Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information (ESI)

Intracluster Proton Transfer in Protonated Benzonitrile-$(H_2O)_{n\leq6}$ Nanoclusters: Hydrated Hydronium Core for $n \geq 2$

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Figure S1. Optimized structures of BN, W, and different H^+BN isomers calculated at the B3LYP-D3/aug-cc-pVTZ level. Bond lengths are given in Å. Relative energies (E_0) are given in kJ mol^{-1}.

Figure S2. NBO atomic charge distribution (in e) of BN, H^+BN, H^+BN-L(H) (L=Ar and N_2), and most stable branched isomers of H^+(BN-$W_{n\leq6}$) obtained at the B3LYP-D3/aug-cc-pVTZ level at room temperature.

Figure S3. NBO interactions of donor-acceptor orbitals ($E^{(2)}$ in kJ mol^{-1}) involved in the H-bonds of the type NH…L in H^+BN-L(H) with L=Ar, N_2, and W, and the type OH…N and OH…O in the most stable isomers of BN-$H^+W_{n\leq6}$ calculated at the B3LYP-D3/aug-cc-pVTZ level at room temperature.

Figure S4. NCI analysis for the H-bonds (ρ* in a.u.) of the type NH…L in H^+BN-L(H) with L=Ar, N_2, and W, and the type OH…N and OH…O in the most stable isomers of BN-$H^+W_{n\leq6}$ calculated at the B3LYP-D3/aug-cc-pVTZ level at room temperature.

Figure S5. Potential energy barrier (E_e in cm^{-1}) for internal rotation of the W ligand in H^+BN-W(H) calculated at the B3LYP-D3/aug-cc-pVTZ level in cm^{-1}. Bond lengths are given in Å.

Figure S6. Optimized structures of various H^+BN-W isomers obtained at the B3LYP-D3/aug-cc-pVTZ level. Binding energies (D_0) and bond lengths are given in cm^{-1} and Å, respectively. Numbers in parentheses correspond to relative energies and free energies in cm^{-1} (E_0, G).

Figure S7. Comparison of experimental IRPD spectrum of H^+(BN-W) with linear IR absorption spectra of the CH-bonded H^+BN-W isomers calculated at the B3LYP-D3/aug-cc-pVTZ level.

Figure S8. Potential energy barrier (E_e in cm^{-1}) between two equivalent H^+BN-W(m/p) local minima calculated at the B3LYP-D3/aug-cc-pVTZ level in cm^{-1}. Bond lengths are given in Å.

Figure S9. Optimized structures of various BN-H^+W_2 isomers obtained at the B3LYP-D3/aug-cc-pVTZ level. Binding energies (D_0) and bond lengths are given in cm^{-1} and Å, respectively. Numbers in parentheses correspond to relative energies and free energies in cm^{-1} (E_0, G).

Figure S10. Structures and IR spectra of most stable isomers of W and H^+W_n obtained at the B3LYP-D3/aug-cc-pVTZ level. Binding energies (D_0) and bond lengths are given in cm^{-1} and Å, respectively. Numbers in parenthesis correspond to relative energies and free energies in cm^{-1} (E_0, G). The total binding energies are evaluated for dissociation into H_3O^+ and neutral W fragments. For n=5, we consider the B, R, and C isomers reported in Fagiani et al. (2016). For n=6, the E and Z isomers correspond to the 6E and 6Z isomers in Heine et al. (2013). For n=7, the E/c, E/4r, E/5R, and Z/5r isomers correspond to the $7E_C$, $7E_{4R}$, $7E_{5R}$, and 7Z isomers in Heine et al. (2015).

Figure S11. Comparison of experimental IRPD spectrum of H^+(BN-W_2) with linear IR absorption spectra of the CH-bonded H^+BN-W_2 isomers (m/p and o/m) calculated at the B3LYP-D3/aug-cc-pVTZ level.

Figure S12. Comparison of experimental IRPD spectrum of H^+(BN-W_5) with linear IR absorption spectra of the linear H^+BN-W_5(I) isomer calculated at the B3LYP-D3/aug-cc-pVTZ level. The binding energy (D_0) and bond lengths are given in cm^{-1} and Å, respectively. Numbers in parenthesis correspond to relative energies and free energies in cm^{-1} (E_0, G).

Figure S13. Comparison of experimental IRPD spectrum of H^+(BN-W_6) with linear IR absorption spectra of the linear H^+BN-W_6(I) isomer calculated at the B3LYP-D3/aug-cc-pVTZ level. The binding energy (D_0) and bond lengths are given in cm^{-1} and Å, respectively. Numbers in parenthesis correspond to relative energies and free energies in cm^{-1} (E_0, G).

Table S1. CH stretch frequencies (cm^{-1}) of $H^+(BN\text{-}W_n)$ clusters with n=0-3 calculated at the B3LYP-D3/aug-cc-pVTZ level.

	Calc.[a]	Isomer
H^+BN	3080 (0.2, a_1) 3076 (3, b_2) 3067 (2, a_1) 3064 (0.2, b_2) 3057 (0.2, a_1)	
$H^+(BN\text{-}W)$	3079 (0.02, a') 3075 (0.5, a') 3066 (0.1, a') 3062 (0.2, a') 3055 (0.1, a')	$H^+BN\text{-}W(H)$
$H^+(BN\text{-}W_2)$	3076 (0.3) 3072 (0.4) 3063 (0.2) 3059 (0.1) 3052 (0.02)	$BN\text{-}H^+W_2$
$H^+(BN\text{-}W_3)$	3075 (0.5, a'), 3075 (0.6) 3070 (1, a'), 3071 (1) 3062 (1, a'), 3063 (0.6) 3057 (0.1, a'), 3058 (0.1) 3050 (0.01, a'), 3050 (0.01)	$BN\text{-}H^+W_3$(b), $BN\text{-}H^+W_3$(I)

[a] Vibrational symmetry species and IR intensities (in km mol^{-1}) are listed in parentheses.

Table S2. Experimental structural parameters of BN (in Å, °) compared to calculated values obtained at the B3LYP-D3/aug-cc-pVTZ level.

structural parameter	exp [a]	calc
r_{C1C2}	1.396	1.3989
r_{C2C3}	1.391	1.3869
r_{C3C4}	1.399	1.3914
r_{C1C7}	1.444	1.4300
r_{C7N8}	1.156	1.1523
r_{C2H9}	1.088	1.0805
r_{C3H10}	1.087	1.0811
r_{C4H11}	1.084	1.0814
∠C6C1C2	121.8	120.1
∠C1C2C3	119.0	119.7
∠C2C3C4	120.1	120.2
∠C3C4C5	120.1	120.1
∠C1C2H9	120.4	119.6
∠C2C3H10	120.0	119.7

[a] Taken from Casado et al. (1970).

Table S3. Selected experimental and calculated vibrational frequencies (B3LYP-D3/aug-cc-pVTZ) of H^+BN and H^+BN-L (L=Ar, N_2, W) in cm^{-1}.

	Exp.[a]	Vibration	Calc.[b]	Isomer
H^+BN	3555±3	ν_{NH}[f]	3560 (1221, a_1)	
		ν_{CN}	2223 (613, a_1)	
H^+BN-Ar	3556 (11)	ν_{NH}[f]	3561 (1212, a')	H^+BN-Ar(π)
	3500 (33)	ν_{NH}[b] + ν_s	3486	H^+BN-Ar(H)
	3414 (44)	ν_{NH}[b]	3415 (2546, a_1)	H^+BN-Ar(H)
		ν_{CN}	2222 (454, a_1) 2223 (603, a')	H^+BN-Ar(H) H^+BN-Ar(π)
H^+BN-N_2	3351 (24)	ν_{NH} + ν_s	3357	H^+BN-N_2(H)
	3221 (30)	ν_{NH}	3229 (3583, a_1)	H^+BN-N_2(H)
		ν_{CN}	2215 (284, a_1)	H^+BN-N_2(H)
H^+BN-W	3710 (b)	ν_3	3708 (173, a")	H^+BN-W(H)
	3620 (34)	ν_1	3621 (84, a')	H^+BN-W(H)
		ν_{NH}[b] + ν_s	3060	H^+BN-W(H)
	2750 (b)	ν_{NH}[b]	2505 (5246, a')	H^+BN-W(H)
		ν_{CN}	2065 (1043, a')	H^+BN-W(H)

[a] Values in parentheses correspond to fwhm of the bands in cm^{-1}. The notation (b) indicates broad bands for which it is difficult to extract the widths.

[b] Values in parentheses correspond to IR intensities in km mol^{-1} and vibrational symmetries.

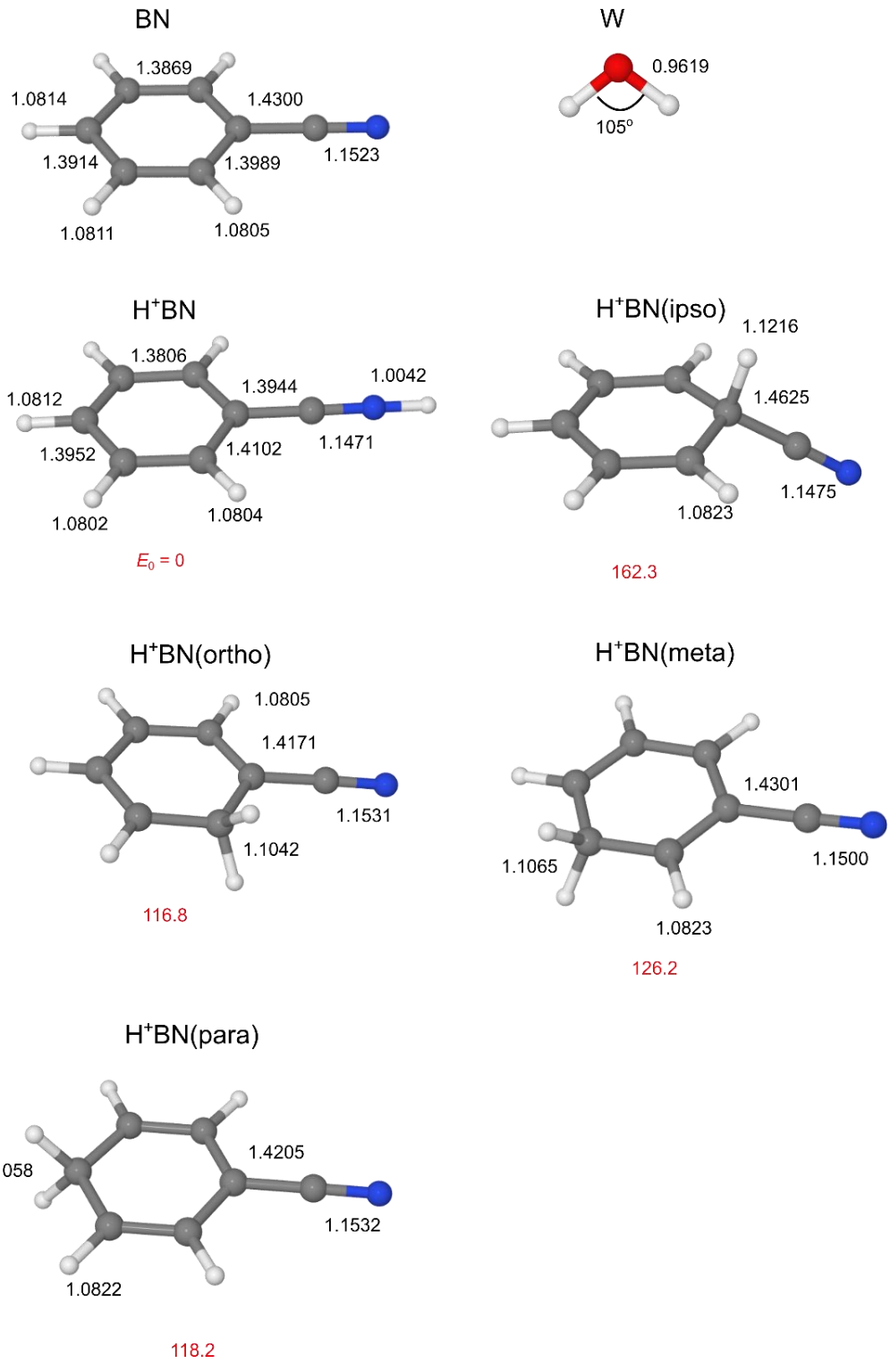
BN
1.3869
1.0814
1.4300
1.3914
1.3989
1.1523
1.0811
1.0805
W
0.9619
105°
H+BN
1.3806
1.0812
1.3944
1.0042
1.3952
1.4102
1.1471
1.0802
1.0804
E0 = 0
H+BN(ipso)
1.1216
1.4625
1.1475
1.0823
162.3
H+BN(ortho)
1.0805
1.4171
1.1531
1.1042
116.8
H+BN(meta)
1.4301
1.1065
1.1500
1.0823
126.2
H+BN(para)
1.4205
1.1058
1.1532
1.0822
118.2

Figure S1

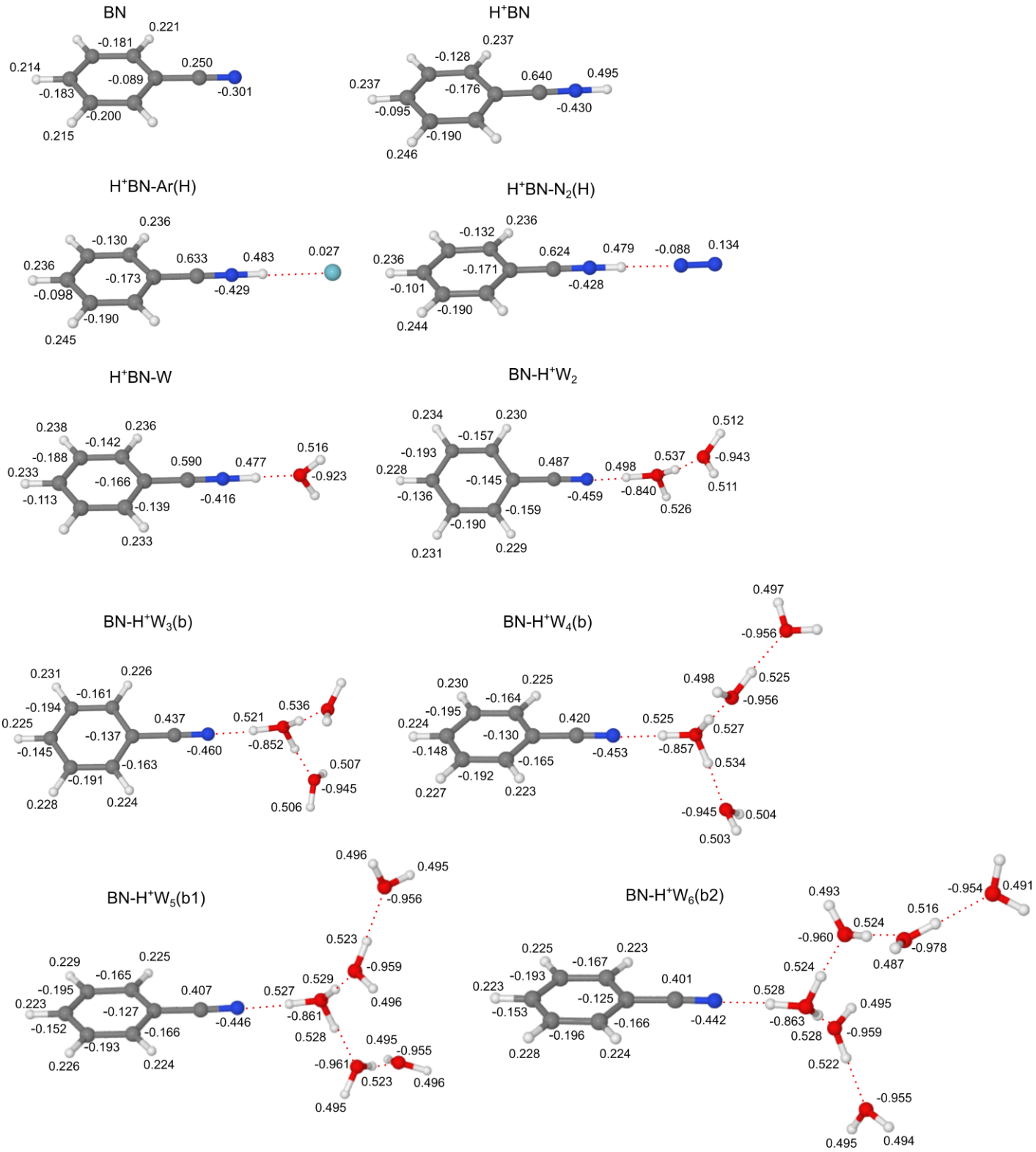
BN
0.221
-0.181
0.214
0.250
-0.089
-0.183
-0.301
-0.200
0.215
H+BN
0.237
-0.128
0.237
0.640
0.495
-0.176
-0.095
-0.430
-0.190
0.246
H+BN-Ar(H)
0.236
-0.130
0.236
0.633
0.483
0.027
-0.173
-0.098
-0.429
-0.190
0.245
H+BN-N2(H)
0.236
-0.132
0.236
0.624
0.479
-0.088
0.134
-0.171
-0.101
-0.428
-0.190
0.244
H+BN-W
0.238
0.236
-0.142
-0.188
0.590
0.477
0.516
0.233
-0.166
-0.923
-0.113
-0.139
-0.416
0.233
BN-H+W2
0.234
0.230
-0.157
0.512
-0.193
0.537
0.228
0.487
0.498
-0.943
-0.145
-0.136
-0.840
0.511
-0.459
-0.159
0.526
-0.190
0.231
0.229
BN-H+W3(b)
0.231
0.226
-0.161
-0.194
0.225
0.437
0.521
0.536
-0.137
-0.852
-0.145
-0.460
0.507
-0.163
-0.945
-0.191
0.506
0.228
0.224
BN-H+W4(b)
0.497
-0.956
0.230
0.225
0.498
0.525
-0.164
-0.956
-0.195
0.420
0.224
0.525
0.527
-0.130
-0.857
-0.148
-0.453
0.534
-0.165
-0.192
-0.945
0.504
0.227
0.223
0.503
BN-H+W5(b1)
0.496
0.495
-0.956
0.523
0.229
0.225
-0.165
-0.959
-0.195
0.407
0.529
0.527
0.223
-0.127
0.496
-0.861
-0.446
-0.152
-0.166
0.528
0.495
-0.193
-0.955
-0.961
0.226
0.224
0.523
0.496
0.495
BN-H+W6(b2)
0.493
-0.954
0.491
0.516
0.524
-0.960
-0.978
0.487
0.524
0.225
0.223
-0.167
0.528
0.495
-0.193
0.401
0.223
-0.125
-0.863
-0.959
-0.153
-0.442
0.528
0.522
-0.166
-0.196
-0.955
0.228
0.224
0.495
0.494

