Partial atomic charge calculation of small molecules
TP*ACM*4

README FILE

A SAMPLE PDB FILE IS SHOWN HERE

HIGHLIGHT THE MAIN FORMAT FEATURES

```
000000000100000000020000000003000000000400000000050000000006000000000700000000
123456789012345678901234567890123456789012345678901234567890123456789012345678

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 Cl   UNK     1      -2.059  -1.281   0.431 -0.048000         cl
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	Record Name	"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 X 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 13^{th} or 14^{th} 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.