

z14xcotrin.f
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A set of subroutines to interpolate the OPAL opacity tables in the six input variables Z, X, exC, exO, T6, and R (where $R = \text{RHO} / T6^3$). Optionally, this can be extended by allowing interpolation in opacities for compositions where the C, N, O, and Ne in the metallicity Z have been interconverted by nuclear burning, and/or the OPAL opacity tables can be extended by molecular opacities (at low temperatures) and/or conductive opacities (at high densities).

Send any questions/comments/bug-reports to boothroy@cita.utoronto.ca

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INTRODUCTION AND UPDATE HISTORY
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-----Arnold I. Boothroyd: VERSION of SEPTEMBER 7, 2007-----z14xcotrin21.f
(Default version of this program needs 23.9 Mb of matrix storage.)

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OPAL 1995: Reference: C.A. Iglesias & F.J. Rogers (1996), ApJ, 464, 943-953
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Note OPAL opacities are available at http://www-phys.llnl.gov/Research/OPAL/
This program is from http://www.cita.utoronto.ca/~boothroy/kappa.html
*****
1995 OPAL opacities for arbitrary metallicity Z (in the range 0.0 to 0.1),
including C,O-rich opacities. Interpolation in Z can be performed when the
opacities are read in and/or when the opacity-calculation routine is called;
this choice is under user control. It is possible to obtain opacities at
arbitrary values of [O/Fe] by using the non-CO-rich opacity files 'GN93hz'
and (one of) 'Aldr96a2', 'C95hz', or 'W95hz' (but this can only be done at
the time when the opacities are being read in, not subsequently when the
opacity-calculation routine is called). Arbitrary hydrogen abundances and
arbitrary amounts of excess carbon and oxygen are always allowed. Uses the
40 OPAL opacity files Gz???.x?? (also checks for earlier names Gx??z* ).
--ALSO: accurate opacity values can be interpolated as a function of varying
relative C, N, O, and Ne abundances (and/or a user-specified element).
--ALSO: molecular opacities may be read in and used (at low T).
--ALSO: conductive opacities may be read in and used (at high density).

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*****
Based on the old OPAL routines xcotrin.f and xcotrinz.f, modified to use
the new (1995) opacity tables Gz???.x?? and GN93hz --- similar to xcotrin21.f
(but with a significantly different interface, as described further below).
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*** UPDATED SEPTEMBER 7, 2007: from version of AUGUST 26, 2007:
--Added automatic handling of the new alpha-enhanced GS98 molecular opacities
that are now available from http://webs.wichita.edu/physics/opacity/
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*** UPDATED AUGUST 26, 2007: from version of APRIL 6, 2007:
--Fixed a bug so that FZEDGE is now set correctly to 0.0 for Z out-of-range
(previous version incorrectly set FZEDGE = 1.0 in such a case, and returned
the conductive opacity [if available], rather than a value of 1.0E+35 to
indicate that the opacity could not be computed; this bug is now fixed).
--Smoother switch-off of non-exC,O-opacity-shifts for 0.2 < exC+exO < 0.3
(this change only affects 0.2 < exC+exO < 0.3 at X > 0.03 [such compositions
should seldom actually occur], and even there has almost negligible effect).
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*** UPDATED APRIL 6, 2007: from version of MARCH 29, 2007:
--Minor modifications, for smoother extrapolation in temperature and density
(this will also improve the switchover from OPAL to conductive opacities).
--Fixed a bug that caused incorrect CNO-interpolation at X = 0.03 (actually,
for 0.029999 < X < 0.030001), yielding errors (usually, small ones) there.
--Fixed a bug that could yield an incorrect name for the default [O/Fe] file.
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*** UPDATED MARCH 29, 2007: from version of MARCH 24, 2007:
--Added updated conductive opacities: from 'Potekhin et al.' (2006).
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*** UPDATED MARCH 24, 2007: from version of FEBRUARY 2, 2007:
--Simplified quadratic interpolation routines to reduce call overhead.
--Added option to print out the names of the opacity files that were read in.
--Fixed bug in Hubbard & Lampe conductive opacity interpolation (that had

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been introduced by quadratic-interpolation formula of FEBRUARY 2, 2007).

*** UPDATED FEBRUARY 2, 2007: from version of DECEMBER 16, 2006:

--Added support for Ferguson et al. 2005 molecular opacities (essentially, updated versions of the Alexander and Ferguson 1994 molecular opacities).
 --Fixed bug in exC- and exO-interpolation at small helium abundances.
 --Modified quadratic-interpolation formulae to reduce roundoff error.

*** UPDATED DECEMBER 16, 2006: from version of NOVEMBER 23, 2006:

--Allow bzip2 (de)compression of input files (suffix '.bz2') as well as gzip (suffix '.gz') and compress (suffix '.Z').

*** UPDATED NOVEMBER 23, 2006: from version of SEPTEMBER 21, 2006:

--Some updates in the comments below, and a minor bug-fix.

*** UPDATED SEPTEMBER 21, 2006: from versions of SEPTEMBER 6 and 13, 2006:

--Fixed the (allowed) extension of OPAL opacities using conductive opacities; such extension now works correctly, when specified by the user.

*** UPDATED SEPTEMBER 6, 2006: from previous version of OCTOBER 20, 2004:

 * NOTE that BINARY OPACITY DUMPS of previous versions are INCOMPATIBLE with *
 * this new version, due to changes in the arrays: any such binary dumps *
 * MUST BE RECOMPUTED using DUMP_OPAL_OPAC with this new program version. *

--New, simpler subroutines have been added for reading in the opacities.
 --Alexander & Ferguson (1994) molecular opacity routines and storage added, with relevant subroutines to control its use (by default, it is NOT used).
 --Conductive opacity routines added, allowing use of Hubbard & Lampe (1969), & Itoh et al. (1983), Mitake et al. (1984) [by default these are NOT used].
 --Common block /opalGS98mixes/ revised, to hold the meteoritic Z-mix as well.
 --Minor bug fixed in computation of opacities that require the user-defined (nonCNO-interpolation) file CF_USER.
 --Added new routines: ASK_OPAL_Z_MIX to return abundances of components of the metallicity Z, and a few others involving opacity filename control.

*** UPDATED OCTOBER 20, 2004: from version of JUNE 30, 2004:

--Common blocks revised, to reduce the file-size of the compiled program (by refraining from initializing any parts of very large common blocks).

*** UPDATED JUNE 30, 2004: from version of MARCH 9, 2004:

--Some redundant variables removed, to avoid compiler warning messages.

*** UPDATED MARCH 9, 2004: from version of FEBRUARY 1, 2004:

--Minor bug-fix in subroutine OPAL_X_CNO_FU, to handle more correctly the previously-ignored possibility that N+Ne may have decreased relative to Z (the bug-fix does its best to prevent exC and exO from becoming negative).

*** UPDATED FEBRUARY 1, 2004: from version of JANUARY 9, 2004:

--Added subroutines DUMP_OPAL_OPAC and READ_OPAL_DUMP which allow one to store a set of opacities in unformatted binary form for future re-use (gives a large speed advantage when later one wishes to read opacities with the same inputs, at the cost of some disk space for the opacity dumpfile).
 --Added subroutines ASK_KHIGHZ_OFE and ASK_MAIN_OPAL_FILE.
 --Moved all initializations of common block variables into a BLOCK DATA, as required by some compilers; fixed a few other minor bugs.

*** UPDATED JANUARY 9, 2004: from version of AUGUST 2, 2003: minor changes:

--Added subroutines ASK_LAST_OPAC and ASK_LAST_XCNOU (which just return values contained in common blocks /E_OPAL_Z/ and /X_OPAL_Z/, respectively).
 --Fixed subroutine OPAL_X_CNO_FU so that it no longer yields an error if one calls this subroutine OPAL_X_CNO_FU before calling the subroutine READZEXCO.
 --Fixed the places where some compilers objected to the use of the string

concatenation operator.

*** UPDATED AUGUST 2, 2003: from version of APRIL 27, 2001: Add the option of using an alternate set of OPAL files (e.g., 'GS98hz' rather than 'GN93hz') to get opacities appropriate to an updated solar composition (e.g., Grevesse and Sauval 1998) --- note that the files Gz???.x?? need not be updated, as their opacities are shifted to agree with those from the file 'GS98hz'. ALSO, add the option of interpolating the opacities as a function of varying relative C, N, O, and Ne abundances (as well as in the "excess" C and O). ALSO, increase the allowed file-plus-directory name length to 255 characters (rather than 80); this affects common /opdir/ and the alternate OPAL file set, but not common /opalmixes/ (default OPAL files, 8 characters long). Also, maximum allowed T6,R extrapolation is now just over one grid spacing (instead of just under); this latter change should have negligible effect. Also, an approximation used previously when computing the abundances for mixes that are interpolated in [O/Fe] has been replaced by the exact formula (this change should also have little effect: none at all for [O/Fe]=0.0).

*** UPDATED APRIL 27, 2001: from version of MARCH 4, 2001: for more accurate X-interpolation at $X > 0.1$ (with a LARGE improvement in the accuracy as X approaches 1-Z), using the added X-values available in the file GN93hz. Also fixed a minor bug in the CO-interpolation (that could have caused small errors in the interpolated opacity, but only in the seldom-encountered situation of near-maximal CO-enrichment combined with a non-zero hydrogen abundance: $X > 0.0$ with C+O just less than 1-X-Z).

*** UPDATED MARCH 4, 2001: from version of MAY 28, 1999: add the metallicity Z to the list { X, C, O, T6, R } of variables in which the OPAL opacities can be interpolated (rather than being restricted to only a single metallicity, defined when the opacities were read in). This is required if gravitational settling of metals takes place. Also, newly added subroutines allow easier opacity-directory specification, and easier user control of how Z, T, and R edges and extrapolation are handled. Also, the opacity files Gz???.x?? and GN93hz are allowed to be in compressed form (they must have suffix .gz if they were compressed using 'gzip', or suffix .Z if they were compressed using 'compress'); any compressed opacity files will be decompressed, read in, and compressed again.

Updated MAY 28, 1999: from version of JUNE 26, 1997: to look for the CO-rich opacity file names in the newer format Gz???.x?? before trying the old format Gx??z*. Note that some opacity values in Gz001.x35 Gz004.x70 Gz050.x35 Gz100.x70 differ by roundoff amounts (+/- 0.001 in log10[kappa]) from corresponding older files Gx35z001 Gx70z004 Gx35z05 Gx70z10; also, Gz050.x35 and Gz100.x70 each omit a redundant duplicate composition table present in Gx35z05 and Gx70z10. In all other cases, the newer OPAL files Gz???.x?? are identical to the corresponding older files Gx??z*. ***** ALSO: the name of the common block that returns the opacity values has been changed from common/e/ to common/e_opal_z/ in order to avoid compilation errors when compiling using f2c (Fortran to C conversion).

 TEMPERATURES AND DENSITIES CONTAINED IN OPAL OPACITY TABLES:

The OPAL opacities are tabulated in terms of logT and logR, where
 $\log R = \log \text{RHO} - 3 * (\log T - 6)$, i.e., $R = \text{RHO} / T6^3$
 (with T being temperature in Kelvins and RHO being density in g/cm³)
 The "density" and temperature ranges contained in the tables are:
 logR : -8.0 to 1.0 [at logR = -8.0 (0.5) 1.0, i.e., delta_logRHO = 0.5]
 logT : 3.75 to 8.70 [at logT = 3.75 (0.05) 6.00 (0.10) 8.10 (0.20) 8.70]

COMPOSITIONS FOR WHICH OPACITY TABLES ARE AVAILABLE:

Type 2 OPAL Tables - including enhanced C & O (40 files):

=====

These are 40 files of the form Gz???.x?? , where the "z???" part may be any of { "z000", "z001", "z004", "z010", "z020", "z030", "z050", "z100" } and the "x??" part may be any of { "x00", "x03", "x10", "x35", "x70" }. These have 8 metallicities $Z = \{ 0.0, .001, .004, .01, .02, .03, .05, .1 \}$ and 5 hydrogen abundances $X = \{ 0.0, 0.03, 0.1, 0.35, 0.7 \}$; each pair of { X, Z } has up to 60 different compositions with varying amounts of "excess" carbon and oxygen (above that contained in Z), i.e., mixes having $\text{exC,exO} = \{ 0.0, .01, .03, .1, .2, .4, .6, 1-X-Z \}$ (such that no mix has $X+Z+\text{exC}+\text{exO} > 1.0$). These files allow fairly good interpolated opacities for $X < 0.75$ and $Z < 0.12$, with any amount of excess carbon and oxygen. This may suffice if there is not much diffusion (to yield high X values), but these opacities are NOT AT ALL ACCURATE for $X > 0.75$ (very high hydrogen abundances); opacities at $X = 1-Z$ may be off by up to an order of magnitude (unless corrected by including the Type 1 tables below).

The above files are ALWAYS read in, for one or more Z-values (as determined by your call to one of the opacity-reading subroutines).

Type 1 OPAL Tables - fixed metal distribution (by default, 4 files):

=====

file 'GN93hz' [O/Fe]=0.0: solar composition, Grevesse and Noels (1993)
 file 'Alrd96a2' [O/Fe]=0.3: alpha enhanced elements, Allard (1996)
 file 'C95hz' [O/Fe]=0.4: alpha enhanced elements, Chaboyer (1995)
 file 'W95hz' [O/Fe]=0.5: alpha enhanced elements, Weiss (1995)

Each of these 4 files contains 126 compositions: opacities at 13 Z-values $Z = \{ 0.0, 0.0001, 0.0003, 0.001, 0.002, 0.004, 0.01, 0.02, 0.03, 0.04, 0.06, 0.08, 0.1 \}$ and at 10 X-values $X = \{ 0.0, 0.1, 0.2, 0.35, 0.5, 0.7, 0.8, 0.9, 0.95, 1-Z \}$; they do NOT have enhanced-CO ("excess-C,O") compositions.

One or two of these Type 1 files will typically be read in (as determined by your call to one of the opacity-reading subroutines). For non-CO-rich cases this allows slightly improved Z-interpolation (for $Z < 0.12$) and slightly improved X-interpolation (for $0.03 < X < 0.75$); for high hydrogen abundances ($X > 0.75$), such as may result from diffusion (e.g., helium settling), the accuracy is GREATLY IMPROVED.

NOTE THAT additional Type 1 tables can be computed at the OPAL website, or may be available elsewhere. By default, this program allows for counterparts of the above 4 files with a different composition (e.g., for the Grevesse & Sauval 1998 mix: 'GS98hz', 'GS98hz_OFe.3_Alrd96a2', 'GS98hz_OFe.4_C95', and 'GS98hz_OFe.5_W95', or the more recent Asplund, Grevesse, & Sauval 2004 mix: 'AGS04hz', etc.). This program also allows for the existence of files where C, N, O, and Ne abundances are interconverted (as by nuclear burning: e.g., 'GN93hz.CtOaN', 'GN93hz.COtoN', 'GN93hz.CNotoNe'); such files can be used to enable the program to return accurate opacity values as a function of varying relative C, N, O, and Ne abundances. Some other user-specified element (or set of elements) can also be interpolated (e.g., 'GN93hz.user').

The program can also be set to use 'AGS04hz' etc., instead of the above.

Additional (OPTIONAL) non-OPAL tables: conductive and molecular opacities:
 ***** =====

-- They are available for the sake of convenience (to allow extension of the OPAL opacities to lower T and higher R), and some testing has been done to check that the switchover between tables works reasonably, but the USER MUST CHOOSE whether to read in (and use) these extensions or not.

```
'Potekhin et al.' (2006) CONDUCTIVE OPACITIES: opacity file 'condall06.d'
=====
-- Conductive opacities available: http://www.ioffe.rssi.ru/astro/conduct/
*****
***** NOTE: as of March 9, 2007: the revised/updated file condall06.d *****
***** containing conductive opacities is available on the website. *****
***** This should be an improvement over the Hubbard & Lampe (1969) *****
***** plus Itoh (1984) conductive opacities described further below. *****
*****
These 'condall06.d' electron conductivities are available in the ranges:
-6 < logRHO < 9.75      in density RHO, with spacing delta logRHO = 0.25
 3 < logT < 9          in temperature T, with spacing delta logT = 1/3
Zion = {1,2,3,4,6,8,12,16,20,26,30,36,42,48,60} mean nuclear charge

-----FROM THE ABOVE WEBPAGE: "The plasma is assumed fully ionized (electron
collisions with neutrals are neglected, the ions are assumed pointlike).
This model may be still useful for evaluation of conductivities of partially
ionized plasmas, if one uses a mean-ion model. Then the ion charge Zion
should be replaced by an effective (or average) ion charge Zeff. For
nondegenerate plasmas, the results are based on a continuation from the
degenerate domain (using Fermi-Dirac averaging) and can be considered as
order-of-magnitude estimates. For degenerate plasmas, on the contrary, the
results come from the exact theory and should be much more accurate."
"Non-magnetic conductivities have been updated 18 July 2006. The updated
codes and table have been put at this site 9 September 2007. There are two
modifications. 1. The electron-electron (ee) scattering contribution is
now included in such a way that both the cases of strongly degenerate and
nondegenerate plasmas are recovered accurately. Now the high-T limit of our
data matches the numerical tables of Hubbard & Lampe, 1968, ApJS 18, 297
(which remain the most accurate calculations of conductive opacities for
astrophysical use in nonmagnetic, nondegenerate, weakly coupled plasma).
2. The ee contribution is updated according to the results by Shternin and
Yakovlev (2006)."
```

-----References for the above (non-magnetic) electron thermal conductivities:

A. Y. Potekhin, D. A. Baiko, P. Haensel, D. G. Yakovlev (1999), "Transport properties of degenerate electrons in neutron star envelopes and white dwarf cores", *Astron. Astrophys.* 346, 345

O. Y. Gnedin, D. G. Yakovlev, A. Y. Potekhin (2001), "Thermal relaxation of young neutron stars", *Mon. Not. R. Astron. Soc.* 324, 725

P. S. Shternin, D. G. Yakovlev (2006), "Electron thermal conductivity owing to collisions between degenerate electrons", *Phys. Rev. D* 74, 043004

S. Cassisi, A. Y. Potekhin, A. Pietrinferni, M. Catelan, M. Salaris (2007) "Updated electron-conduction opacities: the impact on low-mass stellar models", *Astrophys. J.*, in press [astro-ph/0703011]

-----NOTE: the last reference above suggests that the rms ionic charge is the appropriate one for use in plasmas not so dense as to be crystalline, i.e.,

$$Z_{ion} = (\langle z^2 \rangle)^{0.5} = \sqrt{\frac{\sum_i \{ z_i * z_i * n_i \}}{\sum_i \{ n_i \}}}$$

$$= \sqrt{\frac{\sum_i \{ z_i * z_i * X_i / A_i \}}{\sum_i \{ X_i / A_i \}}}$$

where z_i is the ionic charge of element i and n_i is its number density; n_i is proportional to X_i / A_i , the mass fraction over the atomic mass.