Figure S2

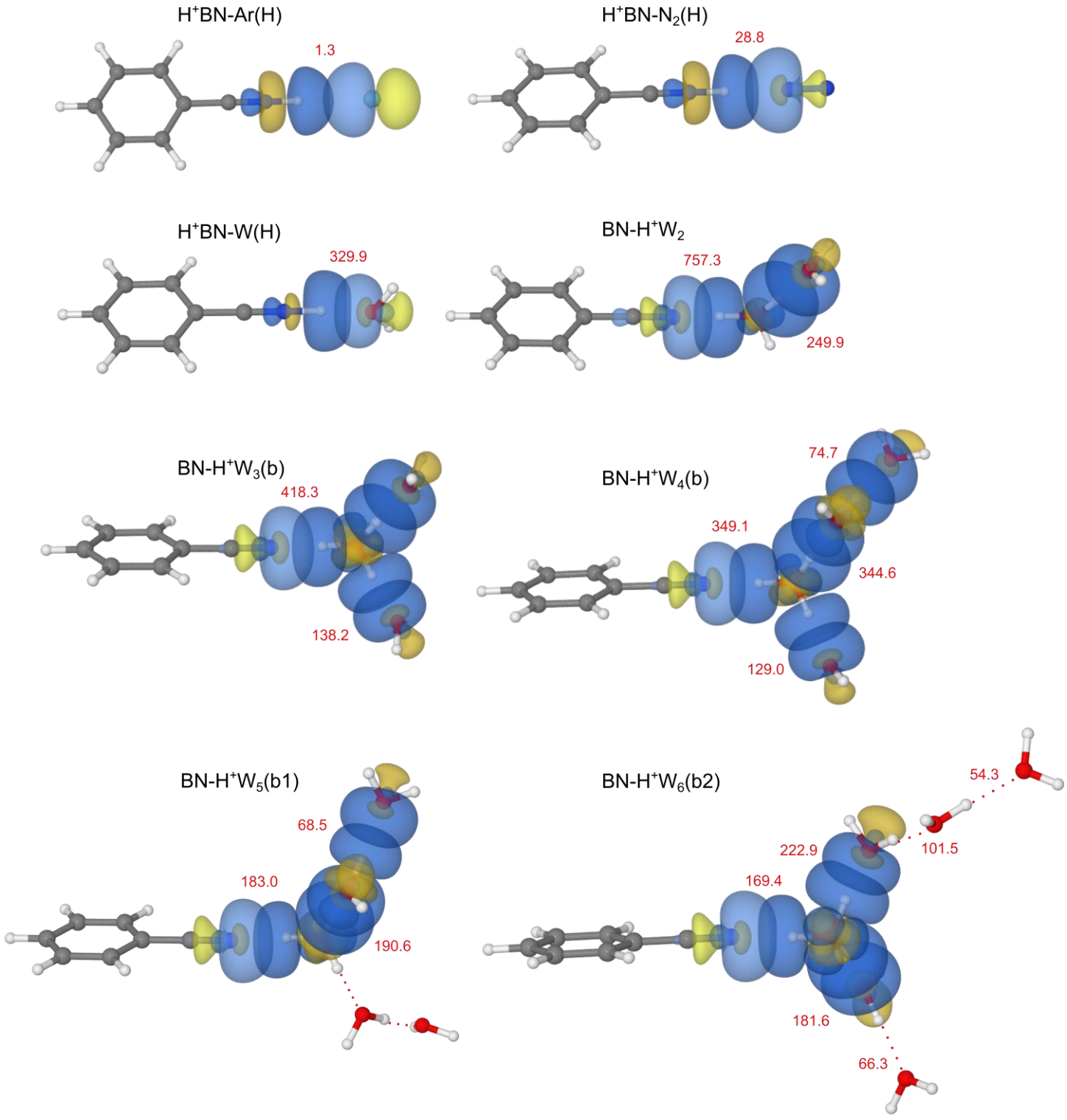
H+BN-Ar(H)
1.3
H+BN-N2(H)
28.8
H+BN-W(H)
329.9
BN-H+W2
757.3
249.9
BN-H+W3(b)
418.3
138.2
BN-H+W4(b)
74.7
349.1
344.6
129.0
BN-H+W5(b1)
68.5
183.0
190.6
BN-H+W6(b2)
54.3
101.5
222.9
169.4
181.6
66.3

Figure S3

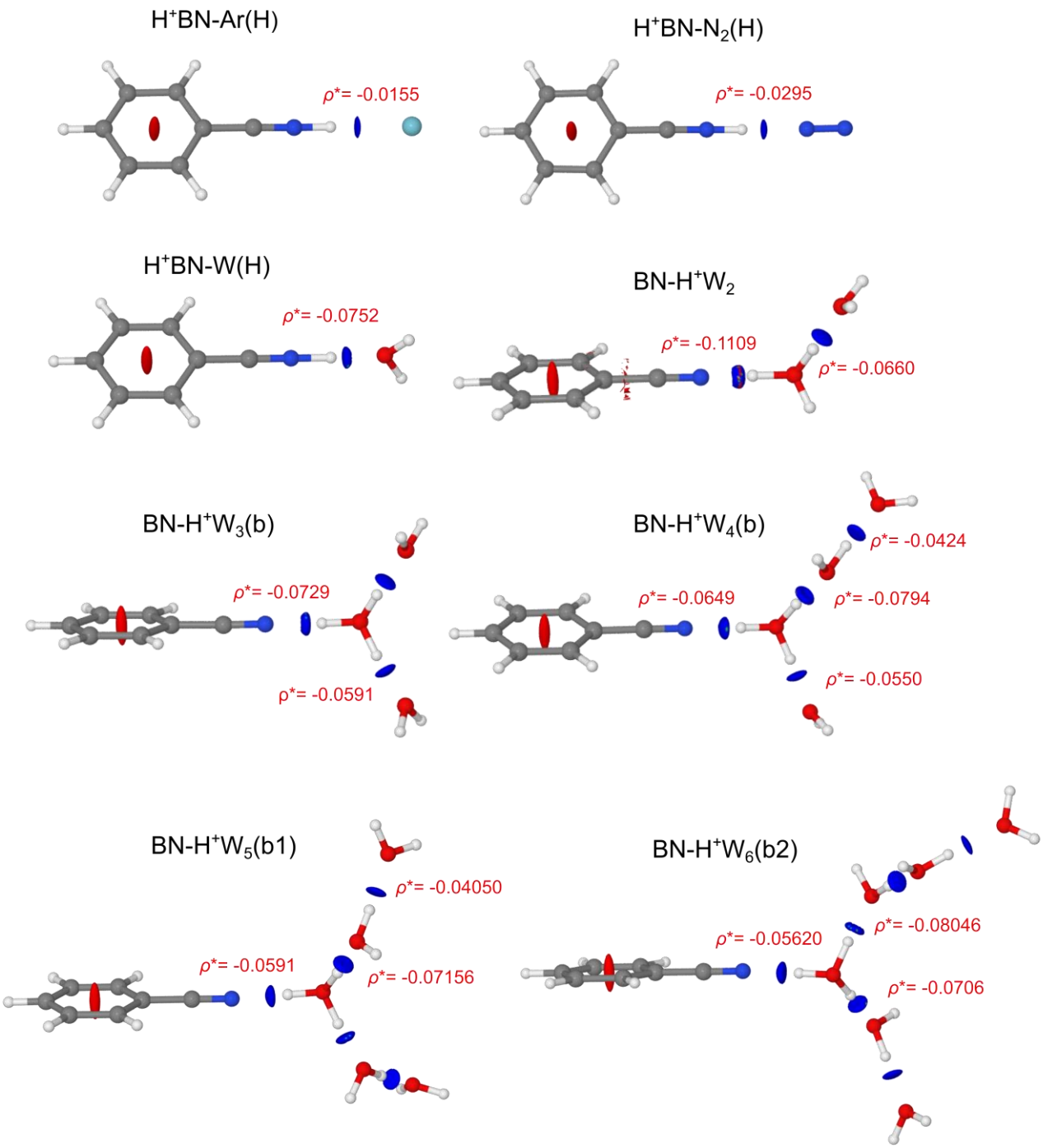
H+BN-Ar(H)
ρ*= -0.0155
H+BN-N2(H)
ρ*= -0.0295
H+BN-W(H)
ρ*= -0.0752
BN-H+W2
ρ*= -0.1109
ρ*= -0.0660
BN-H+W3(b)
ρ*= -0.0729
ρ*= -0.0591
BN-H+W4(b)
ρ*= -0.0424
ρ*= -0.0649
ρ*= -0.0794
ρ*= -0.0550
BN-H+W5(b1)
ρ*= -0.04050
ρ*= -0.0591
ρ*= -0.07156
BN-H+W6(b2)
ρ*= -0.08046
ρ*= -0.05620
ρ*= -0.0706

Figure S4

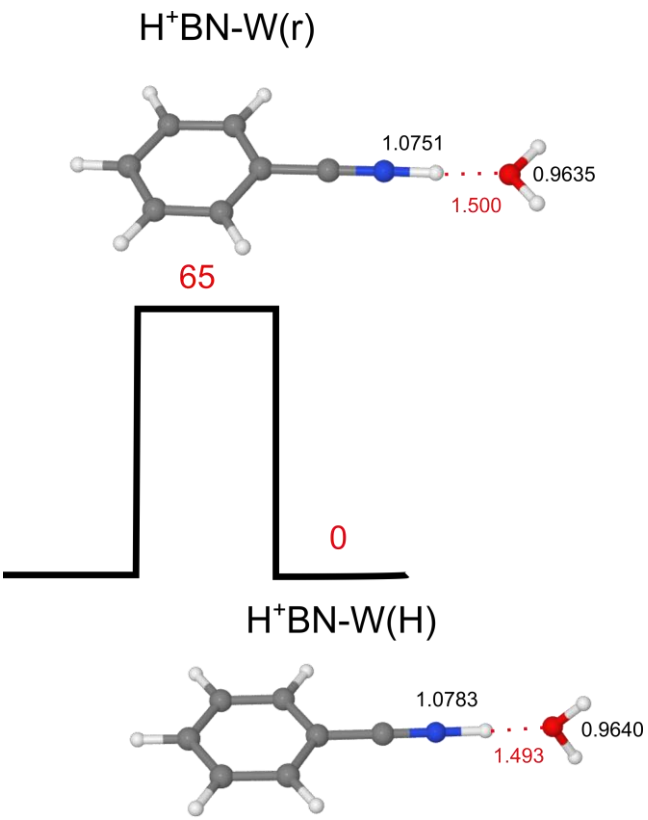

Figure S5

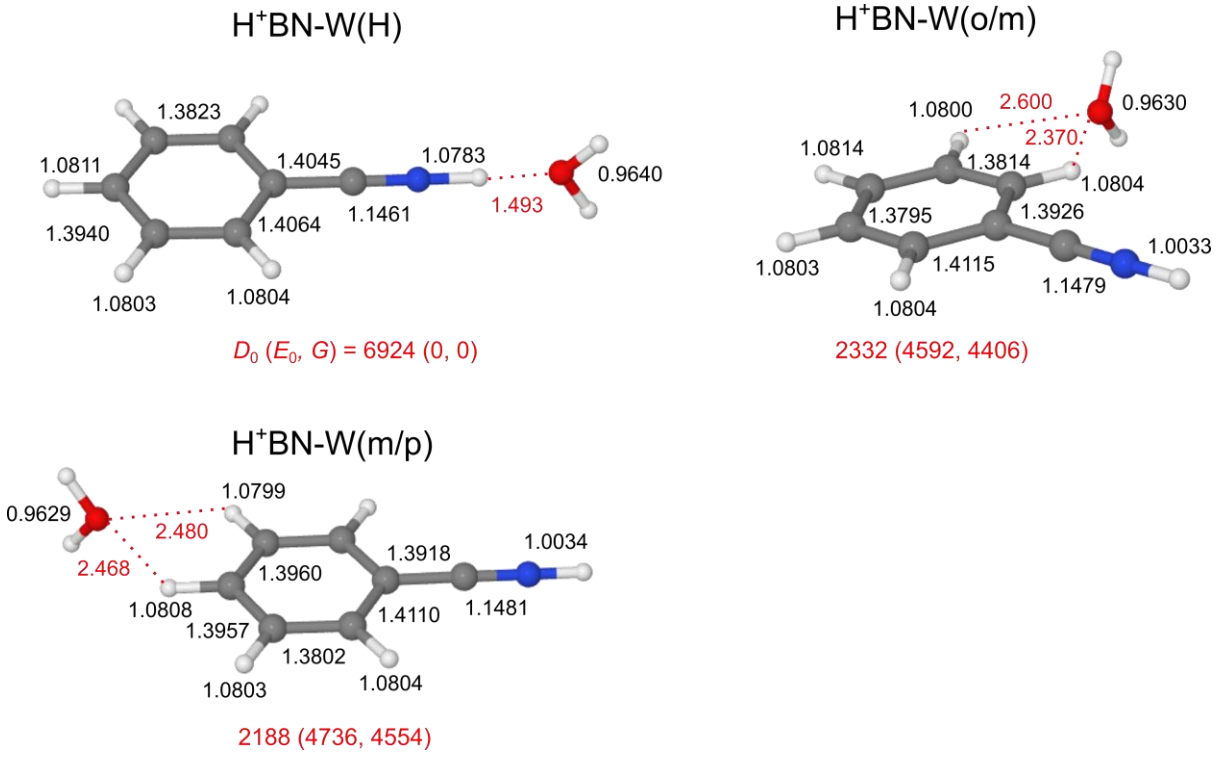
H+BN-W(H)
1.3823
1.0811
1.4045
1.0783
0.9640
1.493
1.3940
1.4064
1.1461
1.0803
1.0804
D0 (E0, G) = 6924 (0, 0)
H+BN-W(o/m)
1.0800
2.600
0.9630
2.370
1.0814
1.3814
1.0804
1.3795
1.3926
1.0033
1.0803
1.4115
1.1479
1.0804
2332 (4592, 4406)
H+BN-W(m/p)
1.0799
0.9629
2.480
2.468
1.3918
1.0034
1.3960
1.0808
1.4110
1.1481
1.3957
1.3802
1.0803
1.0804
2188 (4736, 4554)

