```
!!
!!        ___                    _                       __ _
!!       / __|  _  _   ___ | |_  ___  _ __    __  ___  _ _  / _(_)  __ _
!!       \__ \ | || | (_-< |  _|/ -_)| '  \  / _|/ _ \| ' \|  _|| | / _` |
!!       |___/  \_, | /__/  \__|\___||_|_|_| \__|\___/|_||_||_|  |_| \__, |
!!             |__/                                                   |___/
!!
!! PyRED - http://q4md-forcefieldtools.org
!! Compatible with Python versions 2.5 up to 2.7.18
!!
!!            The System.config file
!! http://q4md-forcefieldtools.org/REDServer-Development/Documentation/System.config
!!    Description of the keywords used by PyRED
!!          Documentation of February 2015
!!        Last update of this documentation:
!!              March 25th, 2025
!!
!! Always reload this file, when reading this file with a web browser to be sure to
!! access to the latest version!
!!
!! The System.config file is optional.
!! It is provided as an input within the archive file to overwrite default tasks.
!! See http://q4md-forcefieldtools.org/Tutorial/Mini-HowTo-InputFiles.pdf
!!      http://q4md-forcefieldtools.org/Tutorial/Tutorial-4.php
!!
!! Keywords provided in the System.config file are related to the tasks carried out by
!! the PyRED program.
!!
!! If an error is made in a keyword, the PyRED job is executed with the default value.
!!
!! The System.config file only contains plain text (no rich text file format).
!! It has to be prepared or modified using a text editor such as the vi, gedit, nedit
!! geany, or the notepad.
!!
!! Note: FF = empirical force field(s)
!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!                                                                                    !!
!!    A KEYWORD IN THE SYSTEM.CONFIG FILE MUST BE ACTIVATED TO BE USED BY PyRED:      !!
!! A KEYWORD IS ACTIVATED BY DELETING THE '#' CHARACTER AT THE BEGINNING OF A LINE    !!
!! ACTIVATE A KEYWORD ONLY WHEN NECESSARY AND AFTER FULLY UNDERSTANDING ITS MEANING !!
!!                                                                                    !!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!
!! Maximal amount of memory available in MegaBytes (MB) for the QM jobs
!!  256 MegaBytes (MB) = 32 MegaWords (MW)
!!    See http://deviceanalytics.com/memcalc.php
!!  2048 MB = 2 GB = 256 MW (64 bits machine)
!! The default of MAXMEMVAL = 8192
!! (The user does NOT control this keyword, which is managed by the queueing system)
# MAXMEMVAL = 8192
!!
!! Number of processor(s) used in parallel (in QM calculations)
!! The default of NP = 8
!! (The user does NOT control this keyword, which is managed by the queueing system)
# NP = 8
!!
!! GAMESS (i. e. GAMESS-US), FIREFLY (i. e. PC-GAMESS), or GAUSSIAN
!!              (g16, g09 or g03) is used in QM calculations
!! GAMESS   https://www.msg.chem.iastate.edu/gamess/
!! FIREFLY  http://classic.chem.msu.su/gran/gamess/
```

```
!! GAUSSIAN https://gaussian.com/
!! This keyword is controlled by the user, through the R.E.D. Server Development
!!    web site during the input submission procedure
!! TO ACCESS TO THE GAUSSIAN PROGRAM, REGISTER AND USE YOUR PRIVATE ACCOUNT
# QMSOFT = GAUSSIAN
!!
!! Language used in the PyRED log file
!! EN (English), FR (French) or CN (Chinese)
!! The default of LANGUAGE = EN
!! Not yet implemented: only the English language is available
# LANGUAGE = EN
!!
!! The PyRED log file in the TXT or HTML format
!! The default of TYPE_LOG = TXT
!! Not yet implemented: only the TXT file format is available
# TYPE_LOG = TXT
!!
!! Directory name where the final data are stored
!! The default of DIR = Data-R.E.D.Server
!! (The user does not control this keyword, which is managed by the queueing system)
# DIR = Data-R.E.D.Server
!!
