Molecular geometries obtained at the level of B3LYP/6-311g(d,p)

BN-Ph neutral

S 2.100000 -3.248000 1.322000

N 3.482000 -1.339000 0.262000

N 2.552000 0.972000 -0.058000

C 3.839000 -3.352000 1.408000

C 4.424000 -2.246000 0.769000

C 5.822000 -2.190000 0.660000

H 6.302000 -1.368000 0.154000

C 6.577000 -3.211000 1.218000

H 7.657000 -3.166000 1.136000

C 5.978000 -4.292000 1.878000

H 6.595000 -5.073000 2.307000

C 4.598000 -4.377000 1.972000

H 4.119000 -5.217000 2.461000

C 2.223000 -1.760000 0.415000

C 1.068000 -0.975000 0.058000

C 1.305000 0.414000 -0.038000

C -0.281000 -1.408000 0.020000

C 2.375000 2.352000 0.003000

C 0.989000 2.667000 0.070000

C 0.595000 4.000000 0.296000

H -0.449000 4.226000 0.440000

C 1.533000 5.023000 0.361000

C 2.895000 4.681000 0.192000

H 3.646000 5.461000 0.217000

C 3.328000 3.377000 0.024000

H 4.382000 3.162000 -0.064000

C 1.149000 6.492000 0.612000

C -0.367000 6.679000 0.798000

H -0.927000 6.372000 -0.090000

H -0.588000 7.735000 0.977000

H -0.745000 6.113000 1.654000

C 1.853000 7.001000 1.892000

H 1.552000 6.411000 2.762000

H 1.589000 8.047000 2.081000

H 2.940000 6.943000 1.809000

C 1.594000 7.354000 -0.593000

H 2.673000 7.298000 -0.756000

H 1.335000 8.404000 -0.427000

H 1.101000 7.022000 -1.511000

C 5.141000 0.765000 0.222000

C 5.201000 0.994000 1.607000

H 4.350000 0.728000 2.227000

C 6.319000 1.563000 2.210000

H 6.334000 1.726000 3.282000

C 7.418000 1.932000 1.433000

H 8.290000 2.380000 1.898000

C 7.383000 1.724000 0.057000

H 8.230000 2.013000 -0.557000

C 6.259000 1.147000 -0.536000

H 6.248000 0.992000 -1.609000

C 3.889000 -0.116000 -2.058000

C 3.577000 0.928000 -2.947000

H 3.249000 1.885000 -2.555000

C 3.671000 0.774000 -4.329000

H 3.419000 1.603000 -4.982000

C 4.080000 -0.442000 -4.873000

H 4.151000 -0.567000 -5.948000

C 4.392000 -1.496000 -4.018000

H 4.706000 -2.451000 -4.426000

C 4.296000 -1.329000 -2.637000

H 4.544000 -2.175000 -2.004000

B 3.812000 0.122000 -0.452000

S -2.100000 3.248000 -1.322000

N -3.482000 1.339000 -0.262000

N -2.552000 -0.972000 0.058000

C -3.839000 3.352000 -1.408000

C -4.424000 2.246000 -0.768000

C -5.822000 2.190000 -0.660000

H -6.302000 1.368000 -0.154000

C -6.577000 3.211000 -1.218000

H -7.657000 3.166000 -1.136000

C -5.978000 4.292000 -1.878000

H -6.595000 5.073000 -2.307000

C -4.598000 4.377000 -1.971000

H -4.119000 5.217000 -2.461000

C -2.223000 1.760000 -0.415000

C -1.068000 0.975000 -0.058000

C -1.305000 -0.414000 0.039000

C 0.281000 1.408000 -0.020000

C -2.375000 -2.352000 -0.003000

C -0.989000 -2.667000 -0.070000

C -0.595000 -4.000000 -0.296000

H 0.449000 -4.226000 -0.440000

C -1.533000 -5.023000 -0.362000

C -2.895000 -4.681000 -0.192000

H -3.646000 -5.461000 -0.217000

C -3.328000 -3.377000 -0.024000

H -4.382000 -3.162000 0.064000

C -1.149000 -6.492000 -0.612000

C 0.367000 -6.679000 -0.798000

H 0.927000 -6.372000 0.089000

H 0.588000 -7.735000 -0.978000

H 0.745000 -6.113000 -1.655000

C -1.853000 -7.001000 -1.892000

H -1.552000 -6.411000 -2.762000

H -1.589000 -8.047000 -2.082000

H -2.940000 -6.943000 -1.809000

C -1.594000 -7.354000 0.593000

H -2.673000 -7.298000 0.756000

H -1.336000 -8.404000 0.427000

H -1.101000 -7.022000 1.511000

C -5.141000 -0.765000 -0.222000

C -5.201000 -0.994000 -1.607000

H -4.350000 -0.728000 -2.227000

C -6.319000 -1.563000 -2.210000

H -6.334000 -1.726000 -3.282000

C -7.418000 -1.932000 -1.434000

H -8.290000 -2.380000 -1.898000

C -7.383000 -1.724000 -0.057000

H -8.230000 -2.013000 0.557000

C -6.259000 -1.147000 0.536000

H -6.248000 -0.992000 1.609000

C -3.889000 0.116000 2.058000

C -3.577000 -0.928000 2.947000

H -3.249000 -1.885000 2.555000

C -3.671000 -0.774000 4.329000

H -3.419000 -1.603000 4.982000

C -4.080000 0.442000 4.873000

