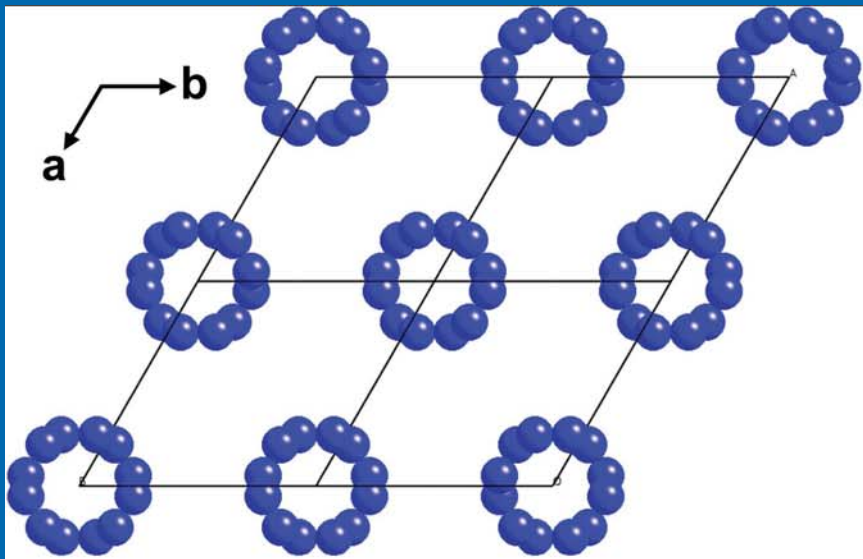


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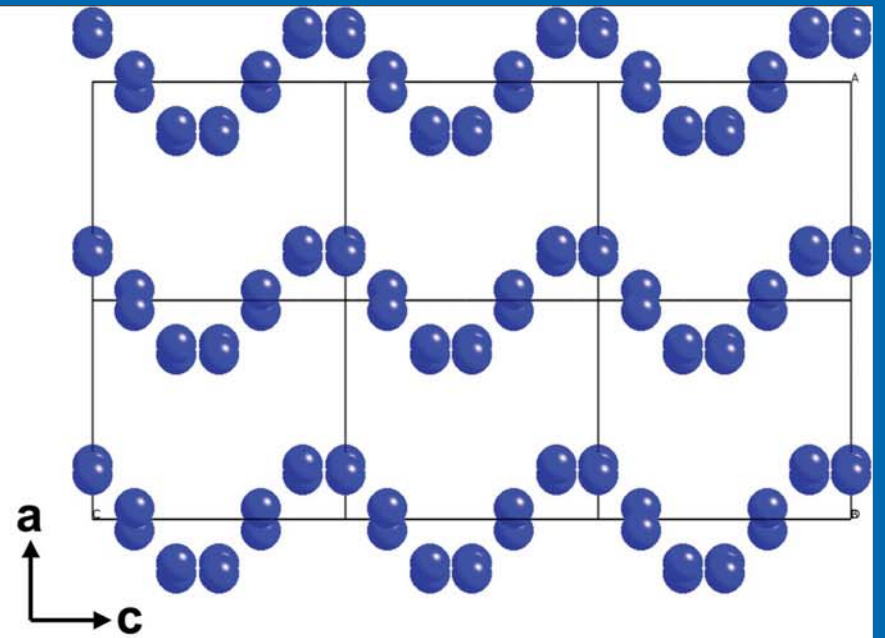


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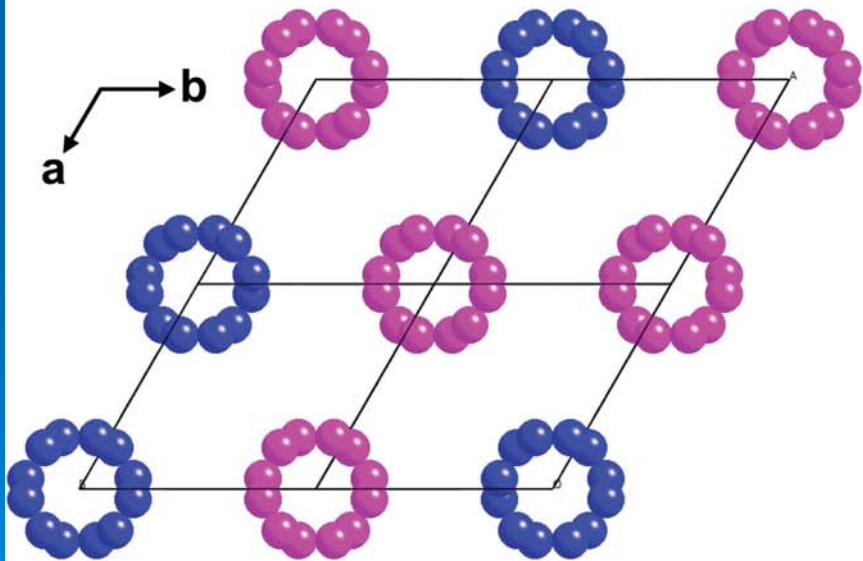