!! Geometry optimization will be carried out if OPT_Calc = ON
!! OFF No geometry optimization is done & QM output file(s) have to be provided
!! OFF1 Geom. opt. is skipped and the PDB input file(s) is(are) directly used in MEP
!!    computation (OFF1 has to be avoided as much as possible)
!! ON  'Tight' geom. opt. (default for charge derivation)
!! ON1 'VeryTight' geom. opt.
!! ON2 'Normal' geom. opt. (default in QM programs; but not in PyRED)
!! ON3 'Loose' geom. opt. (useful only in the debug mode)
!! The default of OPT_Calc = ON
!! Using OPT_Calc = ON is in some circumtances (example: floppy molecules) difficult
!!    to satisfy/time consumming: using OPT_Calc = ON2 is an alternative in these cases
# OPT_Calc = ON
!!
!! MEP & charges will be calculated if MEPCHR_Calc = ON
!! The default of MEPCHR_Calc = ON
!! OFF only geometry optmization is carried out
# MEPCHR_Calc = ON
!!
!! Control the SCF convergence criterion for the MEP computation step
!! The absence of this keyword leads to the use of default values (recommended)
!! Using SCFCONVER_MEP = 6 can help decreasing the cpu time or avoiding
!!     convergence failure in some particular cases (to be used with care)
!! Using SCFCONVER_MEP = 7 (or 8) is the default in PyRED
!! Using SCFCONVER_MEP = 8 is recommended, when using the MP2 method
!! (not applyable if MOD_GAUSSIAN_JOB = Complex)
# SCFCONVER_MEP = 5, 6, 7 or 8
!!
!! Charges are re-fitted & FF libraries re-built from a previous PyRED job.
!!    If Re_Fit = ON then OPT_Calc = OFF & MEPCHR_Calc = OFF
!! A previous job (a 'Data-R.E.D.Server' directory) has to be provioded by the
!!    user in the archive file)
!! The default of Re_Fit = OFF
# Re_Fit = OFF
!!
!! Normal or Complex job when using the Gaussian program
!! - For organic molecules the Normal mode should be enough
!!    (although benzene is a good example to be tested)
!! - For bio-inorganic molecules the Complex mode and DFT based charge models
!!    are recommended
!! The Complex mode involves various additional computation/checking, that are
!!    cpu demanding, and that require more time!
!! To understand the use of the Complex mode, see:
!! http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo21.pdf
```

```
       !! The default of MOD_GAUSSIAN_JOB = Normal
       # MOD_GAUSSIAN_JOB = Normal
       !!
       !! Request frequencies to be computed in an additional step using the theory level
       !!    defined for geometry optimization
       !! Useful to check if the stationary point found during the geometry optimization
       !!    step is a real minimum. The determination of frequencies is cpu demanding,
       !!    and require non-negligible computation time
       !! It is recommended to set Freq_Calc = ON
       !! The default of Freq_Calc = OFF as this computation is cpu demanding
       # Freq_Calc = OFF
       !!
       !! Charge derivation procedure:
       !! Notation: Single point MEP computation//Geometry optimization
       !! RESP-A1:  HF/6-31G(d)//HF/6-31G(d)                          Connolly algo.  2 RESP fit(*1)
       qwt=.0005/.0010
       !!   Used in the Cornell (1995), Kollman (1996), Cheatham (1998), Wang (1999), and Hornak (2006)
       et al. FF
       !! RESP-B1:  B3LYP/cc-pVTZ SCRF(IEFPCM,Solv.=Ether)//HF/6-31G(d,p) Connolly algo.  2 RESP fit(*1)
       qwt=.0005/.0010
       !!   Used in the Duan (2003) et al. FF
       !!   See http://q4md-forcefieldtools.org/REDServer-Development/Documentation/Charge-models.php
       !!   Be sure to use the Gaussian 2003 program because the IEFPCM solvation model has changed in
       Gaussian 2009
       !! RESP-C1: HF/6-31G(d)//HF/6-31G(d)                           CHELPG algo.   2 RESP fit(*1)
       qwt=.0005/.0010
       !!