Figure S6

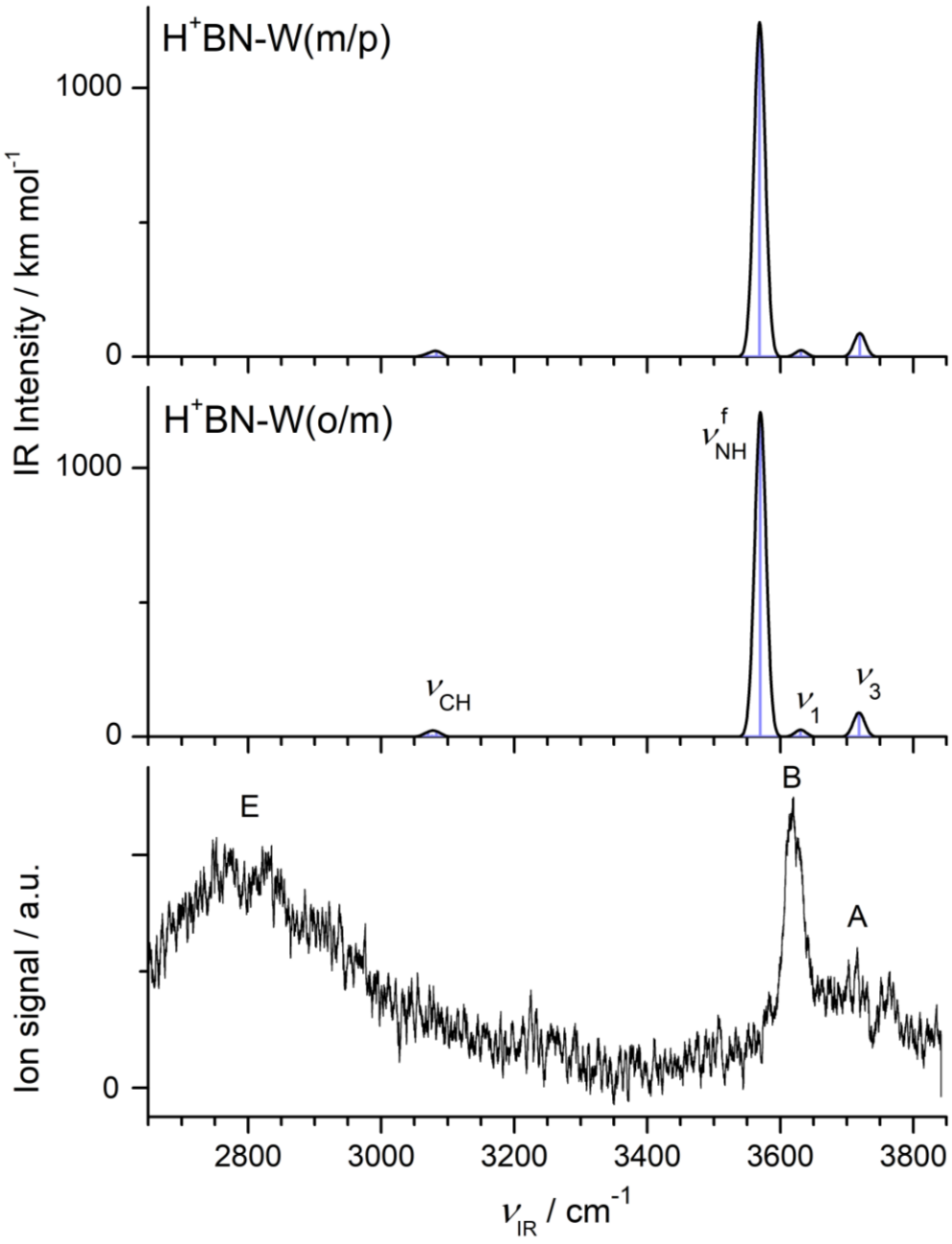
H+BN-W(m/p)
1000
0
IR Intensity / km mol-1
H+BN-W(o/m)
1000
0
νCH
νNHf
ν1
ν3
E
B
A
0
Ion signal / a.u.
2800
3000
3200
3400
3600
3800
νIR / cm-1

Figure S7

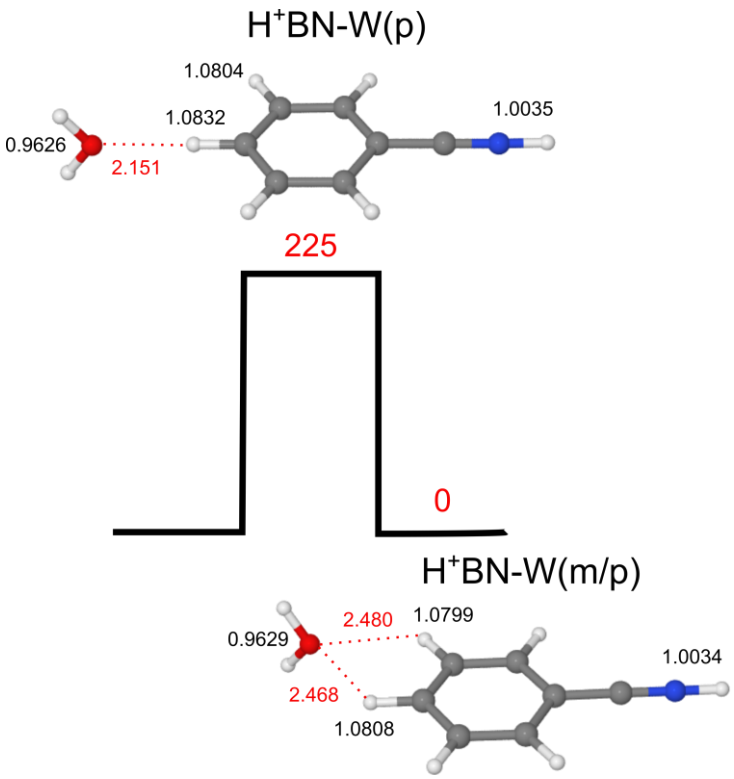
H+BN-W(p)
1.0804
1.0832
1.0035
0.9626
2.151
225
0
H+BN-W(m/p)
2.480
1.0799
0.9629
1.0034
2.468
1.0808

Figure S8

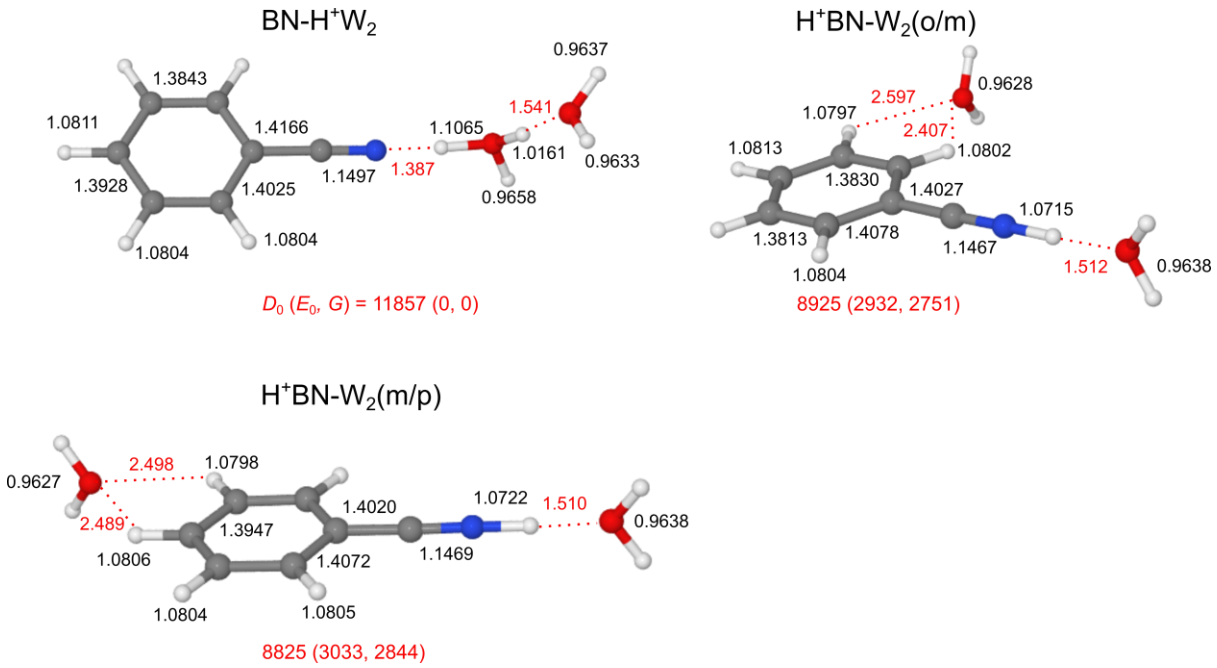
BN-H+W2
1.3843
1.0811
1.4166
1.3928
1.4025
1.1497
1.387
1.1065
1.541
0.9637
1.0161
0.9633
0.9658
1.0804
1.0804
D0 (E0, G) = 11857 (0, 0)
H+BN-W2(o/m)
0.9628
2.597
1.0797
2.407
1.0813
1.0802
1.3830
1.4027
1.0715
1.3813
1.4078
1.1467
1.512
0.9638
1.0804
8925 (2932, 2751)
H+BN-W2(m/p)
0.9627
2.498
1.0798
1.4020
1.0722
1.510
2.489
1.3947
0.9638
1.0806
1.4072
1.1469
1.0804
1.0805
8825 (3033, 2844)

Figure S9

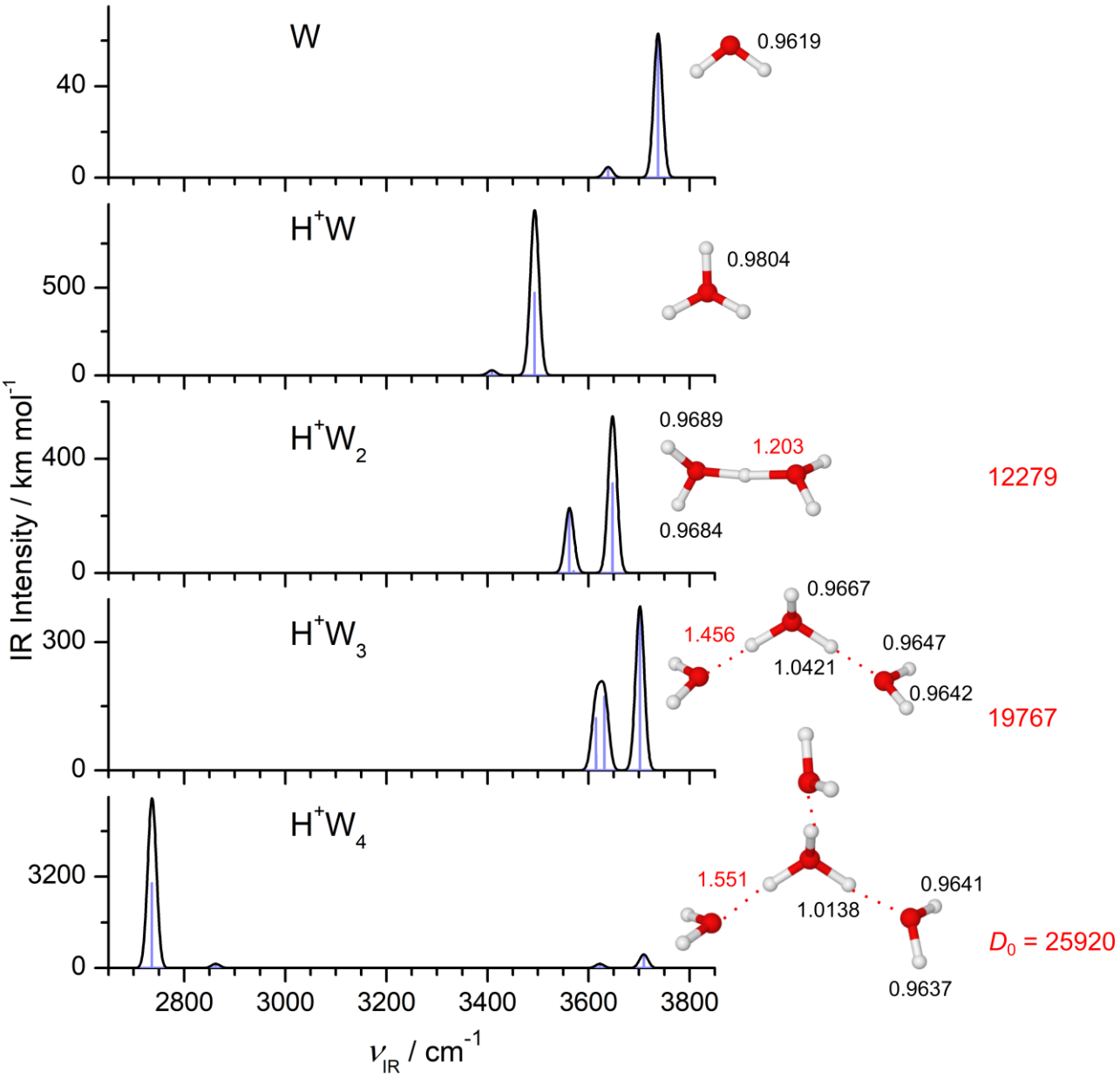
W
H+W
H+W2
H+W3
H+W4
IR Intensity / km mol-1
νIR / cm-1
0.9619
0.9804
0.9689
1.203
0.9684
12279
0.9667
1.456
0.9647
1.0421
0.9642
19767
1.551
0.9641
1.0138
0.9637
D0 = 25920

Figure S10a

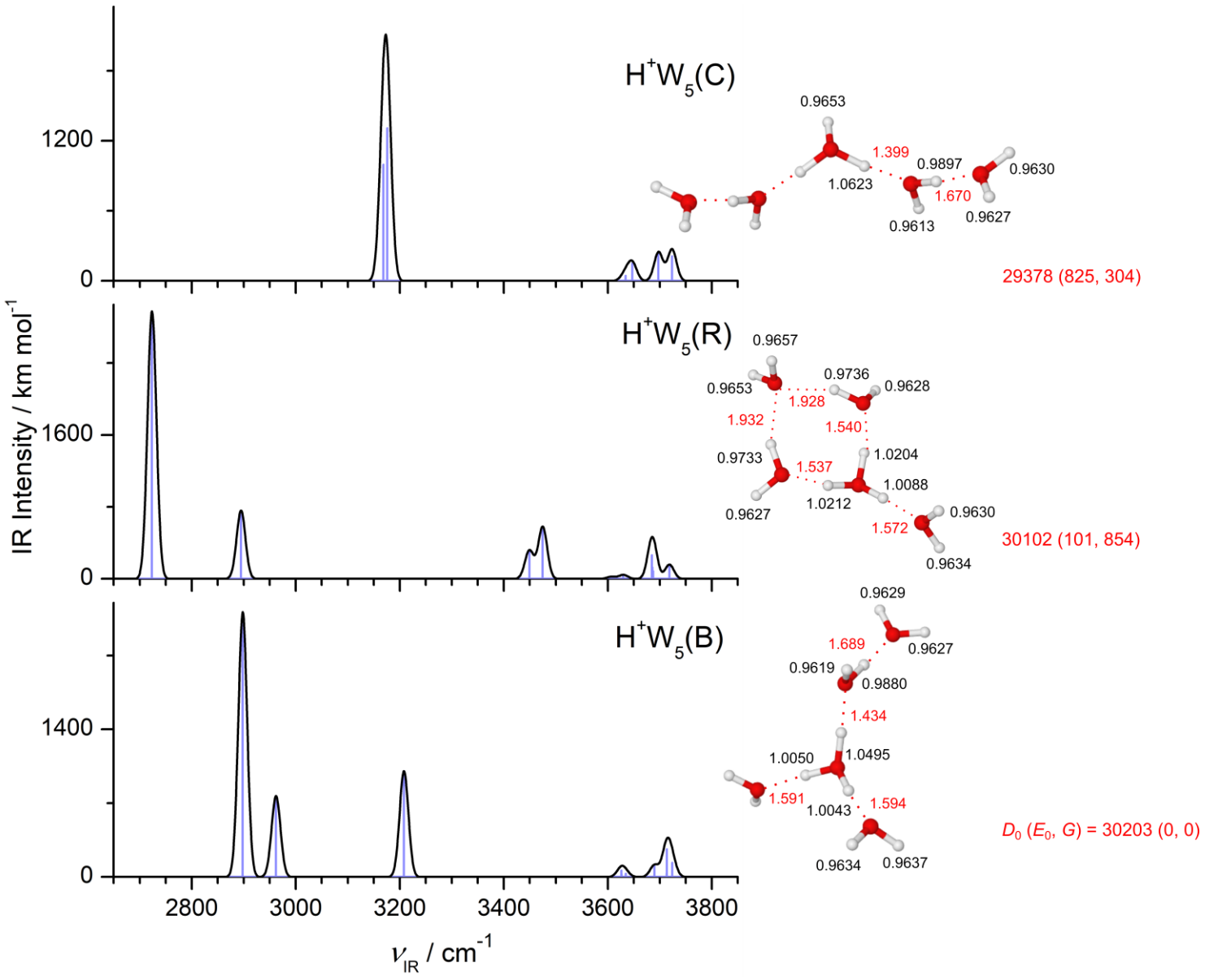
H+W5(C)
H+W5(R)
H+W5(B)
IR Intensity / km mol-1
νIR / cm-1
0
1200
1600
1400
2800
3000
3200
3400
3600
3800
0.9653
1.399
0.9897
0.9630
1.0623
1.670
0.9627
0.9613
29378 (825, 304)
0.9657
0.9653
0.9736
0.9628
1.928
1.932
1.540
0.9733
1.537
1.0204
1.0088
1.0212
0.9627
0.9630
1.572
0.9634
30102 (101, 854)
0.9629
1.689
0.9627
0.9619
0.9880
1.434
1.0050
1.0495
1.591
1.0043
1.594
0.9634
0.9637
D0 (E0, G) = 30203 (0, 0)