[Correctly summing the contributions of different ions in a multicomponent plasma would be "much more complicated", according to the references.]

Also: the log of the electron thermal conductivity logCHI (stored in the file condall06.d) converts to the log of the conductive opacity logKAPPA_c via:

$$\log KAPPA_c = \log(16 * \sigma / 3) + 3 * \log T - \log RHO - \log CHI$$

where

σ = the Stefan-Boltzmann constant.

- By default, if conductive opacities are read in, then the (OPAL) opacity-calculating subroutines will actually return the overall effective opacity $\text{Kappa} = 1 / (1 / \text{Kappa_radiative} + 1 / \text{Kappa_conductive})$. This will be allowed to extend the opacities to the highest densities for which valid conductive opacities are available (significantly higher than the upper density limit of the OPAL opacity table, at most temperatures).

The above are preferable to the older available conductive opacities:

W.B. Hubbard & M. Lampe (1969) ApJS, 163, 297: H&L opacity file 'Condopac'

```
=====
-- In a form usable by these opacity subroutines, this file is available
   only from http://www.cita.utoronto.ca/~boothroy/kappa.html
   (the same website as for this file containing the opacity subroutines).
This file includes 'H&L' conductive opacities for H, He, and C, for somewhat
irregular temperature ranges in the density range  $-6 < \log \text{RHO} < 6$ . When
this file is read in, approximate tables for O and Ne are also stored (by
adding a constant to the table for C).
```

'Itoh' (1984) conductive opacities (to supplement the above input file)

```
=====
- By default, the 'H&L' tables are superseded by the later 'Itoh' conductive
opacities at high density (where the latter are valid), using formulae from
N. Itoh, S. Mitake, H. Iyetomi, & S. Ichimaru (1983), ApJ 273, 774, plus
S. Mitake, S. Ichimaru, & N. Itoh (1984), ApJ 277, 375. [The formulae are
used to get the combined effects of conductive opacities for H, He, C, O,
and Ne, where Ne represents all elements heavier than oxygen.]
```

- "Reasonable" interpolated (and extrapolated) conductive opacity values are computed in regions where neither of the above are valid.

J.W. Ferguson et al. (2005) ApJ, 623, 585: (updated) MOLECULAR OPACITY files

```
=====
-- Opacity files available from http://webs.wichita.edu/physics/opacity/
*****
***** NOTE that these 2005 molecular opacities should supersede and *****
***** replace those of Alexander & Ferguson (1994) below; the authors *****
***** state that the accuracy should be significantly better. *****
*****
```

The Ferguson et al. (2005) molecular opacity table ranges are:

2.7 < logT < 4.5 in temperature T [one table may be missing logT < 2.8]
at logT = 4.5 (-0.05) 3.5 (-0.01) 2.9 (-0.05) 2.7

-8.0 < logR < 1.0 in R = RHO / T6^3 [this is same range as OPAL tables]
at logR = -8.0 (0.5) 1.0

Z = { 0.0 0.00001 0.00003 0.0001 0.0003 0.001 0.002 0.004 0.01 0.02 0.03
0.04 0.05 0.06 0.08 0.1 }

X = { 0.0 0.1 0.2 0.35 0.5 0.7 0.8 0.9 0.95 1-Z }

Each of the 155 (X,Z) cases has its own ASCII file of opacity values, with the file name reflecting the values of X and Z (as per examples below).

Several different mixes are available, each with its set of 155 (X,Z) cases (contained in a gzip-compressed tar archive on the above web page); for most of these, compositions are also specified:

--- GN93 mix (Grevesse & Noels 1993): tar archive f05.g93.tar.gz contains
g0.0.tron g0.00001.tron ... g99999.00001.tron g10.0.tron

--- GS98 mix (Grevesse & Sauval 1998): f05.gs98.tar.gz contains
g98.0.0.tron g98.0.00001.tron ... g98.99999.00001.tron g98.10.0.tron

--- L03 mix (Lodders 2003): f05.l03.tar.gz contains
l03.0.0.tron l03.0.00001.tron ... l03.99999.00001.tron l03.10.0.tron

--- AGS04 mix (Asplund, Grevesse & Sauval 2004): f05.ags04.tar.gz contains
ags04.0.0.tron ags04.0.00001.tron ... ags04.99999.00001.tron ags04.one.tron

Compositions are listed on the website for these mixes. There are also two

```

mixes for which opacities are available but the composition is not listed:
--- S92 mix (Seaton 1992) -- composition unspecified, but mix is presumably
very similar to GN93 (opacities are very similar): f05.s92.tar.gz contains
s92.0.0.tron s92.0.00001.tron ... s92.99999.00001.tron s92.one.tron
--- S92AE mix (alpha-element-enhanced version of S92) -- composition not
specified, except for [alpha/Fe] = [O/Fe] = 0.3: f05.s92ae.tar.gz contains
s92ae.0.0.tron s92ae.0.00001.tron ... s92ae.99999.00001.tron s92ae.one.tron
--- alpha-enhanced mixes for Grevesse & Sauval 1998 (the compositions for
these are listed on the website):
--- GS98-.2 with [alpha/Fe] = [O/Fe] = -0.2: f05.gs98-.2.tar.gz contains
gs98-.2.0.0.tron ... gs98-.2.99999.00001.tron gs98-.2.one.tron
--- GS98+.2 with [alpha/Fe] = [O/Fe] = 0.2: f05.gs98+.2.tar.gz contains
gs98+.2.0.0.tron ... gs98+.2.99999.00001.tron gs98+.2.one.tron
--- GS98+.4 with [alpha/Fe] = [O/Fe] = 0.4: f05.gs98+.4.tar.gz contains
gs98+.4.0.0.tron ... gs98+.4.99999.00001.tron gs98+.4.one.tron
--- GS98+.6 with [alpha/Fe] = [O/Fe] = 0.6: f05.gs98+.6.tar.gz contains
gs98+.6.0.0.tron ... gs98+.6.99999.00001.tron gs98+.6.one.tron
--- GS98+.8 with [alpha/Fe] = [O/Fe] = 0.8: f05.gs98+.8.tar.gz contains
gs98+.8.0.0.tron ... gs98+.8.99999.00001.tron gs98+.8.one.tron
    
```

***Any excess C or O is simply added to Z, yielding LESS ACCURATE OPACITIES.

- Opacities are considered to be O.K. for Ztotal < 0.10, and Ztotal > 0.12 is considered to be "unavailable" (where Ztotal = Z + exC + exO).

- By default, the switchover from OPAL to Ferguson et al. 2005 opacities will occur smoothly as logT is reduced from 4.4 to 4.2 (this is the temperature range in the overlap region where the two opacity tables seem to be the closest to being equal).

D.R. Alexander & J.W. Ferguson (1994) ApJ, 437, 879: opacity file 'Alexopac'

-- In a form usable by these opacity subroutines, this file is available only from <http://www.cita.utoronto.ca/~boothroy/kappa.html> (the same website as for this file containing the opacity subroutines).

***** NOTE that these 1994 molecular opacities are SUPERSEDED by the *****
***** 2005 opacities from <http://webs.wichita.edu/physics/opacity/> *****
***** (see Ferguson et al. 2005, ApJ, 623, 585), as DESCRIBED ABOVE. *****

This file includes molecular opacities and dust opacity; table ranges are:
3.0 < logT < 4.1 in temperature T,
-12.0 < logRHO < -6.0 in density RHO (not R, unlike OPAL), for
Z = { 0.0001, 0.0003, 0.001, 0.002, 0.004, 0.01, 0.02, 0.03, 1.0 } and
X = { 0.0001, 0.03, 0.10, 0.35, 0.70, 0.80 } .

[note that the Z = 1.0 table is of course only available for X = 0.0].

Extensions of this table:

- The X = 0.0001 tables are treated as having X = 0.0 (the difference is negligible for the above metallicity range 0.0001 < Z < 0.03).
- Unlike the OPAL 'GN93hz' opacities, these must be extrapolated for X > 0.8 but this yields errors no larger than the difference between Alexander and OPAL opacities even up to X = 1 - Z.
- To match the available OPAL tables, tables at Z = 0.05 and Z = 0.10 were extrapolated from the Z = 0.02 and 0.03 cases, taking the average of the result of extrapolating Kappa in Z and of logKappa in logZ (this yielded the best results in the temperature region of overlap between Alexander and OPAL opacities).
- A set of { Z = 0.0, X = 0.7 } opacities have been obtained using Fig. 1 of Alexander & Ferguson 1994, and the OPAL opacities at logT = 3.75 or higher.
- A rough approximation of opacities for { Z = 0.0, X = 0.0 } was obtained by using the OPAL opacities at high-T, and extrapolating logKappa downwards in logT by fitting a least-squares quadratic.

- For other X-values at Z=0.0 these two opacity sets were interpolated in X.
- ***This extends the tables of low-temperature opacities from $0.0001 < Z < 0.03$ to the full available metallitic range $0.0 < Z < 0.1$ of the OPAL tables; but THE ACCURACY OF THE EXTENSIONS MAY BE POOR (especially for $Z < 0.0001$); it is better to use the Ferguson et al. (2005) molecular opacities instead.
- ***Also, any excess carbon or oxygen is simply added to Z: for significant "excess-C,O" (exC,exO comparable to Z) this yields LESS ACCURATE OPACITIES, and for large "excess-C,O" ($0.1 < Z + \text{exC} + \text{exO} < 1.0$) one must interpolate between the $Z = 0.1$ and $Z = 1.0$ mixes, yielding VERY INACCURATE OPACITIES.
- By default, if 'Alexopac' is read in, then the switchover from OPAL to Alexander opacities will occur smoothly as logT is reduced from 3.97 to 3.87 (this is the temperature range in the overlap region where the two opacity tables seem to be the closest to being equal).
- By default, Alexander opacities are considered to be O.K. for $Z < 0.10$ at all X, and for all Z at $X = 0.0$; they are considered to be "unavailable" in the region where $Z > 0.15$ at $X > 0.03$ (this constraint be tightened by the user at the time when the opacities are read in).

=====
 List of subroutines contained in this file
 =====

This file contains the following subroutines; the nine subroutines marked with ** are those the user is most likely to wish to use (and are the first subroutines described below), while those marked with * can be called by the user (and are described in the comments further below):

```

BLOCK DATA OPAL_OPAC_DATA
SUBROUTINE OPALINIT( KHIGHZ, OFEBRACK, Z, KZ, KMET )
SUBROUTINE GET_ZAVAIL
SUBROUTINE GET_TRVALS
** SUBROUTINE OPAC( Z, XH, EXC, EXO, T6, R )
** SUBROUTINE OPAL( Z, XH, EXC, EXO, SLT, SLR )
** SUBROUTINE OPAL_X_CNO_FU( XH, SLT, SLR, XMET, NMET, FU )
* SUBROUTINE OPAL_F_CNOU( Z, XH, EXC, EXO, SLT, SLR, FCN, FCON, FCNONE, FU )
SUBROUTINE OPAL_F_XCON_CNOU( Z, XH, EXC, EXO, Y, XCN, XON, XNEHEAVY,
    FMUAINV, FMUEINV, ZSQBAR, SLT, SLR, FCN, FCON, FCNONE, FU )
SUBROUTINE Z_FCNO( XH, XMET, NMET, FU, Z, EXC, EXO, Y, XCN, XON, XNEHEAVY,
    FMUAINV, FMUEINV, ZSQBAR, FCN, FCON, FCNONE, FUSE )
* SUBROUTINE KAPFERG( SLT, SLR, XH, Z, EXC, EXO, FLKA, DLKATR, DLKARO, DLKAT, FKAEDGE )
* SUBROUTINE CACHEFERG( KSTO, XH, XZCO )
* SUBROUTINE KAP_MOL( SLT, SLR, XH, Z, EXC, EXO, FLKA, DLKATR, DLKARO, DLKAT, FKAEDGE )
* SUBROUTINE KAPALEX( FLT, FLRO, X, XZCO, FLKA, DLKAT, DLKARO, FKAEDGE )
* SUBROUTINE ASK_LAST_ALEX_EDGE( FKAEDGE, FTRA, FTRA_LO, FTRA_HI, FZKAEDGE )
* SUBROUTINE KAPCOND( FLRO, FLT, X, Y, XCN, XON, XNEHEAVY, FMUAINV, FMUEINV,
    ZSQBAR, IDER, FLKC, FLKCT, FLKCRO, FKCEGE, FKCOK )
* SUBROUTINE KAP_COND_POT( FLRO, FLT, ZION, IDER,
    FLKC, FLKCT, FLKCRO, FKCEGE, FKCOK )
* SUBROUTINE OPAL_K_ONLY( Z, XH, EXC, EXO, SLT, SLR, FCN, FCON, FCNONE, FU )
** SUBROUTINE ASK_LAST_OPAC( OP, DOPT, DOPR, DOPTD, FEDGE, FTREDGE, FZEDGE )
* SUBROUTINE ASK_LAST_XCNOU( Z, X, XC, XO, SLT, SLR, FCN, FCON, FCNONE, FU )
* SUBROUTINE ASK_OPAL_Z_MIX( IMIX, XIZ, N_X, FNINZ, N_N )
* SUBROUTINE ASK_OPAL_MIX_WT( ATWT, NWT, ATWTHHE, NHHE, ATZ, NZ )
** SUBROUTINE SET_OPAL_DIR( CDIRIN )
** SUBROUTINE SET_MOL_DIR( CDIR_MOL )

