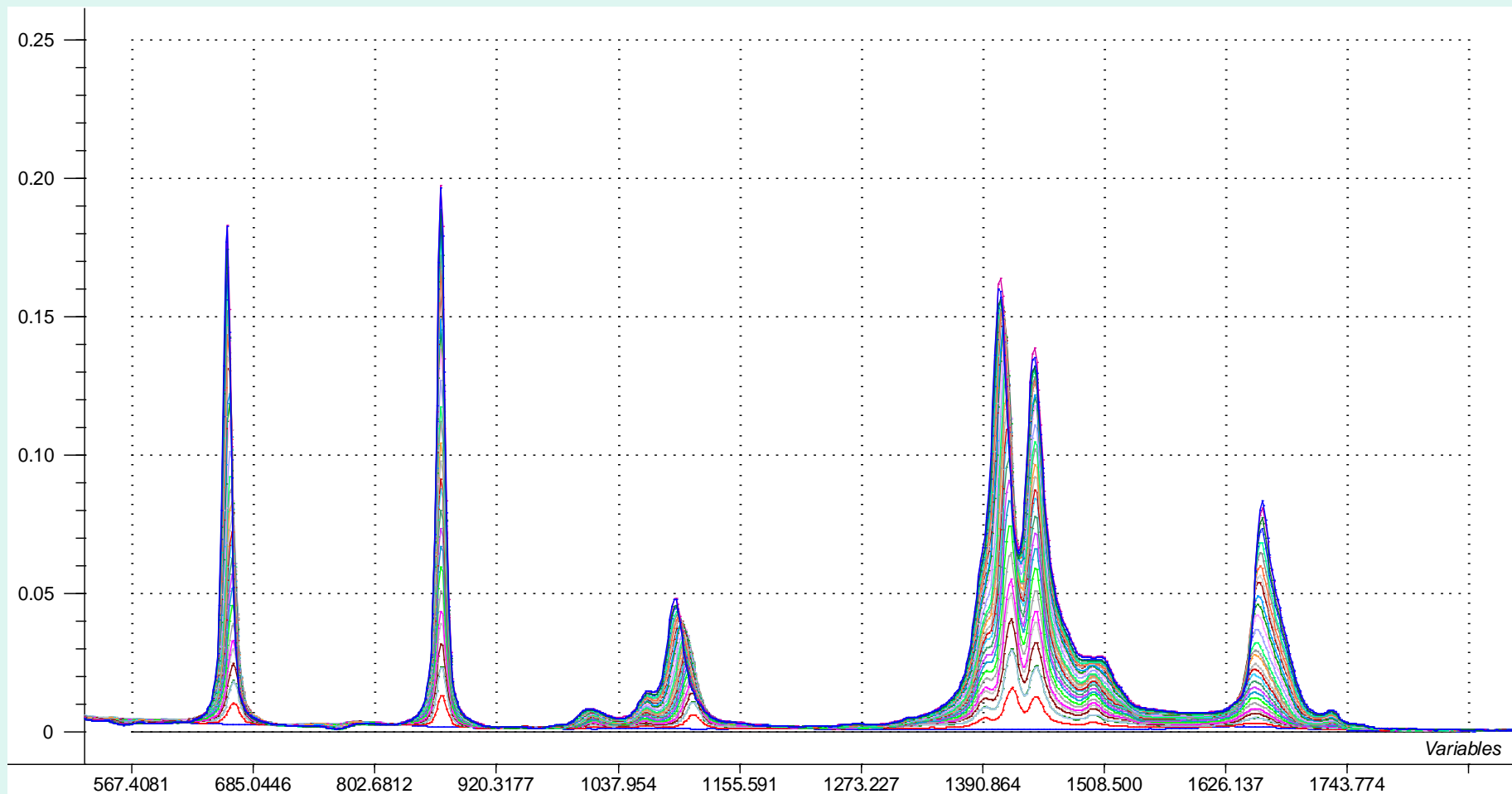