Figure S10b

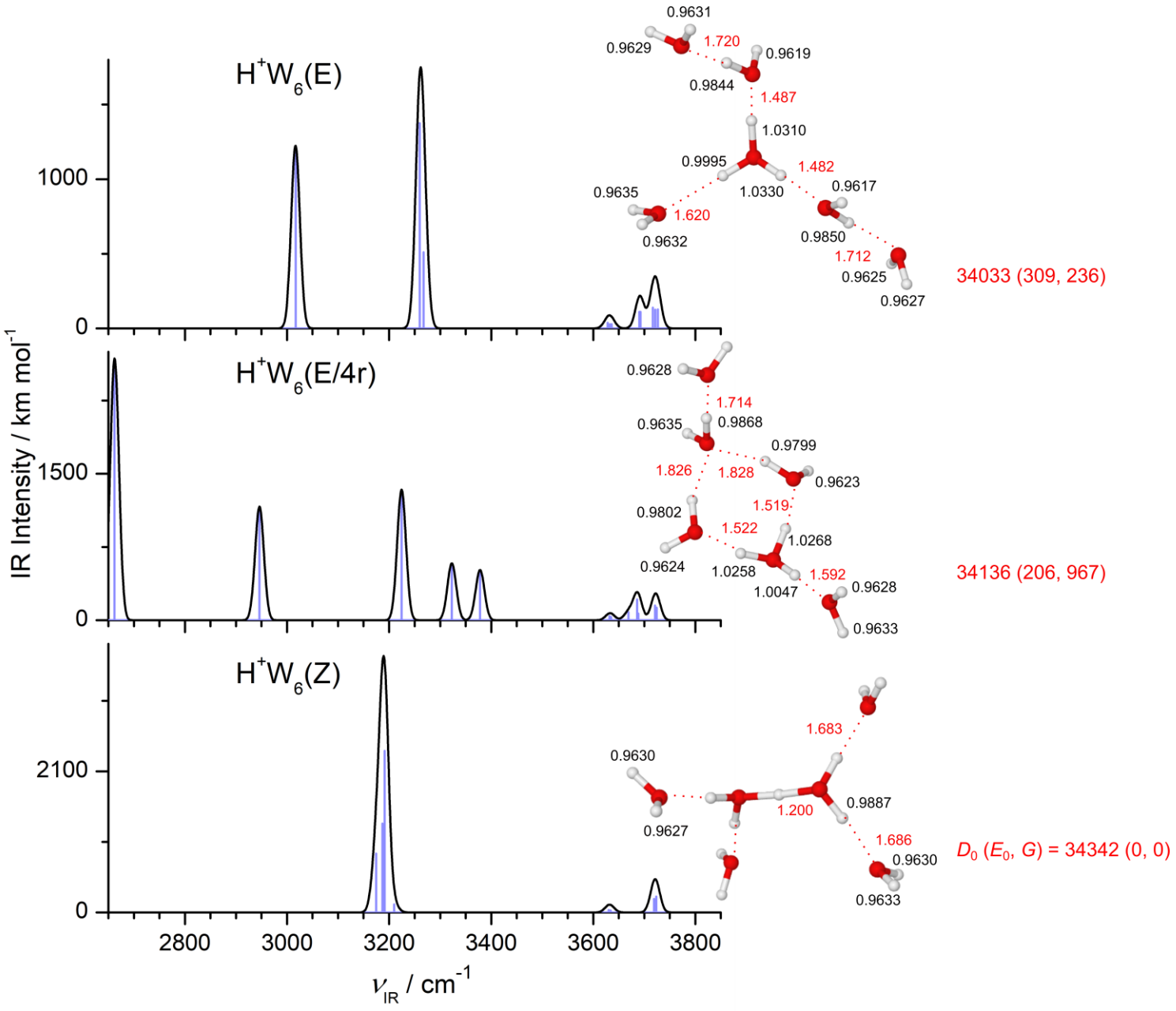
H+W6(E)
H+W6(E/4r)
H+W6(Z)
IR Intensity / km mol-1
νIR / cm-1
0
1000
1500
2100
2800
3000
3200
3400
3600
3800
0.9631
0.9629
1.720
0.9619
0.9844
1.487
1.0310
0.9995
1.482
0.9635
1.0330
0.9617
1.620
0.9632
0.9850
1.712
0.9625
0.9627
34033 (309, 236)
0.9628
1.714
0.9635
0.9868
0.9799
1.826
1.828
0.9623
0.9802
1.519
1.522
1.0268
0.9624
1.0258
1.592
1.0047
0.9628
0.9633
34136 (206, 967)
1.683
0.9630
0.9887
1.200
0.9627
1.686
0.9630
0.9633
D0 (E0, G) = 34342 (0, 0)

Figure S10c

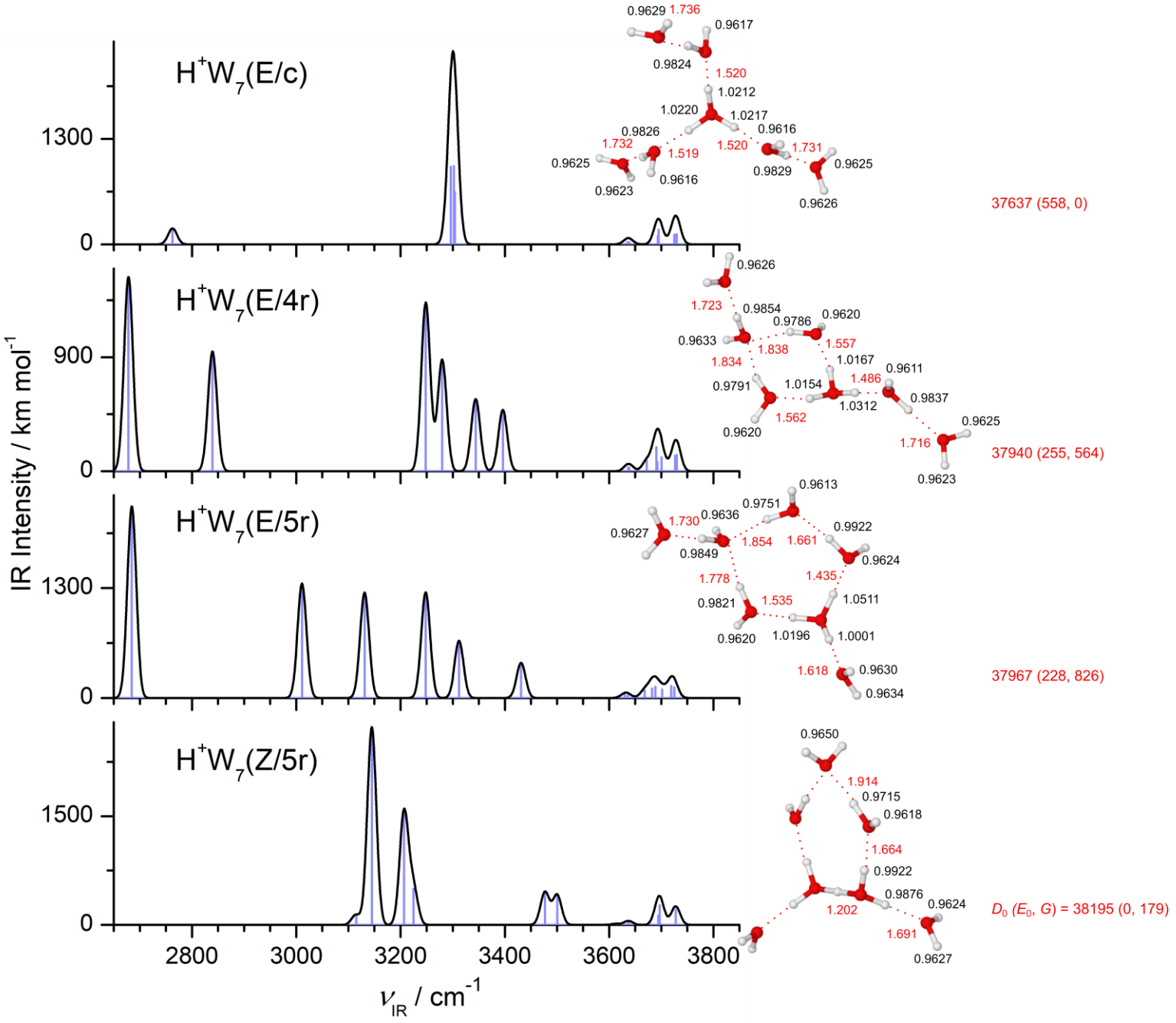
H+W7(E/c)
H+W7(E/4r)
H+W7(E/5r)
H+W7(Z/5r)
IR Intensity / km mol-1
νIR / cm-1
37637 (558, 0)
37940 (255, 564)
37967 (228, 826)
D0 (E0, G) = 38195 (0, 179)

Figure S10d

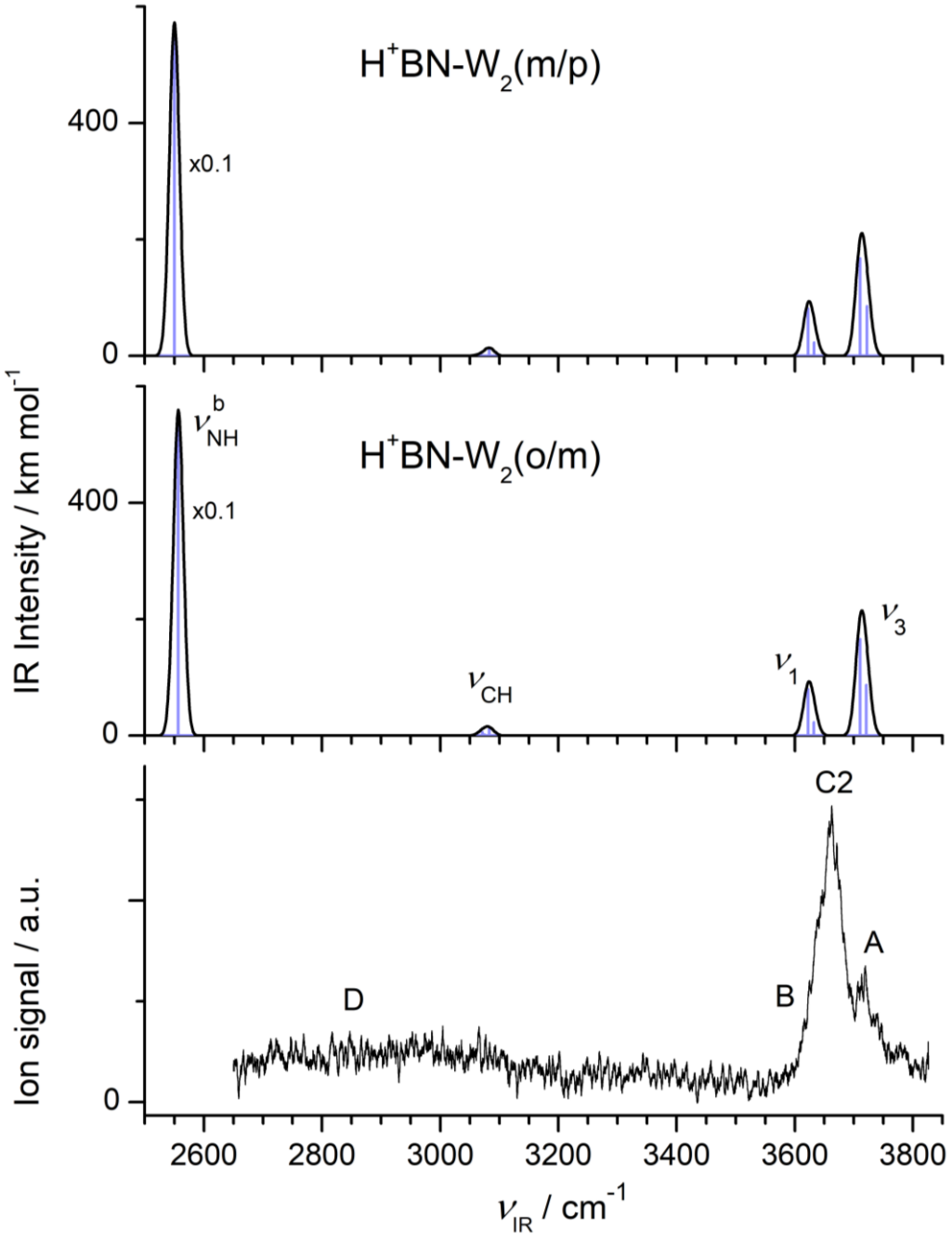
H+BN-W2(m/p)
400
x0.1
0
H+BN-W2(o/m)
400
x0.1
0
IR Intensity / km mol-1
ν b NH
ν CH
ν 1
ν 3
C2
A
B
D
0
Ion signal / a.u.
2600
2800
3000
3200
3400
3600
3800
ν IR / cm-1

Figure S11

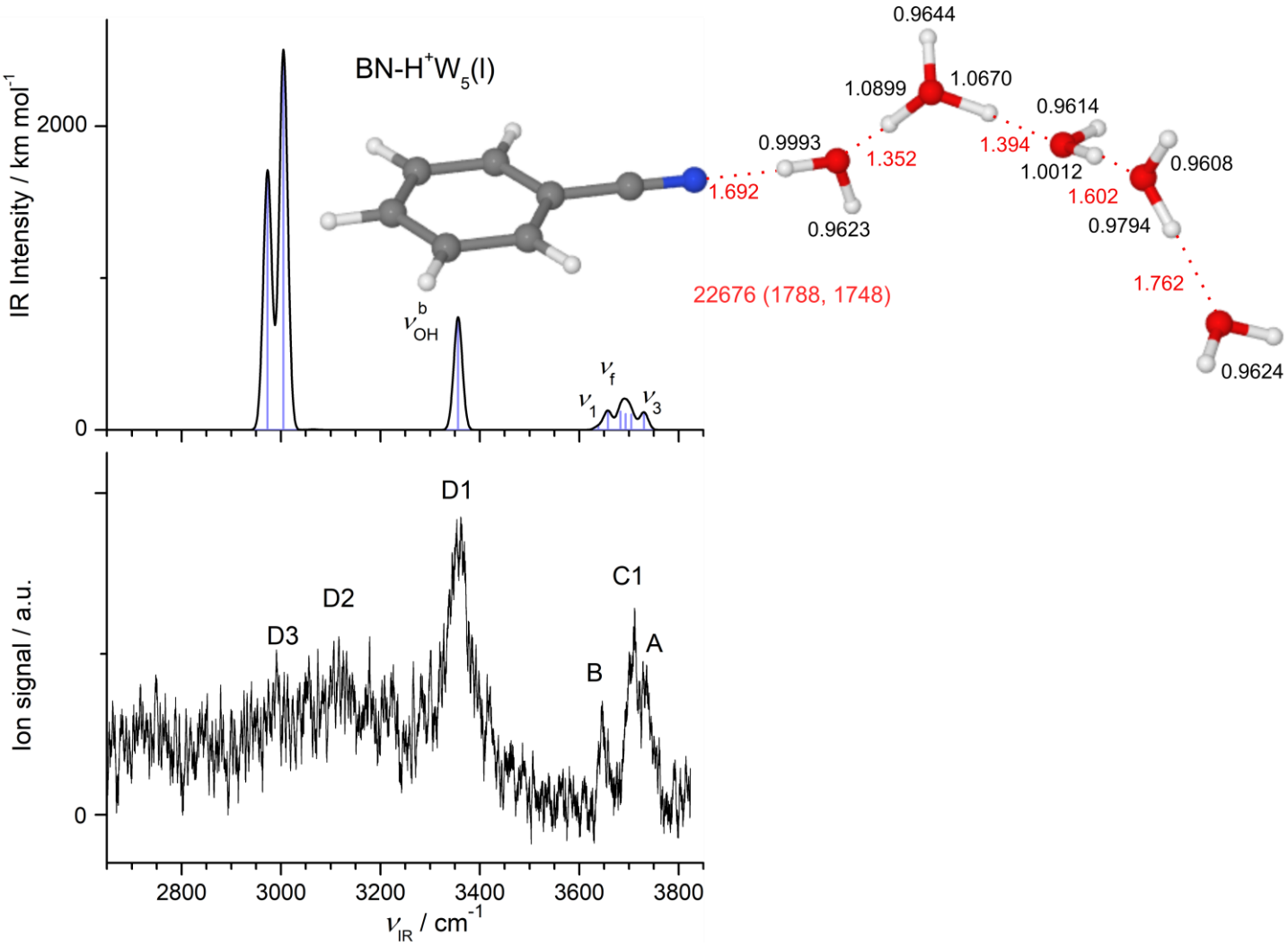
BN-H+W5(I)
IR Intensity / km mol-1
2000
0
ν_{OH}^{b}
ν_f
ν_1
ν_3
0.9644
1.0899
1.0670
0.9614
0.9993
1.352
1.394
1.0012
0.9608
1.692
1.602
0.9623
0.9794
1.762
22676 (1788, 1748)
0.9624
Ion signal / a.u.
D1
D2
D3
C1
A
B
0
2800
3000
3200
3400
3600
3800
ν_{IR} / cm-1