```

```
** SUBROUTINE SET_COND_DIR( CDIR_COND )
** SUBROUTINE SET_OPAL_LIST_LEVEL( LIST_LEVEL )
* SUBROUTINE SET_OPAL_LIST_UNIT( LIST_IU )
** SUBROUTINE READ_BASIC_OPAL_OPAC( IU, Z, CF_HZ, OFEBRACK, CF_OFE )
** SUBROUTINE READ_EXTENDED_OPAC( IU, Z, CF_HZ, OFEBRACK, CF_OFE,
    I_MOL, I_COND, I_CNO, CF_USER )

* SUBROUTINE SET_OFE_FILE( CFILEOFE )
* SUBROUTINE SET_ALTMIX_OFE_FILE( CFILEOFE )
* SUBROUTINE SET_METEOR_MIX_FILE( CFILEMET )
* SUBROUTINE SET_ALTMIX_MAIN_FILE( CFILE_HZ )
* SUBROUTINE SET_CNO_FILES( CF_HZ, CF_C, CF_O, CF_N, CF_U )
* SUBROUTINE SET_CNO_EXT( IE, CE_HZ, CE_C, CE_O, CE_N, CE_U )
* SUBROUTINE SET_COND_FILE( CFILECOND, I_FULL_PATH )
* SUBROUTINE SET_COND_USE( KCOND, KREPLACE_ITOH )
* SUBROUTINE SET_COND_INFLAGS( KCOND_FIX, KCOND_GAP, KCOND_HAVE )
* SUBROUTINE ASK_COND_USE( KCOND, KCOND_AVAIL, KREPLACE_ITOH )
* SUBROUTINE ASK_COND_INFLAGS( KC_FIX, KC_GAP, KC_FIX_N, KC_GAP_N )
* SUBROUTINE SET_FERG_USER( CBEG_FERG )
* SUBROUTINE ASK_FERG_USER( CBEG_FERG )
* SUBROUTINE SET_FERG_ACC( IACC )
* SUBROUTINE ASK_FERG_ACC( IACC )
* SUBROUTINE SET_ALEX_FILE( CFILEALEX, I_FULL_PATH )
* SUBROUTINE SET_ALEX_USE( KALEX )
* SUBROUTINE SET_ALEX_DO_RHOSW( IRHOSW )
* SUBROUTINE ASK_ALEX_USE( KALEX, KALEX_AVAIL, ITYPE )
* SUBROUTINE ASK_KHIGHZ_OFE( KHIGHZ_USED, OFEBRACK_USED )
* SUBROUTINE ASK_OPAL_FILE_USED( ITYPE, CF_USED )
* SUBROUTINE SET_XHI( KXHI )
* SUBROUTINE ASK_XHI( KXHI, KAVAIL )
* SUBROUTINE SET_CNO_INTERP( KCNO, KUSER )
* SUBROUTINE ASK_CNO_INTERP( KCNO, KUSER, KCNO_AVAIL, KUSER_AVAIL )
* SUBROUTINE SET_ERR_CHECK( LEVEL )
* SUBROUTINE ASK_ERR_CHECK( LEVEL )
* SUBROUTINE SET_LOGT6_LIMITS( VLO, DVLO, VHI, DVHI )
* SUBROUTINE SET_LOGR_LIMITS( VLO, DVLO, VHI, DVHI )
* SUBROUTINE RESET_Z_LIMITS( VLO, DVLO, VHI, DVHI )
* SUBROUTINE ASK_LOGT6_LIMITS( VLO, DVLO, VHI, DVHI )
* SUBROUTINE ASK_LOGR_LIMITS( VLO, DVLO, VHI, DVHI )
* SUBROUTINE ASK_Z_LIMITS( NZMAX, ZMIN, ZMAX )
* SUBROUTINE ASK_Z_USE( NZUSE, ZLO, ZMID, ZHI, ZLOEX, ZHIEX )
* SUBROUTINE ASK_Z_ARRAY( KZSTART, KARRAYSTART, ZARRAY, NARRAY )
* SUBROUTINE SET_SMOOTH( INITSMOOTH, LOWCOSMOOTH, INTERPCOSMOOTH )
* SUBROUTINE ASK_SMOOTH( INITSMOOTH, LOWCOSMOOTH, INTERPCOSMOOTH )
* SUBROUTINE SET_LOGT_SW_FERG( FLTSW_LO, FLTSW_HI )
* SUBROUTINE ASK_LOGT_SW_FERG( FLTSW_LO, FLTSW_HI )
* SUBROUTINE SET_LOGT_SW_ALEX( FLTSW_LO, FLTSW_HI )
* SUBROUTINE SET_LOGRHO_SW_ALEX( FLRHOSW_LO, FLRHOSW_HI )
* SUBROUTINE SET_LOGT_RHOSW_ALEX( FLTSW_R_LO, FLTSW_R_HI )
* SUBROUTINE ASK_LOGT_SW_ALEX( FLTSW_LO, FLTSW_HI )
* SUBROUTINE ASK_LOGRHO_SW_ALEX( FLRHOSW_LO, FLRHOSW_HI )
* SUBROUTINE ASK_LOGT_RHOSW_ALEX( FLTSW_R_LO, FLTSW_R_HI )
* SUBROUTINE READCO( Z, KALLRD, KHIGHZ, IULOW )
* SUBROUTINE READEXCO( Z, KALLRD, KHIGHZ, IULOW, OFEBRACK )
* SUBROUTINE READZEXCO( NZIN, ZLO, Z, ZHI, KHIGHZ, IULOW, OFEBRACK )
* SUBROUTINE READ_BEST_MOL( IU, I_MOL, CF_HZ, OFEBRACK )
* SUBROUTINE READFERG( IU )
* SUBROUTINE ADDFILE_FERG( IU, F_STO, F_READ, CFILEFERG, I_FULL_PATH )
* SUBROUTINE READ_ADD_FERG( IU, F_STO, F_READ, KTYPE_FERG )
SUBROUTINE FIND_FERG( KTYPE_FERG, LEN_BEG, CFILE_USE )
SUBROUTINE INIT_FERG_INDICES
* SUBROUTINE READALEX( IU )
* SUBROUTINE READ_COND_POT( IU )
* SUBROUTINE READCOND( IU )
```

```

SUBROUTINE FIND_RJUMP_HL_COND
** SUBROUTINE DUMP_OPAL_OPAC( IU, CF_D )
** SUBROUTINE READ_OPAL_DUMP( IU, CF_D )
SUBROUTINE READ_KZ( KZ, Z, KALLRD, KHIGHZ, IULOW, OFEBRACK )
SUBROUTINE REVISE_HITR_FOR_INITSMOOTH
SUBROUTINE COINTSMO( XXC, XXO, KZ )
SUBROUTINE COINTERP( XXC, XXO, KZ )
SUBROUTINE T6RINTERP( SLR, SLT )
SUBROUTINE SNGL_CINTERP3( ZM, Z0, Z1, ZP, Z, N0, MXNV, VM, V0, V1, VP, VF, DF, D2, XH )
SUBROUTINE QZLOG4INT( ZLOGD )
FUNCTION QUADSL( IC, I, X, Y1, Y2, Y3, X1, X2, X3 )
FUNCTION QDERSL( IC, I, X, Y1, Y2, Y3, X1, X2, X3 )
FUNCTION QCHKSL( IC, I, X, Y1, Y2, Y3, X1, X2, X3 )
FUNCTION QUAD( IC, I, X, Y1, Y2, Y3, X1, X2, X3 )
FUNCTION QDER( IC, I, X, Y1, Y2, Y3, X1, X2, X3 )
FUNCTION QCHK( IC, I, X, Y1, Y2, Y3, X1, X2, X3 )
FUNCTION QZINTER( IC, I, Z, NMOREZ, F1, F2, F3, F4, Z1, Z2, Z3, Z4, ZDEL )
FUNCTION MIXFIND( IU, IOFE, IGETZXI, IREW, ITAB, LINE, Z, X, C, O )
SUBROUTINE CHK_DIR_NAME( CDIRIN, COPDIR, KOPE )
SUBROUTINE CHK_OFE_ALT_FILE( K_OFE )
SUBROUTINE INDEX_CO_DELTAS( ISET, KXHZ, JX, JC, JO )
SUBROUTINE FINISH_CNO
SUBROUTINE SPLINE( X, Y, N, Y2 )
SUBROUTINE SPLINT( XA, YA, N, Y2A, X, Y, YP )
SUBROUTINE FITY
SUBROUTINE FITX
SUBROUTINE GETD( F, N, D, FP1, FPN )
SUBROUTINE INTERP( FLT, FLRHO, G, DGDT, DGDRHO, IERR )
SUBROUTINE SMOOTH
SUBROUTINE OPALTAB
SUBROUTINE OPEN_CHK_ZIP( IU, FNAME, IGZIP, CMSG )
SUBROUTINE CLOSE_CHK_ZIP( IU, FNAME, IGZIP )
SUBROUTINE QUADSLSTO( I, X, X1, X2, X3 )
FUNCTION QUADSLGET( I, Y1, Y2, Y3 )
SUBROUTINE QDERSLSTO( I, X, X1, X2, X3 )
SUBROUTINE QDERSLGET( I, Y1, Y2, Y3, Y, DYDX )
SUBROUTINE QCHKSLSTO( I, X, X1, X2, X3 )
FUNCTION QCHKSLGET( I, Y1, Y2, Y3 )
SUBROUTINE QCHKSTO( I, X, X1, X2, X3 )
FUNCTION QCHKGET( I, Y1, Y2, Y3 )
SUBROUTINE QDERNSTO( I, NMORE, X, X1, X2, X3, X4 )
SUBROUTINE QDERNGET( I, NMORE, Y1, Y2, Y3, Y4, Y, DYDX )
SUBROUTINE QUADNSTO( I, NMORE, X, X1, X2, X3, X4 )
FUNCTION QUADNGET( I, NMORE, Y1, Y2, Y3, Y4 )
SUBROUTINE QDER4STO( I, X, X1, X2, X3, X3 )
SUBROUTINE QDER4GET( I, Y1, Y2, Y3, Y4, Y, DYDX )
SUBROUTINE QUAD4STO( I, X, X1, X2, X3, X3 )
FUNCTION QUAD4GET( I, Y1, Y2, Y3, Y4 )
SUBROUTINE QDERSTO( I, X, X1, X2, X3 )
SUBROUTINE QDERGET( I, Y1, Y2, Y3, Y, DYDX )
SUBROUTINE QUADSTO( I, X, X1, X2, X3 )
FUNCTION QUADGET( I, Y1, Y2, Y3 )
FUNCTION NUM_BLANKS_CONTAINED( FNAME )
FUNCTION NON_BLANK_BEGIN( FNAME )
SUBROUTINE OPOLDR( IU, FNAME )
SUBROUTINE OPOLUF( IU, FNAME )
SUBROUTINE OPNEUF( IU, FNAME )
SUBROUTINE INQFIL( FNAME, LXST )
SUBROUTINE LINUX_GET_HOME_DIR( FNAME, FNALT, IALT )
FUNCTION LNBLNK( FNAME )

```

The last 6 of the above subroutines contain file-handling routines; if one is using VMS rather than some flavor of Unix or Linux, then one may have to

comment out some statements in these subroutines and uncomment others, as well as in the "data cb" statement at the end of BLOCK DATA OPAL_OPAC_DATA. (The last 2 routines should be needed only if you are using fort77 under Linux, but should still work correctly on any flavor of Unix/Linux system.)

Note that the above routines have been tested on several Linux systems (and Unix, for some earlier versions), but have NOT been tested on a VMS system.

 NOTE THAT ALL REAL VARIABLES ARE SINGLE PRECISION (real*4)

 NOTE THAT NO FILENAME MAY EXCEED 255 CHARACTERS IN LENGTH.

 =====
 The subroutines that interpolate among the OPAL opacities:
 =====

----NOTE that the following four opacity-calculating subroutines CAN extend the OPAL opacities to lower temperatures (by using molecular opacities) or to higher densities (using conductive opacities); whether they do either (or both) of these extensions DEPENDS ON HOW YOU READ IN THE OPACITIES via the subroutines described further below.

*** OPAC(z, xh, exC, exO, T6, R) The purpose of the subroutines OPAC or
 ----- OPAL is to perform up to 6-variable
 *** OPAL(z, xh, exC, exO, slt, slr) interpolation on log10(kappa), to yield
 ----- the opacity (and also its temperature
 and density derivatives) at the given composition, temperature, and density values (the details of how this interpolation is performed are discussed further below). The user can control how the opacities are initially read in via subroutines discussed further below; otherwise, the first time OPAC or OPAL is called, opacities will be read in for an estimated "optimum" range of Z-values (that encompass the input value z). These subroutines actually call OPAL_F_CNOU(z, xh, exC, exO, slt, slr, 0.0, 0.0, 0.0, 0.0) (see description below) to perform the opacity interpolation.

The SINGLE-PRECISION REAL interpolation variables are:

z	The metallicity, Z (excluding any "excess" C and O)
xh	The hydrogen mass fraction, X
exC	The enhanced ("excess") carbon mass fraction, exC. The total carbon mass fraction, Xc, is the sum of exC and the initial amount included in the metal mass fraction Z
exO	The enhanced ("excess") oxygen mass fraction, exO.
OPAC:	
T6	The temperature in millions of degrees Kelvin, T6
R	= { rho(gm/cc) / T6**3 }, the temperature-shifted density value
OPAL:	
slt	log10(T6) = log10(T) - 6
slr	log10(R) = log10(rho) - 3 * slt = log10(rho) - 3 * [log10(T)-6]

(by definition, the helium mass fraction is Y = 1.0 - z - xh - exC - exO). Note that, while z and xh must be non-negative, small NEGATIVE values for exC and/or exO are allowed, provided that the sums { z + exC , z + exO ,

$z + exC + exO$ } are non-negative; this leads to (linear) extrapolation in $\log(z+exC+0.001)$ and/or $\log(z+exO+0.001)$, unlike the earlier version of MAY 28, 1999 (where negative exC or exO values were treated as being zero).

Your routine that calls to OPAC or OPAL should either include the statement:

```
common/e_opal_z/ opact,dopact,dopacr,dopactd,fedge,ftredge,fzedge
```

OR ELSE, after calling the opacity-calculation routine (e.g., OPAC or OPAL):

```
call ASK_LAST_OPAC(OPACT,DOPACT,DOPACR,DOPACTD,FEDGE,FTREDGE,FZEDGE)
-----
```

(this subroutine ASK_LAST_OPAC just returns the values from the common block /e_opal_z/ in its user-supplied arguments).

These SINGLE-PRECISION REAL variables have the following meanings:

OPACT	returns the Log of the Rosseland mean opacity: $\text{Log}_{10}(\text{kappa})$
DOPACT	returns $d\text{Log}(\text{kappa})/d\text{Log}(T_6)$ at constant R (NOT rho!)
DOPACR	returns $d\text{Log}(\text{kappa})/d\text{Log}(R)$ at constant T_6 , which is = $d\text{Log}(\text{kappa})/d\text{Log}(\text{rho})$ at constant temperature
DOPACTD	returns $d\text{Log}(\text{kappa})/d\text{Log}(T_6)$ at constant density, which is = $d\text{Log}(\text{kappa})/d\text{Log}(T)$ at constant density = $\text{DOPACT} - 3.0 * \text{DOPACR}$
FEDGE	returns the degree-of-extrapolation product $\text{FTREDGE} * \text{FZEDGE}$ or, in some cases, A SMALLER VALUE (even zero): - If you have read in conductive opacities, then FEDGE is reduced in switchover regions (radiative to conductive or one conductive table to another) where one or both of the opacities requires some extrapolation (FTREDGE, described below, is NOT reduced, to indicate that the opacities should still be quite accurate there). - If the 'GN93hz' opacities are NOT available, then FEDGE reduces to zero as X increases from 0.76 to 0.8 (but the opacity is still calculated out to $X = 1 - Z$); you should ALWAYS SUPPLY the file 'GN93hz', since errors can be quite large in some cases if you do not (up to an order of magnitude for $Z < 0.001$ at $X = 1 - Z$).
FTREDGE	returns 1.0 for T_6, R inside table boundaries, reduces to 0.0 as T_6, R moves more than one grid spacing outside table (except, in general, in switchover regions).
FZEDGE	returns 1.0 for Z inside the available range [zlow,zhigh], reduces to 0.0 as Z moves out to the boundaries of the extreme-Z-extrapolation range [zlo_ex,zhi_ex].

BY DEFAULT, the OPAL-opacity calculating routines set $\text{OPACT} = 1.0\text{E}+35$ and return without actually calculating the opacity IF:

(1) $\text{FZEDGE} = 0.0$, or

(2) $\text{FTREDGE} = 0.0$ and ($\log R < -6$ or $\log T < 3.97$) .

Otherwise, even if $\text{FTREDGE} = 0.0$, the radiative opacity is extrapolated (linearly) without limit to high T or R, since an estimate of the radiative opacity may be needed in such regions to determine whether the conductive opacity suffices there or not.

IF YOU HAVE READ IN CONDUCTIVE OPACITIES, then FTREDGE will be non-zero where they are valid and dominate, even if the radiative opacities are not valid there: i.e., conductive opacities can be used to EXTEND the radiative opacities, as well as being combined with them via the relevant formula

$$\text{Kappa} = 1 / (1 / \text{Kappa}_{\text{rad}} + 1 / \text{Kappa}_{\text{cond}}) .$$

Also: FTREDGE will be unity in the density region where opacities switch over from fully-valid radiative to fully-valid conductive ones, even if

part of this switchover region requires some extrapolation of one or both of these. However, FEDGE will be less than unity (possibly even zero) in switchover regions where such such extrapolation is required, and also in density gaps where different conductive opacity tables do not quite meet. (Also, at high T and R, an extrapolated conductive opacity value is returned even in regions where FTREDGE is zero.)

NOTE THAT, if you have set the error-checking level to 2 (see SET_ERR_CHECK below), then ANY "out-of-range" case (where the final value of FEDGE = 0.0) is considered a fatal error and the program halts.

If FZEDGE = 0.0, then the given Z-value lay too far outside the available Z-range to be extrapolated (this is checked first, before T6 and R).

If FTREDGE = 0.0 (and FZEDGE > 0.0), then the given T6 and/or R values lay too far outside the available table for reasonable extrapolation.

Details of the extrapolation, and of subroutines allowing user control over the boundaries, are discussed further below.

*** OPAL_X_CNO_FU(xh, slt, slr, xmet, nmet, fu) This subroutine adds any
----- opacity shifts due to the
interconversions C --> N, O --> N, and/or N --> Ne (which can arise from
nuclear burning) to the opacities interpolated in the 6 basic variables
{ z, xh, exC, exO, slt, slr }. USE OF THIS SUBROUTINE CAN BE TRICKY.

---WARNING--- This subroutine estimates Z from the mass fraction of elements heavier than Ne. UNLESS (1) you keep track of the mass fractions at least of C, N, O, Ne, and "heavies", and (2) your initial Z-composition, namely {C, N, O, Ne, "heavies"}, is THE SAME as that in the "solar" opacity table (e.g., 'GN93hz', 'GS98hz', or 'AGS04hz'), this subroutine will obtain an ERRONEOUS Z value and thus an INCORRECT OPACITY.

---WARNING--- If nmet = 19 in your array, then you must have initialized ALL of {C,N,O,Ne,Na,Mg,Al,Si,P,S,Cl,Ar,K,Ca,Ti,Cr,Mn,Fe,Ni} to a "solar" opacity table mix (e.g., from 'GN93hz' or 'GS98hz'), OTHERWISE you will get ERRONEOUS Z and CNO-interpolation factors (since the program uses stored atomic weight values to convert xmet into number fractions in this case), and thus an INCORRECT OPACITY. If you include either fewer or more heavy elements, e.g., if you combine some of these elements into a collective "Xheavy", then you MUST use a value of nmet NOT EQUAL TO 19.

---WARNING--- OPAL_X_CNO_FU implicitly assumes that elements heavier than Ne are negligibly affected by nuclear burning. IF ANY ELEMENTS HEAVIER THAN Ne ARE PRODUCED VIA NUCLEAR BURNING, this will cause the Z-value estimated by OPAL_X_CNO_FU to increase by roughly 5 to 6 times as much as the increase in heavy element abundance. This may give LESS GOOD OPACITY values, or even yield estimated Z-values so large as to be OUT OF RANGE (this will occur for Xheavy > 0.02, roughly; in the worst case, Xheavy > 0.015 may give estimated Z > 0.1, i.e., beginning to be out of range). If any elements heavier than Ne are produced via nuclear burning, you may wish to assign all or most of the newly-nucleosynthesized "heavies" to the Ne abundance, for purposes of opacity calculation (or else use some other subroutine).

The input variables are:

xh	The hydrogen mass fraction, X (as for OPAL or OPAC above)
slt	$\log_{10}(T6) = \log_{10}(T) - 6$ (as for OPAL above)
slr	$\log_{10}(R) = \log_{10}(\rho) - 3 * slt$ (as for OPAL above)
xmet	SINGLE-PRECISION REAL ARRAY of size nmet, giving the mass fractions of the "metals", i.e., of C, N, O, Ne, ... NOTE that these are the actual mass fractions (NOT the mass fractions relative to Z), and any "excess" C or O should be

included in the values of `xmet(1)` or `xmet(3)`, respectively. By definition, the mass fraction `Y` of helium is given by $Y = 1 - x_h - \text{SUM}\{x_{\text{met}}(i)\}$, where $i=1, \dots, \text{nmet}$ in the SUM.

