Predicted compounds of Radon with Acetylene and Water

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Supplementary Information

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Harmonic Frequencies

The computed harmonic vibrational spectrum of HRnCCH and HRnOH, as calculated at the AVDZ/MP2 level, are shown in Table 1 and Table 2.

Table 1: Harmonic IR frequencies and intensities for HRnOH (AVDZ/MP2)

Vibration mode	Frequency [cm-1]	Intensity [Km mol-1]
HO-Rn stretch	437.36	133.04
H−Rn−O−H symmetric bend	535.82	5.75
H−Rn−O oop bend	560.00	1.29
H−Rn−O−H antisymmetric bend	791.03	5.94
H-Rn stretch	1738.61	1034.39
H-O stretch	3775.39	60.14

Table 2: Harmonic IR frequencies and intensities for HRnCCH (AVDZ/MP2)

Vibration mode	Frequency [cm^{-1}]	Intensity [Km mol-1]
C-H stretch	3443.86	30.88
C-C stretch	1932.44	3.28
H-Rn stretch	1656.62	1183.78
Bend	614.33	3.52
	614.33	3.55
Bend	592.06	19.1
	592.04	24.8
Rn-C stench	313.91	149.25
H-Rn-C bend	155.4	12.7
	155.34	12.68

Geometrical structures

HRnCCH

Equilibrium structure (1)

Basis set: aug-cc-pvtz

Theory: CASPT2

Energy (Hartree): -364.67277893

No. of imaginary frequencies: 0

Geometry:

H	0.0000000000	-0.0000049234	-4.4175831705
C	0.0000000000	-0.0000024974	-3.3549561513
C	0.0000000000	0.0000047333	-2.1250160369
Rn	0.0000000000	-0.0000001105	0.3065769257
H	0.0000000000	0.0000026141	2.1897753241

Equilibrium structure (2)

Basis set: aug-cc-pvtz

Theory: MP2

Energy (Hartree): -364.67709116

No. of imaginary frequencies: 0

Geometry:

H	0.0000000000	-0.0000208384	-4.3928342832
C	0.0000000000	-0.0000075553	-3.3282496863
C	0.0000000000	0.0000138222	-2.0977502335
Rn	0.0000000000	-0.0000001722	0.3037371069
H	0.0000000000	-0.0000159002	2.1473949763

3B transition structure

Basis set: aug-cc-pvdz

Theory: CCSD(T)

Energy (Hartree): -364.56516927

No. of imaginary frequencies: 1

Geometry:

H	0.0000000000	0.0000000000	-4.8561047256
C	0.0000000000	0.0000000000	-3.7764233282
C	0.0000000000	0.0000000000	-2.5368189125
Rn	0.0000000000	0.0000000000	0.3494978102
H	0.0000000000	0.0000000000	3.1037409800

2B transition structure

Basis set: aug-cc-pvdz

Theory: MP2

Energy (Hartree): -364.47832024

No. of imaginary frequencies: 1

Geometry:

H	0.0000000000	1.2342469971	3.9000240889
C	0.0000000000	0.4061384467	3.2018294136
C	0.0000000000	-0.6725689545	2.5260280034
Rn	0.0000000000	0.0013380827	-0.3276677816
H	0.0000000000	1.6459036580	0.0195408317

2B Reaction products

Basis set: aug-cc-pvtz

Theory: MP2

Energy (Hartree): -364.83813314

No. of imaginary frequencies: 0

Geometry:

H	0.0000000000	0.0000012134	-6.0201227211
C	0.0000000000	0.0000011214	-4.9582707784
C	0.0000000000	-0.0000014428	-3.7457389222
Rn	0.0000000000	0.0000000230	0.5103943077
H	0.0000000000	-0.0000024507	-2.6833791737

HRnOH

Equilibrium structure (1)

Basis set: aug-cc-pvtz

Theory: CASPT2

Energy (Hartree): -363.81968479

No. of imaginary frequencies: 0

Geometry:

H	-0.7970329827	0.0000000000	2.5175278523
O	0.0631176162	0.0000000000	2.0800554325
Rn	-0.0011957842	0.0000000000	-0.1522112479
H	0.0585376549	0.0000000000	-2.0076544077

Equilibrium structure(2)

Basis set: aug-cc-pvtz

Theory: MP2

Energy (Hartree): -363.8461381

No. of imaginary frequencies: 0

Geometry:

H	-0.8302445448	0.0000000000	2.4774335305
O	0.0636311737	0.0000000000	2.1087276149
Rn	-0.0010692778	0.0000000000	-0.1543009582
H	0.0557319605	0.0000000000	-1.9623866074

3B transition structure

Basis set: aug-cc-pvdz

Theory: CASPT2

Energy (Hartree): -363.69652555

No. of imaginary frequencies: 1

Geometry:

H	0.0000000000	2.7290119200	0.9231237478
O	0.0000000000	2.6430159263	-0.0502016490
Rn	0.0000000000	-0.1895964091	-0.0012997045
H	0.0000000000	-2.9204402240	0.1600294214

2B transition structure

Basis set: aug-cc-pvdz

Theory: MP2

Energy (Hartree): -363.65709551

No. of imaginary frequencies: 1

Geometry:

H	-0.1226339700	0.0000000000	3.3111468202
O	0.0121012834	0.0000000000	2.3516237124
Rn	0.0072802384	0.0000000000	-0.1838229993
H	-1.6730618118	0.0000000000	-0.1489007378

2B reaction products

Basis set: aug-cc-pvtz

Theory: MP2

Energy (Hartree): -364.00311180

No. of imaginary frequencies: 0

Geometry:

H	-0.8513381253	0.0000000000	-4.0053860946
O	0.0588150443	0.0000000000	-3.6952636819
Rn	-0.0002771003	0.0000000000	0.2969001413
H	-0.0212180757	0.0000000000	-2.7361117749