H -4.151000 0.567000 5.948000

C -4.392000 1.496000 4.018000

H -4.707000 2.451000 4.426000

C -4.296000 1.329000 2.637000

H -4.544000 2.175000 2.004000

B -3.812000 -0.122000 0.452000

BN-Ph radical anion

S 2.092000 -3.273000 1.317000

N 3.498000 -1.326000 0.298000

N 2.563000 0.965000 -0.119000

C 3.838000 -3.369000 1.405000

C 4.424000 -2.241000 0.796000

C 5.825000 -2.189000 0.715000

H 6.314000 -1.357000 0.235000

C 6.581000 -3.220000 1.263000

H 7.662000 -3.163000 1.198000

C 5.982000 -4.318000 1.886000

H 6.591000 -5.109000 2.307000

C 4.594000 -4.401000 1.950000

H 4.107000 -5.254000 2.410000

C 2.204000 -1.753000 0.423000

C 1.081000 -0.991000 0.056000

C 1.307000 0.411000 -0.094000

C -0.298000 -1.399000 0.062000

C 2.396000 2.341000 -0.057000

C 1.007000 2.655000 0.029000

C 0.620000 3.987000 0.273000

H -0.422000 4.208000 0.435000

C 1.561000 5.010000 0.329000

C 2.919000 4.674000 0.135000

H 3.672000 5.455000 0.152000

C 3.347000 3.368000 -0.045000

H 4.400000 3.154000 -0.147000

C 1.178000 6.478000 0.594000

C -0.335000 6.661000 0.818000

H -0.915000 6.348000 -0.053000

H -0.555000 7.717000 1.005000

H -0.687000 6.090000 1.681000

C 1.909000 6.990000 1.857000

H 1.631000 6.395000 2.731000

H 1.646000 8.035000 2.057000

H 2.994000 6.932000 1.748000

C 1.589000 7.348000 -0.617000

H 2.663000 7.291000 -0.808000

H 1.333000 8.399000 -0.443000

H 1.073000 7.015000 -1.522000

C 5.140000 0.771000 0.276000

C 5.155000 1.006000 1.661000

H 4.291000 0.721000 2.254000

C 6.241000 1.602000 2.295000

H 6.218000 1.769000 3.368000

C 7.356000 1.992000 1.553000

H 8.204000 2.460000 2.043000

C 7.367000 1.776000 0.178000

H 8.227000 2.079000 -0.413000

C 6.273000 1.173000 -0.446000

H 6.298000 1.014000 -1.519000

C 3.990000 -0.158000 -2.034000

C 3.702000 0.867000 -2.952000

H 3.332000 1.819000 -2.586000

C 3.864000 0.698000 -4.326000

H 3.624000 1.514000 -5.001000

C 4.320000 -0.516000 -4.835000

H 4.442000 -0.654000 -5.905000

C 4.607000 -1.553000 -3.952000

H 4.953000 -2.510000 -4.331000

C 4.443000 -1.371000 -2.578000

H 4.668000 -2.204000 -1.920000

B 3.831000 0.092000 -0.426000

S -2.092000 3.273000 -1.317000

N -3.498000 1.326000 -0.298000

N -2.563000 -0.965000 0.119000

C -3.838000 3.369000 -1.405000

C -4.424000 2.241000 -0.796000

C -5.825000 2.189000 -0.715000

H -6.314000 1.357000 -0.235000

C -6.581000 3.220000 -1.263000

H -7.662000 3.163000 -1.198000

C -5.982000 4.318000 -1.886000

H -6.591000 5.109000 -2.307000

C -4.594000 4.401000 -1.950000

H -4.107000 5.254000 -2.410000

C -2.204000 1.753000 -0.423000

C -1.081000 0.991000 -0.056000

C -1.307000 -0.411000 0.094000

C 0.298000 1.399000 -0.062000

C -2.396000 -2.341000 0.057000

C -1.007000 -2.655000 -0.029000

C -0.620000 -3.987000 -0.273000

H 0.422000 -4.208000 -0.435000

C -1.561000 -5.010000 -0.329000

C -2.919000 -4.674000 -0.135000

H -3.672000 -5.455000 -0.152000

C -3.347000 -3.368000 0.046000

H -4.400000 -3.154000 0.147000

C -1.178000 -6.478000 -0.594000

C 0.335000 -6.661000 -0.818000

H 0.915000 -6.348000 0.053000

H 0.555000 -7.717000 -1.005000

H 0.687000 -6.090000 -1.681000

C -1.909000 -6.990000 -1.857000

H -1.631000 -6.395000 -2.731000

H -1.647000 -8.035000 -2.057000

H -2.994000 -6.932000 -1.748000

C -1.589000 -7.348000 0.617000

H -2.663000 -7.291000 0.808000

H -1.333000 -8.399000 0.443000

H -1.073000 -7.015000 1.522000

C -5.140000 -0.771000 -0.276000

C -5.155000 -1.006000 -1.661000

H -4.291000 -0.721000 -2.254000

C -6.241000 -1.602000 -2.296000

H -6.218000 -1.769000 -3.368000

C -7.356000 -1.992000 -1.553000

H -8.204000 -2.460000 -2.043000

C -7.367000 -1.777000 -0.178000

H -8.227000 -2.079000 0.413000

C -6.272000 -1.173000 0.446000

H -6.298000 -1.014000 1.519000

C -3.990000 0.158000 2.034000

C -3.702000 -0.867000 2.952000