Figure S12

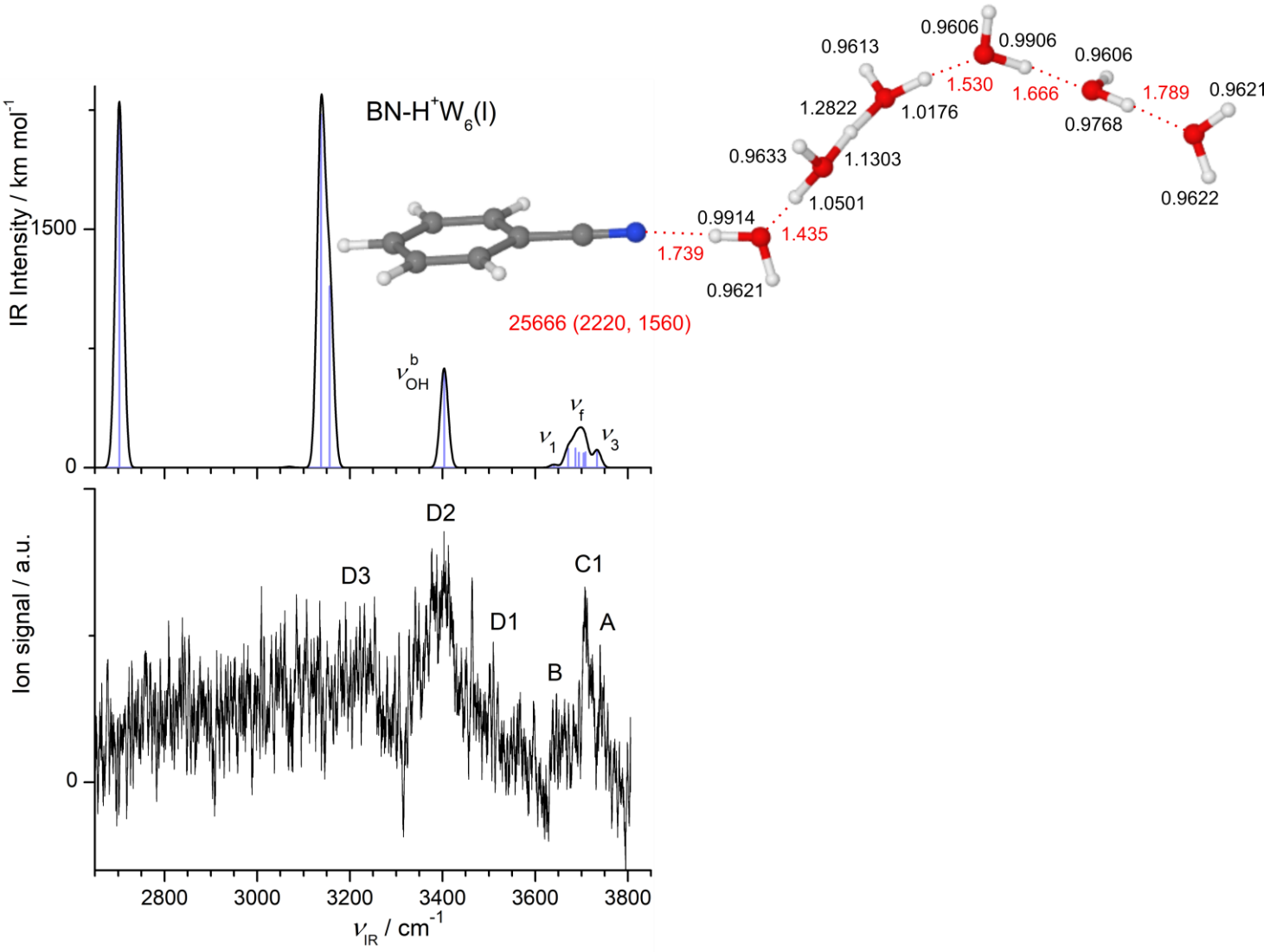
BN-H+W6(I)
IR Intensity / km mol-1
1500
0
25666 (2220, 1560)
0.9606
0.9906
0.9606
0.9613
1.530
1.666
1.789
0.9621
1.2822
1.0176
0.9768
0.9633
1.1303
1.0501
0.9622
0.9914
1.435
1.739
0.9621
νb OH
νf
ν1
ν3
Ion signal / a.u.
D2
D3
C1
D1
A
B
0
2800
3000
3200
3400
3600
3800
νIR / cm-1

Figure S13

Cartesian Coordinates of Relevant Structures (in Å) and Energies (in hartree)

BN

C	0.00000000	1.20583500	-1.47716800
C	0.00000000	1.21219100	-0.09024300
C	0.00000000	0.00000000	0.60806200
C	0.00000000	-1.21219100	-0.09024300
C	0.00000000	-1.20583500	-1.47716800
C	0.00000000	0.00000000	-2.17130600
H	0.00000000	2.14261900	-2.01678500
H	0.00000000	2.14391800	0.45693500
H	0.00000000	-2.14391800	0.45693500
H	0.00000000	-2.14261900	-2.01678500
H	0.00000000	0.00000000	-3.25267300
C	0.00000000	0.00000000	2.03806500
N	0.00000000	0.00000000	3.19033800

Sum of electronic and zero-point Energies= -324.517964
Sum of electronic and thermal Energies= -324.511874
Sum of electronic and thermal Enthalpies= -324.510930
Sum of electronic and thermal Free Energies= -324.547572

H^+BN

C	0.00000000	1.21558500	-1.53610000
C	0.00000000	1.23201600	-0.15563500
C	0.00000000	0.00000000	0.53051000
C	0.00000000	-1.23201600	-0.15563500
C	0.00000000	-1.21558500	-1.53610000
C	0.00000000	0.00000000	-2.22089700
H	0.00000000	2.14728700	-2.08273000
H	0.00000000	2.16425200	0.39045700
H	0.00000000	-2.16425200	0.39045700
H	0.00000000	-2.14728700	-2.08273000
H	0.00000000	0.00000000	-3.30212800
C	0.00000000	0.00000000	1.92491300
N	0.00000000	0.00000000	3.07201200
H	0.00000000	0.00000000	4.07625600

Sum of electronic and zero-point Energies= -324.833754
Sum of electronic and thermal Energies= -324.826953
Sum of electronic and thermal Enthalpies= -324.826009
Sum of electronic and thermal Free Energies= -324.863934

W

O	0.00000000	0.00000000	0.11698300
H	0.00000000	0.76357100	-0.46793200
H	0.00000000	-0.76357100	-0.46793200

Sum of electronic and zero-point Energies= -76.444969
Sum of electronic and thermal Energies= -76.442134
Sum of electronic and thermal Enthalpies= -76.441190
Sum of electronic and thermal Free Energies= -76.462611

N_2

N	0.00000000	0.00000000	0.54558200
N	0.00000000	0.00000000	-0.54558200

Sum of electronic and zero-point Energies= -109.565010
Sum of electronic and thermal Energies= -109.562650
Sum of electronic and thermal Enthalpies= -109.561706
Sum of electronic and thermal Free Energies= -109.583435

Ar

HF=-527.5600021

H^+BN-W(H)

C	-1.16241900	2.45584500	0.00000000
C	-1.21016200	1.07439100	0.00000000
C	0.00000000	0.35783000	0.00000000
C	1.24377700	1.01442600	0.00000000
C	1.26352700	2.39659100	0.00000000
C	0.06733600	3.11238400	0.00000000
H	-2.08145600	3.02356500	0.00000000
H	-2.15560000	0.55151600	0.00000000
H	2.16248100	0.44587500	0.00000000
H	2.20922600	2.91869100	0.00000000
H	0.09373200	4.19319000	0.00000000
C	-0.03334800	-1.04628600	0.00000000
N	-0.05959500	-2.19211200	0.00000000
H	-0.07737000	-3.27025200	0.00000000
O	-0.04057600	-4.76245000	0.00000000
H	-0.21075400	-5.30464700	0.77866800
H	-0.21075400	-5.30464700	-0.77866800

Sum of electronic and zero-point Energies= -401.310271
Sum of electronic and thermal Energies= -401.300326
Sum of electronic and thermal Enthalpies= -401.299382
Sum of electronic and thermal Free Energies= -401.346681

H^+BN-W(o/m)

C	1.37596000	-0.67218900	0.00000000
C	0.00000000	-0.55008300	0.00000000
C	-0.55677700	0.74520700	0.00000000
C	0.24954900	1.90372200	0.00000000
C	1.62021100	1.74760200	0.00000000
C	2.17886400	0.46747100	0.00000000
H	1.80677500	-1.66230300	0.00000000
H	-0.61899500	-1.43552800	0.00000000
H	-0.20015100	2.88606000	0.00000000
H	2.25838800	2.61919400	0.00000000
H	3.25487500	0.36012600	0.00000000
C	-1.94273900	0.88067400	0.00000000
N	-3.08542700	0.98977700	0.00000000
H	-4.08436100	1.08374900	0.00000000
O	0.15939400	-3.67398700	0.00000000
H	0.17795000	-4.26113300	0.76303200
H	0.17795000	-4.26113300	-0.76303200

Sum of electronic and zero-point Energies= -401.289348
Sum of electronic and thermal Energies= -401.278495
Sum of electronic and thermal Enthalpies= -401.277550
Sum of electronic and thermal Free Energies= -401.326606

H^+BN-W(m/p)

C	-1.15843200	0.30983800	0.00000000
C	0.00000000	1.05939200	0.00000000
C	1.23915500	0.38298400	0.00000000
C	1.31571500	-1.02596100	0.00000000
C	0.13907500	-1.74744600	0.00000000
C	-1.08902100	-1.08440000	0.00000000
H	-2.12753700	0.78629600	0.00000000
H	-0.03322400	2.13941800	0.00000000
H	2.27539800	-1.52231500	0.00000000
H	0.17424100	-2.82721100	0.00000000
H	-2.01482500	-1.64212600	0.00000000

C	2.41662900	1.12509400	0.00000000
N	3.38737900	1.73806500	0.00000000
H	4.23595000	2.27361500	0.00000000
O	-4.22288100	-0.54048100	0.00000000
H	-4.80866300	-0.58365200	0.76298600
H	-4.80866300	-0.58365200	-0.76298600

Sum of electronic and zero-point Energies= -401.288694
Sum of electronic and thermal Energies= -401.277783
Sum of electronic and thermal Enthalpies= -401.276838
Sum of electronic and thermal Free Energies= -401.325932

BN-H^+W_2

C	3.19065100	1.27408400	-0.06058400
C	1.82189200	1.20061100	-0.25368100
C	1.17933000	-0.03709900	-0.10435800
C	1.90054900	-1.19123700	0.23508500
C	3.26864600	-1.09646200	0.42393800
C	3.91066600	0.13061000	0.27677500
H	3.69756200	2.22153300	-0.17298600
H	1.25294800	2.08078100	-0.51618500
H	1.39142600	-2.13771600	0.34587900
H	3.83559000	-1.97819300	0.68541800
H	4.97941500	0.19620900	0.42566600
C	-0.22082000	-0.12541500	-0.30068700
N	-1.35703800	-0.19974300	-0.45948200
H	-2.72069600	-0.34938900	-0.66308100
O	-3.80253200	-0.51674300	-0.82423400
H	-4.41972500	-0.09027300	-0.13898800
H	-4.08683800	-0.31361000	-1.72459600
O	-5.34256900	0.46120800	0.96566700
H	-5.61416200	1.37681400	1.09139200
H	-5.96092800	-0.09421800	1.45345500

Sum of electronic and zero-point Energies= -477.777718
Sum of electronic and thermal Energies= -477.765240
Sum of electronic and thermal Enthalpies= -477.764296
Sum of electronic and thermal Free Energies= -477.819832

H^+BN-W_2(o/m)

C	2.29664200	-0.13734900	0.00003100
C	0.94697800	-0.43913500	0.00003000
C	0.02180600	0.61989600	0.00000300
C	0.43772300	1.96480500	-0.00002300
C	1.79190600	2.23738200	-0.00002000
C	2.71542400	1.19135200	0.00000600
H	3.00822600	-0.94941800	0.00005000
H	0.62683900	-1.47077300	0.00005000
H	-0.29006900	2.76330900	-0.00004500
H	2.13185200	3.26280500	-0.00003900
H	3.77283600	1.41731100	0.00000700
C	-1.34969800	0.32594600	0.00000000
N	-2.47070800	0.08469500	-0.00000200
H	-3.51731300	-0.14504700	0.00000000
O	2.09293400	-3.37968000	-0.00001600
H	2.30043600	-3.92885000	0.76309500
H	2.30050400	-3.92878100	-0.76315700
O	-4.98115300	-0.52392400	0.00001300
H	-5.54870300	-0.48076200	0.77779100
H	-5.54858500	-0.48121700	-0.77787600

Sum of electronic and zero-point Energies= -477.764358
Sum of electronic and thermal Energies= -477.750324
Sum of electronic and thermal Enthalpies= -477.749380
Sum of electronic and thermal Free Energies= -477.807298

H^+BN-W_2(m/p)

C	0.30913100	-1.88911600	0.00000000
C	-0.54875900	-0.80609400	0.00000000
C	0.00000000	0.49045600	0.00000000
C	1.39142100	0.70048200	0.00000000
C	2.22689600	-0.40043900	0.00000000
C	1.68911100	-1.68699700	0.00000000
H	-0.07340800	-2.89891300	0.00000000
H	-1.62041900	-0.94449700	0.00000000
H	1.79247700	1.70374600	0.00000000
H	3.29794900	-0.25868100	0.00000000
H	2.33489400	-2.55343800	0.00000000
C	-0.85989100	1.59778000	0.00000000
N	-1.56442500	2.50270300	0.00000000
H	-2.22746800	3.34528500	0.00000000
O	1.44905100	-4.87928300	0.00000000
H	1.55078900	-5.45739900	0.76309100
H	1.55078900	-5.45739900	-0.76309100
O	-3.20662500	4.49461300	0.00000000
H	-3.42074800	5.02165000	0.77800500
H	-3.42074800	5.02165000	-0.77800500

Sum of electronic and zero-point Energies= -477.763900
Sum of electronic and thermal Energies= -477.749807
Sum of electronic and thermal Enthalpies= -477.748863
Sum of electronic and thermal Free Energies= -477.806875

BN-H^+W_3(b)

C	-0.80079200	3.92713200	0.00000000
C	-0.91279400	2.54668800	0.00000000
C	0.25171000	1.76710500	0.00000000
C	1.51858400	2.36638300	0.00000000
C	1.61121900	3.74830600	0.00000000
C	0.45627100	4.52580200	0.00000000
H	-1.69260500	4.53715800	0.00000000
H	-1.88336800	2.07196200	0.00000000
H	2.40833400	1.75344200	0.00000000
H	2.58331400	4.21997500	0.00000000
H	0.53618900	5.60390600	0.00000000
C	0.14915000	0.35004700	0.00000000
N	0.06972400	-0.79760800	0.00000000
H	0.06787300	-2.34540600	0.00000000
O	0.10395600	-3.37905600	0.00000000
H	-0.27589600	-3.79057500	0.83563000
H	-0.27589600	-3.79057500	-0.83563000
O	-0.80079200	-4.52553300	-2.13628700
O	-0.80079200	-4.52553300	2.13628700
H	-0.21395100	-5.00635800	-2.73008000
H	-0.21395100	-5.00635800	2.73008000
H	-1.59358900	-4.30586200	-2.63680400
H	-1.59358900	-4.30586200	2.63680400

Sum of electronic and zero-point Energies= -554.246132
Sum of electronic and thermal Energies= -554.230050
Sum of electronic and thermal Enthalpies= -554.229106
Sum of electronic and thermal Free Energies= -554.294676

BN-H$^+$W$_3$(I)

C	-3.78487800	1.54356200	0.15241100
C	-2.44555700	1.23698700	0.32555800
C	-2.01101600	-0.07554500	0.09594600
C	-2.91094900	-1.07300300	-0.30380700
C	-4.24651100	-0.74752100	-0.47188400
C	-4.68182800	0.55535300	-0.24473600
H	-4.13068200	2.55218400	0.32709800
H	-1.74092900	1.99572600	0.63399900
H	-2.56209700	-2.08082800	-0.47677400
H	-4.94871400	-1.50887000	-0.77953900
H	-5.72596900	0.80194000	-0.37764900
C	-0.64036100	-0.40171400	0.27170600
N	0.46920200	-0.66886200	0.41359700
H	1.89742700	-1.09809800	0.59571500
O	2.88376000	-1.43996200	0.71802300
H	3.60641500	-0.98129100	0.07185500
H	3.14843900	-1.41287000	1.64577100
O	4.49083900	-0.42097500	-0.83121600
H	5.14430400	0.27240500	-0.56369100
H	4.89875100	-0.99437300	-1.48791000
O	6.15912300	1.50364800	-0.04632500
H	6.12968600	2.38065700	-0.44377900
H	7.05577000	1.38505300	0.28470700

