Files generated by R.E.D. Server/R.E.D. IV
Charge derivation & force field library building for the central fragment of a new amino acid.

Programs interfaced: Gaussian 2003 & RESP

Parent_directory	**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	
JOB2-gau_m1-1-3.com	
JOB2-gau_m1-1-3.out	
JOB2-gau_m1-1-4.com	
JOB2-gau_m1-1-4.out	
JOB2-gau_m1-2-1.com	Gaussian input: *m1*-2-1: molecule 1; conformation 2; orientation 1
JOB2-gau_m1-2-1.out	Gaussian output
JOB2-gau_m1-2-2.com	
JOB2-gau_m1-2-2.out	
JOB2-gau_m1-2-3.com	
JOB2-gau_m1-2-3.out	
JOB2-gau_m1-2-4.com	
JOB2-gau_m1-2-4.out	
Mol_m1-o1-qmra.pdb	conformation 1; Orientation of opt. geometry based on the Gaussian program
Mol_m1-o1-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 1;orientation 1
Mol_m1-o1-rbra2.pdb	
Mol_m1-o1-rbra3.pdb	
Mol_m1-o1-rbra4.pdb	
Mol_m1-o1.mol2	*conformation 1; Force field library (without intra-molecular charge constraint)*
Mol_m1-o1-sm.mol2	***conformation 1; Force field library (with intra-molecular charge constraint)***
Mol_m1-o2-qmra.pdb	conformation 2; Orientation of opt. geometry based on the Gaussian program
Mol_m1-o2-rbra1.pdb	Rigid-body re-orientation algorithm: conformation 2;orientation 1
Mol_m1-o2-rbra2.pdb	
Mol_m1-o2-rbra3.pdb	
Mol_m1-o2-rbra4.pdb	
Mol_m1-o2.mol2	*conformation 2; Force field library (without intra-molecular charge constraint)*
Mol_m1-o2-sm.mol2	***conformation 2; Force field library (with intra-molecular charge constraint)***
esout_m1	RESP output (without intra-molecular charge constraint)
esout_m1.sm	RESP output (with intra-molecular charge constraint)
espot_m1	Eight 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	
espot_m1-1-3	
espot_m1-1-4	
espot_m1-2-1	*m1*-1-1: molecule 1; conformation 2; orientation 1
espot_m1-2-2	
espot_m1-2-3	
espot_m1-2-4	
input1_m1	RESP input - single molecule (stage 1) (without intra-molecular charge constraint)
input1_m1.sm	RESP input - single molecule (stage 1) (with intra-molecular charge constraint)
input2_m1	RESP input - single molecule (stage 2) (without intra-molecular charge constraint)
input2_m1.sm	RESP input - single molecule (stage 2) (with intra-molecular charge constraint)
output1_m1	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
output1_m1.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)
output2_m1	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
output2_m1.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
punch1_m1	RESP output - single molecule (stage 1) (without intra-molecular charge constraint)
punch1_m1.sm	RESP output - single molecule (stage 1) (with intra-molecular charge constraint)
punch2_m1	RESP output - single molecule (stage 2) (without intra-molecular charge constraint)
punch2_m1.sm	RESP output - single molecule (stage 2) (with intra-molecular charge constraint)
qout1_m1	RESP output (charge values - stage 1) (without intra-molecular charge constraint)
qout1_m1.sm	RESP output (charge values - stage 1) (with intra-molecular charge constraint)
qout2_m1	RESP output (charge values - stage 2) (without intra-molecular charge constraint)
qout2_m1.sm	RESP output (charge values - stage 2) (with intra-molecular charge constraint)