H -3.332000 -1.819000 2.586000

C -3.864000 -0.699000 4.326000

H -3.624000 -1.515000 5.001000

C -4.320000 0.516000 4.835000

H -4.442000 0.654000 5.905000

C -4.607000 1.553000 3.952000

H -4.953000 2.510000 4.331000

C -4.443000 1.371000 2.578000

H -4.668000 2.204000 1.920000

B -3.831000 -0.092000 0.426000

BN-Ph dianion

S 2.108000 -3.283000 1.336000

N 3.522000 -1.307000 0.328000

N 2.574000 0.965000 -0.167000

C 3.864000 -3.382000 1.380000

C 4.439000 -2.232000 0.789000

C 5.843000 -2.188000 0.702000

H 6.333000 -1.347000 0.239000

C 6.608000 -3.233000 1.221000

H 7.689000 -3.169000 1.148000

C 6.020000 -4.346000 1.819000

H 6.631000 -5.150000 2.217000

C 4.625000 -4.424000 1.887000

H 4.138000 -5.288000 2.328000

C 2.195000 -1.739000 0.437000

C 1.098000 -1.003000 0.061000

C 1.310000 0.412000 -0.142000

C -0.311000 -1.393000 0.104000

C 2.411000 2.339000 -0.106000

C 1.015000 2.645000 -0.012000

C 0.628000 3.976000 0.243000

H -0.415000 4.188000 0.415000

C 1.567000 5.004000 0.293000

C 2.926000 4.679000 0.086000

H 3.677000 5.463000 0.100000

C 3.355000 3.371000 -0.101000

H 4.409000 3.162000 -0.206000

C 1.177000 6.470000 0.565000

C -0.332000 6.642000 0.819000

H -0.927000 6.315000 -0.038000

H -0.559000 7.697000 1.006000

H -0.661000 6.069000 1.690000

C 1.926000 6.993000 1.813000

H 1.669000 6.394000 2.692000

H 1.659000 8.038000 2.018000

H 3.010000 6.939000 1.684000

C 1.557000 7.344000 -0.653000

H 2.628000 7.289000 -0.865000

H 1.299000 8.396000 -0.475000

H 1.025000 7.005000 -1.546000

C 5.135000 0.791000 0.350000

C 5.092000 1.016000 1.736000

H 4.208000 0.710000 2.286000

C 6.141000 1.623000 2.419000

H 6.069000 1.782000 3.491000

C 7.282000 2.034000 1.729000

H 8.103000 2.511000 2.257000

C 7.353000 1.827000 0.354000

H 8.234000 2.143000 -0.199000

C 6.293000 1.214000 -0.318000

H 6.367000 1.061000 -1.390000

C 4.095000 -0.164000 -2.003000

C 3.978000 0.895000 -2.922000

H 3.689000 1.877000 -2.562000

C 4.202000 0.724000 -4.287000

H 4.091000 1.568000 -4.962000

C 4.549000 -0.530000 -4.790000

H 4.717000 -0.670000 -5.854000

C 4.662000 -1.601000 -3.907000

H 4.915000 -2.589000 -4.282000

C 4.436000 -1.415000 -2.542000

H 4.516000 -2.273000 -1.884000

B 3.853000 0.083000 -0.396000

S -2.108000 3.283000 -1.336000

N -3.522000 1.307000 -0.328000

N -2.574000 -0.965000 0.167000

C -3.864000 3.382000 -1.380000

C -4.439000 2.232000 -0.789000

C -5.844000 2.188000 -0.702000

H -6.333000 1.347000 -0.239000

C -6.608000 3.233000 -1.221000

H -7.689000 3.169000 -1.148000

C -6.020000 4.346000 -1.819000

H -6.631000 5.150000 -2.217000

C -4.625000 4.424000 -1.887000

H -4.138000 5.288000 -2.328000

C -2.195000 1.739000 -0.437000

C -1.098000 1.003000 -0.061000

C -1.310000 -0.412000 0.142000

C 0.311000 1.393000 -0.104000

C -2.411000 -2.339000 0.106000

C -1.015000 -2.645000 0.012000

C -0.628000 -3.976000 -0.243000

H 0.415000 -4.188000 -0.415000

C -1.567000 -5.004000 -0.293000

C -2.926000 -4.679000 -0.086000

H -3.677000 -5.463000 -0.100000

C -3.355000 -3.371000 0.101000

H -4.409000 -3.162000 0.206000

C -1.177000 -6.470000 -0.565000

C 0.332000 -6.642000 -0.819000

H 0.927000 -6.315000 0.038000

H 0.559000 -7.697000 -1.005000

H 0.661000 -6.069000 -1.690000

C -1.926000 -6.993000 -1.813000

H -1.669000 -6.394000 -2.692000

H -1.659000 -8.038000 -2.018000

H -3.010000 -6.939000 -1.684000

C -1.557000 -7.344000 0.653000

H -2.628000 -7.289000 0.865000

H -1.299000 -8.396000 0.475000

H -1.025000 -7.005000 1.546000

C -5.135000 -0.791000 -0.350000

C -5.092000 -1.016000 -1.736000

H -4.208000 -0.710000 -2.286000

C -6.141000 -1.623000 -2.419000

H -6.069000 -1.782000 -3.491000

C -7.282000 -2.034000 -1.729000

H -8.103000 -2.511000 -2.257000

C -7.353000 -1.827000 -0.354000

H -8.234000 -2.143000 0.199000