`nmet` INTEGER size of the array `xmet`: ideally it should be the case that `nmet = nel_zmix = 19`, in which case `xmet` is assumed to hold the mass fractions of the elements of the OPAL mix, namely, {C,N,O,Ne,Na,Mg,Al,Si,P,S,Cl,Ar,K,Ca,Ti,Cr,Mn,Fe,Ni}. If the array size `nmet` is not 19, then the sum of `xmet(5)` through `xmet(nmet)` is used as the total mass fraction of all elements heavier than Ne, i.e., the array `xmet` must contain at least {C,N,O,Ne,Xheavy}.

NOTE that if `Xheavy` contains any part of the abundances from C, N, O, or Ne, then the calculated `Z` value will be in error! (Also, if you have set the error level to 3 or higher [see the subroutine `SET_ERR_CHECK`] and CNO-interpolation is available, then it is a fatal error if `nmet` is not equal to 19.)

`fu` SINGLE-PRECISION REAL variable, giving the fraction of the opacity shifts to be applied from any user-specified file: `fu` multiplies opacity differences between the files `CF_USER` and `CF_HZ` (as specified by the subroutine `READ_EXTENDED_OPAC`: see below).

If NO user-specified opacity file `CF_USER` has been read in, then the value of `fu` is ignored (a value of 0.0 is used).

This subroutine uses the array `xmet(nmet)` to calculate the metallicity `Z`, the excess carbon and oxygen `EXC` and `EXO`, and the fractions `FCN`, `FCON`, and `FCNONE` (to apply the C --> N, O --> N, and N --> Ne opacity shifts --- the CNO-interpolation of `logKappa` is linear in the CNO number fractions). In general, it sets `FUSE = fu` (except that the value of `FUSE` is restricted so that it does not correspond to a reduction by more than a factor of 2 in the total number density of elements heavier than Ne). This subroutine then does the equivalent of calling

```
OPAL_F_CNOU( Z, xh, EXC, EXO, slt, slr, FCN, FCON, FCNONE, FUSE ) .
```

NOTE that there would usually be little point in using `OPAL_X_CNO_FU` unless you have called `READ_EXTENDED_OPAC` with a non-zero value of `I_CNO` (to allow CNO-interpolation in the opacities) and/or a non-blank `CF_USER` value (the user-specified opacity correction filename).

If the CNO-interpolation opacity files have not been read in, then this subroutine approximates the opacity effects of C,N,O,Ne interconversion by applying small negative and/or positive values of `exC` and `exO` ("excess-C,O") which may or may not be better than nothing.

NOTE that interconversion of C,N,O,Ne via CNO-cycle burning changes slightly the value of `Z` that this subroutine will compute, for a given set of mass fractions of elements heavier than Ne: the total number density in C,N,O,Ne is constant, but the total mass in these elements changes. Thus this subroutine `OPAL_X_CNO_FU` should only be used if one has read in a RANGE of `Z`-values (see opacity-reading subroutines below): if one has read in only a single `Z`-value, then `OPAL_X_CNO_FU` is likely to yield out-of-range `Z` values.

Note that the subroutine `SET_CNO_FILES(cf_hz, cf_c, cf_o, cf_n, cf_user)` (discussed below) can be used to set the names of the opacity files that are used to get the opacity shifts for CNO-interconversion (files `cf_hz` through `cf_n`) and any user-specified opacity shifts (`cf_user`, relative to `cf_hz`). NOTE that the first four of these files (`cf_hz`, `cf_c`, `cf_o`, `cf_n`) are those used for CNO-interpolation, and should all have the SAME number fractions for the elements heavier than Ne in their compositions (only C,N,O,Ne should be interconverted in these CNO-interpolation files).

```
*** OPAL_F_CNOU( z, xh, exC, exO, slt, slr, fcn, fcon, fcnone, fu ) For users
----- who want
```

to use their own methods to compute the metallicity Z, the "excess" carbon and oxygen mass fractions EXC and EXO, and CNO-interpolation factors FCN, FCON, and FCNONE (as well as any user-factor FU) from their composition.

This interface is similar to OPAL(z, xh, exC, exO, slt, slr) except for the added CNO/user-interpolation factors:

```

fcn      Multiplies opacity differences between files cf_c and cf_hz
fcon     Multiplies opacity differences between files cf_o and cf_hz
fcnone   Multiplies opacity differences between files cf_n and cf_hz
fu       Multiplies opacity differences between files cf_user and cf_hz

```

Note that the inputs supplied to the opacity-reading subroutines (described below) control whether CNO-interpolation and/or user-interpolation opacity files are read in. If no CNO-interpolation files were read in, then the values of fcn, fcon, fcnone are ignored; if no user-interpolation file was read in, then the value of fu is ignored.

NOTE that all the previous opacity-calculating interfaces above ultimately call the subroutine OPAL_F_XCON_CNOU (described further below); the values of Z, XH, EXC, EXO, SLT, SLR, FCN, FCON, FCNONE, FU actually used can be checked by calling the subroutine ASK_LAST_XCNOU described below.

```
*** ASK_LAST_XCNOU( Z, X, XC, XO, SLT, SLR, FCN, FCON, FCNONE, FU )
```

This subroutine just returns the last-used OPAL_F_CNOU input values: it can be used to check these values, rather than including common /x_opal_z/ in the calling program.

```
*** ASK_LAST_OPAC( OPACT, DOPACT, DOPACR, DOPACTD, FEDGE, FTREDGE, FZEDGE )
```

This subroutine just returns the last-computed opacity values, taken from common /e_opal_z/ (as an alternative to including this common block in the calling program), as described above (under the OPAC and OPAL routines).

```
*** ASK_OPAL_Z_MIX( IMIX, XIZ, N_X, FNINZ, N_N )
```

For the mix specified by IMIX , this subroutine returns the components of the metallicity Z, in the arrays XIZ(N_X) and FNINZ(N_N) ; note that up to 19 components are returned, the ratios by mass and by number respectively of {C,N,O,Ne,Na,Mg,Al,Si,P,S,Cl,Ar,K,Ca,Ti,Cr,Mn,Fe,Ni}. Mix specs are:

```

IMIX = 9 (actually, any IMIX > 5 or < -10) : return the actual mixture used
IMIX = 1 : return the 'GN93hz' main solar mix
IMIX = 2 : return the 'Alrd96a2' [O/Fe] = 0.3 mix
IMIX = 3 : return the 'C95hz' [O/Fe] = 0.4 mix
IMIX = 4 : return the 'W95hz' [O/Fe] = 0.5 mix
IMIX = 5 : return the user-specified [O/Fe] > 0 mix
IMIX = 0 : return the meteoritic mix
IMIX = -1 : return the alternate main solar mix (default 'GS98hz')
IMIX = -2 : return the corresponding version of 'Alrd96a2' [O/Fe] = 0.3 mix
IMIX = -3 : return the corresponding version of 'C95hz' [O/Fe] = 0.4 mix
IMIX = -4 : return the corresponding version of 'W95hz' [O/Fe] = 0.5 mix
IMIX = -5 : return the corresponding user-specified [O/Fe] > 0 mix
IMIX = -6 : return the "default-CNO" mix (for CNO-interpolation)
IMIX = -7 : return the CtoN mix (for CNO-interpolation)
IMIX = -8 : return the CtoNe mix (for CNO-interpolation)
IMIX = -9 : return the CNOtoNe mix (for CNO-interpolation)
IMIX = -10 : return the user-defined nonCNO-interpolation mix

```

```

*** ASK_OPAL_MIX_WT( ATwt, Nwt, ATwtHHe, NHHe, ATz, Nz ) This subroutine
----- returns the atomic
weights and nuclear charges used for the components of the metallicity Z:

ATwt(Nwt) = real array returning up to 19 atomic weight values, as used
            for {C,N,O,Ne,Na,Mg,Al,Si,P,S,Cl,Ar,K,Ca,Ti,Cr,Mn,Fe,Ni};
            if Nwt < 19 then only Nwt values will be returned, and
            if Nwt < 1 then no atomic weight values will be returned.
ATwtHHe(NHHe) = real array returning up to 2 atomic weight values, as used
               for H and He.
ATz(Nz) = real array returning up to 19 atomic numbers (nuclear charges),
          for {C,N,O,Ne,Na,Mg,Al,Si,P,S,Cl,Ar,K,Ca,Ti,Cr,Mn,Fe,Ni}.

=====
The subroutines that read in the OPAL opacities:
=====

*** READ_OPAL_DUMP( IU, CF_D ) If a binary opacity file was created at some
----- earlier time by DUMP_OPAL_OPAC below, then
this subroutine can read it in again; note that ALL opacities and user
settings are restored from this unformatted binary file.
NOTE that the only advantage of this is speed: reading such an opacity
dumpfile is MUCH faster than using READ_BASIC_OPAL_OPAC (or its alternates).

IU = integer Fortran unit number: from 1 to 99, and not equal to 5 or 6;
    negative value means "use previous/default value" (if no positive
    Fortran unit number was ever given earlier, the default is 23).
CF_D = character string: name of opacity dumpfile to be read in (INCLUDING
    THE DIRECTORY, if it is not a local file). NOTE that this file
    must exist, and must not be in compressed form.

----[NOTE that the format of this dumpfile is INCONSISTENT with those produced
by program versions between FEBRUARY 1, 2004 and SEPTEMBER 6, 2006; any such
dumpfiles must be re-created by the present version.]

*** DUMP_OPAL_OPAC( IU, CF_D ) AFTER you have read in the opacities (from the
----- plain-text OPAL opacity files) via one of the
subroutines below, this subroutine can be used to dump an unformatted binary
file of the current opacities and user settings (just as read in) for future
re-use by the subroutine READ_OPAL_DUMP above. Note that if you have read
in conductive and/or molecular opacities as well (e.g., via the subroutine
READ_EXTENDED_OPAC below), then these will also be stored in the dumpfile.

IU = integer Fortran unit number: from 1 to 99, and not equal to 5 or 6;
    negative value means "use previous/default value".
CF_D = character string: name of opacity dumpfile to be created (INCLUDING
    THE DIRECTORY, if it is not a local file); this file will be
    overwritten if it already exists.

The size of this opacity dumpfile will depend on the number of Z-values
stored; typically, 'z14xcotrin21.f' will store the maximum number of 14, for
a size of about 24 Mb (while 'z5xcotrin21.f' can store at most 5, for 9 Mb;
'z1xcotrin21.f' will always store 1, for 2.7 Mb) [if no molecular opacities
were read in, these sizes will be 23 Mb, 8 Mb, and 1.7 Mb, respectively].

[But if you read opacities using READZEXCO (rather than one of the simpler
subroutines READ_BASIC_OPAL_OPAC or READ_EXTENDED_OPAC described below),
then the input argument NZIN determines how many Z-values are used.]

```

*** SET_OPAL_DIR(cdirin) The input character variable cdirin can be used
 ----- to specify the directory where the OPAL-opacity
 ASCII files will subsequently be looked for (default is the local directory,
 which can also be specified by supplying a blank argument to SET_OPAL_DIR).
 Note: the total length of the directory name MUST NOT exceed 246 characters.

Example: call set_opal_dir('/home/username/opal_directory/')

OR: to specify "look in local directory": call set_opal_dir(' ')

OR: for a local subdirectory: call set_opal_dir('opal_directory/')

*** SET_MOL_DIR(cdir_mol) The input character variable cdir_mol specifies
 ----- the directory where the molecular-opacity ASCII
 files will subsequently be looked for (blank input means "use the default":
 i.e., try both the OPAL directory and the local directory).

*** SET_COND_DIR(cdir_cond) The input character variable cdir_cond gives
 ----- the directory where conductive-opacity ASCII
 files will subsequently be looked for (blank input means "use the default":
 i.e., try both the OPAL directory and the local directory).

*** SET_OPAL_LIST_LEVEL(LIST_LEVEL) This subroutine can be used to make the
 ----- opacity-reading routines print out the
 ASCII opacity files that are actually read in (this can be useful when one
 uses a subroutine such as READ_EXTENDED_OPAC to read in the "best available"
 Ferguson molecular opacities, for example):

LIST_LEVEL = integer flag to determine whether names of the ASCII opacity
 files that are read in are printed out as they are read in
 (note that binary opacity dump-files are NEVER printed).
 The input value of LIST_LEVEL has the following effect:
 0 : (default) NO listing (printout) of opacity file names.
 1 : print the first Type 2 OPAL opacity (Gz???.x??) file,
 the first of each Ferguson molecular opacity case
 (or Alexander file), any conductive opacity file(s),
 and any Type 1 OPAL opacity file(s) (e.g., 'GN93hz',
 'GS98hz', 'AGS04hz', 'W95hz', 'AGS04hz_Ofe.5_W95',
 'GS98hz.Ct0N', 'GS98hz.COtoN', 'GS98hz.CNOtoNe'...).
 > 1 : up to LIST_LEVEL Type 2 OPAL opacity files will be
 printed, and up to LIST_LEVEL of each Ferguson
 case read in (this is seldom useful, but for
 example one might use LIST_LEVEL of 9999 to
 print out EVERY opacity file that is read in).

*** SET_OPAL_LIST_UNIT(LIST_IU) Set the integer Fortran unit number for the
 ----- above list output (default is 6, i.e., the
 standard output). An input value of 5, of more than 99, or less than 0,
 will be reset to the default of 6 (standard output). [Note that if the
 value of LIST_IU coincides with one of the Fortran units used to actually
 read in an opacity file, a warning will be printed to the standard output,
 and all subsequent list output will be printed to the standard output.]

*** READ_BASIC_OPAL_OPAC(IU, Z, CF_HZ, OFEBRACK, CF_OFE) Read in the basic
 ----- OPAL opacities,
 possibly for non-solar alpha-element abundances (i.e., non-zero [O/Fe]):

IU = integer Fortran unit number: from 7 to 96; note IU through IU+3 may be used (negative value means "use previous/default value"). Note that values from 0 to 6 will be reset to 7, and values greater than 96 will be reset to 96.

Z = (real) "typical" metal-mass-fraction value; opacities will be read in for as wide a range around Z as possible (negative means "use the default value of 0.02"). For the version z14xcotrin21.f of these subroutines, the value of Z is irrelevant, as ALL of the available metallicities will be read in (from 0.0 to 0.1). For z5xcotrin21.f metallicities within about a factor of two of Z will be available; for z1xcotrin21.f on the the single metallicity Z will be read in.

CF_HZ = character variable (or string constant) giving the "main" opacity file to read in, typically 'GN93hz', 'GS98hz', or 'AGS04hz' (but one can specify any Type-1 OPAL opacity file having a solar mix; blank means "use the default of 'GN93hz'"). NOTE that not only will this file CF_HZ be read in, but ALSO the file 'GN93hz' and the 40 Type-2 files (Gz???.x??).

OFEBRACK = (real) value of $[O/Fe] = \log\{ (n_O/n_{Fe}) / (n_O/n_{Fe})_{Sun} \}$; if this is non-zero, then opacities are interpolated between the file CF_HZ and the file CF_OFE to get opacities for the given $[O/Fe]$ value.

CF_OFE = character variable (or string constant) giving the name of the OPAL opacity file with non-zero $[O/Fe]$; if OFEBRACK = 0.0, then this argument is ignored (blank means "use the default": for CF_HZ = 'GN93hz' the default is CF_OFE = 'W95hz', otherwise the default is to append '_Ofe.5_W95' to the value of CF_HZ).

----- NOTE that if the opacity files on disk are in compressed form (suffix '.gz', '.Z', or '.bz2'), then they will be uncompressed (by gunzip, uncompress, or bunzip2, respectively), read in, and compressed again; however, this slows down the input and MAY LEAD TO INPUT ERRORS if more than one instance of this program is running.

*** READ_EXTENDED_OPAC(IU,Z,CF_HZ,OFEBRACK,CF_OFE,I_MOL,I_COND,I_CNO,CF_USER)

This is an extended version of the above subroutine READ_BASIC_OPAL_OPAC:

IU, Z, CF_HZ, OFEBRACK, CF_OFE : as in READ_BASIC_OPAL_OPAC above.

I_MOL = flag controlling whether the low-temperature molecular opacities will be used. The most useful values are as follows:

I_MOL = 0 : do not read in any molecular opacities

I_MOL = 1 : look for molecular opacities for the same composition as the OPAL opacities (if no matching molecular set of opacities can be found, look for any available set of molecular opacities). If OFEBRACK is not zero, try to add opacity-shifts to get opacities appropriate for this input $[O/Fe]$ value.

I_MOL = -1 : read the molecular opacities, but do not use them to extend the OPAL opacities to low T when using the OPAL opacity-calculating subroutines described above [the molecular opacities can be accessed by the subroutine KAP_MOL, described further below].

I_MOL = 21, 31, 41, ... 121 : read ONLY the corresponding set of Ferguson 2005 molecular opacities (21=GN93, 31=GS98, 41=L03, 51=AGS04, 61=S92, 71=S92AE, 81=GS98-.2, 91=GS98+.2, 101=GS98+.4, 111=GS98+.6, 121=GS98+.8).

I_MOL = 991 : read ONLY the molecular opacities specified by a previous call to SET_FERG_USER (described further below).

-----[A more-detailed description of I_MOL than most users will need follows the descriptions of the other input variables.]

