

Supplementary information

Exploration of Free Energy Surface and Thermal Effects on Relative Population and Infrared Spectrum of the $\text{Be}_6\text{B}_{11}^-$ Fluxional Cluster

The XYZ cartesian atomic coordinates $\text{Be}_6\text{B}_{11}^-$

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0.000000000      Be6B11_0000.out
Be  0.871471000000  -2.240509000000  0.377306000000
Be  -1.189569000000  0.091524000000  -1.070090000000
Be  -1.553783000000  -0.035182000000  1.029073000000
Be  0.353918000000  0.927628000000  1.191148000000
B   -2.388865000000  -1.286223000000  -0.191009000000
Be  0.902109000000  0.576938000000  -1.026034000000
B    2.138354000000  1.405375000000  0.186226000000
B    2.104451000000  -1.290639000000  -0.677320000000
B   -0.695071000000  2.012979000000  -0.103576000000
B   -2.937178000000  0.167009000000  -0.293782000000
B   -0.966176000000  -1.813381000000  0.224983000000
B    0.854208000000  2.267959000000  0.001131000000
B    1.541700000000  -0.519470000000  0.705420000000
B   -2.190898000000  1.507723000000  -0.161535000000
B    2.776437000000  0.070546000000  -0.362169000000
Be  0.251303000000  -1.389407000000  -1.254458000000
B    0.054679000000  -0.866672000000  1.274075000000
17  0.617460000      Be6B11_0001.out
Be  -1.462704000000  -0.014249000000  0.967655000000
B    2.728694000000  0.030013000000  -0.619010000000
B   -2.146695000000  -1.259141000000  -0.336682000000
B    2.196858000000  1.375491000000  0.031415000000
B   -0.880491000000  -1.823626000000  0.448212000000
B    1.934511000000  -1.299414000000  -0.736505000000
B   -0.694414000000  1.931806000000  0.025551000000
Be  0.874964000000  0.501056000000  -0.992441000000
B   -2.883951000000  0.123283000000  -0.317897000000
Be  1.826138000000  -0.480368000000  0.902917000000
Be  0.408897000000  0.951482000000  1.344252000000
B    0.772439000000  -1.870483000000  0.277861000000
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B    -2.220982000000    1.503653000000    -0.070210000000
Be   -0.113249000000    -1.338601000000    -1.218981000000
B     0.106145000000    -0.876434000000    1.446090000000
B     0.872097000000    2.199862000000    0.022620000000
Be   -1.264310000000    0.336919000000    -1.217707000000
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0.855910000    Be6B11_0002.out
Be   -0.597631000000    1.124894000000    1.052561000000
Be   -0.597631000000    1.124894000000    -1.052561000000
B    -2.238140000000    -1.547111000000    0.000000000000
B     1.559153000000    1.828212000000    0.000000000000
Be   -0.597631000000    -1.125067000000    1.051152000000
B     0.289604000000    2.707478000000    0.000000000000
B    -2.209386000000    0.001996000000    0.000000000000
B    -1.233725000000    2.689543000000    0.000000000000
B    -2.233185000000    1.551289000000    0.000000000000
Be    1.279363000000    0.001246000000    -1.086218000000
Be    1.279363000000    0.001246000000    1.086218000000
B    -1.242591000000    -2.688862000000    0.000000000000
Be   -0.597631000000    -1.125067000000    -1.051152000000
B     2.675935000000    0.757041000000    0.000000000000
B     0.280383000000    -2.711048000000    0.000000000000
B     2.670570000000    -0.762843000000    0.000000000000
B     1.546820000000    -1.827411000000    0.000000000000

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1.230527500    Be6B11_0003.out

