GAMESS-US EMSL Formatting to GAMESS-US ORCA Formatting

This document is a guide to converting basis sets from GAMESS-US to ORCA’s formatting. This particular example will be for the polarization of bromine. ORCA’s versions of 6-31G\* does not support bromine. Therefore it must be inserted in the %basis section manually.

----------------------------------------------------------------------------------------------------------------------

**ORCA Formatting**

S 6

1 113718.2000000 0.0017176960

2 17074.4400000 0.0131674400

3 3889.5760000 0.0650455300

4 1097.0960000 0.2269505000

5 352.0624000 0.4768357000

6 120.7002000 0.3583677000

S 6

1 2471.1380000 0.0022436870

2 589.3838000 0.0299485300

3 191.8738000 0.1256009000

4 72.9533900 -0.0009832786

5 30.0583900 -0.6013141000

6 12.5292700 -0.4913983000

P 6

1 2471.1380000 0.0037901820

2 589.3838000 0.0299597900

3 191.8738000 0.1318228000

4 72.9533900 0.3432708000

5 30.0583900 0.4642345000

6 12.5292700 0.2079387000

S 6

1 109.6411000 -0.0059756830

2 38.5894800 0.0554212200

3 16.3781800 0.2681200000

4 7.2218360 -0.1543606000

5 3.2636970 -0.7206306000

6 1.4654990 -0.3316437000

P 6

1 109.6411000 -0.0069074830

2 38.5894800 -0.0304143200

3 16.3781800 0.0460272500

4 7.2218360 0.3650689000

5 3.2636970 0.4949232000

6 1.4654990 0.2090394000

S 3

1 2.1036510 0.3029029000

2 0.7547050 -0.2152659000

3 0.3005140 -0.9633941000

P 3

1 2.1036510 -0.0282671400

2 0.7547050 0.3503065000

3 0.3005140 0.7182446000

S 1

1 0.1090710 1.0000000000

P 1

1 0.1090710 1.0000000000

D 3

1 62.2551400 0.0770422900

2 17.3128400 0.3707384000

3 5.6079150 0.7097628000

D 1

1 1.7464860 1.0000000

D 1

1 0.4366000 1.0000000

**GAMESS-US Formatting**

S 6

1 113718.2000000 0.0017176960

2 17074.4400000 0.0131674400

3 3889.5760000 0.0650455300

4 1097.0960000 0.2269505000

5 352.0624000 0.4768357000

6 120.7002000 0.3583677000

L 6

1 2471.1380000 0.0022436870 0.0037901820

2 589.3838000 0.0299485300 0.0299597900

3 191.8738000 0.1256009000 0.1318228000

4 72.9533900 -0.0009832786 0.3432708000

5 30.0583900 -0.6013141000 0.4642345000

6 12.5292700 -0.4913983000 0.2079387000

L 6

1 109.6411000 -0.0059756830 -0.0069074830

2 38.5894800 0.0554212200 -0.0304143200

3 16.3781800 0.2681200000 0.0460272500

4 7.2218360 -0.1543606000 0.3650689000

5 3.2636970 -0.7206306000 0.4949232000

6 1.4654990 -0.3316437000 0.2090394000

L 3

1 2.1036510 0.3029029000 -0.0282671400

2 0.7547050 -0.2152659000 0.3503065000

3 0.3005140 -0.9633941000 0.7182446000

L 1

1 0.1090710 1.0000000000 1.0000000000

D 3

1 62.2551400 0.0770422900

2 17.3128400 0.3707384000

3 5.6079150 0.7097628000

D 1

1 1.7464860 1.0000000

D 1

1 0.4366000 1.0000000

The difference is that GAMESS-US uses “L” to combine the S and P functions, whereas ORCA splits the two apart (highlighted respectively). This must be done in order for the calculation to run in ORCA. An example of how to split them apart is below. The numbers in the middle column represent S, and the ones on the right represent P.

L 3

1 2.1036510 0.3029029000 -0.0282671400

2 0.7547050 -0.2152659000 0.3503065000

3 0.3005140 -0.9633941000 0.7182446000

CONVERTED to:

S 3

1 2.1036510 0.3029029000

2 0.7547050 -0.2152659000

3 0.3005140 -0.9633941000

P 3

1 2.1036510 -0.0282671400

2 0.7547050 0.3503065000

3 0.3005140 0.7182446000

----------------------------------------------------------------------------------------------------------------------

To add a basis set to a calculation, you must add a new section with %basis. The keyword needed to specify the element is “NewGTO X” (X is element). Next the ORCA formatted basis set is inserted. Finally, two “end” statements must be placed at the end or the calculation will not work. Below is an example of the new section.

%basis

NewGTO X

“ORCA formatted basis”

end

end

An example file can be found as “Bromine Solvent Correction Example”, and is being used to run a solvent correction (water) in parallel.