C -6.293000 -1.214000 0.318000

H -6.367000 -1.061000 1.390000

C -4.095000 0.164000 2.003000

C -3.979000 -0.895000 2.922000

H -3.689000 -1.877000 2.562000

C -4.202000 -0.724000 4.287000

H -4.091000 -1.568000 4.962000

C -4.549000 0.530000 4.790000

H -4.717000 0.670000 5.854000

C -4.662000 1.601000 3.907000

H -4.915000 2.589000 4.282000

C -4.436000 1.415000 2.542000

H -4.516000 2.273000 1.884000

B -3.853000 -0.083000 0.396000

BN-Ph radical cation

S 2.093000 -3.317000 1.277000

N 3.463000 -1.403000 0.228000

N 2.539000 0.926000 -0.073000

C 3.829000 -3.454000 1.297000

C 4.411000 -2.340000 0.666000

C 5.804000 -2.300000 0.504000

H 6.279000 -1.471000 0.003000

C 6.559000 -3.347000 1.003000

H 7.635000 -3.322000 0.881000

C 5.965000 -4.437000 1.659000

H 6.586000 -5.237000 2.043000

C 4.590000 -4.506000 1.807000

H 4.119000 -5.351000 2.294000

C 2.210000 -1.815000 0.411000

C 1.051000 -1.004000 0.081000

C 1.300000 0.393000 -0.016000

C -0.287000 -1.411000 0.017000

C 2.400000 2.319000 -0.026000

C 1.027000 2.666000 0.045000

C 0.671000 4.002000 0.260000

H -0.364000 4.266000 0.398000

C 1.645000 5.004000 0.325000

C 2.992000 4.625000 0.168000

H 3.766000 5.383000 0.199000

C 3.387000 3.305000 0.007000

H 4.434000 3.053000 -0.059000

C 1.296000 6.482000 0.567000

C -0.216000 6.708000 0.743000

H -0.780000 6.417000 -0.149000

H -0.408000 7.769000 0.916000

H -0.615000 6.160000 1.601000

C 2.008000 6.974000 1.849000

H 1.691000 6.396000 2.721000

H 1.766000 8.024000 2.032000

H 3.095000 6.894000 1.771000

C 1.774000 7.321000 -0.642000

H 2.853000 7.244000 -0.793000

H 1.537000 8.376000 -0.483000

H 1.282000 6.998000 -1.564000

C 5.116000 0.678000 0.333000

C 5.106000 0.848000 1.728000

H 4.230000 0.554000 2.300000

C 6.192000 1.393000 2.407000

H 6.154000 1.510000 3.485000

C 7.326000 1.792000 1.701000

H 8.173000 2.219000 2.225000

C 7.361000 1.638000 0.317000

H 8.239000 1.945000 -0.241000

C 6.269000 1.086000 -0.354000

H 6.316000 0.971000 -1.432000

C 3.934000 -0.112000 -2.038000

C 3.943000 1.019000 -2.873000

H 3.863000 2.012000 -2.442000

C 4.054000 0.911000 -4.257000

H 4.059000 1.806000 -4.869000

C 4.160000 -0.343000 -4.855000

H 4.248000 -0.432000 -5.931000

C 4.151000 -1.481000 -4.053000

H 4.235000 -2.463000 -4.504000

C 4.036000 -1.362000 -2.668000

H 4.034000 -2.273000 -2.080000

B 3.829000 0.059000 -0.425000

S -2.093000 3.317000 -1.277000

N -3.463000 1.403000 -0.228000

N -2.539000 -0.926000 0.073000

C -3.829000 3.454000 -1.297000

C -4.411000 2.340000 -0.666000

C -5.805000 2.300000 -0.503000

H -6.279000 1.472000 -0.003000

C -6.559000 3.347000 -1.002000

H -7.635000 3.322000 -0.881000

C -5.965000 4.437000 -1.659000

H -6.586000 5.238000 -2.043000

C -4.590000 4.506000 -1.807000

H -4.119000 5.351000 -2.294000

C -2.210000 1.815000 -0.411000

C -1.051000 1.004000 -0.082000

C -1.300000 -0.393000 0.016000

C 0.287000 1.411000 -0.017000

C -2.400000 -2.319000 0.026000

C -1.027000 -2.666000 -0.045000

C -0.671000 -4.002000 -0.260000

H 0.364000 -4.266000 -0.398000

C -1.645000 -5.004000 -0.325000

C -2.992000 -4.625000 -0.168000

H -3.766000 -5.383000 -0.199000

C -3.387000 -3.305000 -0.007000

H -4.434000 -3.053000 0.059000

C -1.296000 -6.482000 -0.566000

C 0.216000 -6.708000 -0.742000

H 0.780000 -6.417000 0.149000

H 0.408000 -7.769000 -0.916000

H 0.615000 -6.160000 -1.600000

C -2.008000 -6.974000 -1.849000

H -1.691000 -6.396000 -2.720000

H -1.766000 -8.025000 -2.031000

H -3.095000 -6.894000 -1.770000

C -1.774000 -7.321000 0.643000

H -2.852000 -7.243000 0.794000

H -1.536000 -8.376000 0.484000

H -1.282000 -6.997000 1.564000

C -5.116000 -0.678000 -0.333000

C -5.106000 -0.848000 -1.728000

H -4.229000 -0.554000 -2.300000

C -6.191000 -1.393000 -2.408000

H -6.154000 -1.511000 -3.485000

