RADDOSE

```
using raddose at Vanderbilt University
 first use sbset to set up ccp4
 then set an alias
> alias raddose '/sb/apps/raddose/raddose'
```

NAME

raddose - calculations of absorbed X-ray dose by protein crystals

SYNOPSIS

raddose
[Keyworded input]

KEYWORDED INPUT

The available keywords are:

CELL, VOLUME, NMON, NRES, NDNA, NRNA, PATM, SATM, SOLVENT, ENERGY, WAVLENGTH,
PHOSEC, BEAM, CRYSTAL, IMAGES, EXPOSURE, REMARK,,CONVH, HEAT, END

In the description below, optional items are in [], keywords are in uppercase, parameters are in lowercase. The input is case-insensitive.

CELL a b c [alpha beta gamma]

Cell dimensions in Angstroms, alpha beta and gamma default to 90 degrees.

VOLUME v

If the CELL card is not given, the unit cell volume may be given in cubic Angstroms.

NMON n

Number of monomers, n in the unit cell. (N.B. NOT the asymmetric unit).

NRES n

Number of amino acid residues in a single chain. The number and types of atoms are calculated assuming an average amino acid content defined as
amino acid = 5 C + 1.35 N + 1.5 O + 8H
Sulfur atoms should be added explicity with the PATM keyword

NRNA n

Number of RNA nucleotides in a monomer. The number and types of atoms are calculated assuming an average nucleotide content defined as.
mean nucleotide = 11.25H + 9.5C + 3.75N + 7O + 1P
If a more accurate estimate is required individual atoms may be entered explicitly with the PATM keyword.

NDNA n

Number of DNA deoxynucleotides in a monomer. The number and types of atoms are calculated assuming an average deoxynucleotide content defined as.
mean Nucleotide = 11.75H + 9.75C + 4N + 6O + 1P
If a more accurate estimate is required individual atoms may be entered explicitly with the PATM keyword.

PATM <Element> no-atoms [<element> no-atoms]...

Define atoms to add to the protein part of the scattering as no. of atoms per monomer

e.g. PATM S 10 Se 2 !Add 10 sulfur and 2 selenium atoms per monomer

SATM <Element> conc-mM [<element> conc-mM]...

Define the concentration of elements (not including water) in the solvent in millimoles per litre. Do not define these for oxygen and lighter elements (ie no PEG, but yes for ammonium sulfate).

e.g. SATM Na 1000 Cl 1000 ! 1M sodium chloride

SOLVENT solv_proportion

The fraction of the unit cell that is occupied by solvent. If not given explicity, this value is estimated from NRES, NRNA and NDNA using 1.35 g/ml for protein, 2.0 g/ml for RNA and DNA.

SPLINOR Element filename

Optional keyword, to use empirical absorption coefficients from a CHOOCH splinor file. Only one SPLINOR keyword may be used.

e.g. SPLINOR Se se_scan.splinor

ENERGY energy_keV

The energy of the beam in keV. The beam energy may also be input with the WAVELENGTH keyword.

RANGE low_keB high_keV [step_keV]

Optional range of energies for which to calculate doses. The step size defaults to 0.01 keV

HENDLI dose_Gray

The radiation dose limit in Gray. Defaults to 2E7 Gray.

WAVELENGTH wavelength

The wavelength of the incident beam in Angstrom.

If no ENERGY or WAVELENGTH card is given, a wavelength of 1.54 A (8.05 keV) is used, corresponding to copper K_alpha radiation.

PHOSEC psec

The flux of the beam in photons per second.

BEAM xbeam ybeam

Beam size in mm

GAUSS x-fwhm y-fwhm

Optional keyword, giving the full-width-half-maxima in mm of a Gaussian beam profile. If this keyword is not given, a uniform beam is assumed.

CRYSTAL xcryst ycryst zcryst

Crystal dimensions x,y,z in mm.

IMAGES no_images

The number of images taken.

EXPOSURE exp_time

Exposure time per image in seconds.

CONV convh

Optional - the convective heat transfer coefficient in W m-2 K-1. Default value 320. Don't change unless you think you know what you are doing.

HEAT cp

Optional - Specific Heat Capacity of the Crystal in J/kg/K. Defaults to 500. Don't change unless you think you know what you are doing.

END

The end of input tokens

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BUILDING

compile with something like.

```
g77 -O -w -fno-second-underscore -fno-globals -fno-automatic -o raddose
name2z.f z2name.f mucal.f upcase.f raddose.f -L$CCP4_LIB  -lccp4
```

A CCP4 environment must be present.

EXAMPLES

```
# HEWL Dose calculations ##################################
#!/bin/sh
raddose <<EOF
REMARK tetragonal HEWL dose calculations
CELL 78 78 38 90 90 90
NMON 8
NRES 129
PATM S 10
SATM Na 1000 Cl 1000
CRYSTAL 0.2 0.2 0.2
BEAM 0.15 0.15
ENERGY 12.65
PHOSEC 1E12
IMAGES 100
EXPOSURE 1
END

EOF
```