       !! RESP-O1: HF/6-31G(d)//HF/6-31G(d)                           Connolly algo.  2 RESP fit(*2)
       qwt=.000184/.000184
       !!   Defined for the OPLS FF
       !! RESP-P1:  HF/6-31G(d)//HF/6-31G(d)                          CHELPG algo.   2 RESP fit(*2)
       qwt=.000184/.000184
       !!
       !! RESP-A2:  HF/6-31G(d)//HF/6-31G(d)                          Connolly algo.  1 RESP fit(*1)
       qwt=.0100
       !! RESP-C2:  HF/6-31G(d)//HF/6-31G(d)                          CHELPG algo.   1 RESP fit(*1)
       qwt=.0100
       !!   Used in the Glycam FF
       !! ESP-A1:   HF/6-31G(d)//HF/6-31G(d)                          Connolly algo.  1 ESP fit(*3)
       qwt=.0000
       !!   Used in CHARMM and OPLS FF parameterization
       !! ESP-C1:   HF/6-31G(d)//HF/6-31G(d)                          CHELPG algo.   1 ESP fit(*3)
       qwt=.0000
       !!   Used in CHARMM and OPLS FF parameterization
       !!
       !! ESP-A2:   HF/STO-3G//HF/STO-3G                              Connolly algo.  1 ESP fit(*4)
       qwt=.0000
       !!   Used in the Weiner et al. FF
       !! ESP-C2:   HF/STO-3G//HF/STO-3G                              CHELPG algo.   1 ESP fit(*4)
       qwt=.0000
       !!
       !! RESP-X1:  B3LYP/6-31G(d)//B3LYP/6-31G(d)                    Connolly algo.  2 RESP fit(*1)
       qwt=.0005/.0010      i.e. fit = RESP-A1
       !! RESP-Y1:  B3LYP/6-31G(d)//B3LYP/6-31G(d)                    CHELPG algo.   2 RESP fit(*1)
       qwt=.0005/.0010      i.e. fit = RESP-C1
       !!
       !! RESP-X2:  B3LYP/6-31G(d)//B3LYP/6-31G(d)                    Connolly algo.  1 RESP fit(*1)
       qwt=.0100            i.e. fit = RESP-A2
       !! RESP-Y2:  B3LYP/6-31G(d)//B3LYP/6-31G(d)                    CHELPG algo.   1 RESP fit(*1)
       qwt=.0100            i.e. fit = RESP-C2
       !!
       !! ESP-X1:   B3LYP/6-31G(d)//B3LYP/6-31G(d)                    Connolly algo.  1 ESP fit(*3)
       qwt=.0000            i.e. fit = ESP-A1
       !! ESP-Y1:   B3LYP/6-31G(d)//B3LYP/6-31G(d)                    CHELPG algo.   1 ESP fit(*3)
       qwt=.0000            i.e. fit = ESP-C1
```

```
        !!
        !! RESP-X11: B3LYP/6-31G(d)//B3LYP/6-31G(d)                          Connolly algo.  3 RESP fit(*5)
        qwt=.0000/.0005/.0010 i.e. fit = 1 ESP + RESP-A1
        !! RESP-Y11: B3LYP/6-31G(d)//B3LYP/6-31G(d)                          CHELPG algo.    3 RESP fit(*5)
        qwt=.0000/.0005/.0010 i.e. fit = 1 ESP + RESP-C1
        !!
        !! RESP-X22: B3LYP/6-31G(d)//B3LYP/6-31G(d)                          Connolly algo.  2 RESP fit(*5)
        qwt=.0000/.0100      i.e. fit = 1 ESP + RESP-A2
        !! RESP-Y22: B3LYP/6-31G(d)//B3LYP/6-31G(d)                          CHELPG algo.    2 RESP fit(*5)
        qwt=.0000/.0100      i.e. fit = 1 ESP + RESP-C2
        !!