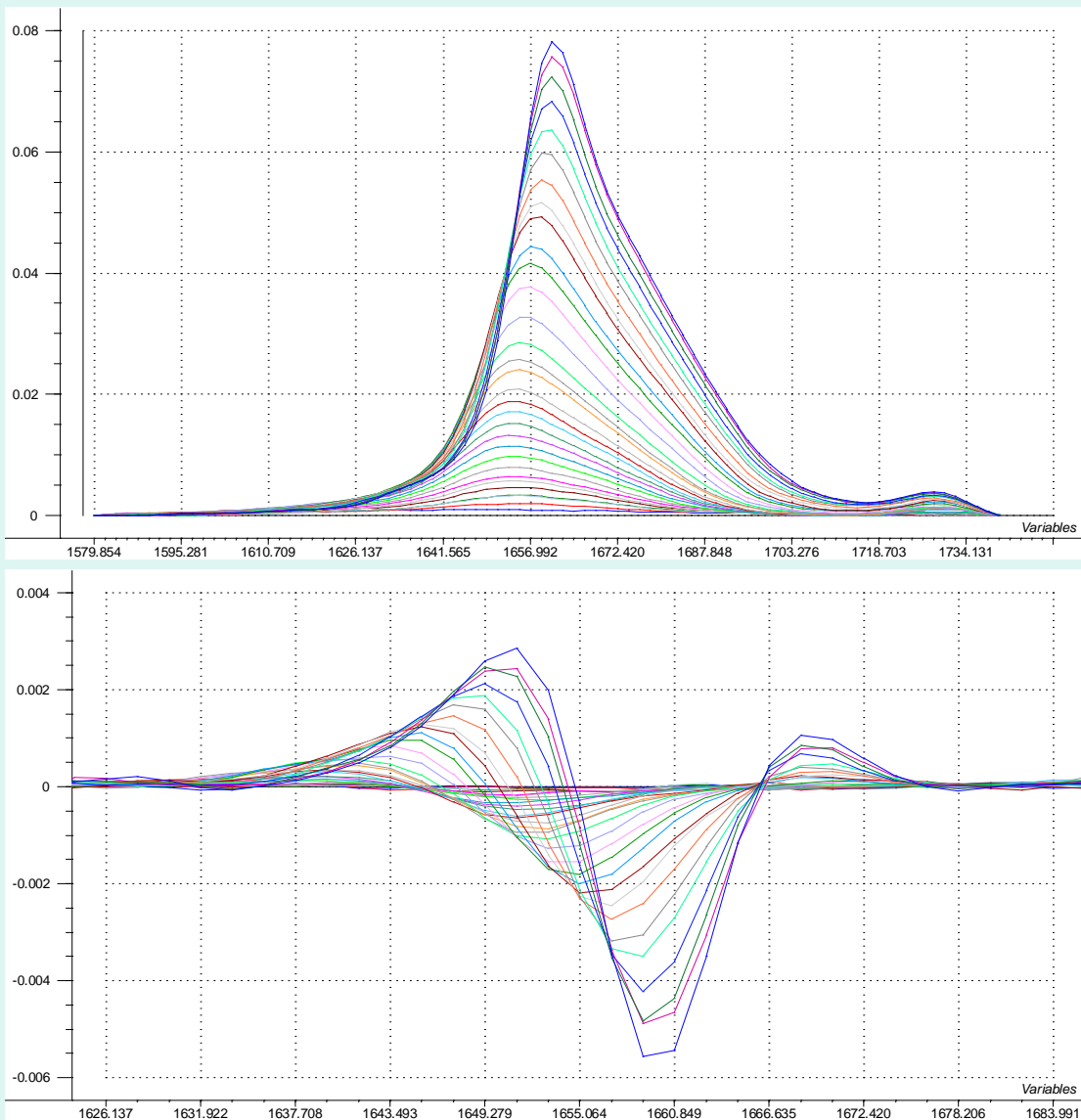


