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Diffuse Reflectance Spectrum of Nickel Monoxide

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Diffuse reflectance spectra of pure and diluted samples of nickel monoxide powder have been studied in the region 200–1000 nm. Three bands have been observed. The bands near 710, 450, and 227 nm have been assigned to $^3A_{2g} \rightarrow {}^3T_{1g}(^3F)$, $^3A_{2g} \rightarrow {}^3T_{1g}(^3P)$, and electron transfer transitions, respectively.

A large number of complexes of Ni^{2+} have been studied (*1*, *2*). The absorption spectra of nickel monoxide in different lattice sites and in thin films have been investigated (*3–7*). The study of its diffuse reflectance spectrum has been limited to its pure powder in the region 300–1000 nm only (*8*). No such investigations below 300 nm and in the case of diluted samples have been reported so far. The present investigations have been done for both pure and diluted powder samples of nickel monoxide extended down to 200 nm.

Experimental

The diffuse reflectance, R, from the samples has been measured with Hilger's UVISPEK spectrophotometer fitted with an annular ring type of diffuse reflectance attachment. Lithium fluoride for the reasons given earlier (*9*, *10*) has been used both as reference standard and dilutant. The preparation of the samples has also been discussed earlier (*11*). The Kubelka Munk remission function (*12*), $F\ [=(1-R)^2/2R]$ has been used as a measure of absorption by the sample.

Results

The plots of F versus wave numbers (cm^{-1}) have been shown in Fig. 1. Three bands have been observed. They have been numbered I, II, and III starting with lowest energy. Their characteristics have been collected in Table I.

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Discussion

The nickel atom has the electronic structure (*A*) $(3d)^8(4s)^2$. The oxidation state of nickel monoxide is Ni^{2+}. The common Ni^{2+} complexes are octahedral ones (*1*). The ground state of Ni^{2+} in octahedral coordination (*13*) is $^3A_{2g}(t_{2g})^6(e_g)^2$. Three absorption bands corresponding to the transitions (*1*) $^3A_{2g} \rightarrow {}^3T_{2g}$, $^3A_{2g} \rightarrow {}^3T_{1g}\ (^3F)$, and $^3A_{2g} \rightarrow {}^3T_{1g}\ (^3P)$ are reported (*14–16*).

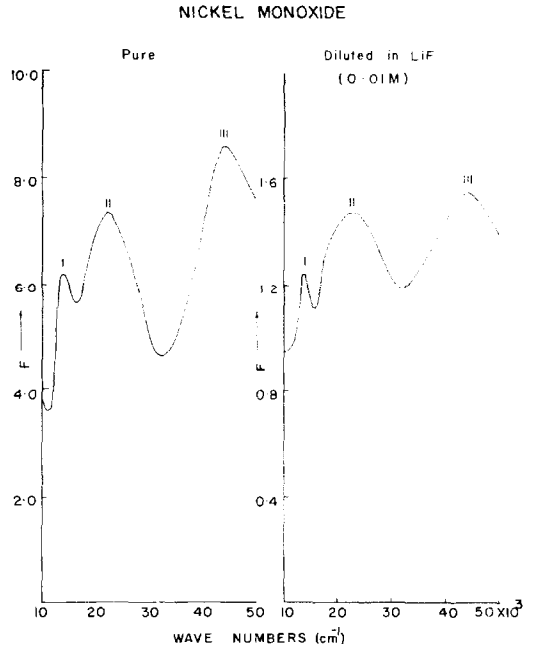

FIG. 1. Diffuse reflectance spectrum of nickel monoxide pure and diluted in LiF (0.01 *M*).

TABLE I

CHARACTERISTICS OF DIFFUSE REFLECTANCE BANDS OF NICKEL MONOXIDE PURE AND DILUTED IN LiF (0.01 *M*)

Sample	Band	Position of peaks λ_{max} nm	ν_{max} cm^{-1}	E_{max} eV	Intensity F_{max}	F_{max}/conc
Pure	I	710	14080	1.74	6.20	
Diluted		720	13890	1.68	1.26	126
Pure	II	450	22220	2.76	7.40	
Diluted		440	22730	2.82	1.74	147
Pure	III	227	44050	5.46	9.30	
Diluted		227	44050	5.46	1.55	155

The two intense bands I and II, in agreement with those of other Ni^{2+} complexes (*13*) may be assigned to the allowed $^3A_{2g} \rightarrow {}^3T_{1g}$ (^3F) and $^3A_{2g} \rightarrow {}^3T_{1g}$ (3p) transitions, respectively. The low-energy band corresponding to the transition $^3A_{2g} \rightarrow {}^3T_{2g}(^3F)$ is not observed in the present study because this energy is less than 10000 cm^{-1}, beyond the range of the instrument.

The intense band III may be attributed to the electron transfer transition. It is of interest to point out that the lowest band to band ($3d^8 \rightarrow 3d^7 4p$) allowed transition is expected to have energy 13.7 eV in the case of isolated Ni^{2+} (*13*) and 11.7 eV in the case of crystals (*3*, *6*). So the band III cannot be assigned to an allowed band to band transition.

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