        !! (1*) RESP fit: Hyperbolic restraint; Charge equivalencing is carried out during the fit.
        !!    Bayly et al. J.Phys.Chem. 1993, 97, 10269.
        !! (2*) RESP fit: Quadratic restraint; Charge equivalencing is carried out during the fit.
        !!    Henchman & Essex J.Comput.Chem. 1999, 20, 483.
        !! (3*) ESP fit:  Charge equivalencing is carried out during the fit.
        !! (4*) ESP fit:  Charge averaging is carried during the fit.
        !!    Weiner et al. J.Comput.Chem. 1986, 7, 230.
        !! (5*) ESP fit followed by one or two hyperbolic restraint fits
        !!
        !! DEBUG, DEBUG1, DEBUG2:
        !! Do not use the DEBUG modes for generating charge values!
        !! The DEBUG modes can be used to (i) quickly get an idea of what is done,
        !! (ii) debug the source code & (iii) create new functionalities.
        !! The default of CHR_TYP = RESP-A1
        # CHR_TYP = RESP-A1
        !!
        !! Method used in geometry optimization
        !! Limited to the use of the Gaussian program by now
        !! Default i.e. the method implemented for the selected charge model
        !! HF
        !! MP2
        !! OPBE   i.e. DFT
        !! PBEPBE i.e. DFT
        !! BP86   i.e. DFT
        !! B3P86  i.e. DFT
        !! B3PW91 i.e. DFT
        !! B3LYP  i.e. DFT
        !! O3LYP  i.e. DFT
        !! X3LYP  i.e. DFT
        !! BLYP, WB97XD, M06, M062X, B97D, B97D3,
        !! PW6B95, PW6B95D3 (i.e. DFT) were added after user requests
        !! Do you need another option?
        !!   contact us: contact_at_q4md-forcefieldtools.org
        # METHOD_OPTCALC = Default
        !!
        !! Basis set for geometry optimization
        !! Limited to the use of the Gaussian program by now
        !! Default i.e. the basis set implemented for the selected charge model
        !! STO-3G
        !! STO-6G
        !! 3-21G
        !! 6-31G(d)
        !! 6-31G(d,p)
        !! 6-31+G(d)
        !! 6-31+G(d,p)
        !! 6-31++G(d,p)
        !! 6-311G(d)
        !! 6-311G(d,p)
        !! 6-311+G(d)
        !! 6-311+G(d,p)
        !! 6-311++G(d,p)
        !! cc-pVDZ
        !! cc-pVTZ
        !! SCRF(IEFPCM,Solvent=Water) or SCRF(IEFPCM,Solvent=Ether) can also be
```

```
!!    added to 6-31G(d) -> cc-pVTZ
!! Do you need another option?
!!    contact us: contact_at_q4md-forcefieldtools.org
# BASSET_OPTCALC = Default
!!
!! Method used in MEP computation
!! Limited to the use of the Gaussian program by now
!! Default i.e. the method implemented for the selected charge model
!! HF
!! MP2
!! OPBE   i.e. DFT
!! PBEPBE i.e. DFT
!! BP86   i.e. DFT
!! B3P86  i.e. DFT
!! B3PW91 i.e. DFT
!! B3LYP  i.e. DFT
!! O3LYP  i.e. DFT
!! X3LYP  i.e. DFT
!! BLYP, WB97XD, M06, M062X, B97D, B97D3,
!! PW6B95, PW6B95D3 (i.e. DFT) were added after user requests
!! Do you need another option?
!!    contact us: contact_at_q4md-forcefieldtools.org
# METHOD_MEPCALC = Default
!!
