Electric field in Mn_{12} crystal

Electric field from +*e* point charge:

$$E = \frac{1}{4\pi\varepsilon_0}\frac{e}{r^2} \tag{1.1}$$

where vacuum permittivity

$$\varepsilon_0 = \frac{1}{\alpha}\frac{e^2}{2hc} = \frac{1}{\alpha}\frac{e^2}{4\pi\hbar c} \tag{1.2}$$

If *r* in Å, then

$$E = k\frac{1}{r^2} \tag{1.3}$$

where $k = \alpha\left(\frac{\hbar c}{e}\right) = 14.39965$ VÅ.

The electric field in the crystal can be calculated as summation over all periodic counterions and other periodic SMMs $[Mn_{12}]^-$:

$$\mathbf{E} = \sum_{\mathbf{L}} k\frac{1}{r_+^2}\left(\frac{\mathbf{r}_+}{r_+}\right) - \sum_{\mathbf{L}} k\frac{1}{r_-^2}\left(\frac{\mathbf{r}_-}{r_-}\right) \tag{1.4}$$

where **L** is lattice vector. In summation (1.4) we do not include the SMM molecule itself.