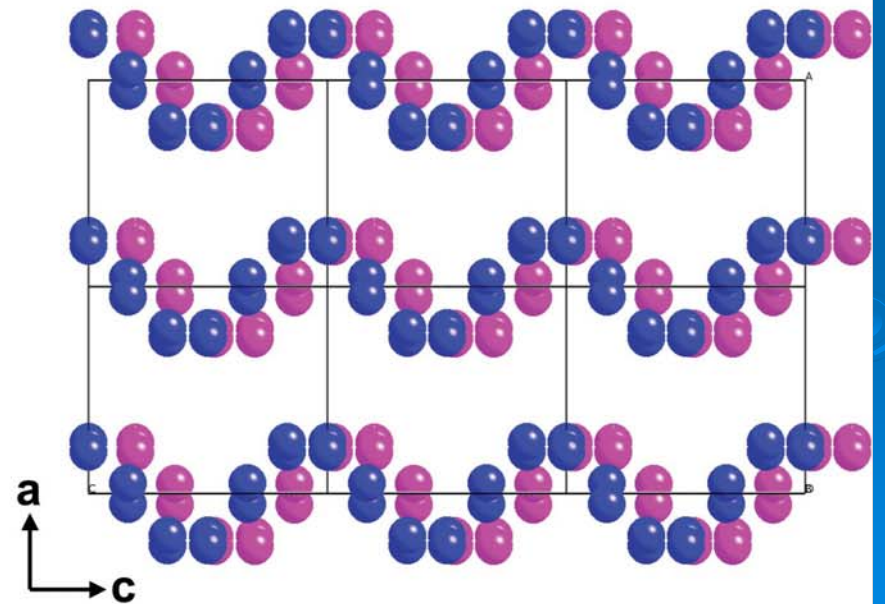
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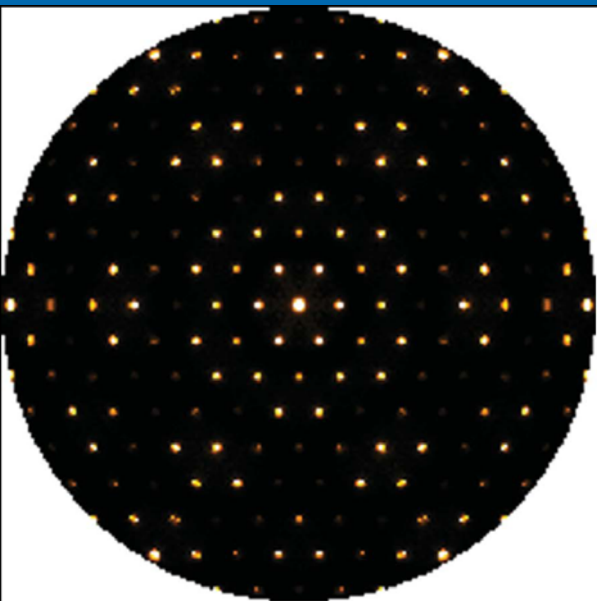
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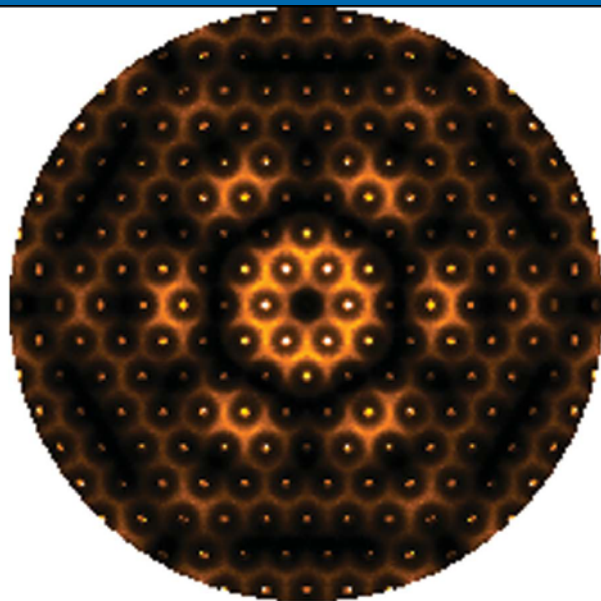
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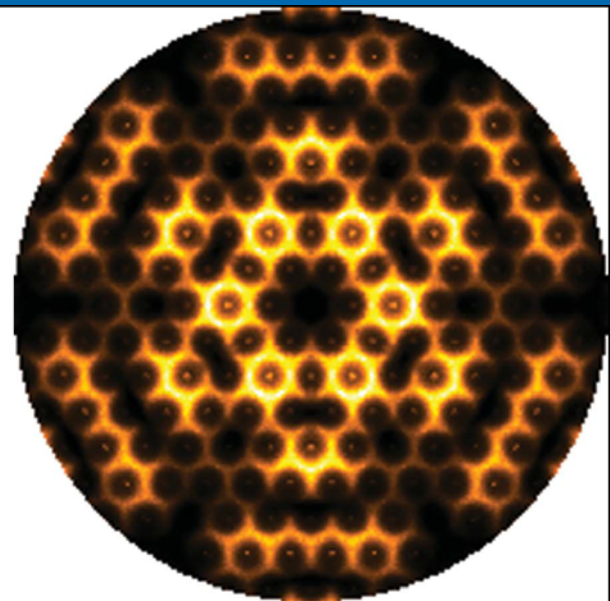
