**substance: NiO**
**property: crystal structure**

Only the monoxide NiO has been well characterized though other oxides, e.g. $Ni_3O_4$, $Ni_2O_3$ and $NiO_2$ have been suggested on the basis of electrochemical evidence [72B]. However, no higher phases have been prepared using conventional solid-state techniques, even under very high oxygen partial pressures [71D, 72S]. As normally synthesized, NiO is cation deficient, the colour varying from green near the stiochiometric limit to black as $\delta$ increases in $Ni_{1-\delta}O$.

**crystal structure:** NaCl-type, cubic, space group $O_h^5$ – Fm3m, $Z = 4$.

Below the Néel temperature ($T_N \approx 522$ K) there is a small rhombohedral distortion derived from exchange striction.

**rhombohedral distortion**

(at $T = 300$ K) (see Fig. 1)

| | | |
|---|---|---|
| $\Delta$ | 3.5' | 71B |
| | 3.5' | 48R |
| | 4.2' | 60S |
| | 3.8' | 54S |
| | 3.8' | 70V |
| | 4.2' | 63G |
| | 4.5' | 71T |

NiO can be doped with Li, with marked effect on many physical properties. Structurally, doping with Li causes a contraction in the lattice consistent with the presence of $Ni^{3+}$.

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**Fig. 1.**

NiO. Angle $\Delta$ of the pseudocubic cell, $\alpha = \pi/2 + \Delta$, vs. temperature for $T$ below $T_N$. Symbols, dashed line: experimental data from [71B, 60S, 54S, 70V], solid line: theory [71B].