Files generated by R.E.D. Server/R.E.D. IV
Charge derivation & force field library building for ten “independent” molecules.

Programs interfaced: Gaussian 2003 & RESP

Parent_directory

Mol_m1 — **Single molecule charge derivation**

File4REDDB_m1.pdb	*m1 = molecule 1*
JOB2-gau_m1-1-1.com	Gaussian input: *m1-1-1*: molecule 1; conformation 1; orientation 1
JOB2-gau_m1-1-1.out	Gaussian output
JOB2-gau_m1-1-2.com	
JOB2-gau_m1-1-2.out	
Mol_m1-o1-qmra.pdb	Orientation of opt. geometry based on the Gaussian program
Mol_m1-o1-rbra1.pdb	Rigid-body re-orientation algorithm: orientation 1
Mol_m1-o1-rbra2.pdb	
Mol_m1-o1.mol2	***Force field library***
esout_m1	RESP output
espot_m1	Two espots of molecule 1 concatenated in a single file
espot_m1-1-1	*m1-1-1*: molecule 1; conformation 1; orientation 1
espot_m1-1-2	
input1_m1	RESP input - single molecule (stage 1)
input2_m1	RESP input - single molecule (stage 2)
output1_m1	RESP output - single molecule (stage 1)
output2_m1	RESP output - single molecule (stage 2)
punch1_m1	RESP output - single molecule (stage 1)
punch2_m1	RESP output - single molecule (stage 2)
qout1_m1	RESP output (charge values - stage 1)
qout2_m1	RESP output (charge values - stage 2)

Mol_m2

Similar listing of files as that found in Mol_m1
Except that “m2” replaces “m1” in the file names.

[...]

Mol_m10

Similar listing of files as that found in Mol_m1
Except that “m10” replaces “m1” in the file names.

Mol_MM — **Multiple molecules charge derivation**

esout_mm	
espot_mm	Contains the “espot” of the 10 molecules concatenated one after the others
input1_mm	RESP input - multiple molecules (stage 1)
input2_mm	RESP input - multiple molecules (stage 2)
mm1-o1.mol2	***Force field library*** *mm1-o1: multiple molecules 1; o1 = conformation 1*
mm2-o1.mol2	
mm3-o1.mol2	
mm4-o1.mol2	
mm5-o1.mol2	
mm6-o1.mol2	
mm7-o1.mol2	
mm8-o1.mol2	
mm9-o1.mol2	
mm10-o1.mol2	
output1_mm	RESP output - multiple molecules (stage 1)
output2_mm	RESP output - multiple molecules (stage 2)
punch1_mm	RESP output - multiple molecules (stage 1)
punch2_mm	RESP output - multiple molecules (stage 2)
qout1_mm	
qout2_mm	