!! Basis set for MEP computation
!! Limited to the use of the Gaussian program by now
!! Default i.e. the basis set implemented for the selected charge model
!! STO-3G
!! STO-6G
!! 3-21G
!! 6-31G(d)
!! 6-31G(d,p)
!! 6-31+G(d)
!! 6-31+G(d,p)
!! 6-31++G(d,p))
!! 6-311G(d)
!! 6-311G(d,p)
!! 6-311+G(d)
!! 6-311+G(d,p)
!! 6-311++G(d,p)
!! cc-pVDZ
!! cc-pVTZ
!! aug-cc-pVDZ
!! aug-cc-pVTZ
!! SCRF(IEFPCM,Solvent=Water) or SCRF(IEFPCM,Solvent=Ether) can also be
!!    added to 6-31G(d) -> aug-cc-pVTZ
!! Do you need another option?
!!    contact us: contact_at_q4md-forcefieldtools.org
# BASSET_MEPCALC = Default
!!
!! Surface options when using the Connolly surface algo. in MEP computation
!! Limited to the use of the Gaussian program by now
!! Default is to use 4 surfaces (1.4, 1.8, 2.0 and 2.2 Ang.) with a density
!!    of 0.28 pt per square au
!! See 'Overlay 6' in the Gaussian doc. https://gaussian.com/overlay6/
!!    for other options:
!! IOp(6/33=2,6/41=X,6/42=Y); X = 4,6,8,10; Y = 1-6,12,18
!!    Replace X by 4, 6, 8 or 10 and Y by 1, ..., 6, 12 or 18
!! IOp(6/33=2,6/41=10,6/42=17) by U. Ryde
!!    http://signe.teokem.lu.se/ulf/Methods/resp.html
!! 6/33=2 (already implemented in PyRED): print the MEP in the output (not documented)
!! Do you need another option?
!!    contact us: contact_at_q4md-forcefieldtools.org
# SURFMK_MEPCALC = Default
!!
```

```
!! Strip Gaussian output in agreement with our licence with Gaussian Inc.
!! The default of STRIP = ON
!! (The user does not control this keyword, which is managed by the queueing system)
# STRIP = ON
!!
!! STATS = ON or OFF for running the statistics module, which analyze atomic charges
!! values (ESP, RESP, Mulliken...)
!! The default of STATS = ON
# STATS = ON
!!
!! Correct charge value rounding off errors at an accuracy defined by the user
!! 6: correction at +/- 1.10-6 e
!! 5: correction at +/- 1.10-5 e
!! 4: correction at +/- 1.10-4 e
!! 3: correction at +/- 1.10-3 e (pay attention)
!! 2: correction at +/- 1.10-2 e (pay a lot of attention)
!! 1: correction at +/- 1.10-1 e (do not use)
!! 0: no correction is performed
!! The default of COR_CHR = 4
# COR_CHR = 4
!!
!! FF library file format generated by PyRED
!! MOL2: See http://q4md-forcefieldtools.org/Tutorial/leap-mol2.php
!! MOL3: See http://q4md-forcefieldtools.org/Tutorial/leap-mol3.php
!! MOL2-TYPEATOM: MOL2 file format with atom names and types inverted
!! The default of OUTPUT_FORMAT = MOL3
# OUTPUT_FORMAT = MOL3
!!
!! LMTFRG-INTRAMCC = ON or OFF
!! Limit the number of generated molecular fragments when requesting
!!    intra-molecular charge constraints (with the 'R' flag)
!! The default of LMTFRG-INTRAMCC = ON
!! LMTFRG-INTRAMCC = ON allows generating a single molecular fragment
!!    i.e. that corresponding to all the requested intra-molecular charge
!!    constraints (the user is generally only interested in this fragment)
!! LMTFRG-INTRAMCC = OFF allows generating all the combinations of molecular
!!    fragments corresponding to the different intra-molecular charge
!!    constraints. This can lead to an important number (and often useless)
!!    of molecular fragments
# LMTFRG-INTRAMCC = ON
!!
!! Generation of atom types in agreement with the following FF
!! GLYCAMFF04:     Glycam04 from the Amber10 distribution
!!                 Kirschner & Woods, Proc.Natl.Acad.Sci.USA 2001, 98, 10541.
!!                 Basma et al. J.Comput.Chem. 2001, 22, 1125.