I_COND = flag controlling whether the high-density conductive opacities will be read in and/or used:

- 0 = do not use these high-RHO conductive opacities at all.
- 1 = read these opacities in, and use them to extend the OPAL opacities to high RHO when using opacity-calculating subroutines described above. By default, the file 'condall06.d' (Potekhin et al. 2006) is used; if not found, 'condall06' is tried; if not found, then the OLD file 'Condopac' (Hubbard & Lampe 1969) is used; if none of these are found, it is a fatal error.
- 2 = same as 1, except that only the Potekhin et al. (2006) file ('condall06.d' or 'condall06') is looked for.
- 1 = same as 1, but do not use conductive opacities to extend the OPAL opacities when using the opacity-calculating subroutines described above (they can be accessed by the subroutine KAPCOND, described further below).
- 2 = same as -1, except that only the Potekhin et al. (2006) file ('condall06.d' or 'condall06') is looked for.

I_CNO = flag controlling whether the varied-CNO opacities will be used:

- 0 = these varied-CNO opacities will neither be read in nor used.
- 1 = these varied-CNO opacities will be read in from files with names given by appending '.CtoN', '.COtoN', and '.CNOtoNe' to the name given by the input CF_HZ, and will be available to use with the opacity-calculating subroutine OPAL_X_CNO_FU (or OPAL_F_CNOU) described above.

CF_USER = character variable (or string constant) giving the name of a user-specified Type-1 OPAL opacity file to read in, for use with OPAL_X_CNO_FU (or OPAL_F_CNOU); a blank input string means that no such file will be read in or used.

----- A more detailed description of I_MOL and its allowed values

(MOST USERS WILL NOT NEED TO BOTHER WITH THIS):

I_MOL = flag controlling whether the low-temperature molecular opacities will be used. IF IT IS NON-ZERO, then if possible Ferguson et al. (2005) molecular opacities MATCHING the OPAL opacity file will be read in; IF no such matching files are found, then all possible molecular opacity files are checked for, and the first one found is read in -- looking first for a user-specified case (see SET_FERG_USER below), next for a case specified by a prior call to the subroutine SET_ALEX_FILE (see below), next for the cases AGS04, L03, GS98, GN93, S92, S92AE, GS98-.2 ... GS98+.8; if none of these are found, the Alexander & Ferguson (1994) opacities will be read in from the file 'Alexopac'; if not even this file is found, then it is a fatal error.

--- If one of the non-alpha-enhanced Ferguson et al. 2005 cases was read in, and $\text{abs}(I_MOL) < 10$ and the input value of OFEBRACK is non-zero, then an attempt will be made to read in files so as to obtain opacity-shifts to yield opacities for this specified [O/Fe] value, using the GS98 GS98-.2 ... GS98+.8 cases if these are available, or if not then the S92 and S92AE cases are tried.

--- The input value of I_MOL also has the following effects:

For the (DEFAULT) Ferguson et al. 2005 case:

- 0 = do not use low-T molecular opacities at all.
- 1 = the molecular opacities are read in, and will be used to extend the OPAL opacities to low T when using the opacity-calculating subroutines described above; the edge factor FKAEDGE will be unity for $XZCO < 0.1$ (where $XZCO = Z + \text{exC} + \text{exO}$ is the total metal mass fraction), and FKAEDGE will go to zero for $XZCO > 0.12$;
- 2 = same as I_MOL = 1
- 3 = same as I_MOL = 1
- 4 = similar to I_MOL = 1, but set edge factor FKAEDGE to zero for too much "excess-CO": $\text{abs}(\text{exC}) + \text{abs}(\text{exO}) > \text{CO_lim}$ where $\text{CO_lim} = 0.2 * \max(Z, 0.0001, Z + \text{exC} + \text{exO})$

[this will not be done if you just call the subroutine KAPFERG (which does not know what Z, exC, and exO are), but it WILL be done for any other subroutine, including KAP_MOL, KAPFERG, and any calls to molecular opacity routines from OPAL-opacity calculating subroutines].

For the (OLD) Alexander & Ferguson 1994 case:

- 0 = do not use low-T molecular opacities at all.
- 1 = the molecular opacities are read in; arbitrary values of XZCO will be allowed at $X = 0$, and $XZCO < 0.1$ will be allowed at all X (the edge factor FKAEDGE will go to zero for $XZCO > 0.15$ at $X > 0.03$).
- 2 = similar to $I_MOL = 1$, but always reduce the edge factor FKAEDGE to zero as XZCO increases from 0.1 to 0.15, even for $X = 0$.
- 3 = similar to $I_MOL = 2$, but restrict to regions where the Alexander tables were available ($0.0001 < XZCO < 0.03$, the original table range), and set the edge factor FKAEDGE to zero for $XZCO < 0.00005$ or $XZCO > 0.05$.
- 4 = similar to $I_MOL = 3$, but set edge factor FKAEDGE to zero for too much "excess-CO".

For both types of molecular opacities:

- 1 = read in the molecular opacities, but do not use them to extend the OPAL opacities to low T when using the OPAL opacity-calculating subroutines described above [the molecular opacities can be accessed by the subroutine KAP_MOL (or KAPFERG or KAPALEX), described further below]. Otherwise, same as $I_MOL = 1$.
- 2 = same as $I_MOL = -1$, with Z-constraints as for $I_MOL = 2$
- 3 = same as $I_MOL = -1$, with Z-constraints as for $I_MOL = 3$
- 4 = same as $I_MOL = -1$, with Z-constraints as for $I_MOL = 4$

Other input values of I_MOL allow one to specify precisely which Ferguson et al. 2005 case to read in (note that for the following cases, NO [O/Fe]-molecular-opacity-shifts will be done):

- 11 thru 14, or -11 thru -14 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson et al. 2005 case specified by a previous call to SET_ALEX_FILE is looked for.
- 21 thru 24, or -21 thru -24 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson GN93 case is looked for ...
- 31 thru 34, or -31 thru -34 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson GS98 case is looked for ...
- 41 thru 44, or -41 thru -44 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson L03 case is looked for ...
- 51 thru 54, or -51 thru -54 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson AGS04 case is looked for ...
- 61 thru 64, or -61 thru -64 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson S92 case is looked for ...
- 71 thru 74, or -71 thru -74 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson S92AE case is looked for ...
- 81 thru 84, or -81 thru -84 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson GS98-.2 case is looked for ...
- 91 thru 94, or -91 thru -94 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson GS98+.2 case is looked for ...
- 101 thru 104 or -101 thru -104 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson GS98+.4 case is looked for ...
- 111 thru 114 or -111 thru -114 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson GS98+.6 case is looked for ...
- 121 thru 124 or -121 thru -124 : same as 1 thru 4 or -1 thru -4, EXCEPT: only the Ferguson GS98+.8 case is looked for ...
- 991 thru 994 or -991 thru -994 : same as 1 thru 4 or -1 thru -4, EXCEPT: only a user-specified Ferguson case is looked for (as previously set by calling SET_FERG_USER).

 SUBROUTINES TO CONTROL THE DETAILS: MOST USERS WILL NOT NEED TO USE THESE:

***** NOTE that the opacity-reading subroutines described above call various versions of the subroutines described below; for example, calling

```
READ_BASIC_OPAL_OPAC( IU, Z, CF_HZ, OFEBRACK, CF_OFE )
```

does the equivalent of:

```
CALL SET_ALTMIX_MAIN_FILE( CF_HZ )
CALL SET_OFE_FILE( CF_OFE )
CALL SET_ALTMIX_OFE_FILE( CF_OFE )
CALL READZEXCO( -9, -1.0, z, -1.0, khighz, IU, OFEBRACK )
```

with a value of khighz determined by the inputs CF_HZ and OFEBRACK;
likewise, calling

```
READ_EXTENDED_OPAC( IU, Z, CF_HZ, OFEBRACK, CF_OFE, I_MOL, I_COND, I_CNO, CF_USER )
```

does the equivalent of:

```
CALL SET_ALTMIX_MAIN_FILE( CF_HZ )
CALL SET_OFE_FILE( CF_OFE )
CALL SET_ALTMIX_OFE_FILE( CF_OFE )
CALL SET_CNO_FILES( ' ', ' ', ' ', ' ', CF_USER )
CALL READZEXCO( -9, -1.0, Z, -1.0, khighz, IU, OFEBRACK )
CALL READ_BEST_MOL( IU, I_MOL, CF_HZ, OFEBRACK )
IF ( IABS( I_COND ) .GT. 1 ) THEN
  CALL READ_COND_POT( IU )
ELSE IF ( I_COND .NE. 0 ) THEN
  CALL READCOND( IU )
ENDIF
```

```
CALL SET_COND_USE( MIN(1,MAX(0,I_COND)), 99 )
```

where the value of khighz is determined by the various inputs.

Likewise, the opacity-calculating subroutines OPAC, OPAL, OPAL_X_CNO_FU, and OPAL_F_CNOU will call OPAL_F_XCON_CNOU, which then calls one or more of the subroutines OPAL_K_ONLY, KAPCOND, KAPFERG, KAPALEX described below.

```
=====
Other subroutines that interpolate among the OPAL or other opacities:
=====
```

*** OPAL_K_ONLY(Z, XH, EXC, EXO, SLT, SLR, FCN, FCON, FCNONE, FU) This is
 ----- almost
 the same as OPAL_F_CNOU, with the same meaning for the inputs, EXCEPT that
 it will only return the OPAL opacities (i.e., it ignores molecular opacities
 and conductive opacities, whether or not these have been read in).

*** KAPFERG(slt, slr, xh, z, exC, exO, FLKA, DLKATR, DLKARO, DLKAT, FKAEDGE)

This routine interpolates and returns the Ferguson et al. 2005 molecular opacity (provided that a set of these opacities has been read in) [NOTE that if these Ferguson et al. 2005 molecular opacities are available, then the Alexander & Ferguson 1994 molecular opacities are not, and vice versa]:

```
slt, slr, xh, z, exC, exO = (real) input values, as in subroutine OPAL.
FLKA = (real) variable returning Log(kappa), equivalent to OPACT
DLKATR = (real) variable returning dLog(kappa)/dLog(T) at constant R,
         equivalent to DOPACT
DLKARO = (real) variable returning dLog(kappa)/dLog(RHO) at constant T,
```


equivalent to DOPACR
 DLKAT = (real) variable returning $d\log(\kappa)/d\log(T)$ at constant density,
 equivalent to DOPACTD
 FKAEDGE = (real) variable returning the edge factor, equivalent to FEDGE

*** CACHEFERG(ksto, xh, xzco) This subroutine caches Z- and X-interpolated
 ----- Ferguson et al. 2005 molecular opacity values
 for future use [if a LARGE number of low-temperature opacities must be
 evaluated with the same Z and X values, this can speed up the evaluation].
 ksto = (integer) storage index, 1 or 2, of the cache storage area (only
 two sets of Z- and X-interpolated opacities can be cached, at
 X1,Z1 and X2,Z2).
 xh = X, (real) hydrogen mass fraction to use.
 xzco = Z + exC + exO, (real) total metal mass fraction to use.

*** KAP_MOL(slt, slr, xh, z, exC, exO, FLKA, DLKATR, DLKARO, DLKAT, FKAEDGE)

 This routine just calls either KAPFERG (see above) or KAPALEX (see below),
 depending on which type of molecular opacities are available.

*** KAPALEX(FLT, FLRO, X, XZCO, FLKA, DLKAT, DLKARO, FKAEDGE) This routine
 ----- interpolates
 and returns the Alexander & Ferguson 1994 molecular opacities (provided that
 these opacities have been read in from the file 'Alexopac') [NOTE that if
 these Alexander & Ferguson 1994 molecular opacities are available, then the
 Ferguson et al. 2005 molecular opacities are not, and vice versa]:

FLT = $\log(T) = \text{SLT} + 6.0$
 FLRO = $\log(\text{RHO}) = \text{SLR} + 3.0 * \text{SLT}$
 X = hydrogen mass fraction (the same as XH above)
 XZCO = Z + exC + exO = 1 - X - Y = the total mass fraction of elements
 heavier than helium (note that the Alexander & Ferguson 1994
 opacities are available only as a function of temperature,
 density, hydrogen abundance, and metallicity)
 FLKA = (real) variable returning $\log(\kappa)$, equivalent to OPACT
 DLKAT = (real) variable returning $d\log(\kappa)/d\log(T)$ at constant density,
 equivalent to DOPACTD
 DLKARO = (real) variable returning $d\log(\kappa)/d\log(\text{RHO})$ at constant T,
 equivalent to DOPACR
 FKAEDGE = (real) variable returning the edge factor, equivalent to FEDGE

*** ASK_LAST_ALEX_EDGE(FKAEDGE, FTRA, FTRA_LO, FTRA_HI, FZKAEDGE) To give
 ----- access to
 the detailed edge factors for the molecular opacities (which yielded the
 final overall value of FKAEDGE, as returned by KAPFERG or KAPALEX above):

FKAEDGE = real variable returning the final overall edge factor; it is
 defined as $\text{FKAEDGE} = \text{FTRA} * \text{FZKAEDGE}$.
 FTRA = real variable returning the temperature-density edge factor, which
 is defined as $\text{FTRA} = \min(\text{FTRA_LO}, \text{FTRA_HI})$.
 FTRA_LO = real variable returning the edge factor for the low T, low RHO
 edges of the molecular opacity tables.
 FTRA_HI = real variable returning the edge factor for the high T, high RHO
 edges of the molecular opacity tables.
 FZKAEDGE = real variable returning the molecular Z-edge factor, in the
 manner determined by the value of KALEX as set by the
 subroutine READ_EXTENDED_OPAC (or SET_ALEX_USE below).

*** SET_ALEX_USE(KALEX) This allows the user to control whether molecular
 ----- opacities that were read in will actually be used,
 and how; it may be called at any time to change this behavior:

KALEX = integer input flag controlling handling of molecular opacities:
 if KALEX > 0, then the OPAL-opacity-calculating subroutines will
 use the molecular opacities (if they have been
 read in) as an extension to lower T;
 if KALEX < 0 or KALEX = 0, then the OPAL opacity-calculating
 subroutines will ignore the molecular opacities
 whether or not they have been read in (but the
 subroutine KAPFERG or KAPALEX will still work).
 Specific values for KALEX control the molecular-opacity Z-edge
 factor, whether called from OPAL-opacity-calculating subroutines
 or from the subroutines KAPFERG or KAPALEX:

- 1 : (DEFAULT) For Ferguson et al. 2005 opacities, the Z-edge
 factor FZKAEDGE is unity for $XZCO < 0.10$ at all X, and
 goes to zero for $XZCO > 0.12$; but for the Alexander 1994
 opacities, FZKAEDGE is unity for $X = 0$ at all $XZCO$ and for
 $XZCO < 0.10$ at all X, and it goes to zero at $XZCO > 0.15$
 and $X > 0.03$ (note that $XZCO = 1 - X - Y = Z + exC + exO$).
- 2 : For Ferguson et al. 2005, same meaning as KALEX = 1; but
 for Alexander 1994, FZKAEDGE goes to zero for $XZCO > 0.15$
 at all X.
- 3 : For Ferguson et al. 2005, same meaning as KALEX = 1; but
 for Alexander 1994, restrict to the regions where tables
 were available (not extrapolated or otherwise created):
 FZKAEDGE = 1.0 for $0.0001 < XZCO < 0.03$, and goes to
 FZKAEDGE = 0.0 for $XZCO < 0.00005$ or $XZCO > 0.05$.
- 4 : FOR THE OPAL-OPACITY-CALCULATING SUBROUTINES and KAPFERG:
 for BOTH the Ferguson et al. 2005 and the Alexander 1994
 cases: multiply the FZKAEDGE value from case 3 above by a
 factor that is unity if exC and exO are both zero,
 and which goes to zero if $abs(exC) + abs(exO) > CO_lim$
 for $CO_lim = 0.2 * max(Z , 0.0001 , Z + exC + exO)$.
 [Note that this constraint cannot be applied in KAPALEX,
 which does not know the separate values of Z, exC , exO
 (but only their sum $XZCO$); thus, for calls to KAPALEX
 itself, KALEX = 4 has the same effect as KALEX = 3.]
- 0 : Same as KALEX = -1.
- 1 thru -4 : molecular opacities should NOT be used by the OPAL
 opacity-calculating routines, even if they are read in;
 same as 1 thru 4 when KAPFERG is called explicitly;
 same as 1 thru 3 when KAPALEX is called explicitly.
- 9 : Set KALEX to its default value of 1.
- 99 : Leave the current value of KALEX unchanged.

*** ASK_ALEX_USE(KALEX, KALEX_AVAIL, ITYPE) This subroutine returns the
 ----- current value of these integer
 flags that control the use of molecular opacities (see SET_ALEX_USE above):

KALEX = integer variable returning the value of KALEX as in SET_ALEX_USE.
 KALEX_AVAIL = integer variable returning a flag value telling whether (and
 which) molecular opacities are actually available:

- 0 : not available (molecular opacities never read in).
- 1 : Alexander & Ferguson 1994 molecular opacities are
 available (the file 'Alexopac' has been read in):
 subroutine KAPALEX can be used to return Alexander
 opacities, and if KALEX > 0 then these will be
 used to extend the OPAL opacities to low T.
- 2 : some set of Ferguson et al. 2005 molecular opacities
 is available; subroutine KAPFERG can be used to

return these, and if KALEX > 0 then these will be used to extend the OPAL opacities to low T.

ITYPE = integer variable returning a flag value, whose meaning depends on which type of molecular opacities are available:

ITYPE = ITYPE_FERG for Ferguson et al. 2005 molecular opacities: the index of the (last) type of Ferguson opacities that were read in (note that if several types of Ferguson opacities were combined using READ_ADD_FERG or ADDFILE_FERG, the index refers to the last type to be read in and combined):

1 = case specified by CFILE_ALEX (see SET_ALEX_FILE below),
 2 = GN93 case, 3 = GS98 case, 4 = L03 case,
 5 = AGS04 case, 6 = S92 case, 7 = S92AE case,
 8 = GS98-.2 case, 9 = GS98+.2 case, 10 = GS98+.4 case,
 11 = GS98+.4 case, 12 = GS98+.8 case,
 99 = user-specified case (see SET_FERG_USER above).

