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{ Definition to access to MXD objects for MXD-V4.1.0.0 }

type $lsq_coef  is [lsq_vexp,baselex] float,
   $int_cte  is [no_lsq,readonly,baselex] integer,
   $int_fix  is [no_lsq]           integer,
   $word_int  is [word]           integer,
   $byte_int  is [byte]           integer,
   $flt_fix  is [no_lsq]           float,
   lsq_var    is [lsq_var]         float,
   sfloat     is [sigma]          float,
   data_field is [dat_field]      float,
   lsq_parm   is [lsq_parm]       wild_object,
   trans_mat  is                 array[12] of float;

begin
  include $sys_mxdlib||'mxd_lsq.mxd_env';

  item lsqblock:I$lsqblock is
    dmp*, mrq*: $flt_fix
  end;

  item item_block phase:I$phase is
    scale, aa, bb*, cc*, al*, be*, ga*: float
  end;

  item wavevect( rat*: $int_cte ):I$wavevect is
    qx*, qy*, qz*: float
  end for phase;

  item npoladir:I$npoladir is
    hx*, hy*, hz*, efu*, efd*, f2_corr*: float
  end for phase;

  item symtry:-I$symtry is
    m11, m12, m13: $int_fix; t1: $flt_fix;
    m21, m22, m23: $int_fix; t2: $flt_fix;
    m31, m32, m33: $int_fix; t3: $flt_fix
  end for phase;

  item item_block atom_group:I$atmgroup is
    transf*: trans_mat
  end for phase, atom_group;

  item atom:I$atom is
    rdf, idf*,
    pop,
    x, y, z,
    b11, b22*, b33*, b12*, b23*, b31*: float
  end for phase, atom_group;

  item catom = atom:I$catom;

  item moment( atm: atom; qv*: wavevect ):I$moment is
    frm,
    rmx, rmy, rmz,
    imx*, imy*, imz* : float
  end for phase, atom_group;

  item pmoment = moment:I$moment for phase;

  item mdsdsp( atm: atom; qv: wavevect ):I$mdsdsp is
    rux*, ruy*, ruz*,
    iux*, iuy*, iuz* : float
  end for phase, atom_group;

  item pmdsdsp = mdsdsp:I$mdsdsp for phase;

  item lsq_constraint:I$constraint is
    calc, obs, sg, we*: float
  end;

  lsq_directive center:D$center for phase;
  lsq_directive lattice( string ):D$lattice for phase;
  lsq_directive space_group( string ):D$space_group for phase;

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lsq_directive fixed( lsq_var& * ):D$fixed;
lsq_directive unfixed( lsq_var& * ):D$unfixed;
lsq_directive limits( float, float, lsq_var& * ):D$limits;

lsq_directive lsq_option[ float, float ]:D$option;
lsq_directive parm_display( lsq_parm& * ):D$dsplpar;

$lsq_coef      $h:C$h,          $k:C$k,          $l:C$l,
               $rh:C$rh,          $rk:C$rk,          $rl:C$rl,
               $hh:C$hh,          $kk:C$kk,          $ll:C$ll, $sithsl:C$sithsl,
               $sh:C$sh,          $sk:C$sk,          $sl:C$sl,
               $qx:C$qx,          $qy:C$qy,          $qz:C$qz,
               $hx:C$hx,          $hy:C$hy,          $hz:C$hz,
               $fnr:C$fnr,         $fni:C$fnri,
$fmxr:C$fmxr, $fmyr:C$fmyr, $fmzr:C$fmzr,
$fmxi:C$fmxi, $fmyi:C$fmyi, $fmzi:C$fmzi,
$npola:C$npola, $obs:C$obs,   $sig:C$sig, $weight:C$weight,
$calc:V$dat$calc,   $fn2:V$dat$fn2,   $fm2:V$dat$fm2, $f2pola:V$dat$f2pola;

item hkl_xf2( scale*, lambda*, fn2_corr*, fm2_corr*, dyn_weight*: float ):I$dathkl_xf2 data is
    ih, ik, il, nq*, mul*, npola*: integer;
    nvw*: wavevect; npadir*: npoladir; npha*: phase;
    isent*?, selnb*: integer;
    obs, sg*, we*: float
end + 16;

item hkl_xsf = hkl_xf2:I$dathkl_xsf;
item hkl_xray = hkl_xf2:I$dathkl_xray;

item hkl_nf2 = hkl_xf2:I$dathkl_nf2;
item hkl_nsf = hkl_xf2:I$dathkl_nsf;
item hkl_nray = hkl_xf2:I$dathkl_nray;

$lsq_coef $x0:C$y_x, $yobs:C$y_obs, $ysg:C$y_sg, $ywe:C$y_weight;

item curve:I$datcurve data is
    x0: float;
    isent*?: integer;
    yobs, sg*, we*: float
end + 16;

$lsq_coef $lchi2:C$lchi2, $cchi2:C$cchi2, $lmaxf:C$lmaxf, $cmaxf:C$cmaxf;

end;

lsqblock^      c$lsqblock:-1;
phase^          c$phase:-1;
wavevect^       c$wavevect:-1;
npoladir^       c$npoladir:-1;
symtry^         c$symtry:-1;
atom_group^    c$atom_group:-1;
atom^           c$atom:-1;
catom^          c$catom:-1;
moment^         c$moment:-1;
mdsdsp^         c$mdsdsp:-1;

$int_cte no     := 0, yes     := 1, always := 2;
{ End of mxd environment file }

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