

# Singular Value Decomposition (SVD) applied to determination of acidity constants of the Me-BDBD acid

Teleson N. Teles

Depto de Química e Exatas, UESB  
45201-560, Jequié, BA  
E-mail: teleson@uesb.br

Regina T. Yamaki

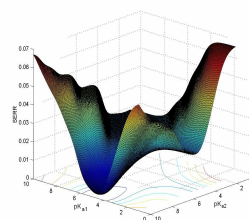
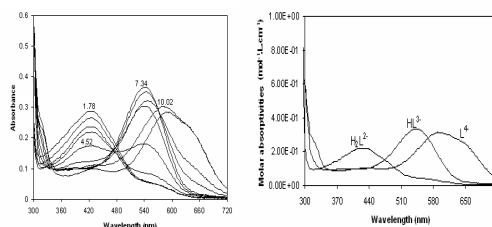
Depto de Química e Exatas, UESB  
45201-560, Jequié, BA  
E-mail: yamaki@uesb.br

## RESUMO

The usual techniques for determination of acidity constants [1,2] are based on hard modelling methods, where the mass-action law and mass balance equation are required, as well as an initial proposal of a chemical equilibrium model of species. Least-squares curve fitting procedures are also presented in all these methods. Recently, some works [3, 4] have introduced new methods, which combine/explore the hard and soft modeling methodologies.

In this work, we use the idea of the physical constraints approach [3] for determining acidity constants of the Me-BDBD acid, which were not yet investigated. The pH-Absorbance spectrophotometric data matrices of the Me-BDBD acid are analyzed by using singular value decomposition (SVD) instead of the techniques used in the cited works. The number of independent spectroscopic components (rank of the problem) and the acidity constants, concentration and spectral response of each specie (parameters of the model) are obtained by means of a SVD based method, where a unified hard-soft modeling is used. The method shows that the model parameters can be extracted from certain subspaces (obtained by SVD analysis). The dimension of these subspaces is a measure of the complexity (rank) of the model. The results show the good performance (computational efficiency and robustness) of the proposed method. For illustration, the figures below show the input spectrophotometric data, the estimated spectral response of each component and the objective function (in which the minimum point corresponds to the solution for acidity

constants) of the problem, respectively. The method is general and can be applied not only for the quantitative spectral analysis of the Me-BDBD acid, but on any multicomponent chemical equilibrium analysis.



## References

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