ITYPE = IRHOSW for Alexander & Ferguson 1994 molecular opacities: integer variable returning a flag value telling whether there is a density switchover between OPAL and Alexander opacity tables (as well as the temperature switchover which must be present) [see subroutine SET_ALEX_DO_RHOSW described further below; note Ferguson et al. 2005 opacities NEVER have a density switchover].

```
*** KAPCOND( FLRO, FLT, X, Y, XCN, XON, XNEHEAVY, FMUAINV, FMUEINV,
            ZSQBAR, IDER, FLKC, FLKCT, FLKCRO, FKCEGE, FKCOK )
```

 This subroutine calculates and returns the conductive opacities.

If the file 'condall06.d' was read in, use the Potekhin et al. 2006 tables; whether RMS or linear mean ionic charge is used depends on IDER (see below), where

$$\text{Zion(rms)} = (\langle z^2 \rangle)^{0.5} = \text{sqrt}(\text{ZSQBAR} / \text{FMUAINV})$$

$$\text{Zion(linear)} = \langle z \rangle = \text{FMUEINV} / \text{FMUAINV}$$

Alternatively, if the file 'Condopac' was read in instead, use the Hubbard & Lampe 1969 tables, possibly extended and modified by formulae of Itoh et al. 1983 and Mitake et al. 1984, depending on the value of IDER (see below).

FLRO = log(RHO) = SLR + 3.0 * SLT

FLT = log(T) = SLT + 6.0

X = hydrogen mass fraction (the same as XH above).

Y = helium mass fraction.

XCN = Xc + Xn / 2 = effective total carbon mass fraction.

XON = Xo + Xn / 2 = effective total oxygen mass fraction.

XNEHEAVY = Xne + Xheavy = mass fraction of elements heavier than oxygen [by definition, X + Y + XCN + XON + XNEHEAVY = 1].

FMUAINV = 1 / mu_A = SUM_i{ X_i / A_i } (for all elements i in the mix -- note that X_i is the mass fraction and A_i the atomic weight); if FMUAINV < 0.0, then an approximate value is calculated from the input values of X, Y, XCN, XON, and XNEHEAVY.

FMUEINV = 1 / mu_e = SUM_i{ X_i * z_i / A_i } (for all elements i in the mix -- note that z_i is the atomic number of element i); if FMUEINV < 0.0, then an approximate value is calculated.

ZSQBAR = $\langle z^2 \rangle / \text{mu}_A = \text{SUM}_i\{ X_i * (z_i)^2 / A_i \}$ (for all elements i in the mix); this is the mean square ionic charge $\langle z^2 \rangle$ divided by mu_A (i.e., multiplied by FMUAINV) for the mixture; if ZSQBAR < 0.0, then an approximate value is calculated.

IDER = flag controlling which conductive opacities are returned.

For the (DEFAULT) Potekhin 2006 ('condall06.d') case:

1 : bi-quadratic interp, Zion = $(\langle z^2 \rangle)^{0.5}$, with derivatives;

NOTE: Zion(rms) = $(\langle z^2 \rangle)^{0.5} = \text{sqrt}(\text{ZSQBAR} / \text{FMUAINV})$;

if it is necessary to extrapolate in log(Zion), do linear extrapolation using the (quadratic) slope at the edge of the matrix; if it is necessary to extrapolate in logT or

logRHO, do linear extrapolation using the slope of the 2 points at the edge of the matrix (this linear formula is mixed with a quadratic if one moves inside the edge of the matrix; full bi-quadratic occurs one grid-spacing inside the edge).

- 0 : bi-quadratic interp, $Zion = (\langle z \rangle^2)^{0.5}$, no derivatives.
 - 1 : use the Potekhin-website formulae, $Zion = (\langle z \rangle^2)^{0.5}$, with derivatives [uses linear interpolation in $\log(Zion)$]; extrapolate linearly using slope at edge of matrix. (This cubic interpolation from the Potekhin-website file 'condint.f' is slower than bi-quadratic interpolation, and may be slightly noisier when using single precision real variables, but yields similar results).
 - 2 : bi-quadratic interp, $Zion = \langle z \rangle$, with derivatives;
NOTE: $Zion(\text{linear}) = \langle z \rangle = FMUEINV / FMUAINV$.
 - 3 : bi-quadratic interp, $Zion = \langle z \rangle$, no derivatives.
 - 4 : Potekhin-website formulae, $Zion = \langle z \rangle$, with derivatives.
- For the (OLD) H&L ('Condopac') case:

- 1 : combine as necessary, with derivatives: use "H&L" at lower density, "Itoh" at higher density, with switchover region
- 0 : combine as necessary (no derivatives).
- 1 : get "Itoh" conductive opacities only (no derivatives)
- 2 : get possibly-modified "H&L" opacities only (no derivatives)
- 3 : get "Itoh" conductive opacities only (with derivatives)
- 4 : get possibly-modified "H&L" only (with derivatives)

NOTE: "H&L" is W. B. Hubbard & M. Lampe 1969, ApJS 163, 297; "Itoh" is N. Itoh, S. Mitake, H. Iyetomi, & S. Ichimaru 1983, ApJ 273, 774 plus S. Mitake, S. Ichimaru, & N. Itoh 1984, ApJ 277, 375.

FLKC = (real) variable returning $\log(Kappa_cond)$, equivalent to OPACT

FLKCT = (real) variable returning $d\log(kappa_cond)/d\log(T)$ at constant density, equivalent to DOPACTD (note that a value of 0.0 will be returned if IDER indicates derivatives should not be calculated)

FLKCRO = (real) variable returning $d\log(kappa_cond)/d\log(RHO)$ at constant temperature, equivalent to DOPACR

FKCEDGE = (real) variable returning the edge factor, equivalent to FEDGE or FTREDGE (note that conductive opacities have no metallicity restrictions); but a negative value is returned for regions more than one grid-spacing off the edge of the matrix, and a value of -99999.0 is returned if conductive opacities are not available.

FKCOK = (real) variable returning a somewhat less restrictive edge factor, which is a better indicator of whether the returned conductive opacity is good enough to combine with (or extend) the radiative OPAL opacity.

*** KAP_COND_POT(FLRO, FLT, ZION, IDER, FLKC, FLKCT, FLKCRO, FKCEDGE, FKCOK)

This subroutine calculates and returns the Potekhin et al. (2006) conductive opacities (if they were not read in, it returns, indicating out-of-range).

FLRO = $\log(RHO) = SLR + 3.0 * SLT$ (density, logarithm to the base 10)

FLT = $\log(T) = SLT + 6.0$ (temperature, logarithm to the base 10)

ZION = Zion, the mean ionic charge (the user must calculate this for their mixture, e.g. the rms nuclear charge weighted by number density).

It is a fatal error if $Zion < 0.1$ or $Zion > 130$.

IDER = flag controlling which conductive opacities are returned:

- 1 : bi-quadratic interpolation, with derivatives; switched over to linear extrapolation at matrix edge.
- 0 : bi-quadratic interpolation, no derivatives.
- 1 : use the Potekhin-website formulae, with derivatives [linear interpolation in $\log(Zion)$, cubic interpolation in $\log T$, $\log RHO$]; linear extrapolation via slope at matrix edge.

FLKC, FLKCT, FLKCRO, FKCEDGE, FKCOK : (real) variables returning values as in KAPCOND above.

*** SET_COND_USE(KCOND, KREPLACE_ITOH) This subroutine allows the user to control the way conductive opacities will be handled; it may be called at any time to change this behavior:

KCOND = integer input flag controlling handling of conductive opacities:

1 : (DEFAULT): if a conductive-opacity file has been read in, then the conductive opacity will be combined with the OPAL opacity to yield the overall opacity value when OPAL opacity routines are called (and also used to extend the OPAL opacity to higher density).

0 : even if a conductive-opacity file has been read in, the conductive opacities will be ignored when computing OPAL opacities (i.e., the conductive opacities can only be accessed by the subroutine KAPCOND described above).

-9 : reset to the default value of 1.

-99 : leave the present stored value of this flag unchanged.

KREPLACE_ITOH = integer input flag controlling how conductive opacities are calculated:

99 : (DEFAULT) use the most recent/best conductive opacities available.

-9 : reset to the default value of 99.

-99 : leave the present stored value unchanged.

For Potekhin 2006:

2 : use bi-quadratic interpolation in logRHO, logT, and log(Zion), where Zion = $(\langle z^2 \rangle)^{0.5}$ (rms).

1 : use the formulae from the website: i.e., cubic interpolation in logRHO, linear interpolation in log(Zion), and cubic interpolation in logT, where Zion = $(\langle z^2 \rangle)^{0.5}$ (rms).

0 : use bi-quadratic interpolation in logRHO, logT, and log(Zion), where Zion = $\langle z \rangle$ (linear mean).

-1 : use the formulae from the website: i.e., cubic interpolation in logRHO, linear interpolation in log(Zion), and cubic interpolation in logT, where Zion = $\langle z \rangle$ (linear mean).

For H&L 1969:

2 : reserved (at present, means the same as 0).

1 : reserved (at present, means the same as 0).

0 : use the 1983/1984 'Itoh' conductive opacities to modify and extend the 'H&L' ones.

-1 : use only these 'H&L' conductive opacities, not the 1983/1984 'Itoh' ones.

*** ASK_COND_USE(KCOND, KCOND_AVAIL, KREPLACE_ITOH) This returns the values of these integer flags that control the use of conductive opacities (see SET_COND_USE above):

KCOND = integer variable returning the value of KCOND as in SET_COND_USE.

KCOND_AVAIL = integer variable returning a flag value telling whether the conductive opacities are actually available:
0 : not available (NO conductive opacities have ever been read in).

1 : H&L 1969 conductive opacities have been read in.

2 : Potekhin 2006 conductive opacities have been read in.

KREPLACE_ITOH = integer variable returning the value of KREPLACE_ITOH as in SET_COND_USE above.

[NOTE: if KCOND_AVAIL > 0, then the subroutine KAPCOND can be used to get

conductive opacities, and if KCOND > 0 then these conductive opacities will be used to extend the OPAL opacities to high RHO.]

```
=====
Other subroutines that may be used when reading in opacities:
=====
```

*** SET_ALEX_FILE(CFILEALEX, I_FULL_PATH) This subroutine allows the user
----- to specify a molecular opacity
file whose name has been changed, or which is in a different directory.
---NOTE: ANY DIRECTORY that you specified via SET_MOL_DIR will be DISCARDED.

CFILEALEX = character variable or string constant giving a non-default
name for the molecular opacity file(s); NOTE that if the
input string CFILEALEX ends with a slash ('/'),
then it will be treated as a directory (or subdirectory)
specification and the default filename will be appended.
For Ferguson et al. (2005) molecular opacities, the
(optional) directory specification may be followed by a
filename beginning-part (as in SET_FERG_USER just below).

I_FULL_PATH = integer flag indicating how this should be interpreted:
0 : (DEFAULT): look for molecular opacity file(s) in the
same directory as the OPAL opacity files (or a
subdirectory thereof, if CFILEALEX contains a
subdirectory specification).
1 : just look for file(s) called (or whose names start
with) CFILEALEX (i.e., either the file(s) are in
the local directory, or else the string CFILEALEX
includes any required directory pathname).

*** SET_FERG_USER(CBEG_FERG) This subroutine allows the user to set the
----- beginning-part of the names for a non-default
set of the Ferguson et al. (2005) molecular opacities:

CBEG_FERG = character variable or string constant giving the beginning of
the file names, including at the end any dot ('.') that
separates beginning part from the X-value in the filename
(for the default mixes, CBEG_FERG would be 'g' 'g98.'
'l03.' 'ags04.' 's92.' 's92ae.' 'gs98-.2.' 'gs98+.2.'
'gs98+.4.' 'gs98+.6.' or 'gs98+.8.' for GN93, GS98, L03,
AGS04, S92, S92AE, GS98-.2, GS98+.2, GS98+.4, GS98+.6, or
GS98+.8 mixes, respectively --- note that the GN93 mix is
the only one of these that would not have the separating dot
'.' at the end of the CBEG_FERG value).

[Note that this mix-specification may optionally be preceded
by a subdirectory-specification, e.g., 'f05_gs98/g98.']

*** ASK_FERG_USER(CBEG_FERG) This subroutine returns the value stored by
----- calling SET_FERG_USER as described just above.

CBEG_FERG = character variable, to return the file-name beginning.

*** SET_FERG_ACC(IACC) This subroutine allows one to change the accuracy
----- with which the Ferguson et al. (2005) molecular
opacities are interpolated (YOU SHOULD NOT DO SO):

IACC = (integer) flag value controlling the accuracy:

- 1 : (DEFAULT): when there is a large opacity jump between two adjacent grid-points at low temperature ($\log T < 3.48$), avoid the large overshoot that would result just outside these grid-points from the usual biquadratic interpolation.
- 0 : (NOT RECOMMENDED!): just use usual biquadratic interpolation, which yields somewhat faster computations at $\log T < 3.48$, but which can lead to errors of order a factor of 2, or even occasionally of more than an order of magnitude.

*** ASK_FERG_ACC(IACC) This subroutine returns the value of IACC presently
----- in use, as per the subroutine SET_FERG_ACC above.

IACC = integer variable to return the value of the flag IACC.

*** READ_BEST_MOL(IU, I_MOL, CF_HZ, OFEBRACK) If I_MOL is non-zero, this
----- subroutine tries to read the molecular opacities that best match the OPAL opacities specified by CF_HZ and OFEBRACK (see subroutine READ_EXTENDED_OPAC further above):

IU, I_MOL, CF_HZ, OFEBRACK : same as in READ_EXTENDED_OPAC further above.

*** READFERG(IU) This subroutine reads in the default set of Ferguson et
----- al. (2005) molecular opacities. This subroutine just calls the subroutine READ_ADD_FERG(IU, 0.0, 1.0, 0) below:

IU = (integer) Fortran unit number to use; a value of 5 or of 6 will be reset to 7, and a negative value means "use the default of 23 or the previous specified Fortran unit".

*** ADDFILE_FERG(IU, F_STO, F_READ, CFILEFERG, I_FULL_PATH) This subroutine
----- reads in a set of Ferguson et al. (2005) molecular opacities, as specified by the user, optionally combining them with a previously-input set (it is a fatal error if the specified Ferguson opacity files are not found):

IU = (integer) Fortran unit number (as in READFERG above).

F_STO = (real) value by which to multiply already-stored $\log K$ values, before adding the $\log K$ values newly read in; use $F_STO = 0.0$ to just read in a new set of opacities (if no Ferguson molecular opacities have been read in previously, then the input value of F_STO is ignored, and a value of 0.0 is used).

F_READ = (real) value by which to multiply the $\log K$ values read in from the specified files; typically, $F_READ = 1.0$ is combined with $F_STO = 0.0$ to just read in a new set of opacities (a value of $F_READ = 0.0$ returns without reading anything).

CFILEFERG = character variable or string constant giving the beginning of the Ferguson et al. (2005) molecular opacity filenames (as in SET_ALEX_FILE or SET_FERG_USER above); this specifies which set to use.

I_FULL_PATH = integer flag indicating how this should be interpreted (as in SET_ALEX_FILE above):

0 : (DEFAULT): look for molecular opacity file(s) in the same directory as the OPAL opacity files (or a subdirectory thereof, if CFILEFERG contains a subdirectory specification).

1 : just look for files whose names start with CFILEFERG (i.e., either the files are in the local directory, or else the string CFILEFERG includes any required directory pathname).

*** READ_ADD_FERG(IU, F_STO, F_READ, KTYPE_FERG) This subroutine reads in
 ----- a set of either default or
 non-default Ferguson et al. (2005) molecular opacities, as specified by the
 user, optionally combining them with a previously-input set (it is a fatal
 error if no Ferguson opacity files are found):

IU, F_STO, F_READ = as in subroutine ADDFILE_FERG just above.

KTYPE_FERG = flag indicating which molecular opacities should be read in:

- 0 : look for the first available set of Ferguson opacities,
 in the order 99,1,5,4,3,2,6,7,8,... of cases below:
- 1 : read the Ferguson mix that was specified previously by
 a call to SET_ALEX_FILE or ADDFILE_FERG (see above).
- 2 : read the GN93 Ferguson mix 'g' --- if this is not found
 in the directory specified by SET_OPAL_DIR above (or
 by SET_ALEX_FILE above), look in the subdirectory
 'f05_g93/' as well.
- 3 : read the GS98 Ferguson mix 'g98.' (also look in the
 subdirectory 'f05_gs98/')
- 4 : read the L03 Ferguson mix 'l03.' (also look in the
 subdirectory 'f05_l03/')
- 5 : read the AGS04 Ferguson mix 'ags04.' (also look in the
 subdirectory 'f05_ags04/')
- 6 : read the S92 Ferguson mix 's92.' (also look in the
 subdirectory 'f05_s92/')
- 7 : read the S92AE Ferguson mix 's92ae.' (also look in the
 subdirectory 'f05_s92ae/')
- 8 : read the GS98-.2 Ferguson mix 'gs98-.2.' (also look in
 the subdirectory 'f05_gs98-.2/')
- 9 : read the GS98+.2 Ferguson mix 'gs98+.2.' (also look in
 the subdirectory 'f05_gs98+.2/')
- 10 : read the GS98+.4 Ferguson mix 'gs98+.4.' (also look in
 the subdirectory 'f05_gs98+.4/')
- 11 : read the GS98+.6 Ferguson mix 'gs98+.6.' (also look in
 the subdirectory 'f05_gs98+.6/')
- 12 : read the GS98+.8 Ferguson mix 'gs98+.8.' (also look in
 the subdirectory 'f05_gs98+.8/')
- 99 : (actually, any value larger than 12): read the Ferguson
 mix specified previously by a call to SET_FERG_USER.
- 1 to -99 : first try the case abs(KTYPE_FERG) ; if it is
 not found, behave as if case 0 was specified.

