3.2.4 Larger non-linear free radicals

3.2.4.1 Preliminary remarks

1 Introduction

In the present edition, there are twenty two free radicals in this category (larger non-linear free radicals) compared with seven in the previous supplement. Once again, this is a significant increase, driven to a large extent by the need to obtain information for the identification of species in astrophysical sources.

All the molecules in this section are asymmetric rotors in doublet open-shell states. The effective Hamiltonian is the same as that used for the triatomic asymmetric rotors in section 3.2.2 with the sole exception that the centrifugal distortion of the rotational kinetic energy have been extended for some molecules to higher degree terms [00Bre]. For example, in the Watson S-reduction [77Wat], the extended centrifugal distortion Hamiltonian has the form

$$\begin{aligned} H_{\mathrm{cd}} = & -D_N\left(N^2\right)^2 - D_{NK}N^2N_z^2 - D_KN_z^4 + d_1N^2\left(N_+^2+N_-^2\right) + d_2\left(N_+^4+N_-^4\right) \\ & + H_N\left(N^2\right)^3 + H_{NK}\left(N^2\right)^2N_z^2 + H_{KN}N^2N_z^4 + H_KN_z^6 \\ & + h_1\left(N^2\right)^2\left(N_+^2+N_-^2\right) + h_2N^2\left(N_+^4+N_-^4\right) + h_3\left(N_+^6+N_-^6\right) \\ & + L_{NNK}\left(N^2\right)^3N_z^2 + L_{NK}\left(N^2\right)^2N_z^4 + L_{KKN}N^2N_z^6 + \ldots \\ & + P_{NNK}\left(N^2\right)^3N_z^4 + P_{NKK}\left(N^2\right)^2N_z^6 + P_{KN}N^2N_z^8 + \ldots \end{aligned}$$

The operators involved are defined in section 3.2.3.1.

2 List of tabulated parameters

These are the same as those listed in section 3.2.3.2. In addition:

P_{NNK}, P_{NKK}, P_{KN}	decadic centrifugal distortion parameters
v_i, i=1, 2, 3, …, $3N-6$	vibrational quantum number of the i-th normal mode of a radical consisting of N atoms

3 List of symbols used

See section 3.2.3.1, non-linear triatomic radicals

4 Arrangement of molecules

1.	c-C_3H	9.	CH_2C_4H	17.	HC_4O
2	CH_2F	10.	CH_2CN	18.	HOCO
3.	CHF_2	11.	CH_2CCCN	19.	HNCN
4.	CH_2Cl	12.	CH_2CP	20.	$MgNH_2$
5.	CH_2Br	13.	H_2NS	21.	$CaNH_2$
6.	CH_2N	14.	H_2PO	22.	$SrNH_2$
7.	CH_2P	15.	HCCO		
8.	CH_2CCH	16.	HCCCO		

5 References

77Wat Watson, J.K.G.:Aspects of Quartic and Sextic Centrifugal Effects on Rotational Energy Levels, in: Vibrational spectra and Structure, Vol.6, Durig, J.R., (ed), Amsterdam: Elsevier, 1977.

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