
Contents

Preface	v
List of Tables	ix
List of Figures	xi
Acronyms	xiii
1 Introduction	1
1.1 Previous experimental and theoretical results for $\text{l-C}_3\text{H}^+$	1
1.2 Previous experimental and theoretical results for C_4	2
2 Theoretical methods	7
2.1 Electronic structure methods	7
2.1.1 Single reference methods	7
2.1.2 Multi-reference methods	9
2.1.3 Inclusion of smaller effects	11
2.2 Vibrational Perturbation Theory	13
3 Results for $\text{l-C}_3\text{H}^+$	19
4 Results for C_4 in its $X^3\Sigma_g^-$ ground state	31
5 Conclusion and outlook	45
6 References	47
A Appendix	53
A.1 Description of 4Lin	53
A.2 Force fields for $\text{l-C}_3\text{H}^+$	58
A.3 Additional tables and force fields for C_4	61

<http://www.springer.com/978-3-658-14829-4>

Highly Accurate Spectroscopic Parameters from Ab
Initio Calculations

The Interstellar Molecules $\text{l-C}_3\text{H}^+$ and C_4

Stein, C.

2016, XIV, 63 p. 24 illus., Softcover

ISBN: 978-3-658-14829-4