*** READALEX(IU) This subroutine just reads in the file 'Alexopac' (with
 ----- Alexander & Ferguson 1994 molecular opacities), using the
 Fortran unit IU (provided that this file has not already been read in).

*** SET_COND_FILE(CFILECOND, I_FULL_PATH) This subroutine allows the user
 ----- to specify a which conductive
 opacity file should be read in, and/or a file whose name has been changed,
 or which is in a different directory.

----NOTE: ANY DIRECTORY that you specified via SET_COND_DIR will be DISCARDED.

----NOTE: Calling this subroutine SET_COND_FILE causes any previously-stored
 conductive opacities to be DISCARDED at once.

CFILECOND = character variable or string constant giving the revised name

I_FULL_PATH = integer flag indicating how this should be interpreted:

- 0 : (DEFAULT): look in same directory as for OPAL files.
- 1 : just look for a file called CFILECOND.

*** SET_COND_INFLAGS(KCOND_FIX, KCOND_GAP, KCOND_HAVE) This subroutine sets
 ----- flags controlling
 how the 'H&L' conductive opacity tables are modified when they are read in
 (this will have an effect only if called BEFORE you read in the opacities):

KCOND_FIX = integer input flag controlling an error-fix:

- 1 : (DEFAULT): remove an anomalously low Hydrogen conductive opacity value (at $\log T = 5.4$, $\log \rho = -0.5$).
- 0 : do not do this (NOT RECOMMENDED).
- 9 : reset to the default value of 1.
- 99 : leave the present stored value unchanged.

KCOND_GAP = integer input flag controlling the "gap" in the 'H&L' tables, i.e., the density region where they do not extend to such low temperatures as they do at higher or lower densities:

- 1 : (DEFAULT): high-density 'Itoh' conductive opacities are used in this "gap" to improve the 'H&L' opacity there (beyond the edge of the 'H&L' tables) in order to improve the H&L-to-Itoh switchover at increasing density and low temperature (note that no input H&L values are modified, only the extrapolation region).
- 0 : this is not done: H&L tables are just extrapolated.
- 9 : reset to the default value of 1.
- 99 : leave the present stored value unchanged.

KCOND_HAVE = integer input flag controlling whether the file 'Condopac' (or 'condall06.d') will be read in again:

- 1 : (DEFAULT): it will NOT be read in again (unless it has never been read in at all), even if you call the subroutine READCOND a second time, unless you change the filename by calling SET_COND_FILE.
- 0 : re-read the file 'Condopac' the next time you call the subroutine READCOND.
- 9 : if and only if you have changed the stored value(s) of KCOND_FIX or KCOND_GAP, re-read the file 'Condopac' the next time you call the subroutine READCOND.
- 99 : (equivalent to specifying the default value of 1).

*** ASK_COND_INFLAGS(KC_FIX, KC_GAP, KC_FIX_N, KC_GAP_N) This subroutine
 ----- returns integer
 flag values (as may be set by the subroutine SET_COND_INFLAGS above):

KC_FIX = integer variable returning the value of KCOND_FIX that was used the last time 'Condopac' was read in.

KC_GAP = integer variable returning the value of KCOND_GAP that was used the last time 'Condopac' was read in.

KC_FIX_N = integer variable returning the value of KCOND_FIX that will be used the NEXT time 'Condopac' is read in.

KC_GAP_N = integer variable returning the value of KCOND_GAP that will be used the NEXT time 'Condopac' is read in.

*** READ_COND_POT(IU) This subroutine just reads in the Potekhin 2006
 ----- conductive opacity file 'condall06.d', using Fortran
 unit IU (provided that it has not already been read in).

*** READCOND(IU) This subroutine just reads in either the Potekhin 2006
 ----- conductive opacity file 'condall06.d' or the older H&L
 file 'Condopac', using Fortran unit IU (provided that conductive opacities
 have not already been read in).

*** SET_OFE_FILE(cfileofe) The input character variable cfileofe can be

----- used to set a user-specified filename containing non-CO-rich opacities with $[O/Fe] > 0.0$, similar to 'Alrd96a2', 'C95hz', or 'W95hz'. Only the filename (not the directory pathname) should be specified and the length of the filename MUST NOT exceed 8 characters. This filename is only used in the case $khhighz = 5, 15, 25, \text{ or } 35$ (see READZEXCO below).

*** SET_ALTMIX_OFE_FILE(cfileofe) The input character variable cfileofe
----- can be used to set a user-specified filename containing non-CO-rich GS98 opacities with $[O/Fe] > 0.0$; the length of the name is only restricted by the fact that filename plus OPAL directory name cannot exceed 255 characters in total. This filename is only used in the case $khhighz = -5, -15, -25, \text{ or } -35$ (see READZEXCO below).

*** SET_ALTMIX_MAIN_FILE(cfile_hz) The input character variable cfile_hz
----- can be used to replace the alternate main file 'GS98hz' with a user-specified filename; this new file will be assumed to have $[O/Fe] = 0.0$, i.e., a solar mix. The length of the name is only restricted by the fact that filename plus OPAL directory name cannot exceed 255 characters in total. This filename is used whenever $khhighz < 0$ (see description in READZEXCO below); note that $khhighz = -2, -3, \text{ and } -4$ should NOT be used subsequently, unless this file replacing 'GS98hz' also has the Grevesse & Sauval 1998 mix.

*** SET_CNO_FILES(cf_m, cf_c, cf_o, cf_n, cf_user) This subroutine can be
----- used to set the five alternate opacity filenames that can be used to obtain the CNO-interpolation opacity shifts (plus a user-specified case); the input character variables are only restricted by the fact that filename plus OPAL directory name can't exceed 255 characters in total (blank values mean "use default filenames"):

cf_m = a standard opacity file (with standard composition); the default used in READZEXCO is 'GN93hz' if $khhighz > 0$, or else cfile_hz (e.g., 'GS98hz': see SET_ALTMIX_MAIN_FILE above) if $khhighz < 0$
 cf_c = an opacity file where most or all C (by number) has been converted to N; the default filename is cf_hz with '.CtoN' appended
 cf_o = an opacity file where most/all of both C and O have been converted to N; the default filename is cf_hz with '.CotoN' appended
 cf_n = an opacity file where all CNO has been converted to Ne; the default filename is cf_hz with '.CNotoNe' appended
 cf_user = a user-specified opacity file, with a composition that can be arbitrarily different from that in the file cf_hz; the default filename is cf_hz with '.user' appended

NOTE that the first four of these files (cf_m, cf_c, cf_o, cf_n) should all have the SAME number fractions for the elements heavier than Ne (only C,N,O, Ne should be interconverted in these CNO-interpolation files).

Note that as long as the files cf_m, cf_c, cf_o, and cf_n have compositions that are not linearly dependent (or close to it) in the 3-dimensional space of interconversion of C, N, O, and Ne, the CNO-interpolation should still work correctly. However, it has been tested only for the specific case described above.

*** SET_CNO_EXT(ie, ce_hz, ce_c, ce_o, ce_n, ce_u) This subroutine can
----- be used to change the default extensions for the CNO-interpolation files (which are used to decide on the default CNO-filenames); this can be used as an alternative to calling the subroutine SET_CNO_FILES. As noted above, these default extensions are ' ', '.CtoN', '.CotoN', '.CNotoNe', '.user' respectively. Calling this

subroutine sets these default extensions to the values of the character variables `ce_hz`, `ce_c`, `ce_o`, `ce_n`, `ce_u` respectively. The integer `ie` controls the meaning of a blank input character value:

`ie = 0` : in all cases, a blank input character value means do not change the corresponding default extension (UNLESS YOU HAVE SOME VERY PECULIAR NAMING CONVENTIONS FOR CNO FILES, THIS IS THE ONLY CASE YOU ARE LIKELY TO NEED)

`ie = 1` : if `ce_hz` is blank, reset the corresponding extension to blank (i.e., the default filename remains 'GN93hz' or `cfile_hz`); but if any of the other input character values are blank, do not change these other corresponding default extension

`ie = 2` : if `ce_c` is blank, reset the corresponding extension to blank

`ie = 3` : if `ce_o` is blank, reset the corresponding extension to blank

`ie = 4` : if `ce_n` is blank, reset the corresponding extension to blank

`ie = 5` : if `ce_u` is blank, reset the corresponding extension to blank

`ie = 6` thru `10` : same as `ie = 1` thru `5`, respectively

Note that an extension longer than 80 characters cannot be accommodated.

*** `SET_METEOR_MIX_FILE(cfilemet)` The input character variable `cfilemet` ----- can be used to set a user-specified filename containing a meteoritic mixture. This file is used ONLY to set the components of Z for a meteoritic mixture, which are available to the user but are not used in calculating any opacities.

*** `ASK_OPAL_FILE_USED(ITYPE, CF_USED)` This subroutine returns the name of ----- the specified type of opacity file that was (or will be) used to read in the opacities:

`ITYPE` = integer input flag controlling which file name is returned:

-1 : the name of the OPAL directory `CDIRIN`.

0 : meteoritic-mix file `CFILEMET` (this file may not exist).

1 : the main mix file `CF_HZ`.

2 : molecular opacities file `CFILEALEX`, including directory.

3 : conductive opacities file `CFILECOND`, including directory.

4 : the file 'GN93hz' (needed to correct Gz???x?? files).

5 : the non-zero-[O/Fe] file `CF_OFE`.

6 : the CNO-interpolation main mix file `CF_M`.

7 : the CNO-interpolation C --> N file `CF_C`.

8 : the CNO-interpolation CO --> N file `CF_O`.

9 : the CNO-interpolation CNO --> Ne file `CF_N`.

10 : the user-mix file `CF_USER`.

`CF_USED` = character variable returning the filename specified by `ITYPE`.

*** `ASK_KHIGHZ_OFE(KHIGHZ_USED, OFEBRACK_USED)` This subroutine returns the ----- values that were used when the subroutine `READZEXCO` was called to read in the opacities (directly or via `READ_BASIC_OPAL_OPAC` or `READ_EXTENDED_OPAC`):

`KHIGHZ_USED` = integer variable returning the value of `KHIGHZ` (see below).

`OFEBRACK_USED` = real variable returning the value of [O/Fe] that was used.

*** `READZEXCO(Nzin, Zlo, Z, Zhi, khighz, iulow, ofebrack)` This subroutine ----- is used to read in the OPAL opacity files, allowing the user to control whether and how opacities will subsequently be interpolated in Z. Note that a new set of opacities (at a new Z-range or Z-value) can be read in at any time.

The controlling input variables are:

Nzin INTEGER: the number of metallicity values Z_i to be stored, for subsequent Z-interpolation when OPAL or OPAC is called; this is discussed just below. Nzin = -9 means "use the widest available Z-range around the input Z-value".

Zlo SINGLE-PRECISION REAL: the lowest metallicity value that will be required; this is discussed just below.

Z SINGLE-PRECISION REAL: the "typical" or central metallicity value; this is discussed just below.

Zhi SINGLE-PRECISION REAL: the highest metallicity value that will be required; this is discussed just below.

khighz INTEGER: controls the use of the C=O=0.0 opacity file 'GN93hz' (and/or its equivalents with newer mixes, such as 'GS98hz' and 'AGS04hz'), and of the similar files having [O/Fe] > 0.0:

khighz = 0: use of the file 'GN93hz' is prevented; only for $X < 0.75$ is accurate X-interpolation available.

khighz = 1: the file 'GN93hz' is used to obtain opacities for the C=O=0.0 mixes (i.e., opacities with better Z-interpolation), including the added X-values $X=\{0.2,0.5,0.8,0.9,0.95,1-Z\}$ (i.e., allowing accurate X-interpolation up to $X = 1-Z$); for the mixes with C+O > 0.0, corresponding opacity shifts are applied, for consistency.

khighz = 2: file 'Alrd96a2' with [O/Fe] = 0.3 \ is used in

khighz = 3: file 'C95hz' with [O/Fe] = 0.4 } addition to

khighz = 4: file 'W95hz' with [O/Fe] = 0.5 / 'GN93hz',
if READZEXCO was called with a non-zero value of ofebrack, in order to interpolate in the excess oxygen/alpha-element enrichment [O/Fe].

khighz = 5: the name of a file with non-zero [O/Fe] must have been set already, by calling the subroutine SET_OFE_FILE described below; it will be used instead of 'Alrd96a2', 'C95hz', or 'W95hz' when interpolating in [O/Fe] (its [O/Fe] value will be computed when it is read in; if it actually has [O/Fe] = 0.0, the resulting behavior is not defined and will surely be erroneous).

khighz = -1 thru -5: similar to khighz = 1 thru 5, except that a different set of OPAL opacity files is used, defining a different set of heavy-element abundances to comprise the solar metallicity Z. THE OLD FILE 'GN93hz' IS STILL REQUIRED AS WELL, but the opacities now stored are those from the new file with the same format (called 'GS98hz', by default), and this is the composition that is assigned a value of [O/Fe] = 0.0; khighz = -2 thru -5 likewise implies the use of files with [O/Fe] > 0.0 relative to the mix in 'GS98hz': by default 'GS98hz_OFe.3_Alrd96a2' at [O/Fe] = 0.3, 'GS98hz_OFe.4_C95' at 0.4, 'GS98hz_OFe.5_W95' at 0.5, or user-defined for khighz = -5 via the subroutine SET_ALTMIX_OFE_FILE (see below). The main alternate solar-composition [O/Fe]=0.0 file name can be changed from 'GS98hz' by calling the subroutine SET_ALTMIX_MAIN_FILE (see below); if this is done, khighz = -2 thru -4 should not be used subsequently unless the replacement main file still uses the Grevesse & Sauval 1998 mix; rather, if one wishes opacities with a non-zero [O/Fe] value, one should do something such as:

call set_altmix_main_file('AGS04hz')
call set_altmix_ofe_file('AGS04hz_OFe.5_W95')
and then use khighz = -5.

khighz = -11 thru -15, OR

11 thru 15: same as khighz = -1 thru -5 OR 1 thru 5, except that CNO-interpolation opacity files are read in (if possible: uses the filenames "CF_HZ, CF_C, CF_O, CF_N" that can be set by calling SET_CNO_FILES: see below)

khighz = -21 thru -25, OR

21 thru 25: same as khighz = -1 thru -5 OR 1 thru 5, except that a user-specified (OPAL) opacity interpolation file is read in (if possible: uses the filenames "CF_HZ, CF_U" that can be set by calling SET_CNO_FILES: see below)

khighz = -31 thru -35, OR

31 thru 35: same as khighz = -1 thru -5 OR 1 thru 5, except that BOTH the CNO- and user-specified opacity interpolation files are read in (if possible)

iulow INTEGER: the beginning Fortran unit number for reading opacity files; Fortran units iulow through iulow + 3 may be used. Zero or negative iulow values mean "use previous (or default) value", where the default value is iulow = 23. A fatal error will result if iulow < 7 or iulow > 96 (unless you have set the error level to 0, in which case these values are ignored). (Note: unless the user explicitly calls READZEXCO, READEXCO, READCO, or READ_OPAL_DUMP, the default-setup call to READZEXCO in OPAL will be executed, yielding the default iulow of 23).

ofeback SINGLE-PRECISION REAL: the value of [O/Fe], the logarithmic oxygen (or alpha-element) enhancement factor, relative to the Sun: $ofeback = \log_{10}\left\{ \frac{O_{mix}/Fe_{mix}}{O_{sun}/Fe_{sun}} \right\}$, where O_{mix} , Fe_{mix} , O_{sun} , and Fe_{sun} are number densities. If khighz = 0, 1, or -1, then ofeback is ignored; otherwise, READZEXCO interpolates (or extrapolates) $\log(Kappa)$ linearly between mix 1 (or -1) and mix mod(khighz,10), interpolation factors being such as to yield the desired [O/Fe] by combining these mixes. Note: 'GN93hz' has [O/Fe] = 0.0 by definition, 'Alrd96a2' has [O/Fe] = 0.3, 'C95hz' has [O/Fe] = 0.4, and 'W95hz' has [O/Fe] = 0.5, but they have different patterns of enhancements for elements other than oxygen; their elemental abundances and the corresponding opacity shifts are discussed further below.

Discussion of Nz, Zlo, Z, Zhi in calling the above subroutine READZEXCO:

Z-interpolation of opacity is actually carried out in terms of $\log(Z+0.001)$. The maximum number of z-values that can be stored (to interpolate among) is given by the value of the constant NZ in the parameter statements that begin as "parameter (nz=" . The maximum sensible value is NZ = 14, which requires about 22.7 Mb of opacity matrix storage space. Other reasonable values include NZ = 8 (13.0 Mb) and NZ = 5 (8.1 Mb); a value of NZ = 3 (4.9 Mb) still allows quadratic Z-interpolation, while NZ = 2 (3.2 Mb) allows only linear interpolation in $\log(Z+0.001)$; for NZ = 1 (1.6 Mb), the program behaves much the same as the earlier version of MAY 28, 1999 (or as if the subroutines READCO or READEXCO were used instead of READZEXCO).

If you have reduced the error-checking level to 0 (using SET_ERR_CHECK), then the input value of Nz will be decreased if necessary so that it does not exceed NZ, the maximum available number of Z-storage values; otherwise, a value of Nz > NZ or of Nz < 1 is a fatal error, EXCEPT THAT Nz = -9 means "use maximum possible value, i.e., as if Nz = NZ". If necessary, the subroutine ASK_Z_LIMITS can be called to check the value of this hard-wired limit NZ, or the subroutine ASK_Z_USE can be called after READZEXCO to check the number of Z-values actually used (see below).

Values of Z_{lo} , Z , Z_{hi} that are within $1.E-6$ of one of the file z -values { 0.0, 0.0001, 0.0003, 0.001, 0.002, 0.004, 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.08, 0.1 } are generally reset to be exactly equal to that value (except that only the range [$-1.E-6$, $1.E-8$] is reset to be exactly zero). Any value of Z_{lo} , Z , or Z_{hi} greater than 0.1 is always a fatal error.