# **THE STUDY OF THE INTERACTION BETWEEN DIMETHYL FORMAMIDE AND WATER IN BINARY MIXTURES BY MEANS OF RAMAN SPECTROSCOPY AND CHEMOMETRIC TECHNIQUES**

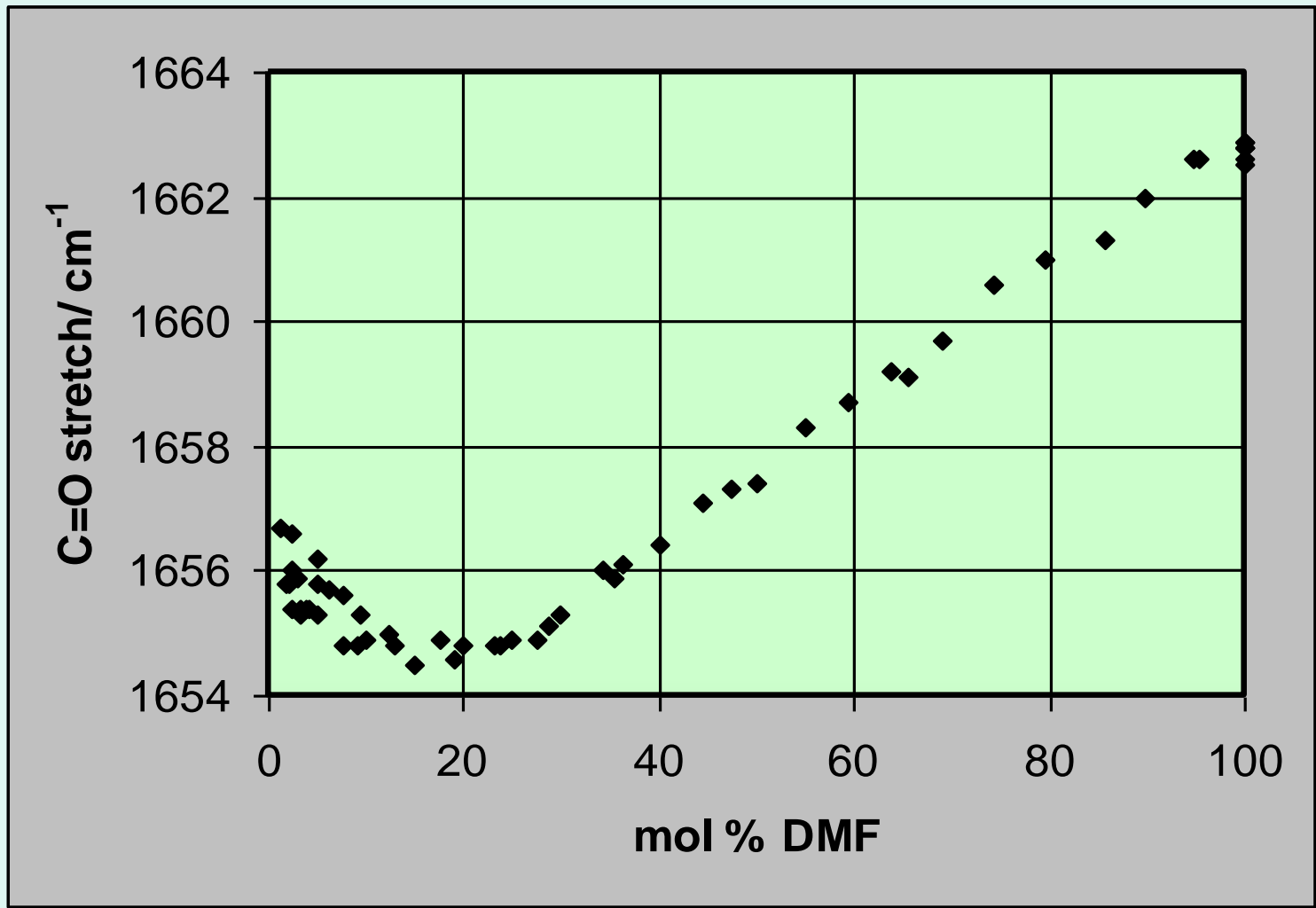
SO Paul, Department of Chemistry, University of South Africa,  
PO Box 392, PRETORIA, 0003, South Africa.  
paulso@unisa.ac.za



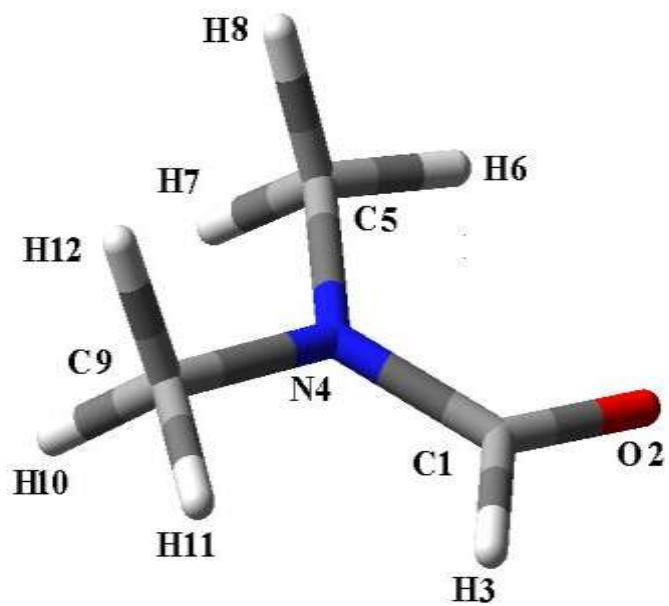
**FIG. 1 RAMAN SPECTRA OF DMF-WATER MIXTURES**