C -7.326000 -1.792000 -1.701000

H -8.173000 -2.219000 -2.226000

C -7.361000 -1.638000 -0.318000

H -8.239000 -1.945000 0.240000

C -6.269000 -1.086000 0.354000

H -6.316000 -0.971000 1.431000

C -3.934000 0.112000 2.037000

C -3.943000 -1.019000 2.873000

H -3.863000 -2.012000 2.442000

C -4.054000 -0.911000 4.257000

H -4.059000 -1.806000 4.869000

C -4.160000 0.343000 4.854000

H -4.249000 0.431000 5.931000

C -4.152000 1.480000 4.053000

H -4.235000 2.463000 4.504000

C -4.036000 1.362000 2.668000

H -4.034000 2.273000 2.079000

B -3.829000 -0.059000 0.425000

BN-Ph dication

S 2.076000 -3.396000 1.224000

N 3.440000 -1.473000 0.189000

N 2.529000 0.873000 -0.090000

C 3.806000 -3.563000 1.175000

C 4.386000 -2.437000 0.553000

C 5.774000 -2.412000 0.339000

H 6.243000 -1.578000 -0.158000

C 6.526000 -3.484000 0.781000

H 7.597000 -3.477000 0.619000

C 5.936000 -4.582000 1.433000

H 6.559000 -5.401000 1.772000

C 4.567000 -4.638000 1.633000

H 4.104000 -5.488000 2.118000

C 2.187000 -1.873000 0.404000

C 1.034000 -1.040000 0.103000

C 1.301000 0.369000 -0.003000

C -0.297000 -1.417000 0.019000

C 2.432000 2.277000 -0.060000

C 1.072000 2.661000 0.013000

C 0.757000 4.001000 0.223000

H -0.267000 4.305000 0.358000

C 1.768000 4.980000 0.289000

C 3.100000 4.561000 0.141000

H 3.897000 5.292000 0.179000

C 3.452000 3.224000 -0.014000

H 4.491000 2.936000 -0.058000

C 1.458000 6.465000 0.522000

C -0.049000 6.734000 0.684000

H -0.613000 6.461000 -0.213000

H -0.209000 7.800000 0.853000

H -0.473000 6.204000 1.543000

C 2.177000 6.936000 1.811000

H 1.838000 6.371000 2.683000

H 1.960000 7.993000 1.988000

H 3.261000 6.831000 1.740000

C 1.974000 7.284000 -0.687000

H 3.052000 7.181000 -0.823000

H 1.761000 8.344000 -0.531000

H 1.485000 6.973000 -1.614000

C 5.084000 0.579000 0.444000

C 4.993000 0.703000 1.841000

H 4.086000 0.395000 2.356000

C 6.041000 1.217000 2.599000

H 5.943000 1.300000 3.676000

C 7.218000 1.625000 1.972000

H 8.037000 2.026000 2.558000

C 7.335000 1.509000 0.589000

H 8.249000 1.819000 0.095000

C 6.280000 0.991000 -0.163000

H 6.396000 0.906000 -1.238000

C 3.965000 -0.101000 -2.016000

C 4.203000 1.053000 -2.784000

H 4.294000 2.020000 -2.304000

C 4.339000 0.995000 -4.169000

H 4.533000 1.903000 -4.729000

C 4.225000 -0.225000 -4.832000

H 4.331000 -0.273000 -5.909000

C 3.975000 -1.380000 -4.097000

H 3.895000 -2.337000 -4.601000

C 3.836000 -1.315000 -2.712000

H 3.650000 -2.240000 -2.178000

B 3.840000 -0.007000 -0.397000

S -2.076000 3.396000 -1.223000

N -3.440000 1.473000 -0.189000

N -2.529000 -0.873000 0.090000

C -3.806000 3.563000 -1.175000

C -4.386000 2.437000 -0.553000

C -5.774000 2.412000 -0.338000

H -6.243000 1.578000 0.158000

C -6.526000 3.484000 -0.781000

H -7.597000 3.477000 -0.619000

C -5.936000 4.582000 -1.433000

H -6.559000 5.401000 -1.772000

C -4.567000 4.638000 -1.633000

H -4.104000 5.488000 -2.118000

C -2.187000 1.873000 -0.404000

C -1.034000 1.040000 -0.103000

C -1.301000 -0.369000 0.003000

C 0.297000 1.417000 -0.019000

C -2.432000 -2.277000 0.060000

C -1.072000 -2.661000 -0.013000

C -0.757000 -4.001000 -0.223000

H 0.267000 -4.305000 -0.358000

C -1.768000 -4.980000 -0.289000

C -3.100000 -4.561000 -0.141000

H -3.897000 -5.292000 -0.179000

C -3.452000 -3.224000 0.014000

H -4.491000 -2.936000 0.058000

C -1.458000 -6.465000 -0.522000

C 0.049000 -6.734000 -0.684000

H 0.613000 -6.461000 0.213000

H 0.209000 -7.800000 -0.853000

H 0.473000 -6.204000 -1.543000

C -2.177000 -6.936000 -1.811000

H -1.838000 -6.371000 -2.683000

H -1.960000 -7.993000 -1.988000

H -3.261000 -6.831000 -1.740000

C -1.974000 -7.284000 0.687000

H -3.052000 -7.181000 0.823000

H -1.761000 -8.344000 0.531000

H -1.485000 -6.973000 1.614000

C -5.084000 -0.579000 -0.444000