!!                 Kirschner & Woods, J.Phys.Chem.A 2001 105, 4150.
!!     Application: Cezard et al. Phys.Chem.Chem.Phys. 2011, 13, 15103.
!!
!! AMBERFF94:      Cornell et al. J.Am.Chem.Soc. 1995, 117, 5179.
!!
!! AMBERFF96:      Cornell et al. J.Am.Chem.Soc. 1995, 117, 5179.
!!                 Kollman et al. Computer Simulation of Biomolecular Systems
!!                   ed. Wilkinson, Weiner & van Gunsteren, Elsevier, Escom,
!!                   The Netherlands, 1997, 3, 83-96.
!!
!! AMBERFF98:      Cornell et al. J.Am.Chem.Soc. 1995, 117, 5179.
!!                 Cheatham et al. J.Biomol.Struct.Dyn. 1999, 16, 845.
!!
!! AMBERFF99:      Cornell et al. J.Am.Chem.Soc. 1995, 117, 5179.
!!                 Wang et al. J.Comput.Chem. 2000, 21, 1049.
!!
!! AMBERFF99SB:    Wang et al. J.Comput.Chem. 2000, 21, 1049.
!!                 Hornak et al. Proteins 2006, 65, 712.
!!
!! AMBERFF99SBBSC: Wang et al. J.Comput.Chem. 2000, 21, 1049.
```

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        !!                     Hornak et al. Proteins 2006, 65, 712.
        !!                     Perez et al. Biophys.J. 2007, 92, 3817.
        !!
        !! AMBERFF03:      Wang et al. J.Comput.Chem. 2000, 21, 1049.
        !!                     Duan et al. J.Comput.Chem. 2003, 24, 1999.
        !!
        !! AMBERFF10:      Wang et al. J.Comput.Chem. 2000, 21, 1049.
        !!                     Hornak et al. Proteins 2006, 65, 712.
        !!                     Perez et al. Biophys.J. 2007, 92, 3817.
        !!                     Banas et al. J.Chem.TheoryComput. 2010, 6, 3836.
        !!                     Zgarbov et al. J.Chem.TheoryComput. 2011, 7, 2886.
        !!
        !! OFF:            No FF atom type is generated
        !! Use the Gaussian 2003 program, when requesting the AMBERFF03 FF:
        !!    (the IEFPCM solvation model has changed in Gaussian 2009)
        !! The default of FFPARM = AMBERFF10
        !! See also:
        !! http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo5.pdf
        !!    To use GAFF, GAFF2 and AmberFF14SB, AmberFF19SB
        !! http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo6.pdf
        !!    To use GLYCAM 2006 or OPLS
        # FFPARM = AMBERFF10
        !!
        !! Rounding off of FF parameters in the generated FF parameter files
        !! The default of FFPARM_ROUND = ON
        # FFPARM_ROUND = ON
        !!
        !! Energy decomposition is carried out using the FF
        !! MM energy values are computed only if no missing FF parameter is found
        !! (see the 'frcmod.unknown' file)
        !! The default of ENERGY_CALC = ON
        # ENERGY_CALC = ON
        !!
        !! Scaling factor for 1-4 electrostatic energy values
        !! The default of SCALE_FACTOR_EEL = 0.8333
        !!    i.e. 1/SCEE = 1/1.2 = 0.8333
        # SCALE_FACTOR_EEL = 0.8333
        !!
        !! Scaling factor for 1-4 vdW energy values
        !! The default of SCALE_FACTOR_VDW = 0.5000
        !!    i.e. 1/SCNB = 1/2 = 0.5
        # SCALE_FACTOR_VDW = 0.5000
        !!
        !! Control the generation of Jmol and/or JSmol applets within the php interface
        !! The default of JAVA_APPLET = OFF
        !!    if JAVA_APPLET = OFF only JSmol applets are generated
        !!    if JAVA_APPLET = ON Jmol and JSmol applets are generated
        # JAVA_APPLET = OFF
```