

Electronic Supplementary Information

Radon Hydrides: Structure and Bonding

Rosalba Juarez,^a Claudia Zavala-Oseguera,^a J. Oscar C. Jimenez-Halla,^{a,*} F.

Matthias Bickelhaupt,^{b,*} and Gabriel Merino^{a,*}

^a *Departamento de Química, Universidad de Guanajuato, Noria Alta s/n C.P.*

36050, Guanajuato, Gto. México.

^b *Department of Theoretical Chemistry and Amsterdam Center for Multiscale*

Modeling, Scheikundig Laboratorium der Vrije Universiteit, De Boelelaan

1083, NL-1081 HV Amsterdam, The Netherlands.

Table 1-SI. Vibrational harmonic frequencies and infrared intensities of the radon hydrides, computed at ZORA-BP86/TZ2P level.^a

System and	Frequency	IR Intensity
H-Rn-F		
Rn-F Stretch	427	119.9
H-Rn-F Bend	511	3.3
H-Rn Stretch	1738	339.3
H-Rn-Cl		
Rn-Cl Stretch	251	53.6
H-Rn-Cl Bend	466	0.3
H-Rn Stretch	1618	798.7
H-Rn-Br		
Rn-Br Stretch	168	23.4
H-Rn-Br Bend	446	0.0
H-Rn Stretch	1561	1043.1
H-Rn-I		
Rn-I Stretch	130	11.7
H-Rn-I Bend	425	0.0
H-Rn Stretch	1474	1440.7
H-Rn-CCH		
Out-of-plane	161	13.0
Rn-C Stretch	296	116.7
H-Rn-C Bend	540	10.4
C-C-H Bend	645	42.0
H-Rn Stretch	1561	823.3
C-C Stretch	2041	5.5
C-H Stretch	3429	62.8
H-Rn-CN		
Out-of-plane	187	0.4
Rn-C Stretch	274	79.1
H-Rn-C Bend	533	3.2
H-Rn Stretch	1621	780.9
C-N Stretch	2205	25.5
H-Rn-NC		
Out-of-plane	148	0.0
Rn-N Stretch	287	65.8
H-Rn-N Bend	507	2.2
H-Rn Stretch	1697	961.2
H-Rn and N-C	2092	219.6

^a Frequencies are in cm⁻¹ and IR intensities in KM/Mole.