C -4.993000 -0.703000 -1.841000

H -4.086000 -0.395000 -2.356000

C -6.041000 -1.217000 -2.599000

H -5.943000 -1.300000 -3.676000

C -7.218000 -1.625000 -1.973000

H -8.037000 -2.026000 -2.558000

C -7.335000 -1.509000 -0.589000

H -8.249000 -1.819000 -0.095000

C -6.280000 -0.991000 0.163000

H -6.396000 -0.906000 1.238000

C -3.965000 0.101000 2.016000

C -4.203000 -1.053000 2.784000

H -4.294000 -2.020000 2.304000

C -4.339000 -0.995000 4.169000

H -4.533000 -1.903000 4.729000

C -4.225000 0.225000 4.832000

H -4.331000 0.273000 5.909000

C -3.975000 1.380000 4.097000

H -3.895000 2.337000 4.601000

C -3.836000 1.315000 2.712000

H -3.650000 2.240000 2.178000

B -3.840000 0.007000 0.397000

Compound 3

C -0.600000 -1.213000 -0.173000

C 0.818000 -1.167000 0.012000

C -1.449000 -0.090000 -0.141000

C -0.818000 1.167000 -0.012000

C 0.600000 1.213000 0.173000

C 1.449000 0.090000 0.142000

C -1.257000 2.555000 -0.074000

C -0.105000 3.352000 0.150000

C -2.466000 3.207000 -0.370000

C -0.161000 4.746000 0.162000

C -2.539000 4.596000 -0.380000

H -3.354000 2.637000 -0.603000

C -1.381000 5.349000 -0.095000

H 0.729000 5.338000 0.346000

H -1.444000 6.432000 -0.096000

C 1.257000 -2.555000 0.074000

C 2.466000 -3.207000 0.369000

C 0.105000 -3.352000 -0.149000

C 2.539000 -4.596000 0.379000

H 3.354000 -2.637000 0.602000

C 0.160000 -4.746000 -0.161000

C 1.381000 -5.349000 0.095000

H -0.729000 -5.338000 -0.345000

H 1.444000 -6.432000 0.096000

C 2.895000 0.335000 0.113000

S 3.974000 -0.571000 -0.985000

C 4.815000 1.430000 0.416000

C -2.895000 -0.335000 -0.113000

S -3.974000 0.571000 0.985000

C -4.815000 -1.430000 -0.416000

N 3.473000 1.332000 0.722000

N -3.472000 -1.332000 -0.722000

N 0.989000 2.528000 0.288000

N -0.989000 -2.528000 -0.287000

C -5.291000 -0.472000 0.506000

C -6.629000 -0.447000 0.903000

C -7.488000 -1.400000 0.371000

H -6.989000 0.291000 1.609000

C -5.699000 -2.380000 -0.945000

C -7.026000 -2.358000 -0.546000

H -8.530000 -1.401000 0.667000

H -5.332000 -3.110000 -1.657000

H -7.720000 -3.087000 -0.948000

C 5.291000 0.472000 -0.506000

C 6.628000 0.447000 -0.904000

C 7.488000 1.400000 -0.371000

H 6.989000 -0.291000 -1.610000

C 5.699000 2.380000 0.945000

C 7.026000 2.358000 0.546000

H 8.530000 1.401000 -0.668000

H 5.332000 3.109000 1.657000

H 7.720000 3.087000 0.948000

C 3.837000 -5.302000 0.695000

H 4.177000 -5.910000 -0.151000

H 4.630000 -4.588000 0.929000

H 3.729000 -5.973000 1.553000

C -3.837000 5.302000 -0.695000

H -4.629000 4.588000 -0.930000

H -4.177000 5.910000 0.150000

H -3.729000 5.973000 -1.553000

H 1.929000 2.779000 0.557000

H -1.929000 -2.779000 -0.557000

Molecular geometries obtained at the level of B3LYP-D3/TZVP

BN-Ph neutral

S -2.14609783 -3.24169986 -1.30735339

N -3.48949130 -1.29038017 -0.26948213

N -2.53157628 1.00424427 0.02440699

C -3.89209798 -3.30262886 -1.39399585

C -4.45086676 -2.17577957 -0.77016039

C -5.84370875 -2.08321353 -0.66423690

H -6.30081587 -1.24314270 -0.16987193

C -6.62379746 -3.08681697 -1.21290291

H -7.70082239 -3.01307767 -1.13497836

C -6.05174177 -4.18991979 -1.85749154

H -6.68647580 -4.95834746 -2.27970159

C -4.67474189 -4.31141450 -1.94744360

H -4.21764676 -5.16867553 -2.42401478

C -2.24125146 -1.73603683 -0.41331137

C -1.08000090 -0.96349890 -0.05899502

C -1.29442822 0.42829507 0.01893816

C 0.26062394 -1.40847624 -0.00480386

C -2.33961340 2.38019627 -0.02767990

C -0.95005055 2.67368499 -0.09028317

C -0.53533789 3.99633201 -0.31019334

H 0.51047478 4.20042086 -0.46130422

C -1.45449114 5.03223383 -0.36118781

C -2.82029468 4.71300691 -0.19484103

H -3.55661527 5.50638371 -0.21088939

C -3.27549805 3.41713513 -0.03996579

H -4.33078479 3.21571182 0.04842562

C -1.04102830 6.49268871 -0.59064290

C 0.47906505 6.65006788 -0.75607550

