Tables of Internal Partition Functions and Thermodynamic Properties of High-Temperature Mars-Atmosphere Species from 50K to 50000K

M. Capitelli\(^1\), G. Colonna\(^1\), D. Giordano\(^2\), L. Marraffa\(^2\), A. Casavola\(^3\), P. Minelli\(^3\), D. Pagano\(^3\), L.D. Pietanza\(^3\) and F. Taccogna\(^3\)

\(^1\) Institute of Inorganic Methodologies and Plasmas CNR, Bari, Italy
\(^2\) European Space Research and Technology Centre (ESTEC), ESA, Noordwijk, the Netherlands
\(^3\) University of Bari, Bari, Italy
CONTENTS

Contents

I General Aspects 1
  1 Nomenclature 3
  2 Introduction 4

3 Method of Calculation 4
  3.1 The Partition Function 4
  3.2 The internal partition function 5
  3.3 Cut-off criteria 5
  3.4 Thermodynamic properties 6
  3.5 The internal partition function of molecular components 7
    3.5.1 Diatomic molecules 7
    3.5.2 Polyatomic molecules 12

4 Results and discussion 14
  4.1 Monoatomic Components 14
  4.2 Diatomic Species 18
  4.3 Triatomic Species 18
  4.4 Thermodynamic data tabulations 19

5 Conclusions 24

6 Acknowledgements 24

A Estimation of energy levels for neutral carbon 25

B Reference States 26

II Tables 29