**Fig. 2 RAMAN SPECTRA OF THE -C=O STRETCHING VIBRATION AND THEIR SECOND DERIVATIVES**

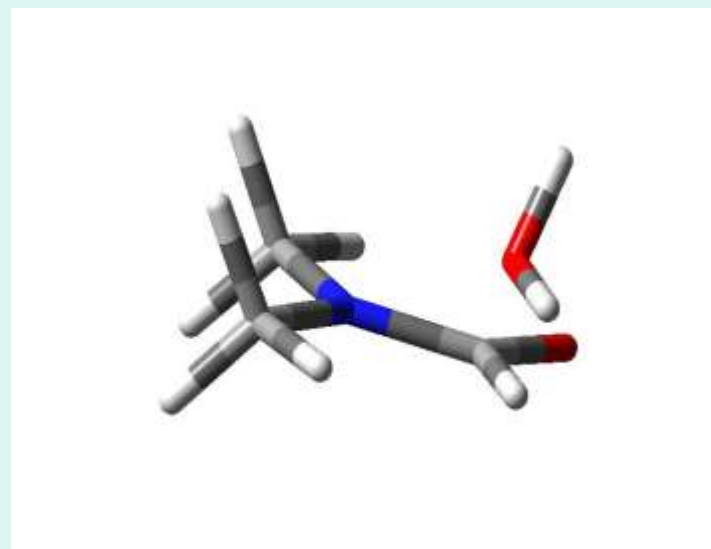
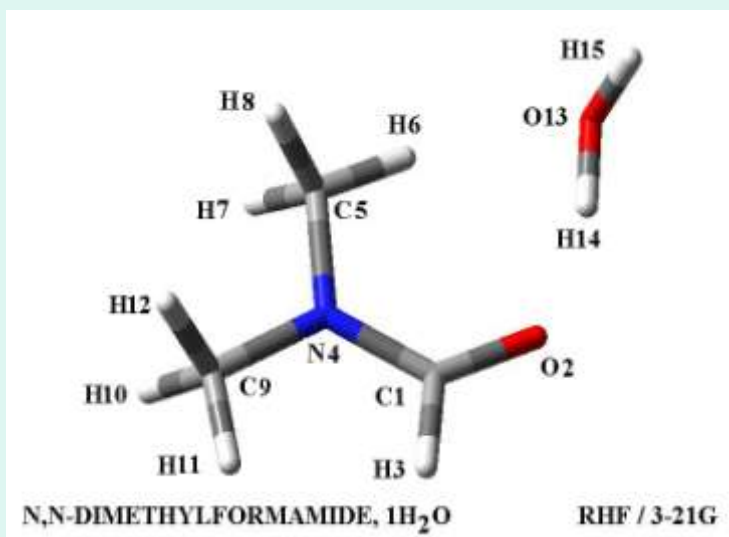