Sum of electronic and zero-point Energies= -554.241506
Sum of electronic and thermal Energies= -554.226297
Sum of electronic and thermal Enthalpies= -554.225353
Sum of electronic and thermal Free Energies= -554.289508

BN-H$^+$W$_4$(b)

C	4.52305400	0.08129500	1.18001600
C	3.15229800	0.27481500	1.13084700
C	2.45335300	-0.07761000	-0.03103400
C	3.12375300	-0.61969000	-1.13539700
C	4.49477000	-0.80626800	-1.06889000
C	5.19211200	-0.45725900	0.08434600
H	5.07056300	0.35035000	2.07185900
H	2.62356300	0.69271000	1.97534700
H	2.57293200	-0.88661200	-2.02573800
H	5.02031400	-1.22341000	-1.91584200
H	6.26204300	-0.60537100	0.12935800
C	1.04614900	0.11791600	-0.09231000
N	-0.09225100	0.27494800	-0.14427100
H	-1.65785500	0.52338300	-0.31566700
O	-2.65845000	0.67496500	-0.45124400
H	-3.24401700	0.07754600	0.15572100
H	-2.90043500	1.64309400	-0.37634200
O	-3.24396900	3.21780600	-0.34487800
O	-4.15656300	-0.73283600	0.99291700
H	-3.53900100	3.69509700	-1.12776800
H	-4.81333200	-1.33090500	0.56787700
H	-3.56795000	3.70497900	0.41986800
H	-3.85614400	-1.15590500	1.80257900
O	-5.99656600	-2.30027800	-0.20179500
H	-6.93996900	-2.25554600	-0.01569600
H	-5.85349600	-3.11049700	-0.70112900

Sum of electronic and zero-point Energies= -630.708355
Sum of electronic and thermal Energies= -630.689230
Sum of electronic and thermal Enthalpies= -630.688285
Sum of electronic and thermal Free Energies= -630.762144

BN-H$^+$W$_4$(c)

C	-1.47982200	4.39175000	0.00000000
C	-1.25771100	3.02451100	0.00000000
C	0.05909000	2.54618700	0.00000000
C	1.14499500	3.43154500	0.00000000
C	0.90424600	4.79566700	0.00000000
C	-0.40305400	5.27426000	0.00000000
H	-2.49189600	4.77021700	0.00000000
H	-2.08601000	2.33078200	0.00000000
H	2.15555000	3.04928300	0.00000000
H	1.73529100	5.48622700	0.00000000
H	-0.58362600	6.34014700	0.00000000
C	0.29842600	1.14479700	0.00000000
N	0.49513000	0.01164000	0.00000000
H	0.84329100	-1.51933400	0.00000000
O	1.11151400	-2.51238400	0.00000000
H	0.75765000	-3.00681300	0.80936700
H	0.75765000	-3.00681300	-0.80936700
O	0.05909000	-3.98207700	-1.82830100
O	0.05909000	-3.98207700	1.82830100
H	0.42740100	-4.22526200	-2.68349500
H	-0.29058300	-4.78679700	1.40884900
H	-0.29058300	-4.78679700	-1.40884900
O	-0.96166100	-5.93681600	0.00000000
H	0.42740100	-4.22526200	2.68349500
H	-1.92504100	-5.99862600	0.00000000
H	-0.64369400	-6.84789800	0.00000000

Sum of electronic and zero-point Energies= -630.707876
Sum of electronic and thermal Energies= -630.690255
Sum of electronic and thermal Enthalpies= -630.689311
Sum of electronic and thermal Free Energies= -630.757812

BN-H$^+$W$_4$(s)

C	-4.60605000	1.13605800	0.18228500
C	-3.25496100	1.03449600	0.47224900
C	-2.56012600	-0.12422200	0.10344200
C	-3.21697000	-1.17375000	-0.55120300
C	-4.56831300	-1.05629600	-0.83394600
C	-5.26101400	0.09451500	-0.46875800
H	-5.14928100	2.02644500	0.46477000
H	-2.73807100	1.83655900	0.97915500
H	-2.67083700	-2.06379900	-0.82860200
H	-5.08224900	-1.86227000	-1.33788100
H	-6.31551300	0.17954400	-0.69133200
C	-1.17225900	-0.23921300	0.40107900
N	-0.05063700	-0.33356500	0.64117400
H	1.54313800	-0.62134100	1.18212800
O	2.46843400	-0.80657700	1.50223500
H	3.54120700	-0.19587000	0.89805400
H	2.45245500	-0.82327700	2.46443600
O	3.96194200	2.47674900	-0.80052000
O	4.41940300	0.22008900	0.43664800
H	4.40887200	3.28686200	-0.53215100
H	4.92562700	-0.44782600	-0.11019200
H	3.70464800	2.59105100	-1.72139500
H	4.24686600	1.06172200	-0.07440300
O	5.79551100	-1.48009300	-0.99501100
H	6.72363300	-1.64693200	-0.79673200
H	5.43979600	-2.29679500	-1.36176200

Sum of electronic and zero-point Energies= -630.706012
Sum of electronic and thermal Energies= -630.687353
Sum of electronic and thermal Enthalpies= -630.686409

Sum of electronic and thermal Free Energies= -630.759420

BN-H$^+$W$_4$(I)

C	4.77032000	1.55641200	-0.08580200
C	3.41982200	1.27282200	-0.20669000
C	2.98773300	-0.05532400	-0.09817100
C	3.90278100	-1.09139900	0.12976000
C	5.24963300	-0.78973300	0.24811300
C	5.68214500	0.52911600	0.14082400
H	5.11286200	2.57788400	-0.16835800
H	2.70382100	2.06251300	-0.38298300
H	3.55642400	-2.11158500	0.21103200
H	5.96262500	-1.58240600	0.42375100
H	6.73472900	0.75740000	0.23399700
C	1.60348900	-0.35727900	-0.22153800
N	0.48434900	-0.60400600	-0.32089400
H	-1.04829000	-1.03700900	-0.46577700
O	-2.01767700	-1.34312300	-0.54986400
H	-2.77575600	-0.85411400	0.21129200
H	-2.29177000	-1.29680200	-1.47279500
O	-3.52172300	-0.36748900	1.04985200
H	-4.28551200	0.20968700	0.70326700
H	-3.85642000	-0.99908500	1.69574900
O	-5.36154300	1.11376600	0.09148900
H	-5.38240000	2.04834900	0.31803400
H	-6.29094700	0.82064800	-0.03673700
O	-7.88813200	0.20004600	-0.29837400
H	-8.31553600	0.22316300	-1.16094100
H	-8.59721000	0.19610900	0.35293100

Sum of electronic and zero-point Energies= -630.703583
Sum of electronic and thermal Energies= -630.685355
Sum of electronic and thermal Enthalpies= -630.684411
Sum of electronic and thermal Free Energies= -630.757514

BN-H$^+$W$_5$(c1)

C	-1.47556800	5.18089800	0.00000000
C	-1.24319900	3.81523100	0.00000000
C	0.07673000	3.34627600	0.00000000
C	1.15564900	4.23976900	0.00000000
C	0.90505900	5.60224700	0.00000000
C	-0.40555800	6.07146200	0.00000000
H	-2.49048700	5.55173500	0.00000000
H	-2.06627700	3.11531500	0.00000000
H	2.16894300	3.86482600	0.00000000
H	1.73114500	6.29876800	0.00000000
H	-0.59395300	7.13600300	0.00000000
C	0.32621700	1.94597200	0.00000000
N	0.53072400	0.81425500	0.00000000
H	0.88845600	-0.73908000	0.00000000
O	1.15547400	-1.72553800	0.00000000
H	0.79197100	-2.22150700	0.81042500
H	0.79197100	-2.22150700	-0.81042500
O	0.07673000	-3.18115600	-1.80226300
O	0.07673000	-3.18115600	1.80226300
H	0.48303800	-3.49858800	-2.61425400
H	-0.30967800	-3.94722800	1.33174900
H	-0.30967800	-3.94722800	-1.33174900
O	-0.99742400	-5.01229300	0.00000000
H	0.48303800	-3.49858800	2.61425400
H	-1.96087200	-5.03323400	0.00000000
H	-0.70468700	-5.95191500	0.00000000
O	-0.12291600	-7.58645300	0.00000000

H	-0.08136500	-8.16295500	0.76995900
H	-0.08136500	-8.16295500	-0.76995900

Sum of electronic and zero-point Energies= -707.170064
Sum of electronic and thermal Energies= -707.149331
Sum of electronic and thermal Enthalpies= -707.148386
Sum of electronic and thermal Free Energies= -707.225974

BN-H^{+}W$_5$(c2)

C	-5.30102500	-0.73502800	0.02814300
C	-3.95690700	-1.06322500	0.09834600
C	-2.99804600	-0.04936100	-0.02404600
C	-3.38423500	1.28337700	-0.21544100
C	-4.73261400	1.59393800	-0.28326600
C	-5.68791000	0.58859300	-0.16195200
H	-6.04735600	-1.51081000	0.12154100
H	-3.64579700	-2.08738200	0.24557200
H	-2.63465000	2.05591900	-0.30853500
H	-5.03961400	2.61942000	-0.43074200
H	-6.73850300	0.83777100	-0.21581700
C	-1.61604500	-0.37959900	0.04702000
N	-0.49967600	-0.65034000	0.10517700
O	3.41736400	-0.90530900	-1.82414100
H	2.52110500	-1.28170400	-0.58366500
O	1.98469400	-1.49926500	0.24369100
H	2.48504000	-1.14673700	1.07374100
H	1.03465300	-1.14283200	0.18331600
O	3.38316700	-0.62512700	2.14283800
H	3.17016600	-0.66014200	3.07954300
H	3.78034500	0.25212700	1.93605200
O	4.42113500	1.63996900	1.14116300
H	4.79649600	2.40662100	1.58415400
H	4.94944400	1.48266900	0.34299700
H	4.22248200	-0.36863200	-1.71178200
H	3.60095900	-1.56714200	-2.49810600
O	5.64890500	0.80643300	-1.35265500
H	6.52236900	0.40493600	-1.26916900
H	5.73916400	1.49251300	-2.02532700

Sum of electronic and zero-point Energies= -707.168946
Sum of electronic and thermal Energies= -707.149156
Sum of electronic and thermal Enthalpies= -707.148212
Sum of electronic and thermal Free Energies= -707.221079

BN-H^{+}W$_5$(b1)

C	4.96217700	0.15124800	-1.11915000
C	3.57704300	0.14663900	-1.14681600
C	2.86971700	-0.09438600	0.03786900
C	3.54668500	-0.32865800	1.24154700
C	4.93206600	-0.32045400	1.25147700
C	5.63770400	-0.08152100	0.07556400
H	5.51565200	0.33644200	-2.02853900
H	3.04312000	0.32680300	-2.06869200
H	2.98935500	-0.51261100	2.14869700
H	5.46220800	-0.50010600	2.17575300
H	6.71867600	-0.07646700	0.09029000
C	1.44681900	-0.10081700	0.01950400
N	0.29662000	-0.10680300	0.00619600
H	-1.33318800	-0.05338000	0.05609100
O	-2.34367800	-0.02558300	0.10585000
H	-2.71944100	0.83704600	-0.29984400
H	-2.76785100	-0.85986600	-0.30462200

O	-3.22359200	2.14597200	-0.85643500
H	-3.67240600	2.20396300	-1.70454900
H	-3.60712800	2.83350800	-0.26895100
O	-3.47551500	-2.05909400	-0.91211500
H	-4.04220000	-2.63701300	-0.35496400
H	-3.04771900	-2.61931200	-1.56606300
O	-5.09048400	-3.59892700	0.63083900
H	-4.83626300	-4.19287900	1.34404200
H	-6.00143000	-3.81444900	0.40695700
O	-4.20878500	4.06477800	0.78685800
H	-3.83121900	4.94653800	0.86554500
H	-5.04333400	4.07993200	1.26553100

Sum of electronic and zero-point Energies= -707.169463
Sum of electronic and thermal Energies= -707.146947
Sum of electronic and thermal Enthalpies= -707.146003
Sum of electronic and thermal Free Energies= -707.230221

BN-H$^+$W$_5$(b2)

C	-4.78357300	-0.36972600	-1.11386900
C	-3.42440400	-0.10203500	-1.08904900
C	-2.77216600	0.01551600	0.14480300
C	-3.47846800	-0.13408600	1.34502000
C	-4.83725000	-0.40159400	1.30237200
C	-5.48799000	-0.51911400	0.07746700
H	-5.29451000	-0.46113600	-2.06162900
H	-2.86873900	0.01703400	-2.00799700
H	-2.96415300	-0.03967600	2.29051200
H	-5.38953700	-0.51775200	2.22384700
H	-6.54852000	-0.72726500	0.05116400
C	-1.37653100	0.29323900	0.18079700
N	-0.24877500	0.51801300	0.21220800
H	1.34006000	0.95621300	0.32489300
O	2.30198200	1.23889300	0.42229500
H	3.01493400	0.46983400	0.13747800
H	2.46337700	2.10105700	-0.04482800
O	2.68399300	3.57413200	-0.75988200
O	3.96332400	-0.43435500	-0.20389100
H	2.81516300	4.37934200	-0.24828600
H	4.54588800	-0.76703700	0.51146000
H	3.09792400	3.71934100	-1.61679500
H	3.70464800	-1.18796700	-0.77608300
O	5.62485700	-1.37513000	1.74218300
H	6.58001700	-1.26297800	1.70045500
H	5.41070500	-1.52852100	2.66782800
O	3.20318900	-2.44850200	-1.87949300
H	3.68087000	-2.59609900	-2.70245800
H	2.89682100	-3.31400700	-1.58995600

Sum of electronic and zero-point Energies= -707.168724
Sum of electronic and thermal Energies= -707.146164
Sum of electronic and thermal Enthalpies= -707.145220
Sum of electronic and thermal Free Energies= -707.228494

BN-H$^+$W$_5$(b3)

C	-5.34793600	-0.15030000	1.19638900
C	-4.00310900	0.17429300	1.12390000
C	-3.27461500	-0.17966500	-0.01897200
C	-3.89027000	-0.85391600	-1.08136600
C	-5.23597500	-1.17076600	-0.99230700
C	-5.96251200	-0.82047600	0.14228600
H	-5.91762900	0.11916700	2.07412900

H	-3.51675700	0.69495900	1.93614900
H	-3.31730400	-1.12052800	-1.95771800
H	-5.71898900	-1.69046300	-1.80728800
H	-7.01239200	-1.07053400	0.20518600
C	-1.89333100	0.15030800	-0.10375700
N	-0.77633800	0.41606300	-0.17442100
H	0.77794500	0.82757900	-0.37469800
O	1.75037900	1.07604900	-0.52269200
H	1.89373300	2.05851600	-0.41923200
H	2.41335700	0.51505600	0.07094600
O	2.08127300	3.67190200	-0.32080700
H	2.45871100	4.13065600	0.43701000
H	2.28014700	4.20601200	-1.09726300
O	3.38168700	-0.18933700	0.85190400
H	4.09348900	-0.70216900	0.37797600
H	3.10252800	-0.70530800	1.61353300
O	5.27105400	-1.47372500	-0.43412700
H	5.14307700	-2.23263600	-1.00914100
H	6.21458900	-1.46331500	-0.17540600
O	7.91749800	-1.38775900	0.30589800
H	8.61194200	-0.98339900	-0.22358200
H	8.35927700	-1.96994500	0.93190200

Sum of electronic and zero-point Energies= -707.167446
Sum of electronic and thermal Energies= -707.145168
Sum of electronic and thermal Enthalpies= -707.144224
Sum of electronic and thermal Free Energies= -707.227852

BN-H^{+}W$_5$(s)