H 1.01912901 6.31139841 0.13116559

H 0.72493032 7.70275023 -0.91063843

H 0.85302482 6.09383438 -1.61829116

C -1.72032212 7.02843760 -1.86879936

H -1.42610031 6.43746081 -2.73870081

H -1.43193098 8.06787708 -2.04676799

H -2.80805393 6.99316397 -1.79362345

C -1.48042580 7.34600121 0.61839285

H -2.56072554 7.31350031 0.76634269

H -1.19559715 8.39106987 0.47055118

H -1.00688628 6.98819971 1.53539925

C -5.11479615 0.83601123 -0.17710703

C -5.20812040 1.06190991 -1.55702245

H -4.38227451 0.76937445 -2.19717720

C -6.32521438 1.66168842 -2.12461096

H -6.37017180 1.82349742 -3.19541932

C -7.38599997 2.06231618 -1.31409010

H -8.25812625 2.53439008 -1.75079301

C -7.31355746 1.85641166 0.05975008

H -8.13081452 2.17059958 0.69880847

C -6.18956334 1.24831683 0.61667222

H -6.14336109 1.09357268 1.68809014

C -3.81381710 -0.07901206 2.04624017

C -3.21799799 0.82809183 2.93149485

H -2.69921152 1.69481895 2.53872560

C -3.27117882 0.64909356 4.31131121

H -2.79673292 1.37008715 4.96738608

C -3.92599056 -0.45443705 4.84820942

H -3.96706129 -0.59914595 5.92130498

C -4.52504918 -1.37283367 3.99126744

H -5.03529169 -2.23967689 4.39586691

C -4.46661264 -1.18179266 2.61396318

H -4.94109841 -1.91560766 1.97206280

B -3.78317002 0.17291121 0.44789891

S 2.14608932 3.24170693 1.30730096

N 3.48947448 1.29038132 0.26943035

N 2.53156588 -1.00424440 -0.02442879

C 3.89209105 3.30261798 1.39395946

C 4.45085297 2.17576642 0.77012386

C 5.84369325 2.08317804 0.66421061

H 6.30078946 1.24309912 0.16984715

C 6.62379095 3.08676963 1.21288524

H 7.70081551 3.01301725 1.13496881

C 6.05174357 4.18987843 1.85747244

H 6.68648480 4.95829580 2.27969036

C 4.67474430 4.31139159 1.94741582

H 4.21765742 5.16865669 2.42398769

C 2.24123678 1.73603788 0.41326825

C 1.07998744 0.96349665 0.05896180

C 1.29441649 -0.42829757 -0.01896596

C -0.26063662 1.40847345 0.00478389

C 2.33960399 -2.38019584 0.02768074

C 0.95004098 -2.67368496 0.09029281

C 0.53533253 -3.99632766 0.31023882

H -0.51047825 -4.20041547 0.46136110

C 1.45448719 -5.03222688 0.36125728

C 2.82028874 -4.71300298 0.19489190

H 3.55661003 -5.50637895 0.21095090

C 3.27548930 -3.41713440 0.03998384

H 4.33077497 -3.21571283 -0.04841889

C 1.04102624 -6.49267755 0.59074129

C -0.47907492 -6.65006624 0.75609308

H -1.01909140 -6.31146260 -0.13120171

H -0.72493545 -7.70274177 0.91071047

H -0.85309281 -6.09378099 1.61825041

C 1.72025134 -7.02837781 1.86895481

H 1.42598613 -6.43736514 2.73881720

H 1.43184564 -8.06780872 2.04695005

H 2.80798713 -6.99311354 1.79383572

C 1.48050311 -7.34602476 -0.61824085

H 2.56080997 -7.31350306 -0.76613655

H 1.19569144 -8.39109463 -0.47037568

H 1.00700210 -6.98826691 -1.53528419

C 5.11479736 -0.83596990 0.17709398

C 5.20811994 -1.06184671 1.55701290

H 4.38226148 -0.76932786 2.19715904

C 6.32522560 -1.66159043 2.12461548

H 6.37017937 -1.82338750 3.19542586

C 7.38602754 -2.06219856 1.31410665

H 8.25816346 -2.53424461 1.75082017

C 7.31359159 -1.85630499 -0.05973584

H 8.13086304 -2.17047394 -0.69878511

C 6.18958620 -1.24824394 -0.61667192

H 6.14338950 -1.09350936 -1.68809173

C 3.81381702 0.07898630 -2.04627491

C 3.21815310 -0.82823597 -2.93151526

H 2.69948063 -1.69502380 -2.53872989

C 3.27134742 -0.64927877 -4.31133550

H 2.79702367 -1.37036328 -4.96739885

C 3.92601735 0.45432706 -4.84825426

H 3.96709741 0.59900415 -5.92135377

C 4.52492037 1.37283852 -3.99132807

H 5.03505016 2.23974070 -4.39594340

C 4.46647103 1.18183854 -2.61401764

H 4.94083113 1.91574542 -1.97212947

B 3.78315962 -0.17290739 -0.44792903

BN-Ph radical cation

S -2.11405500 -3.31921300 -1.26749200

N -3.46169100 -1.37636700 -0.23747100

N -2.52548900 0.94310100 0.03930200

C -3.85830500 -3.42325100 -1.29354300

C -4.42248100 -2.29591500 -0.67476600

