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A. F. Sax (Ed.)

Potential Energy Surfaces

Proceedings of the Mariapfarr Workshop
in Theoretical Chemistry



Springer

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Preface

Mariapfarr, a small place in Lungau in Salzburger Land, is known among (mainly German speaking) quantum chemists for a tradition of winter workshops organized by the theory section of the Austrian Society of Chemists (GÖCh) going back to 1972. The second generation of Mariapfarr workshops started in 1996 with the on on potential energy surfaces (PES), organized by Alexander F. Sax, the proceedings of which are presented here.

Various aspects of PES are reviewed.

The practically important topic of the analytic representation of potential surfaces is treated by Ralph Jaquet.

Brian Sutcliffe discusses fundamental problems related to the separation of electronic and nuclear coordinates and the definition of molecule-fixed frames.

Empirical force fields which are the basis of Molecular Modelling methods are presented by P. Hünenberger and W. F. van Gunsteren.

The Born-Oppenheimer expansion seen from a mathematical point of view is the context of the contribution by Markus Klein.

The basis concepts and the mathematical apparatus of potential energy surfaces are given by A. F. Sax.

Bochum, May 1998

W. Kutzelnigg

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