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B	0.000000000000	1.549129000000	2.235698000000
B	0.000000000000	1.827820000000	−1.553909000000
B	0.000000000000	−0.759893000000	−2.673713000000
B	0.000000000000	−2.707671000000	−0.285066000000
B	0.000000000000	−1.549129000000	2.235698000000
B	0.000000000000	−1.827820000000	−1.553909000000
B	0.000000000000	0.759893000000	−2.673713000000
B	0.000000000000	2.707671000000	−0.285066000000
B	0.000000000000	2.688931000000	1.237960000000
B	0.000000000000	0.000000000000	2.207900000000
B	0.000000000000	−2.688931000000	1.237960000000
Be	1.052108000000	1.124714000000	0.598858000000
Be	1.085258000000	0.000000000000	−1.278866000000
Be	1.052108000000	−1.124714000000	0.598858000000
Be	−1.052108000000	1.124714000000	0.598858000000
Be	−1.085258000000	0.000000000000	−1.278866000000
Be	−1.052108000000	−1.124714000000	0.598858000000

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1.487802500 Be6B11_0004.out

B	−0.809816000000	1.579400000000	0.643022000000
Be	0.596573000000	−0.814845000000	2.010115000000
B	0.051091000000	1.760054000000	−0.791777000000
B	1.580974000000	1.309936000000	−0.966076000000
B	−2.070825000000	0.461623000000	0.890950000000
B	−0.603948000000	0.506270000000	1.857829000000
B	2.628206000000	0.531768000000	−0.066162000000
Be	0.883805000000	0.850245000000	0.737351000000
Be	−0.903703000000	−1.025277000000	0.582096000000
B	−2.628548000000	−0.531967000000	−0.178140000000
B	−1.569501000000	−1.073309000000	−1.210345000000
B	−0.048006000000	−1.595631000000	−1.037654000000
Be	1.608400000000	−0.779034000000	−1.006380000000
Be	0.006693000000	0.158977000000	−1.774212000000
Be	−1.600348000000	0.919041000000	−0.888479000000
B	2.151414000000	−0.709603000000	0.737654000000
B	0.845823000000	−1.685827000000	0.392307000000

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2.377597500 Be6B11_0005.out

B	−1.398792000000	−2.376827000000	−0.608428000000
B	1.860269000000	1.944117000000	0.832486000000

B	0.000000000000	-2.314681000000	-1.284177000000
B	1.398792000000	2.376827000000	-0.608428000000
B	-1.860269000000	-1.944117000000	0.832486000000
B	1.198910000000	1.039826000000	1.873576000000
Be	-0.846279000000	-0.686255000000	-1.602453000000
B	0.000000000000	2.314681000000	-1.284177000000
Be	0.026437000000	-1.647024000000	0.486714000000
Be	1.524481000000	0.000032000000	0.331634000000
B	0.978975000000	-1.100162000000	-1.127179000000
Be	-0.026437000000	1.647024000000	0.486714000000
B	-1.198910000000	-1.039826000000	1.873576000000
B	-0.978975000000	1.100162000000	-1.127179000000
Be	-1.524481000000	-0.000032000000	0.331634000000
Be	0.846279000000	0.686255000000	-1.602453000000
B	0.000000000000	0.000000000000	1.882013000000

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2.383245000 Be6B11_0006.out

Be	0.000000000000	1.524670000000	0.325548000000
Be	0.000000000000	-1.524670000000	0.325548000000
Be	-1.646433000000	0.020113000000	0.488496000000
Be	1.646433000000	-0.020113000000	0.488496000000
B	1.104502000000	-0.972620000000	-1.129209000000
B	-1.104502000000	0.972620000000	-1.129209000000
B	0.000000000000	0.000000000000	1.882165000000
Be	-0.681645000000	-0.847320000000	-1.608316000000
Be	0.681645000000	0.847320000000	-1.608316000000
B	1.033017000000	1.204123000000	1.875487000000
B	-1.033017000000	-1.204123000000	1.875487000000
B	-2.314461000000	-0.012187000000	-1.282308000000
B	2.314461000000	0.012187000000	-1.282308000000
B	-1.936501000000	-1.869964000000	0.837138000000
B	1.936501000000	1.869964000000	0.837138000000
B	2.363598000000	1.412169000000	-0.606771000000
B	-2.363598000000	-1.412169000000	-0.606771000000

