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

Supporting Information

Of

Three – Membered Beryllium Ring, Be_3: Not Just Hydrogen Bond Acceptor

Cartesian coordinates, lowest vibrational frequency (υ_1, cm^{-1}) and total energies (a.u.) of all the optimized geometries.

Be_3

υ_1 = 467.1

E_{B97XD}

Sum of electronic and zero-point Energies = -44.032108

Sum of electronic and thermal Energies = -44.028547

Sum of electronic and thermal Enthalpies = -44.027603

Sum of electronic and thermal Free Energies = -44.055862

$E_{CCSD(T)}$ = -43.8762823

4	-1.103048000	0.636365000	0.000000000
4	1.103048000	0.637030000	0.000000000
4	0.000000000	-1.273395000	0.000000000

HF

υ_1 = 4166.6

E_{B97XD}

Sum of electronic and zero-point Energies = -100.455730

Sum of electronic and thermal Energies = -100.453369

Sum of electronic and thermal Enthalpies = -100.452425

Sum of electronic and thermal Free Energies = -100.472124

$E_{CCSD(T)}$ = -100.3445451

1	0.000000000	0.000000000	-0.824410000
9	0.000000000	0.000000000	0.091601000

HCl

υ_1 = 2965.5

E_{B97XD}

Sum of electronic and zero-point Energies = -460.811540

Sum of electronic and thermal Energies = -460.809180

Sum of electronic and thermal Enthalpies = -460.808235

Sum of electronic and thermal Free Energies = -460.829415

1 0.000000000 0.000000000 -1.206316000

17 0.000000000 0.000000000 0.070960000

H_2O

υ_1 = 1639.9

E_{B97XD}

Sum of electronic and zero-point Energies = -76.419736

Sum of electronic and thermal Energies = -76.416901

Sum of electronic and thermal Enthalpies = -76.415957

Sum of electronic and thermal Free Energies = -76.437361

8 0.000000000 0.000000000 0.116401000

1 0.000000000 0.758516000 -0.465605000

1 0.000000000 -0.758516000 -0.465605000

HCN

υ_1 = 764.1

E_{B97XD}

Sum of electronic and zero-point Energies = -93.408486

Sum of electronic and thermal Energies = -93.405947

Sum of electronic and thermal Enthalpies = -93.405003

Sum of electronic and thermal Free Energies = -93.427841

1 0.000000000 0.000000000 -1.562645000

6 0.000000000 0.000000000 -0.495545000

7 0.000000000 0.000000000 0.647988000

Be_3-HF system

A

υ_1 = 18.5

E_{B97XD}

Sum of electronic and zero-point Energies = -144.495315

Sum of electronic and thermal Energies = -144.489057

Sum of electronic and thermal Enthalpies = -144.488113

Sum of electronic and thermal Free Energies = -144.525740

$E_{CCSD(T)}$ = -144.2252443

4	-1.052942000	1.092403000	0.029818000
4	-1.059897000	-1.095837000	0.029553000
4	-2.922416000	0.003930000	-0.038269000
1	1.171192000	-0.005506000	0.019821000
9	2.107759000	0.000392000	-0.011581000

B

υ_1 = 18.5

E_{B97XD}

Sum of electronic and zero-point Energies = -144.604145

Sum of electronic and thermal Energies = -144.599667

Sum of electronic and thermal Enthalpies = -144.598723

Sum of electronic and thermal Free Energies = -144.629870

$E_{CCSD(T)}$ = -144.3145318

4	1.820920000	-0.007519000	-0.436208000
4	0.159453000	-0.984599000	0.317818000
4	0.168747000	0.990951000	0.306664000
1	0.348974000	0.013787000	1.503418000
9	-0.993939000	-0.001013000	-0.250724000

$TS_{B\text{-}C/D}$

υ_1 = − 410.7

E_{B97XD}

Sum of electronic and zero-point Energies = -144.601072

Sum of electronic and thermal Energies = -144.596393

Sum of electronic and thermal Enthalpies = -144.595448

Sum of electronic and thermal Free Energies = -144.627425

$E_{CCSD(T)}$ = -144.307532

4	1.796813000	0.227874000	-0.238119000
4	0.342500000	-1.020450000	-0.065900000
4	-0.010326000	1.053539000	0.177429000

1	0.860080000	-0.674982000	1.228561000
9	-1.041781000	-0.040986000	-0.080244000

C

υ_1 = 163.0

E_{B97XD}

Sum of electronic and zero-point Energies = -144.644265

Sum of electronic and thermal Energies = -144.639157

Sum of electronic and thermal Enthalpies = -144.638213

Sum of electronic and thermal Free Energies = -144.671261

$E_{CCSD(T)}$ = -144.3678414

4	-0.276229000	0.000129000	0.000041000
4	1.661643000	-1.057222000	-0.000006000
4	1.663511000	1.057277000	-0.000006000
9	-1.665602000	0.000151000	-0.000011000
1	2.794724000	-0.002094000	-0.000016000

D

υ_1 = 247.2

E_{B97XD}

Sum of electronic and zero-point Energies = -144.638988

Sum of electronic and thermal Energies = -144.634018

Sum of electronic and thermal Enthalpies = -144.633074

Sum of electronic and thermal Free Energies = -144.665163

$E_{CCSD(T)}$ = -144.3534475

4	0.365746000	-2.456300000	-0.257642000
4	1.498168000	-0.976392000	0.882416000
4	-0.065559000	-0.328328000	-0.495082000
1	0.116824000	-3.738807000	-0.579303000
9	0.925993000	0.430627000	0.465702000

