

THE RAMAN SPECTRUM OF THE β -QUINOL ACETONITRILE CLATHRATE

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The Raman spectrum of the β -quinol acetonitrile clathrate which was recently reported in this journal is compared to the spectrum reported previously by the author.

In a recent paper Fukushima¹ has reported the results of his reinvestigation of the Raman spectrum of the β -quinol acetonitrile clathrate, a spectrum which has been reported previously by the present author². One of the reasons given by Fukushima for repeating the study was the fact that, in his study, the present author had used the Kr^+ 520.8nm line, with a "rather weak power" of 30 mW at the sample. In his study Fukushima used Ar^+ 488.0 and 514.5nm excitation, but nowhere in his paper does he give a value for the laser power at the sample.

Furthermore comparison of the spectrum illustrated in Fukushima's paper with the spectrum illustrated in the present author's paper³ suggests that the spectrum obtained by the present author is in fact superior to that of Fukushima. The spectrum obtained by Fukushima contained several laser emission lines and these are so intense in the 3000 cm^{-1} region that the present author finds it very difficult to identify, with confidence, the quinol and acetonitrile bands in this region. The spectrum illustrated in ref. 3 does not contain any laser emission lines since an interference filter was used. Fukushima also observed very few of the acetonitrile bands and the band at 3022 cm^{-1} which he assigned in Table 1 to an acetonitrile mode is in fact a quinol band.

Fukushima observed quite substantial differences between the α - and β -quinol spectra below 50 cm^{-1} , and this is not inconsistent with the work reported in

refs. 2 and 3, since it is clearly stated in these papers that the Raman spectra were not studied below 50 cm^{-1} . Fukushima claims that the present author stated in his papers^{2,3} that "the Raman spectra of β -hydroquinone clathrate of acetonitrile in the region below 150 cm^{-1} are similar to those of α -hydroquinone". The present author can find no such sentence in his papers. Fukushima also suggested that the sample used by the present author consisted of a mixture of α -quinol and the clathrate. This possibility can be ruled out since there are marked differences between the Raman spectra of α - and β -quinol in the $50\text{-}3100 \text{ cm}^{-1}$ region² and none of the clathrate samples gave Raman bands characteristic of α -quinol.

In summary it would seem that Fukushima's work has shown very clearly that there are substantial differences between the Raman spectra of α -quinol and the acetonitrile clathrate host lattice in the region below 50 cm^{-1} , but his work in no way invalidates the results reported previously by the present author.

We would also like to report the successful preparation of the β -quinol methyl isocyanide clathrate⁴. The Raman spectrum of this clathrate indicates that the host lattice is distorted, and that there is a reduction in the rotational freedom of the guest molecule about the three fold axis. These observations are similar to those reported previously² for the methyl cyanide and methyl cyanide $-d_3$ clathrates.

References

1. K. Fukushima, Chem.Letters, 1973, 617.
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3. J.E.D. Davies, J.Mol.Struct., 1971, 9, 483.
4. J.E.D. Davies and W.J. Wood, J.Raman Spectry., in the press.

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