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5.164952500 Be6B11_0007.out

Be	-1.140416000000	0.103343000000	1.097260000000
Be	1.140416000000	-0.103343000000	1.097260000000
B	1.806969000000	1.963089000000	-0.386217000000
B	-1.542626000000	-1.932366000000	1.133568000000
Be	0.000000000000	1.577206000000	0.008758000000
B	-0.638597000000	-1.316233000000	2.228919000000

B	1.542626000000	1.932366000000	1.133568000000
B	0.000000000000	0.000000000000	2.724881000000
B	0.638597000000	1.316233000000	2.228919000000
Be	0.000000000000	-1.577206000000	0.008758000000
Be	-1.148876000000	0.082815000000	-1.070831000000
B	1.176139000000	1.697602000000	-1.775334000000
Be	1.148876000000	-0.082815000000	-1.070831000000
B	-1.806969000000	-1.963089000000	-0.386217000000
B	0.326002000000	0.702995000000	-2.591527000000
B	-1.176139000000	-1.697602000000	-1.775334000000
B	-0.326002000000	-0.702995000000	-2.591527000000

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5.631185000 Be6B11_0008.out

B	1.528679000000	1.701700000000	0.509569000000
B	-0.117021000000	-0.964914000000	-1.615283000000
B	-1.648819000000	-0.707237000000	-1.161047000000
Be	-0.302031000000	-1.449462000000	0.175321000000
B	2.641512000000	-0.596366000000	-0.644848000000
Be	-1.789419000000	1.565781000000	0.309923000000
Be	1.619805000000	-0.697074000000	0.999108000000
B	-1.341198000000	-0.925353000000	1.696499000000
B	1.342610000000	-1.332495000000	-1.175056000000
Be	-0.127111000000	0.623224000000	1.414746000000
Be	-0.940410000000	0.987997000000	-1.391875000000
Be	1.010995000000	0.511028000000	-0.864484000000
B	-2.628326000000	0.474501000000	-0.801661000000
B	0.139389000000	-1.127775000000	1.950483000000
B	2.710593000000	0.706957000000	0.147077000000
B	0.040832000000	1.912171000000	0.081513000000
B	-2.245715000000	-0.374385000000	0.498565000000

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10.209425000 Be6B11_0009.out

Be	1.784070000000	-0.881154000000	0.000000000000
Be	-1.178349000000	1.635847000000	0.000000000000
Be	1.064755000000	1.033056000000	0.000000000000
Be	-0.937588000000	-0.323485000000	1.174575000000
B	-2.310757000000	0.242038000000	0.000000000000
B	0.892147000000	-0.081631000000	-1.612675000000
B	0.352235000000	1.385244000000	1.718054000000
Be	-0.937588000000	-0.323485000000	-1.174575000000
Be	-0.817189000000	-2.391480000000	0.000000000000
B	0.892147000000	-0.081631000000	1.612675000000

B	0.621579000000	-1.643571000000	1.185587000000
B	-2.180768000000	-1.259499000000	0.000000000000
B	0.352235000000	1.385244000000	-1.718054000000
B	0.285545000000	2.649292000000	0.765420000000
B	1.006026000000	-2.600648000000	0.000000000000
B	0.621579000000	-1.643571000000	-1.185587000000
B	0.285545000000	2.649292000000	-0.765420000000

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11.904302500 Be6B11_0010.out