TS_{C-E}

υ_1 = −703.7

E_{B97XD}

Sum of electronic and zero-point Energies = -144.638449

Sum of electronic and thermal Energies = -144.633025

Sum of electronic and thermal Enthalpies = -144.632081

Sum of electronic and thermal Free Energies = -144.665551

$E_{CCSD(T)}$ = -144.3456269

4	0.681550000	-0.078400000	0.000020000
4	-3.313231000	-0.026866000	-0.000386000
4	-1.379635000	-0.311428000	0.000439000
9	2.057013000	0.055310000	-0.000085000
1	-2.467851000	1.168990000	0.000475000

TS_{D-E}

$\upsilon_1 = -700.2$

E_{B97XD}

Sum of electronic and zero-point Energies = -144.578889

Sum of electronic and thermal Energies = -144.573548

Sum of electronic and thermal Enthalpies = -144.572604

Sum of electronic and thermal Free Energies = -144.605958

$E_{CCSD(T)}$ = -144.2916339

4	-1.425696000	2.136874000	0.440653000
4	-1.962873000	-1.623186000	-0.601680000
4	-1.693987000	0.247916000	0.219284000
1	-1.073047000	1.517644000	-0.846121000
9	-0.734253000	-1.140115000	0.085243000

E

$\upsilon_1 = 111.6$

E_{B97XD}

Sum of electronic and zero-point Energies = -144.696958

Sum of electronic and thermal Energies = -144.691642

Sum of electronic and thermal Enthalpies = -144.690698

Sum of electronic and thermal Free Energies= -144.718737

$E_{CCSD(T)}$ = -144.4057569

4	-0.017796000	-3.402810000	-0.000006000
4	-0.001965000	-1.275593000	0.000008000
4	0.009700000	0.836536000	0.000014000
1	-0.027910000	-4.751624000	-0.000015000
9	0.017346000	2.218183000	-0.000001000

Be_3-HCl system

A

υ_1 = 41.2

$E_{\square B97XD}$

Sum of electronic and zero-point Energies = -504.848353

Sum of electronic and thermal Energies = -504.841773

Sum of electronic and thermal Enthalpies = -504.840829

Sum of electronic and thermal Free Energies= -504.879658

$E_{CCSD(T)}$ = -504.2105202

4	-1.195560000	1.095548000	0.073373000
4	-1.201157000	-1.098058000	0.072526000
4	-3.069165000	0.003437000	-0.098024000
1	1.204350000	-0.005072000	0.040360000
17	2.505229000	-0.000472000	-0.058893000

E

υ_1 = 99.7

$E_{\square B97XD}$

Sum of electronic and zero-point Energies = -505.037302

Sum of electronic and thermal Energies = -505.031807

Sum of electronic and thermal Enthalpies = -505.030862

Sum of electronic and thermal Free Energies= -505.062776

$E_{CCSD(T)}$ = -504.3781902

4	4.239383000	-0.114239000	0.000000000

4	2.111665000	-0.088922000	0.000000000
4	0.000000000	-0.022316000	0.000000000
1	5.588796000	-0.117482000	0.000000000
17	-1.823117000	0.059964000	0.000000000

Be_3-H_2O system

A

υ_1 = 25.8

$E_{\omega B97XD}$

Sum of electronic and zero-point Energies = -120.455003

Sum of electronic and thermal Energies = -120.447468

Sum of electronic and thermal Enthalpies = -120.446524

Sum of electronic and thermal Free Energies = -120.486946

$E_{CCSD(T)}$ = -120.2159431

4	-1.022416000	1.056573000	0.223546000
4	-1.092503000	-1.136023000	0.082316000
4	-2.922928000	0.037643000	-0.116551000
1	1.472757000	-0.116060000	0.051335000
8	2.430796000	-0.132574000	-0.053625000
1	2.771654000	-0.159274000	0.839655000

E

υ_1 = 112.9

$E_{\omega B97XD}$

Sum of electronic and zero-point Energies = -120.641680

Sum of electronic and thermal Energies = -120.635340

Sum of electronic and thermal Enthalpies = -120.634395

Sum of electronic and thermal Free Energies = -120.668530

$E_{CCSD(T)}$ = -120.377684

4	-0.014202000	-3.445711000	0.000000000
4	-0.007075000	-1.313779000	0.000000000
4	0.000000000	0.799210000	0.000000000

1	-0.017539000	-4.797002000	0.000000000
8	-0.054600000	2.211265000	0.000000000
1	0.539448000	2.948002000	0.000000000

Be_3-HCN system

A

υ_1 = 43.2

E_{B97XD}

Sum of electronic and zero-point Energies = -137.443157

Sum of electronic and thermal Energies = -137.435567

Sum of electronic and thermal Enthalpies = -137.434622

Sum of electronic and thermal Free Energies = -137.476340

$E_{CCSD(T)}$ = -137.1562105

4	-4.028368000	-0.000409000	0.003613000
4	-2.137912000	-1.099456000	-0.001893000
4	-2.138824000	1.099826000	-0.001891000
1	0.803095000	-0.000025000	-0.005239000
6	1.877549000	-0.000007000	-0.001772000
7	3.021718000	0.000032000	0.002365000

E

υ_1 = 79.2

E_{B97XD}

Sum of electronic and zero-point Energies = -137.598524

Sum of electronic and thermal Energies = -137.592083

Sum of electronic and thermal Enthalpies = -137.591139

Sum of electronic and thermal Free Energies = -137.625303

$E_{CCSD(T)}$ = -137.2875259

4	3.082177000	-2.857608000	0.000000000
4	1.556589000	-1.374683000	0.000000000
4	0.000000000	0.060124000	0.000000000
1	4.037951000	-3.808586000	0.000000000

6	-1.267374000	1.172294000	0.000000000
7	-2.141253000	1.923356000	0.000000000