**Fig. 3 THE WAVENUMBER SHIFT WITH COMPOSITION FOR THE -C=O STRETCHING VIBRATION**



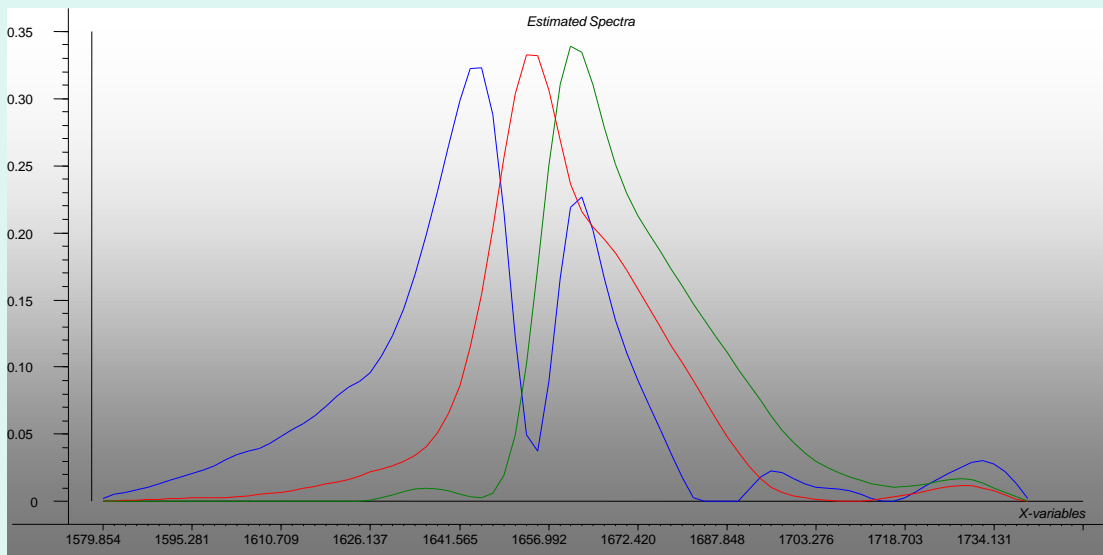
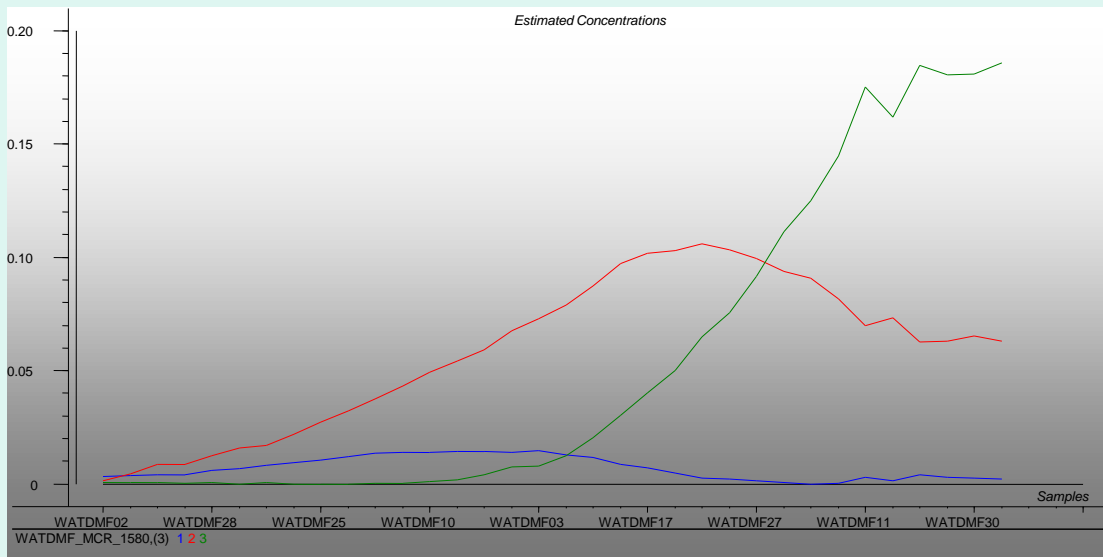
**N,N-DIMETHYLFORMAMIDE (DMF)**