C	4.99674200	0.94431000	-0.83301300
C	3.68168600	0.54707600	-1.01504600
C	3.05089700	-0.21247900	-0.02210300
C	3.73603100	-0.57112000	1.14527600
C	5.05067400	-0.16596000	1.31231900
C	5.67960800	0.58934500	0.32677600
H	5.49024600	1.52936900	-1.59585800
H	3.14383200	0.81565100	-1.91283400
H	3.23977100	-1.15962800	1.90343100
H	5.58582800	-0.44024400	2.21016800
H	6.70580900	0.90125400	0.46240700
C	1.70043800	-0.62925400	-0.20318800
N	0.61000400	-0.96703200	-0.34878200
H	-0.94323400	-1.69887900	-0.62926100
O	-1.81234600	-2.14724200	-0.79262700
H	-3.04695800	-1.41445600	-0.77594300
H	-1.67832500	-2.78665600	-1.49886900
O	-3.84560300	1.55414100	-1.10372900
O	-3.98480100	-0.94650900	-0.73759900
H	-4.19390200	1.92040500	-1.92195000
H	-4.49615500	-1.20847300	0.07736500
H	-3.99076600	2.21817900	-0.39407600
H	-3.94245700	0.07051400	-0.85710800
O	-5.39410300	-1.62607200	1.37725600
H	-6.20932100	-2.12838500	1.27050000
H	-5.00136700	-1.91275200	2.20877200
O	-4.18420000	3.33524400	0.91774300
H	-3.51629900	3.99711200	1.12490700
H	-5.02475700	3.69820900	1.21532900

Sum of electronic and zero-point Energies= -707.166726
Sum of electronic and thermal Energies= -707.144990
Sum of electronic and thermal Enthalpies= -707.144045
Sum of electronic and thermal Free Energies= -707.225871

BN-H^+W_5(I)

C	5.25132700	1.95514200	0.25979500
C	3.96153700	1.48102300	0.08229700
C	3.75485200	0.10729200	-0.09426200
C	4.83481900	-0.78430700	-0.09280700
C	6.11836100	-0.29391900	0.08599200
C	6.32651100	1.07107800	0.26176100
H	5.41898800	3.01389500	0.39632300
H	3.12023900	2.15894900	0.07867400
H	4.66259500	-1.84199100	-0.23071900
H	6.95676200	-0.97564800	0.08796700
H	7.33047000	1.44736900	0.40046300
C	2.43316200	-0.38970700	-0.27878600
N	1.36630400	-0.79385800	-0.42793700
H	-0.15191400	-1.48177300	-0.71973000
O	-1.03720900	-1.91697400	-0.87938600
H	-1.99461900	-1.75850400	0.06175800
H	-1.27807100	-1.77833000	-1.80072300
O	-2.73924200	-1.66403900	0.85202500
H	-3.74173600	-1.54703000	0.50602900
H	-2.66809200	-2.38948100	1.48347400
O	-5.01632100	-1.30979700	-0.00555800
H	-5.55790000	-0.54737400	0.35201400
H	-5.61208600	-2.03832900	-0.20221900
O	-6.37443400	0.71394100	0.90855500
H	-6.76673100	0.77649700	1.78342200
H	-6.84793600	1.34837500	0.33191600
O	-7.65226900	2.48513700	-0.74695700
H	-7.41006400	3.41330000	-0.82509000
H	-8.55164500	2.41132000	-1.08137200

Sum of electronic and zero-point Energies= -707.161919
Sum of electronic and thermal Energies= -707.140490
Sum of electronic and thermal Enthalpies= -707.139546
Sum of electronic and thermal Free Energies= -707.222255

BN-H^+W_6(c1)

C	-5.98656200	0.11264400	0.74811700
C	-4.64581500	0.32911000	1.02214800
C	-3.68381100	-0.05826400	0.08069100
C	-4.06373400	-0.65833100	-1.12642500
C	-5.40874600	-0.86750600	-1.38453500
C	-6.36715200	-0.48349900	-0.45080400
H	-6.73512600	0.40847200	1.46905300
H	-4.33960400	0.79080100	1.94974600
H	-3.31175400	-0.95281900	-1.84417700
H	-5.71058400	-1.32993500	-2.31335200
H	-7.41505100	-0.64960100	-0.65834700
C	-2.30480800	0.16080200	0.35586400
N	-1.19115100	0.33942800	0.58115600
O	2.78953300	-1.29886900	1.20936200
H	1.88308900	-0.04982400	1.28573400
O	1.30905300	0.78898900	1.31187200
H	1.75711800	1.53044400	0.75043400
H	0.36144800	0.60299700	1.00888200
O	2.56809500	2.49629800	-0.04348800
H	2.21958800	3.35042000	-0.31397400
H	3.00717800	2.07356100	-0.82022200
O	3.71786500	1.00756200	-1.94431500
H	4.16817100	1.27349000	-2.75073100
H	4.19301600	0.23461200	-1.58770800
H	3.54604400	-1.31765100	0.58541300
H	3.07762600	-1.71193900	2.02882100
O	4.82450900	-1.25186800	-0.66531100

H	5.73293400	-1.13837600	-0.30619300
H	4.84982000	-2.03557400	-1.22498500
O	7.30241600	-0.87048500	0.40025600
H	7.85812900	-1.52546600	0.83472000
H	7.86801200	-0.11236600	0.22145800

Sum of electronic and zero-point Energies= -783.630626
Sum of electronic and thermal Energies= -783.606736
Sum of electronic and thermal Enthalpies= -783.605792
Sum of electronic and thermal Free Energies= -783.692323

BN-H^{+}W$_6$(c2)

C	5.54494800	-0.43052300	1.45668300
C	4.18054800	-0.41927200	1.21608200
C	3.71149300	-0.03999900	-0.04782200
C	4.60448300	0.32527000	-1.06304800
C	5.96580000	0.30853300	-0.80573900
C	6.43489000	-0.06795400	0.44957400
H	5.91515700	-0.72208400	2.42910400
H	3.48125900	-0.69913700	1.99069300
H	4.22984900	0.61556800	-2.03399500
H	6.66144300	0.58872600	-1.58369500
H	7.49834400	-0.07904900	0.64375800
C	2.31158600	-0.02591900	-0.30502200
N	1.18091000	-0.01390300	-0.51509700
H	-0.41538300	0.00063800	-0.88414700
O	-1.39217000	0.01531400	-1.14507500
H	-1.78394700	-0.91620600	-1.14448400
H	-1.97765500	0.56704600	-0.47064700
O	-2.90160300	1.12435600	0.49474900
O	-2.63015300	-2.22514500	-0.86707900
H	-3.33258800	1.98821600	0.32842800
H	-3.39777200	-2.01475600	-0.29787300
H	-3.59044100	0.46926100	0.71046800
O	-4.50616300	-1.16847600	0.89151600
H	-2.92316600	-2.83130200	-1.55359100
H	-4.45462900	-1.52422800	1.78518900
H	-5.46149500	-1.14179500	0.66355100
O	-7.14093100	-1.06383500	0.18720000
H	-7.70098300	-1.81995200	-0.01608300
H	-7.73585300	-0.33632700	0.39556400
O	-4.12798600	3.54542400	0.09485200
H	-4.19860100	3.98715300	-0.75763900
H	-4.01035100	4.24363500	0.74752500

Sum of electronic and zero-point Energies= -783.629909
Sum of electronic and thermal Energies= -783.605721
Sum of electronic and thermal Enthalpies= -783.604777
Sum of electronic and thermal Free Energies= -783.691658

BN-H^{+}W$_6$(c3)

C	5.54038200	0.16564900	-0.73187900
C	4.19114200	0.22236100	-1.04214900
C	3.24806700	-0.10167100	-0.05877400
C	3.65591300	-0.47996800	1.22640700
C	5.00897800	-0.53156600	1.52029600
C	5.94847300	-0.20993300	0.54479600
H	6.27413400	0.41375400	-1.48535300
H	3.86388800	0.51192100	-2.03030800
H	2.91861600	-0.72832800	1.97614900
H	5.33179300	-0.82286900	2.50955900
H	7.00273400	-0.25251100	0.78034300

C	1.85999900	-0.04693800	-0.37138300
N	0.73937000	-0.00163600	-0.62700000
O	-2.93040300	-2.31124900	-1.33565100
H	-2.20111000	-0.87509800	-1.44637400
O	-1.79634700	0.04096700	-1.46865700
H	-2.42777300	0.71894300	-0.91607800
H	-0.85222300	0.01947600	-1.12686300
O	-3.35207000	1.47188400	-0.23663800
H	-3.22132800	2.43189100	-0.09508700
H	-3.63975800	1.04807900	0.60014500
O	-3.10032800	4.16664000	0.14254100
H	-2.30847400	4.67012400	0.35554100
H	-3.69401900	4.77520200	-0.30898600
O	-4.05926900	-0.10540500	1.85247400
H	-4.45009700	0.13146600	2.69848700
H	-4.49300500	-0.92082800	1.55706300
H	-3.69362700	-2.42934600	-0.74372600
H	-3.09568400	-2.83285500	-2.12686500
O	-5.04504500	-2.52904500	0.58242700
H	-5.95593100	-2.48987600	0.26722600
H	-4.98374800	-3.33565100	1.10827000

Sum of electronic and zero-point Energies= -783.628847
Sum of electronic and thermal Energies= -783.604475
Sum of electronic and thermal Enthalpies= -783.603530
Sum of electronic and thermal Free Energies= -783.690503

BN-H^{+}W$_6$(s1)

C	-5.59714800	0.89289800	-1.18248200
C	-4.34904300	0.29328200	-1.23914700
C	-3.70728200	-0.06878600	-0.04852500
C	-4.31481100	0.16931200	1.19025500
C	-5.56311600	0.76983200	1.23015100
C	-6.20285600	1.13076000	0.04787600
H	-6.09863700	1.17353700	-2.09765400
H	-3.87134800	0.10248400	-2.18931600
H	-3.81105000	-0.11656900	2.10235200
H	-6.03834800	0.95519300	2.18283300
H	-7.17721200	1.59768400	0.08544800
C	-2.42590300	-0.69039400	-0.09975900
N	-1.39185400	-1.19329100	-0.14362600
H	2.17181000	-2.31514300	0.01348800
O	3.15213300	-2.08418300	0.30152900
H	3.71129000	-1.73472400	-0.46663500
H	3.20429600	-1.37905600	1.02402000
O	3.52104100	-0.10826800	1.91121100
O	4.64484200	-0.91469400	-1.43432200
H	3.67495500	-0.15928800	2.85931400
H	5.09220500	-0.19312000	-0.94898800
H	4.25307000	0.40550900	1.51460400
O	5.48483200	1.08092400	0.32312200
H	5.28755800	-1.32546900	-2.02022500
H	5.27242800	1.99266600	0.01898000
H	6.39914600	1.10866900	0.62477900
O	0.86635400	-2.71059700	-0.44608700
H	0.59579900	-3.62444600	-0.31647200
H	0.06445900	-2.14226200	-0.32680000
O	4.88473400	3.58527800	-0.53225900
H	4.97314800	3.91696800	-1.43137200
H	4.56886700	4.32130100	0.00125000

Sum of electronic and zero-point Energies= -783.628725
Sum of electronic and thermal Energies= -783.604895
Sum of electronic and thermal Enthalpies= -783.603951

Sum of electronic and thermal Free Energies= -783.691104

BN-H$^+$W$_6$(s2)

H	3.85453900	0.70586400	-0.41581400
O	3.17863300	-0.03903900	-0.26582700
H	2.36580100	0.05512300	-0.89837100
H	3.61268800	-0.95477900	-0.36286500
O	4.32604100	-2.30791900	-0.51005100
O	1.20277000	0.09068600	-1.81363300
H	4.48559100	-2.87546400	0.27494700
H	0.28695700	0.09686400	-1.43970200
H	4.11037900	-2.89041100	-1.24424300
H	1.20528500	0.68630300	-2.56858600
O	4.82670600	-3.82568100	1.69317600
H	5.68786000	-4.20918400	1.88753500
H	4.18859400	-4.30016600	2.23515700
O	4.81515500	1.87938700	-0.67953900
H	4.92552800	2.60100900	-0.02333400
H	5.66792300	1.74384500	-1.10242800
O	5.05014000	3.90924300	1.11734100
H	5.47610900	3.89152800	1.97999800
H	4.93553500	4.83703700	0.88844700
C	-6.04528000	-0.83579300	-0.30901300
C	-4.71603800	-0.82619400	-0.70094900
C	-3.82548300	0.06158500	-0.08523600
C	-4.26692700	0.93373900	0.91706800
C	-5.59920700	0.91202300	1.29798900
C	-6.48623000	0.03027600	0.68728400
H	-6.73791600	-1.51807600	-0.78075600
H	-4.36419800	-1.49396600	-1.47405500
H	-3.57074300	1.61510800	1.38446900
H	-5.94661400	1.58298700	2.07061000
H	-7.52451600	0.01845800	0.98832000
C	-2.45747100	0.07821900	-0.48494300
N	-1.35350600	0.09019500	-0.80918200

Sum of electronic and zero-point Energies= -783.627479
Sum of electronic and thermal Energies= -783.602169
Sum of electronic and thermal Enthalpies= -783.601225
Sum of electronic and thermal Free Energies= -783.693713

BN-H$^+$W$_6$(b1)

C	5.05545100	0.36499900	1.25831500
C	3.68271500	0.40619100	1.07441000
C	3.14184200	-0.01867100	-0.14542000
C	3.97263200	-0.48123600	-1.17353600
C	5.34332500	-0.51602300	-0.97352600
C	5.88347900	-0.09452000	0.23809300
H	5.48049300	0.69171300	2.19657000
H	3.03130400	0.76224600	1.85945800
H	3.54341800	-0.80518600	-2.11066900
H	5.99090800	-0.87112200	-1.76233900
H	6.95378300	-0.12369400	0.38763400
C	1.73239500	0.02183200	-0.34463000
N	0.59422100	0.05371400	-0.50777600
H	-1.03564300	0.17480000	-0.85779900
O	-2.00525200	0.24481200	-1.10609900
H	-2.62237700	-0.40246300	-0.53854000
H	-2.31844200	1.20830100	-1.08487500
O	-2.73342700	2.70114000	-1.12202500
O	-3.50464100	-1.24461300	0.17243000
H	-2.94824400	3.12123400	-1.95953500
H	-3.93002900	-1.97261500	-0.32381200

H	-3.26299100	3.14366900	-0.42593000
H	-3.21930400	-1.59315500	1.04118200
O	-4.72562700	-3.30294300	-1.18235100
H	-5.68304400	-3.37761200	-1.24759300
H	-4.36728200	-3.77507000	-1.94054800
O	-2.67177000	-2.12478000	2.64282100
H	-3.20803100	-1.95072200	3.42321600
H	-2.25468200	-2.97936000	2.79239100
O	-4.14230800	3.92655900	0.87573800
H	-3.81542500	4.72698600	1.29911700
H	-5.10080200	3.94921100	0.96016000

Sum of electronic and zero-point Energies= -783.627830
Sum of electronic and thermal Energies= -783.602082
Sum of electronic and thermal Enthalpies= -783.601138
Sum of electronic and thermal Free Energies= -783.694012

BN-H^{+}W$_6$(b2)

C	5.62737200	-0.42164000	-1.12443000
C	4.26697300	-0.15907600	-1.12585400
C	3.52189800	-0.40056800	0.03520400
C	4.13710600	-0.90151200	1.18939900
C	5.49846900	-1.15866500	1.17385500
C	6.24143700	-0.91980500	0.02120300
H	6.20943400	-0.23791800	-2.01611800
H	3.78079400	0.22822600	-2.00960600
H	3.55134800	-1.08287200	2.07899200
H	5.98078400	-1.54508900	2.06025300
H	7.30334400	-1.12248700	0.01575800
C	2.12377400	-0.13321300	0.04317500
N	0.99387200	0.08222300	0.05064100
H	-0.61335800	0.45219100	0.12254000
O	-1.59554400	0.67037600	0.18186400
H	-1.79866300	1.58297000	-0.22885100
H	-2.18081700	-0.07587900	-0.23396300
O	-2.05413800	2.96486800	-0.81672400
H	-2.55363400	3.06990000	-1.63161400
H	-2.27844200	3.72519900	-0.23785600
O	-3.08199100	-1.07851500	-0.83340700
H	-3.76499700	-1.52129000	-0.26375400
H	-2.73822000	-1.73921000	-1.44097800
O	-4.92098100	-2.19548700	0.69861600
H	-4.74617200	-2.75276000	1.46138500
H	-5.83095100	-2.39402500	0.40203000
O	-7.49060300	-2.71065500	-0.16339500
H	-8.27577400	-2.27171800	0.17826300
H	-7.80003100	-3.49181600	-0.63225600
O	-2.64768600	5.11278400	0.74226600
H	-3.29775600	5.17626200	1.44877100
H	-2.07862300	5.88464900	0.82344400

Sum of electronic and zero-point Energies= -783.627761
Sum of electronic and thermal Energies= -783.602071
Sum of electronic and thermal Enthalpies= -783.601127
Sum of electronic and thermal Free Energies= -783.694766

BN-H^{+}W$_6$(I)

C	7.00740000	0.88584600	0.83073900
C	5.64452500	1.05280500	0.64397200
C	4.93139100	0.09891600	-0.09243500
C	5.58211200	-1.01451700	-0.63805900
C	6.94543500	-1.16695200	-0.44231500