Be	-0.967864000000	-0.003324000000	-2.025249000000
Be	-0.977869000000	-0.908311000000	1.005310000000
Be	0.977869000000	0.908311000000	1.005310000000
Be	0.967864000000	0.003324000000	-2.025249000000
Be	-1.631200000000	0.684878000000	-0.239010000000
B	0.932498000000	-0.979840000000	1.526020000000
B	-0.932498000000	0.979840000000	1.526020000000
Be	1.631200000000	-0.684878000000	-0.239010000000
B	1.725675000000	1.166405000000	-0.793865000000
B	0.000000000000	-1.306175000000	-1.105711000000
B	0.000000000000	1.306175000000	-1.105711000000
B	0.440133000000	-2.107280000000	0.385744000000
B	-1.725675000000	-1.166405000000	-0.793865000000
B	-0.440133000000	2.107280000000	0.385744000000
B	0.995287000000	2.407450000000	-0.164110000000
B	-0.995287000000	-2.407450000000	-0.164110000000
B	0.000000000000	0.000000000000	2.318162000000

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14.065412500 Be6B11_0011.out

Be	2.136962000000	0.466122000000	-0.136821000000
Be	-2.136962000000	-0.466122000000	-0.136821000000
Be	0.448793000000	1.453418000000	0.501781000000
Be	-0.448793000000	-1.453418000000	0.501781000000
B	-1.013219000000	-1.183852000000	-1.416467000000
B	1.013219000000	1.183852000000	-1.416467000000
B	-1.516619000000	-0.303767000000	1.526878000000
Be	0.858236000000	-0.661623000000	-1.331966000000
Be	-0.858236000000	0.661623000000	-1.331966000000
B	1.516619000000	0.303767000000	1.526878000000
B	0.000000000000	0.000000000000	1.865341000000
B	0.000000000000	2.333754000000	-1.105419000000
B	0.000000000000	-2.333754000000	-1.105419000000
B	1.546339000000	-1.193439000000	0.921284000000

B	-1.546339000000	1.193439000000	0.921284000000
B	-1.178288000000	2.314234000000	-0.085342000000
B	1.178288000000	-2.314234000000	-0.085342000000

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25.153337500 Be6B11_0012.out

Be	-1.277429000000	1.666744000000	0.000000000000
B	-1.541731000000	-2.135511000000	0.000000000000
Be	-0.626280000000	-1.277275000000	1.405826000000
B	-0.006859000000	-2.441749000000	0.000000000000
Be	-0.626280000000	-1.277275000000	-1.405826000000
B	1.212038000000	-1.565687000000	0.808025000000
B	0.037720000000	1.982302000000	1.348142000000
B	-0.811599000000	0.576246000000	1.455720000000
B	1.777627000000	-0.269016000000	0.000000000000
Be	0.926136000000	0.082001000000	-1.658674000000
Be	0.926136000000	0.082001000000	1.658674000000
B	0.037720000000	1.982302000000	-1.348142000000
B	1.212038000000	-1.565687000000	-0.808025000000
Be	-1.878824000000	-0.366759000000	0.000000000000
B	-0.811599000000	0.576246000000	-1.455720000000
B	0.324901000000	2.740038000000	0.000000000000
B	0.614978000000	0.992966000000	0.000000000000

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42.350602500 Be6B11_0013.out

Be	-0.000618000000	1.265154000000	-1.244622000000
Be	0.000618000000	-1.265154000000	-1.244622000000
B	-0.768950000000	-0.000057000000	-2.360234000000
Be	1.577107000000	0.000458000000	1.121963000000
B	0.001596000000	1.217530000000	1.359563000000
B	-1.321661000000	1.600756000000	0.207885000000
B	1.321661000000	-1.600756000000	0.207885000000
Be	-1.852297000000	-0.000057000000	-0.867758000000
B	1.322470000000	1.601879000000	0.207441000000
B	-1.322470000000	-1.601879000000	0.207441000000
B	0.768950000000	0.000057000000	-2.360234000000
B	0.000000000000	0.000000000000	2.355612000000
Be	-1.577107000000	-0.000458000000	1.121963000000
Be	1.852297000000	0.000057000000	-0.867758000000
B	0.000000000000	2.439167000000	0.199873000000
B	-0.001596000000	-1.217530000000	1.359563000000
B	0.000000000000	-2.439167000000	0.199873000000