**RHF / 3-21G**



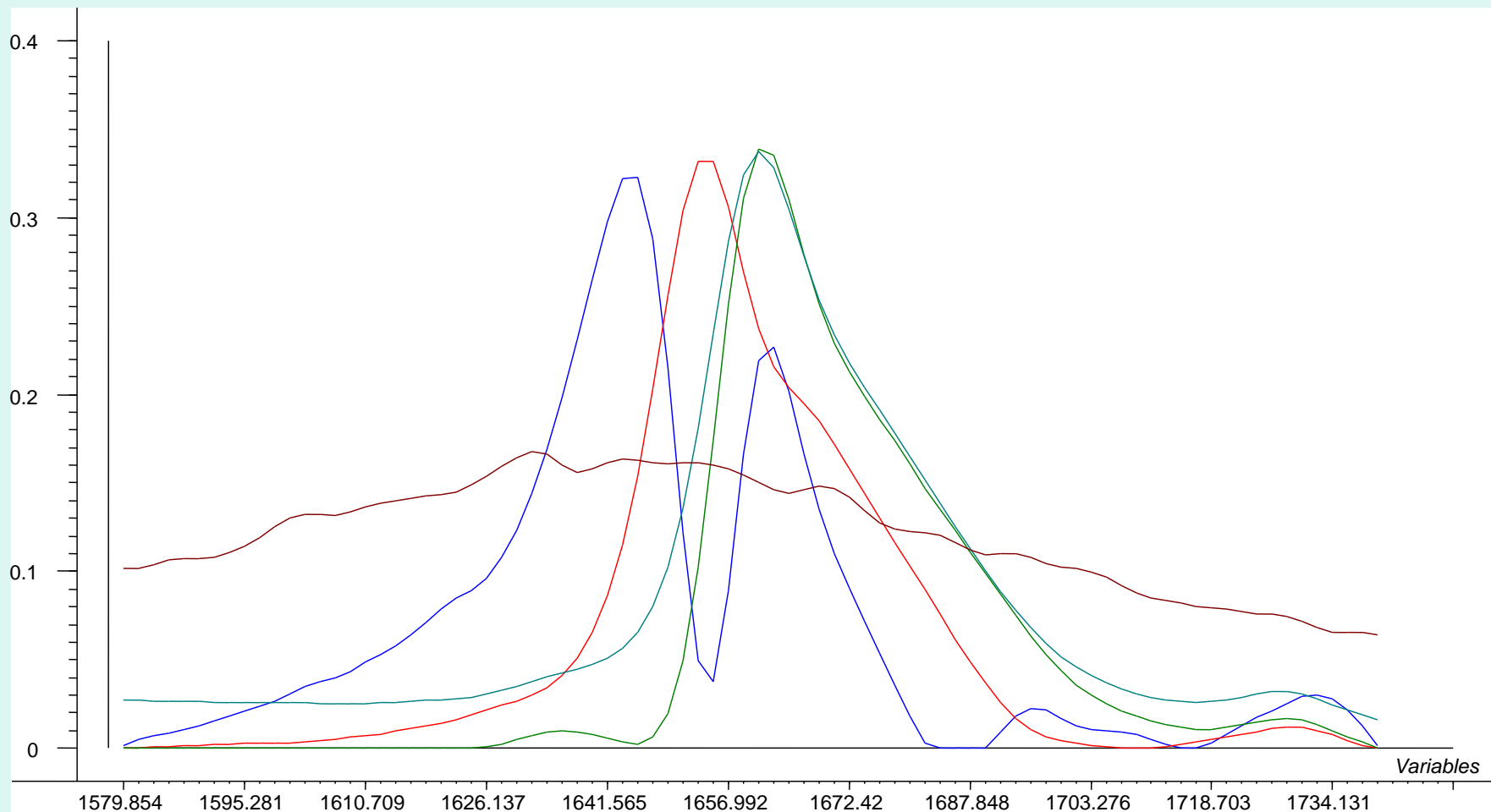
**The vibrational wave numbers of the C=O vibration of the amide group in DMF and its consecutive hydrates. All values in cm<sup>-1</sup>.**

Mode	DMF	DMF.1H <sub>2</sub> O	DMF.2H <sub>2</sub> O	DMF.3H <sub>2</sub> O	DMF.4H <sub>2</sub> O	DMF.5H <sub>2</sub> O	DMF.6H <sub>2</sub> O
23	1876.92						
29		1849.96					
30		1855.27					
36			1866.12				
41				1831.58			
48					1807.06		
53						1806.91	
59							1790.93



**Fig. 4 THE IDENTIFICATION OF THREE MAJOR COMPONENTS CONTRIBUTING TO THE DMF-WATER SPECTRA**





**Fig. 5 THE COMPARISON OF THE RESOLVED SPECTRA WITH THE SPECTRA OF DMF AND WATER. Brown trace: water; cyan: DMF.**

## REFERENCES

- [1] J Zielkiewicz, Phys Chem Chem Phys, 2000, 2, 2925.
- [2] M Chalaris, A Koufou, J Samios, J Mol Liquids 2002, **101, 69.**
- [3] Y-T Lee, J Raman Spectrosc 1997, 28, **45.**
- [4] GI Egorov, AM Kolker, J Mol Liquids 2003,**102, 239**
- [5] G Schultz and I Hargittai, J Phys Chem 1993, **97,** 4966.