C	7.65632500	-0.22030100	0.28969300
H	7.56423600	1.61837500	1.39737600
H	5.13200200	1.90879500	1.05872100
H	5.02154400	-1.74298600	-1.20594100
H	7.45428700	-2.02335600	-0.86110200
H	8.71991100	-0.34459600	0.43838100
C	3.53029100	0.26342000	-0.29148200
N	2.39840200	0.39462000	-0.45294600
H	0.73436500	0.62609700	-0.90324100
O	-0.21871200	0.74824000	-1.14722800
H	-1.23032000	0.69121900	-0.13166500
H	-0.26674500	1.45947300	-1.79330200
O	-2.00709300	0.61674600	0.57103000
H	-2.70094500	-0.26328700	0.42371300
H	-1.66719700	0.68992600	1.46934400
O	-3.53756100	-1.20328700	0.17769700
H	-4.47068000	-1.14756400	0.57967100
H	-3.22518500	-2.11223200	0.19744600
O	-5.87378000	-0.95662300	1.15783200
H	-6.17963100	-1.36540600	1.97154400
H	-6.65713300	-0.86803800	0.55804000
O	-7.94544200	-0.68764600	-0.48334400
H	-8.62235900	0.01214600	-0.40476300
H	-8.32863400	-1.38868800	-1.01673000
O	-9.82748500	1.32592100	-0.25072300
H	-10.62984200	1.30931400	0.27998900
H	-9.94076600	2.03636400	-0.88965800

Sum of electronic and zero-point Energies= -783.620511
Sum of electronic and thermal Energies= -783.595759
Sum of electronic and thermal Enthalpies= -783.594815
Sum of electronic and thermal Free Energies= -783.687658

H^+W

H	0.00000000	0.94274400	-0.19571600
H	-0.81644000	-0.47137200	-0.19571600
H	0.81644000	-0.47137200	-0.19571600
O	0.00000000	0.00000000	0.07339400

Sum of electronic and zero-point Energies= -76.704368
Sum of electronic and thermal Energies= -76.701458
Sum of electronic and thermal Enthalpies= -76.700513
Sum of electronic and thermal Free Energies= -76.722470

H^+W_2

O	0.00000000	-1.20118500	-0.03708300
H	-0.76568700	-1.62417300	-0.45374100
H	0.27629200	-1.71024000	0.73896100
H	0.00000000	0.00000000	0.02289600
O	0.00000000	1.20118500	-0.03708300
H	-0.27629200	1.71024000	0.73896100
H	0.76568700	1.62417300	-0.45374100

Sum of electronic and zero-point Energies= -153.205284
Sum of electronic and thermal Energies= -153.200549
Sum of electronic and thermal Enthalpies= -153.199605
Sum of electronic and thermal Free Energies= -153.229260

H^+W_3

H	-0.56380700	1.66721000	0.00000000
H	-0.02374000	0.34827800	0.88312500

H	-0.02374000	0.34827800	-0.88312500
O	0.02368200	0.89948700	0.00000000
O	0.02368200	-0.44881700	-2.10045500
O	0.02368200	-0.44881700	2.10045500
H	0.76050800	-0.39116200	-2.72044700
H	-0.73904600	-0.79813400	-2.57572900
H	0.76050800	-0.39116200	2.72044700
H	-0.73904600	-0.79813400	2.57572900

Sum of electronic and zero-point Energies= -229.684369
Sum of electronic and thermal Energies= -229.676391
Sum of electronic and thermal Enthalpies= -229.675447
Sum of electronic and thermal Free Energies= -229.715261

H^+W_4

O	0.00000000	0.00000000	0.46027200
H	-0.83003100	-0.51886500	0.19635900
H	0.86436500	-0.45939500	0.19635900
H	-0.03433500	0.97826000	0.19635900
O	0.00000000	2.49306700	-0.13522800
O	2.15905900	-1.24653300	-0.13522800
O	-2.15905900	-1.24653300	-0.13522800
H	-0.41464500	2.90489500	-0.90145200
H	0.03810300	3.16038800	0.55952800
H	2.72303500	-1.09335400	-0.90145200
H	2.71792500	-1.61319200	0.55952800
H	-2.30839000	-1.81154100	-0.90145200
H	-2.75602700	-1.54719600	0.55952800

Sum of electronic and zero-point Energies= -306.157373
Sum of electronic and thermal Energies= -306.146123
Sum of electronic and thermal Enthalpies= -306.145179
Sum of electronic and thermal Free Energies= -306.192700

H^+W_5(B)

H	-1.38223800	-0.78040600	-0.22627500
H	-1.21653500	0.87814800	-0.19752500
H	0.13635200	-0.09852900	0.19942500
O	-0.75678900	-0.00349600	-0.34348900
O	1.38295900	-0.14004700	0.90744700
O	-2.00940300	2.24875400	-0.03802000
H	2.23689300	-0.12780100	0.41075300
H	1.50129500	-0.68351300	1.69222800
H	-2.18823500	2.81869800	-0.79429100
H	-1.97087800	2.81804600	0.73822900
O	-2.29673500	-2.07885200	-0.08474700
H	-3.04492000	-2.16756500	0.51565700
H	-2.47139700	-2.65673500	-0.83594800
O	3.67370800	-0.01746300	-0.47003200
H	4.10313700	-0.72338700	-0.96407300
H	4.34660400	0.65187700	-0.30744400

Sum of electronic and zero-point Energies= -382.621859
Sum of electronic and thermal Energies= -382.607446
Sum of electronic and thermal Enthalpies= -382.606502
Sum of electronic and thermal Free Energies= -382.664360

H^+W_5(R)

H	-1.87278400	-0.02478100	-0.22467300
O	-0.99426900	-0.02075800	-0.72057900

H	-0.42977400	0.80267100	-0.50594300
H	-0.41453600	-0.83165000	-0.50236400
O	0.68329300	-1.82310200	-0.07515000
O	0.64500600	1.81684100	-0.08324600
H	0.82559700	-2.68108500	-0.48813300
H	1.52293300	1.41628800	0.04387200
H	1.54969700	-1.39820700	0.05400700
O	2.81607800	0.02011600	0.37427400
H	0.76136700	2.68247700	-0.48821500
H	3.15219800	0.02748200	1.27954000
H	3.59835200	0.02528300	-0.19131300
O	-3.28631200	0.02538100	0.46218000
H	-4.11532600	-0.02679200	-0.02585500
H	-3.48809000	-0.13952500	1.38924200

Sum of electronic and zero-point Energies= -382.621397
Sum of electronic and thermal Energies= -382.608166
Sum of electronic and thermal Enthalpies= -382.607222
Sum of electronic and thermal Free Energies= -382.660468

H^+W_5(C)

H	0.40735400	-0.71961800	0.90724200
H	1.76152000	-1.10851000	0.00000000
H	0.40735400	-0.71961800	-0.90724200
O	0.94533300	-0.59304700	0.00000000
O	-0.20926700	-0.85270600	-2.15564200
O	-0.20926700	1.13776600	3.91760100
H	-0.24764500	-0.11228300	-2.81125100
H	-0.91217500	-1.47969400	-2.34775600
H	-0.84750500	1.85287000	4.00726100
H	0.28615100	1.10468700	4.74273100
O	-0.20926700	-0.85270600	2.15564200
H	-0.91217500	-1.47969400	2.34775600
H	-0.24764500	-0.11228300	2.81125100
O	-0.20926700	1.13776600	-3.91760100
H	-0.84750500	1.85287000	-4.00726100
H	0.28615100	1.10468700	-4.74273100

Sum of electronic and zero-point Energies= -382.618099
Sum of electronic and thermal Energies= -382.603603
Sum of electronic and thermal Enthalpies= -382.602659
Sum of electronic and thermal Free Energies= -382.662977

H^+W_6(E)

H	0.11332300	1.32628100	-0.31856300
O	-0.12452400	0.39287100	-0.58536800
H	0.70309200	-0.21608600	-0.67012500
H	-0.86120000	-0.00796600	0.01757600
O	-1.95977400	-0.50787300	0.87778000
O	1.83540100	-1.16977700	-0.80661000
H	-2.86703600	-0.61278900	0.50890400
H	2.02395100	-1.56194600	-1.66447000
H	-1.81747900	-1.21844200	1.51003500
H	2.69068600	-1.05705800	-0.33244000
O	-4.44693200	-0.70280000	-0.14509900
H	-5.21993200	-0.29941400	0.26307100
H	-4.77752200	-1.35559300	-0.77045000
O	4.12754300	-0.85172100	0.59011200
H	4.47229200	-1.55309600	1.15294200
H	4.88811700	-0.32963100	0.31427300
O	0.54015800	2.85000600	0.02775100
H	0.36956900	3.56869900	-0.59090500
H	0.50717000	3.23139200	0.91162400

Sum of electronic and zero-point Energies= -459.084278
Sum of electronic and thermal Energies= -459.066758
Sum of electronic and thermal Enthalpies= -459.065813
Sum of electronic and thermal Free Energies= -459.132740

H^+W_6(E/4r)

H	2.54859000	-0.01266400	0.09173600
O	1.88291300	-0.04899400	-0.65994500
H	1.26775000	0.77297200	-0.67593700
H	1.26174800	-0.86293700	-0.59713900
O	0.09492600	-1.83410600	-0.49098800
O	0.11209700	1.75799600	-0.66459500
H	0.07011600	-2.67205500	-0.96360700
H	-0.74209400	1.29079500	-0.77546700
H	-0.75389000	-1.36806100	-0.64268700
O	-1.99609300	-0.03870800	-0.79970800
H	0.09824000	2.55287100	-1.20685900
H	-2.60660800	0.00437500	-0.02568400
H	-2.55883500	-0.07466700	-1.58100700
O	3.67357300	0.10034900	1.21193800
H	4.61616800	0.04334400	1.02183900
H	3.56422000	-0.04417200	2.15755700
O	-3.60381100	0.08272100	1.36641100
H	-4.01995000	0.87812900	1.71438600
H	-4.05429800	-0.66199600	1.77796200

Sum of electronic and zero-point Energies= -459.084747
Sum of electronic and thermal Energies= -459.068476
Sum of electronic and thermal Enthalpies= -459.067532
Sum of electronic and thermal Free Energies= -459.129406

H^+W_6(Z)

O	-0.16060400	1.18924700	0.35961400
H	-0.97128700	1.49193100	0.83795100
H	-0.08657600	1.65509100	-0.50936500
H	0.00000000	0.00000000	0.32745000
O	0.16060400	-1.18924700	0.35961400
H	0.08657600	-1.65509100	-0.50936500
H	0.97128700	-1.49193100	0.83795100
O	2.31708400	-2.08815800	1.65323700
O	-0.16060400	-2.40338600	-1.99993500
O	-2.31708400	2.08815800	1.65323700
O	0.16060400	2.40338600	-1.99993500
H	3.16830900	-1.64889400	1.74942600
H	2.24441600	-2.70844400	2.38628200
H	-0.79412700	-3.12311400	-2.09264300
H	0.53932100	-2.57516500	-2.63870700
H	0.79412700	3.12311400	-2.09264300
H	-0.53932100	2.57516500	-2.63870700
H	-3.16830900	1.64889400	1.74942600
H	-2.24441600	2.70844400	2.38628200

Sum of electronic and zero-point Energies= -459.085686
Sum of electronic and thermal Energies= -459.067684
Sum of electronic and thermal Enthalpies= -459.066740
Sum of electronic and thermal Free Energies= -459.133814

H^+W_7(E/c)

H	-0.17812100	0.71107600	-0.10202300
O	0.16503500	-0.10128800	0.41457200

H	-0.58399200	-0.75198100	0.65621400
H	0.93580400	-0.56734000	-0.06764300
O	2.11093000	-1.18887600	-0.80522500
O	-1.62999900	-1.78393100	1.04587200
H	3.01431700	-1.15465400	-0.41953200
H	-1.83673800	-1.92757800	1.97399300
H	2.02554600	-2.03059900	-1.26219400
H	-2.45487300	-1.92759900	0.53194100
O	4.60482800	-1.01428600	0.24901200
H	5.36801700	-0.69853500	-0.24540800
H	4.95144900	-1.48672700	1.01253200
O	-3.84833000	-2.20502000	-0.46485800
H	-4.09726400	-3.08514200	-0.76578900
H	-4.66053600	-1.68890400	-0.43995000
O	-0.74428800	1.92802700	-0.81299900
H	-0.68854600	2.81509500	-0.39410600
H	-0.63310500	2.04981500	-1.76031800
O	-0.64313200	4.35601800	0.39491200
H	0.12976900	4.90238500	0.56856500
H	-1.41207600	4.91554100	0.54342100

Sum of electronic and zero-point Energies= -535.545670
Sum of electronic and thermal Energies= -535.524673
Sum of electronic and thermal Enthalpies= -535.523729
Sum of electronic and thermal Free Energies= -535.600964

H^+W_7(E/4r)

H	-1.69893400	-0.01829600	0.05677500
O	-0.98513300	-0.07885900	0.79847000
H	-0.37155000	-0.88011100	0.68680900
H	-0.37563600	0.73472400	0.81248000
O	0.81413800	1.73844000	0.77544100
O	0.82792300	-1.86132400	0.49125300
H	0.86590500	2.51779600	1.33695500
H	1.67779400	-1.38951800	0.60857400
H	1.66979500	1.26626200	0.82603900
O	2.93699000	-0.06207400	0.73654600
H	0.89257700	-2.70956600	0.94048800
H	3.49945100	0.00866600	-0.06948400
H	3.54513800	-0.12002100	1.48134200
O	-2.76935600	0.13829600	-0.96129000
O	4.42560300	0.13817500	-1.51655100
O	-5.38080600	0.01963000	-0.28949500
H	-2.66561300	-0.11226200	-1.88336300
H	-3.72351900	0.06983200	-0.73200300
H	4.84729000	-0.58730400	-1.98819200
H	4.78864200	0.95009400	-1.88479900
H	-5.98343600	0.76758200	-0.35168400
H	-5.92277300	-0.75615600	-0.11492000

Sum of electronic and zero-point Energies= -535.547047
Sum of electronic and thermal Energies= -535.527388
Sum of electronic and thermal Enthalpies= -535.526444
Sum of electronic and thermal Free Energies= -535.598396

H^+W_7(E/5r)

O	0.02459200	-1.41691400	1.06480100
H	-1.32030400	-0.71580700	0.82995600
O	-2.19453500	-0.21855000	0.66268600
H	-2.00464300	0.77422800	0.37432600
H	-2.77358100	-0.69733700	0.00260100
O	-1.67488600	2.10119500	-0.06157200
H	-1.99105000	2.84763500	0.45723400

H	-0.70271900	2.22502300	-0.21626600
O	4.11414400	-1.17490900	-0.92799800
H	4.21764600	-2.12694100	-1.02644100
H	4.90196100	-0.77635000	-1.31186000
O	0.94793500	2.24311400	-0.40434700
H	1.39083400	2.66070000	-1.14833100
H	1.51467300	1.51283400	-0.09395900
H	0.87138100	-0.92617300	0.98334300
H	0.11110500	-2.02917600	1.80178000
O	2.32921700	0.05334500	0.70730400
H	2.80223800	0.32433700	1.50188600
H	2.99271900	-0.39481400	0.13376200
O	-3.74709200	-1.52047900	-0.99372200
H	-4.62090000	-1.81745400	-0.71740000
H	-3.78436400	-1.39512300	-1.94783700

Sum of electronic and zero-point Energies= -535.547174
Sum of electronic and thermal Energies= -535.527932
Sum of electronic and thermal Enthalpies= -535.526988
Sum of electronic and thermal Free Energies= -535.597201

$H^{+}W_{7}$(Z/5r)

O	-1.51670400	1.78211700	0.97802400
H	0.07785600	1.38577100	0.71611900
O	1.00270700	1.08063600	0.52626500
H	1.01573600	0.00037100	0.00013400
H	1.49139600	1.78218800	0.03188300
O	1.00324000	-1.08012200	-0.52614000
H	1.49227000	-1.78148600	-0.03186000
H	0.07858300	-1.38573000	-0.71606100
O	2.36264200	-3.01272000	0.73446000
H	3.09785900	-3.47693100	0.32120700
H	2.42995100	-3.17654700	1.68042900
O	-1.51591600	-1.78280900	-0.97806900
H	-1.79228000	-2.31612800	-1.72918700
H	-2.26403300	-1.21264400	-0.73531600
H	-2.26455600	1.21160200	0.73525500
H	-1.79331300	2.31528800	1.72915700
O	-3.55046400	-0.00075800	0.00002400
O	2.36102100	3.01373200	-0.73455000
H	2.42847000	3.17716300	-1.68057800
H	3.09606900	3.47827200	-0.32136100
H	-4.13322600	0.43848600	-0.63132900
H	-4.13299100	-0.44028400	0.63139900

Sum of electronic and zero-point Energies= -535.548209
Sum of electronic and thermal Energies= -535.527905
Sum of electronic and thermal Enthalpies= -535.526961
Sum of electronic and thermal Free Energies= -535.600148