C -5.81141100 -2.23009200 -0.51043000

H -6.26747600 -1.39170100 -0.01209800

C -6.58423400 -3.26286400 -1.00739700

H -7.65857900 -3.21788700 -0.88720900

C -6.00896100 -4.36478100 -1.65618900

H -6.64257900 -5.15457300 -2.03799300

C -4.63593400 -4.46074900 -1.80056800

H -4.18030000 -5.31712100 -2.27927600

C -2.21533100 -1.80419400 -0.40835100

C -1.05677800 -0.99860200 -0.07804900

C -1.29314800 0.39918500 -0.00326100

C 0.27508100 -1.40980300 0.00462500

C -2.37971500 2.33287300 -0.01162500

C -1.00439200 2.66688800 -0.07758900

C -0.63425500 3.99406800 -0.29128900

H 0.40255100 4.24180900 -0.43500400

C -1.59631900 5.00404000 -0.34560400

C -2.94683700 4.64041400 -0.19190600

H -3.71007000 5.40641100 -0.21724500

C -3.35630400 3.32553400 -0.04005100

H -4.40371400 3.08133400 0.03099400

C -1.22690500 6.47537400 -0.56743600

C 0.28890300 6.68151100 -0.71732400

H 0.83201400 6.36473500 0.17648100

H 0.49901800 7.74131300 -0.86838800

H 0.69108300 6.14297500 -1.57829800

C -1.91385500 6.98669800 -1.85227700

H -1.59439500 6.40842300 -2.72163300

H -1.65408900 8.03337800 -2.02468600

H -3.00053500 6.92233300 -1.78614400

C -1.70927300 7.30679300 0.64119700

H -2.79012200 7.24612800 0.77287200

H -1.45178200 8.35847600 0.49868100

H -1.23813800 6.96247000 1.56442300

C -5.09737400 0.71692700 -0.29968700

C -5.12352700 0.87817000 -1.69118000

H -4.27122900 0.55796200 -2.28246300

C -6.21437000 1.44638400 -2.33768800

H -6.21018500 1.55817800 -3.41533100

C -7.31322100 1.87601800 -1.59658800

H -8.16534200 2.32164500 -2.09495300

C -7.30823600 1.73021400 -0.21302400

H -8.15835000 2.06368500 0.37003300

C -6.21101500 1.15498500 0.42476800

H -6.21861700 1.04775700 1.50288400

C -3.87445600 -0.08588500 2.02326300

C -3.67588700 1.01845200 2.86407200

H -3.44358500 1.98699100 2.43757400

C -3.77266000 0.91005500 4.24735800

H -3.61493100 1.78354600 4.86888600

C -4.07158700 -0.31646200 4.83282600

H -4.14790900 -0.40466300 5.90954500

C -4.27216400 -1.42690300 4.02121300

H -4.50736900 -2.38747700 4.46412800

C -4.17216400 -1.30858200 2.63711500

H -4.33801600 -2.19462400 2.03589100

B -3.80263300 0.08661800 0.41648700

S 2.11399700 3.31929700 1.26721800

N 3.46164300 1.37638700 0.23733700

N 2.52544700 -0.94308500 -0.03943000

C 3.85824500 3.42337200 1.29322500

C 4.42242900 2.29600300 0.67451800

C 5.81135000 2.23021700 0.51011500

H 6.26741900 1.39180900 0.01182000

C 6.58416500 3.26304900 1.00697300

H 7.65850600 3.21810100 0.88673600

C 6.00888600 4.36499200 1.65571400

H 6.64249800 5.15482800 2.03743500

C 4.63586300 4.46093200 1.80014100

H 4.18022400 5.31732600 2.27880400

C 2.21527900 1.80423300 0.40815900

C 1.05673400 0.99863300 0.07785000

C 1.29310900 -0.39915700 0.00305900

C -0.27512600 1.40983600 -0.00485500

C 2.37965800 -2.33285800 0.01151200

C 1.00433000 -2.66686400 0.07738000

C 0.63416000 -3.99404100 0.29103100

H -0.40266300 -4.24177500 0.43462900

C 1.59621100 -5.00402200 0.34543500

C 2.94674600 -4.64040500 0.19187800

H 3.70997300 -5.40640700 0.21730200

C 3.35623500 -3.32553000 0.04005000

H 4.40365400 -3.08133800 -0.03088000

C 1.22676000 -6.47535400 0.56721700

C -0.28906300 -6.68148000 0.71697400

H -0.83209600 -6.36467400 -0.17686800

H -0.49920000 -7.74128400 0.86799000

H -0.69130900 -6.14296300 1.57792900

C 1.91359700 -6.98670500 1.85210700

H 1.59406100 -6.40844500 2.72144700

H 1.65381400 -8.03338800 2.02447300

H 3.00028300 -6.92234200 1.78607200

C 1.70922300 -7.30676100 -0.64138700

H 2.79008300 -7.24610700 -0.77296700

H 1.45170700 -8.35844300 -0.49891000

H 1.23817200 -6.96241800 -1.56464900

C 5.09725800 -0.71690000 0.30015400

C 5.12307500 -0.87789300 1.69168000

H 4.27065200 -0.55754000 2.28270500

C 6.21373500 -1.44604900 2.33855100

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