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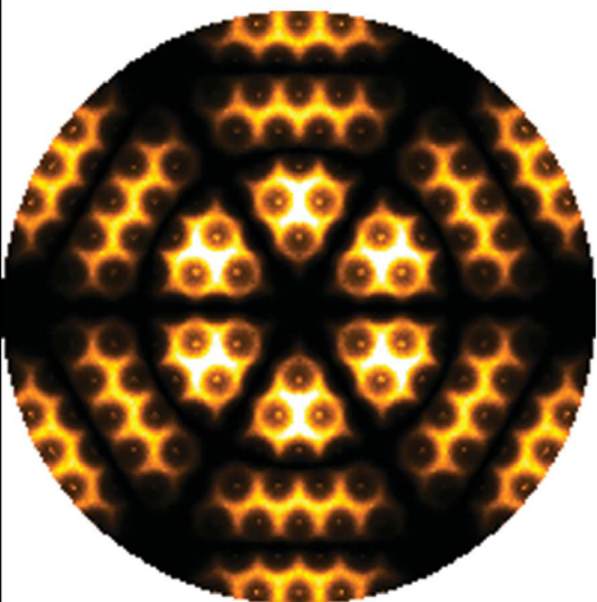
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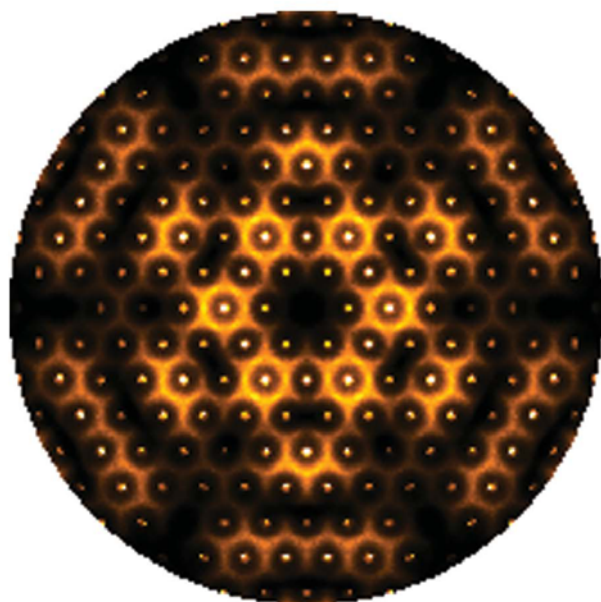
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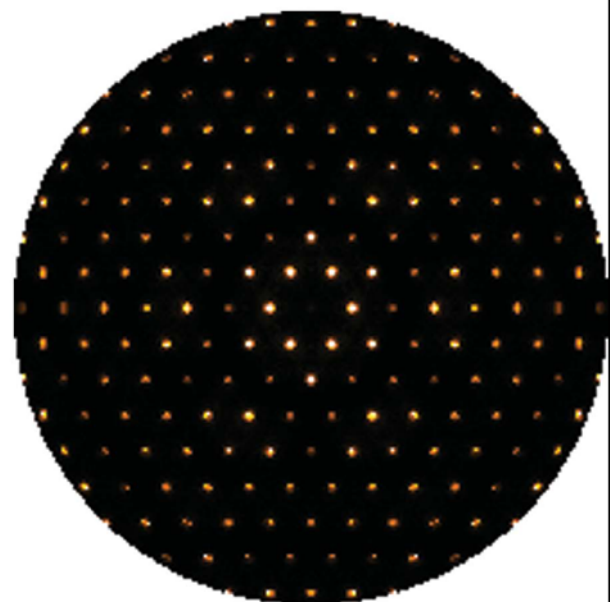
(c)



(d)



(e)



(f)