

Partial atomic charge calculation of small molecules
TPACM4

README FILE

A SAMPLE PDB FILE IS SHOWN HERE

HIGHLIGHT THE MAIN FORMAT FEATURES

000000000100000000020000000003000000000400000000050000000006000000000700000000
12345678901234567890123456789012345678901234567890123456789012345678

```
HETATM  1  C  UNK  0      1.157  0.023  0.831
HETATM  2  N  UNK  0     -0.047 -0.005  0.130
HETATM  3  O  UNK  0     -0.623 -1.007 -0.043
HETATM  4  O  UNK  0     -0.506  0.971 -0.325
HETATM  5  H  UNK  0      1.986 -0.125  0.136
HETATM  6  H  UNK  0      1.294  0.980  1.340
HETATM  7  H  UNK  0      1.191 -0.763  1.588
```

Another example

```
ATOM    1  C1  UNK    1     -2.059 -1.281  0.431 -0.048000      c1
ATOM    2  F   UNK    1     -0.208  0.906 -2.304 -0.128000      f
ATOM    3  F1  UNK    1     -0.868  1.485 -0.256 -0.128000      f
ATOM    4  F2  UNK    1     -1.301 -1.635 -1.970 -0.076000      f
ATOM    5  F3  UNK    1      2.892 -0.315  0.069 -0.186000      f
ATOM    6  F4  UNK    1      1.797  1.550  0.547 -0.186000      f
ATOM    7  O   UNK    1      0.693 -0.237 -0.478 -0.281000      os
ATOM    8  C   UNK    1     -0.465  0.424 -1.038  0.331000      c3
ATOM    9  C1  UNK    1     -1.630 -0.594 -1.134 -0.071000      c3
ATOM   10  C2  UNK    1      1.906  0.532 -0.368  0.438000      c3
ATOM   11  H   UNK    1     -2.518 -0.102 -1.539  0.220000      h2
ATOM   12  H1  UNK    1      2.214  0.938 -1.334  0.111000      h3
```

COLUMNS	DATA TYPE	DEFINITION
1 - 4 / 1-6	RecordName	"ATOM" / "HETATM"
7 - 11	Integer	Atom number
12	Blank space	
13 - 16	Atom symbol	Atom name
17	Blank space	
18 - 20	Residue name	Residue name
21	Blank space	
22 - 26	Integer	Residue number
27	Blank space	
28 - 38	Float	Orthogonal coordinates for X in Å
39 - 46	Float	Orthogonal coordinates for Y in Å
47 - 54	Float	Orthogonal coordinates for Z in Å

SOME IMPORTANT INSTRUCTIONS

1. Only one small molecule at a time is required.
2. The Atom number should increase in serial order starting with '1'.
3. The Residue number should start with '1'.
4. Atom symbol (like C, H, O, Cl) is preferred at 13th or 14th position in the PDB format.
5. The chain should not be specified by any separate variable like 'A' , 'B' etc.
6. TPACM4 required only record name, atom number, atom symbol, residue name, residue number, and X, Y, Z coordinate at proper position as maintained above.