Significantly negative Z -values (below $-1.E-6$) mean "use default values":

- if all three of Z_{lo} , Z , Z_{hi} are negative, then Z is reset to 0.02;
- if only Z is negative, then it is reset to lie between Z_{lo} and Z_{hi} ;
- if Z_{lo} and/or Z_{hi} is negative, then the negative value(s) will be reset to "reasonable" values, according to the values of N_{zin} and Z .

If $N_{zin} = 2$, then the stored z -values are given by the input values of Z_{lo} and Z_{hi} ; if both of these are negative, then a range $\pm 10\%$ in Z is used; if only one of them is negative, a total range of 20% in Z is used, or more if the remaining interval [Z_{lo}, Z] or [Z, Z_{hi}] is larger than this. The minimum allowed range is 1% in Z , or $\Delta Z = 1.E-5$ for small Z values; this is a fatal error, unless you have reduced the error-checking level to 0, in which case the program quietly uses this lower limit. Likewise too large a range: $Z_{lo} < \min\{ 0.6 * Z_{hi} , Z_{hi} - 0.0002 \}$ is a fatal error, unless you have reduced the error-checking level to 0, in which case the ONLY UPPER LIMIT on the linear Z -interpolation range is that it must lie within [0.0,0.1]; BEWARE that large ranges yield inaccurate interpolation.

If $N_{zin} > 2$, then from the set of eight "largest-allowed-spacing" Z -values { $z_1=0.0$, $z_2=0.001$, $z_3=0.004$, $z_4=0.01$, $z_5=0.02$, $z_6=0.03$, $z_7=0.05$, $z_8=0.1$ }, choose the largest z_J and the smallest z_K such that z_J is no greater than Z_{lo} and z_K is no less than Z_{hi} ; it is then a fatal error if $N_{zin} < K - J$, i.e., if the Z -range is too large for the given value of N_{zin} (unless of course you have reduced the error-checking level to 0, in which case arbitrarily large ranges are accepted: BEWARE!). Also...

If $N_{zin} > 2$, then: if a set of N_{zin} adjacent file z -values from the set { 0.0, 0.0001, 0.0003, 0.001, 0.002, 0.004, 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.08, 0.1 } encompasses the range [Z_{lo}, Z, Z_{hi}] , then such a set of N_{zin} z -values is used (as far as possible, it will be centered on Z): for example, for $N_{zin} = 3$, input Z -values [Z_{lo}, Z, Z_{hi}] = [0.01,0.02,0.03] or [0.017,0.018,0.019] or [0.022,0.022,0.024] or [0.019,0.028,0.029] all yield { 0.02, 0.03, 0.04 } , while [0.021,0.028,0.029] yields { 0.02, 0.03, 0.04 } .

If $N_{zin} = 3$ and no set of 3 of the above file z -values will work, then the actual input values are used (except that, if the logarithmic interval from Z_{lo} to Z is sufficiently different from that from Z to Z_{hi} , the value of Z is reset to the logarithmic midpoint of Z_{lo} and Z_{hi}): for example, the input Z -value set [Z_{lo}, Z, Z_{hi}] = [0.012,0.024,0.04] yields { 0.012, 0.024, 0.04 } , while [0.012,0.015,0.04] yields { 0.012, 0.02208679, 0.04 } .

If $N_{zin} > 3$ and no set of N_{zin} of the above file z -values will work, then try whether a similar set that works can be obtained by removing (some of) the z -values that are not present in the C,O-rich OPAL opacity files $Gz???x??$, which are available at { 0.0, 0.001, 0.004, 0.01, 0.02, 0.03, 0.05, 0.1 } ; if such a set is found (with somewhat larger z -intervals), then it is used. Otherwise, endpoints Z_{lo} and Z_{hi} are used, with remaining z -values equally spaced in $\log(Z+0.001)$ between these endpoints.

***** NOTE that if you have set the error-level to 0, then there is NO UPPER LIMIT on the maximum allowed Z -range (except that it must lie in the range [0.0,0.1] where OPAL opacities are available), and thus QUITE INACCURATE Z -interpolation will occur if the input Z -range [Z_{lo} , Z_{hi}] is relatively large and N_{zin} (or NZ) is relatively small.

One or two of the Type-1 OPAL files can be read in (as specified by `khghz`

in your call to the opacity-reading subroutine READZEXCO). For example,
 call readzexco(14, 0.0, -1.0, 0.1, 1, 23, 0.0)
 will read in opacities at all Z-values from 0.0 to 0.1, reading additional opacities from 'GN93hz' (due to the value of khighz=1); Fortran units 23 through 26 will be used for input, and the opacities will have [O/Fe]=0.0 (solar composition for the abundances comprising Z). For non-CO-rich cases, this allows slightly improved Z-interpolation (for $Z < 0.12$) and slightly improved X-interpolation (for $0.03 < X < 0.75$); for high hydrogen abundances ($X > 0.75$), such as may result from diffusion (e.g., helium settling), the accuracy is GREATLY IMPROVED.

NOTE that only the version z14xcotrin21.f allows Nzin = 14 as in the above call; if one is using the less-memory-hogging version z5xcotrin21.f, then the above call would lead to a fatal error, unless you had reduced the error checking level, in which case it would lead to opacities being read in only for the Z-values $Z = \{ 0.0, 0.00217, 0.00905, 0.0309, 0.1 \}$, yielding MUCH LESS ACCURATE Z-interpolation; USER BEWARE!!

For z5xcotrin21.f, only a small Z-range should be read in: for example,
 call readzexco(5, -1.0, 0.02, -1.0, 4, 23, 0.45)
 reads opacities at $Z = .004, .01, .02, .03, .04$, using 'GN93hz' and 'W95hz' to obtain opacities at [O/Fe]=0.45 (the results are then as accurate as with the version z14xcotrin21.f for the restricted Z-range $0.01 < Z < 0.03$: this is described in more detail below).

For z1xcotrin21.f, only a SINGLE Z-value can be read in; the opacities from the files will be interpolated in Z while being read in, if necessary.

To read opacities in the widest available Z-range around some metallicity Z that is compatible with accuracy, one would use Nzin = -9, e.g.,

```
call readzexco( -9, -1.0, Z, -1.0, 11, 23, 0.0 )
```

This would read opacities with [O/Fe] = 0.0 in a range around Z that is determined by the value of NZ in the parameter statements in this file.

NOTE that if opacities have not already been read in, then the first time that an opacity-calculating subroutine is called (e.g., OPAC or OPAL), it will use "call readzexco(-9, -1.0, z, -1.0, 1, 23, 0.0)" to read in the opacities, i.e., basic opacities for the maximum reasonable Z-range (with [O/Fe] = 0.0 and no CNO-interpolation, only interpolation in "excess-C,0").

```
*** READCO( Z, kallrd, khighz, iulow )
```

These subroutines behave the same as the previous

```
*** READEXCO( Z, kallrd, khighz, iulow, ofeback )
```

version of MAY 28, 1999: opacities are read in at

the SINGLE metallicity Z (interpolated among available OPAL opacity files, if necessary), but subsequently opacities are available only at this single metallicity, unless and until the user explicitly reads in a new set of opacities via another call to READCO, READEXCO, or READZEXCO. (For READCO, any positive value of khighz is set to 1, and any negative value to -1).

NOTE THAT the input INTEGER kallrd is ignored (it is included only for backward compatibility).

```
=====
Subroutines used to control the switchover from OPAL to molecular opacities:
=====
```

NOTE that the Ferguson and the Alexander switchover specifications are entirely separate: only one will take effect at any time, namely, the one for which the corresponding molecular opacities have been read in.

*** SET_LOGT_SW_FERG(FLTSW_LO, FLTSW_HI) Set the temperature-boundaries of
 ----- the switchover region from OPAL to
 Ferguson et al. (2005) molecular opacities (this subroutine can be called
 at any time, to change the switchover temperatures):

FLTSW_LO = lowest logT of switchover region, where only Ferguson is used:
 -99.0 : leave current stored logT value unchanged.
 -50.0 : use the default value (of logT = 4.2).
 > -20 : use the input value FLTSW_LO, except that:
 it will not be lower than 3.75 (lowest T for OPAL),
 it will not exceed 4.45 (near highest Ferguson T).
 FLTSW_HI = highest logT of switchover region, where only OPAL is used:
 -99.0 : leave current stored logT value unchanged.
 -50.0 : use the default value (of logT = 4.4).
 > -20 : use the input value FLTSW_HI, except that:
 it will not exceed 4.50 (highest Ferguson T),
 it will not be lower than 3.80 (near lowest OPAL).

Note that in no case will $FLTSW_HI - FLTSW_LO < 0.05$ be allowed to occur
 (the values will be moved further apart if this happens).

*** ASK_LOGT_SW_FERG(FLTSW_LO, FLTSW_HI) Return the current Ferguson logT
 ----- switchover values (as above).

*** SET_LOGT_SW_ALEX(FLTSW_LO, FLTSW_HI) Set the temperature-boundaries of
 ----- the switchover region from OPAL to
 Alexander & Ferguson 1994 molecular opacities (this subroutine can be called
 at any time, to change the switchover temperatures):

FLTSW_LO = lowest logT of switchover region, where only Alexander is used:
 -99.0 : leave current stored logT value unchanged.
 -50.0 : use the default value (of logT = 3.87).
 > -20 : use the input value FLTSW_LO, except that:
 it will not be lower than 3.75 (lowest T for OPAL),
 it will not exceed 4.05 (near highest Alexander T).
 FLTSW_HI = highest logT of switchover region, where only OPAL is used:
 -99.0 : leave current stored logT value unchanged.
 -50.0 : use the default value (of logT = 3.97).
 > -20 : use the input value FLTSW_HI, except that:
 it will not exceed 4.10 (highest Alexander T),
 it will not be lower than 3.80 (near lowest OPAL).

Note that in no case will $FLTSW_HI - FLTSW_LO < 0.05$ be allowed to occur
 (the values will be moved further apart if this happens).

*** ASK_LOGT_SW_ALEX(FLTSW_LO, FLTSW_HI) Return the current Alexander logT
 ----- switchover values (as above).

*** SET_ALEX_DO_RHOSW(IRHOSW) Set the flag controlling whether there is a
 ----- density-switchover too (in the temperature
 region where both OPAL and Alexander 1994 opacities are available, but where
 the OPAL opacities are available up to higher densities):

IRHOSW = input integer flag:
 1 : (DEFAULT): use a density-switchover region too.
 0 : do not do so.
 -9 : use the default value of 1.
 -99 : leave the stored value unchanged.

*** SET_LOGRHO_SW_ALEX(FLRHOSW_LO, FLRHOSW_HI) Set the density-boundaries
 ----- of the switchover region
 (for Alexander 1994 opacities) that is enabled/disabled by SET_ALEX_DO_RHOSW
 above (this can be called at any time, to change the switchover densities):

FLRHOSW_LO = lowest logRHO of switchover region, where only Alexander used:
 -99.0 : leave current stored logRHO value unchanged.
 -50.0 : use the default value (of logRHO = -6.25).
 > -20 : use the input value FLTSW_LO, except that it will lie
 in the range -14.0 < FLRHOSW_LO < -6.0 .
 FLRHOSW_HI = highest logRHO of switchover region, where only OPAL is used:
 -99.0 : leave current stored logRHO value unchanged.
 -50.0 : use the default value (of logRHO = -5.75).
 > -20 : use the input value FLTSW_HI, except that it will lie
 in the range -13.75 < FLRHOSW_HI < -5.75 .

Note that in no case will $FLRHOSW_HI - FLRHOSW_LO < 0.25$ be allowed to occur (the values will be moved further apart if this happens).

*** ASK_LOGRHO_SW_ALEX(FLRHOSW_LO, FLRHOSW_HI) Return current switchover
 ----- logRHO values (as above).

*** SET_LOGT_RHOSW_ALEX(FLTSW_R_LO, FLTSW_R_HI) Set the temperature-bounds
 ----- below which the Alexander-
 to-OPAL density-switchover described above does not take place (due to the
 low-temperature limit of the OPAL opacities):

FLTSW_R_LO = lowest logT of switchover region, where only Alexander used:
 -99.0 : leave current stored logT value unchanged.
 -50.0 : use the default value (of logT = 3.70).
 > -20 : use the input value FLTSW_LO, except that:
 it will not be lower than 3.70 (the lowest
 allowed OPAL-extrapolation logT value),
 it will not exceed $FLTSW_HI - 0.05$ (see the
 subroutine SET_LOGT_SW_ALEX above).
 FLTSW_R_HI = highest logT of switchover region, where only OPAL is used:
 -99.0 : leave current stored logT value unchanged.
 -50.0 : use the default value (of logT = 3.80).
 > -20 : use the input value FLTSW_HI, except that:
 it will not exceed FLTSW_HI,
 it will not be lower than 3.75

Note that in no case will $FLTSW_R_HI - FLTSW_R_LO < 0.05$ be allowed to occur (the values will be moved further apart if this happens).

*** ASK_LOGT_RHOSW_ALEX(FLTSW_R_LO, FLTSW_R_HI) Return density-switchover
 ----- logT-bounds as above.

=====
 The subroutines that control the X-interpolation accuracy:
 =====

*** SET_XHI(kxhi) Set a flag telling whether or not to use the additional
 ----- 'GN93hz' X-values for more accurate X-interpolation
 (provided they are available, i.e., 'GN93hz' or 'GS98hz' has been read in).
 If kxhi = 2 , then a flag is set such that the 'GN93hz' X-values will be

used whenever they are available (this is the DEFAULT case, if you never call SET_XHI). Note that only at $X > 0.03$ will the 'GN93hz' X-values affect the resulting interpolated opacity values.

If $kxhi = 1$, then a flag is set such that the 'GN93hz' X-values will be used whenever they are available, but ONLY for values of $X > 0.7$ (this yields faster but slightly less accurate X-interpolation for $X < 0.7$, while retaining accurate opacities for large X-values up to $X = 1-Z$ (such as may arise from diffusive processes)).

If $kxhi = 0$, then a flag is set such that the 'GN93hz' X-values will NOT be used, even when they are available (this results in only slightly poorer X-interpolation for $X < 0.75$, but yields wildly incorrect opacities for very large X values, i.e., for X approaching 1-Z).

Note that the 'GN93hz' X-values are available for X-interpolation ONLY if the 'GN93hz' file has been read in, i.e., if READZEXCO above has been called with a non-zero value of $khighz$ among its input parameters. Note also that, strictly, the 'GN93hz' X-values are defined only for non-CO-rich mixes ($C=O=0.0$); but corresponding opacity shifts are applied for consistency up to a CO-enhancement of $C+O = 0.2$, these shifts being reduced to zero as $C+O$ increases from 0.2 to 0.3 and being ignored for $C+O$ of 0.3 or more.

*** ASK_XHI($kxhi$, $kavail$) Returns INTEGER VARIABLE flags telling whether
----- 'GN93hz' X-values will be used, and whether they
are actually available at the moment:

Returns $kxhi$ value as set most recently by SET_XHI above (i.e., returns
 $kxhi = 0, 1$, or 2 , with the same meaning as above);
if SET_XHI was never called, then returns $kxhi = 2$.

Returns $kavail = 1$ if the 'GN93hz' files have been read in, i.e., the
'GN93hz' X-values are available, and will be used for
X-interpolation if the value of $kxhi$ so indicates.

$kavail = 0$ if the 'GN93hz' file has NOT (yet) been read in,
i.e., the 'GN93hz' X-values are not available, and
can NOT be used for X-interpolation no matter what
value $kxhi$ has (unless 'GN93hz' is read in later).

=====
The subroutines that control the CNO and/or user-interpolation:
=====

*** SET_CNO_INTERP($kcno$, $kuser$) Set flags telling whether or not to use the
----- CNO/user-interpolation opacity shifts; by
default, both are used, providing they are available (i.e., providing the
relevant opacity files were read in: see flag $khighz$ in READZEXCO above).

If $kcno > 0$, then the CNO-interpolation opacity shifts will be used (if
available); otherwise, they will be ignored

If $kuser > 0$, then the user-specified opacity shifts will be used (if
available); otherwise, they will be ignored

*** ASK_CNO_INTERP($kcno$, $kuser$, $kcno_avail$, $kuser_avail$) Returns INTEGER
----- VARIABLE flags to
indicate whether CNO/user-interpolation opacity shifts will be used when
obtaining opacities.

Returns $kcno$, $kuser$ as set by SET_CNO_INTERP above (or their default
values of 1 if SET_CNO_INTERP was never called)

Returns $kcno_avail$, $kuser_avail$ values of 1 if the corresponding opacity
files have been read in, or 0 if not

```

=====
The subroutines that control the level of error-checking:
=====

```

```

*** SET_ERR_CHECK( LEVEL ) This subroutine sets the error-checking level to
----- the given (integer) input value LEVEL:
Level = 0 : Only minimal error checking is performed on inputs. A Z-value
above 0.1 in the arguments to the opacity-reading subroutine
READZEXCO is a fatal error, as is an inconsistent composition
input to the opacity-calculating subroutines OPAC or OPAL;
most other problematic input is handled or accepted silently,
in a manner that ought to be reasonable (but no guarantees!).
Level = 1 : This is the DEFAULT case (which will occur if you never call the
subroutine SET_ERR_CHECK). At this level, error-checking is
performed on the arguments of the subroutine READZEXCO (which
one calls to read in the opacities). As described above in
the discussion of Nzin, Zlo, Z, Zhi , it is a fatal error
if Nzin < 1 or if Nzin is too large (exceeding the available
number of Z-storage spaces). It is also a fatal error if the
Z-range [Zlo,Zhi] is too small or too large. At this level,
a warning will be issued if you call SET_ALTMIX_MAIN_FILE and
subsequently use khighz = -2, -3, or -4 (see above), or if any
filename exceeds 255 characters (or an extension exceeds 80).
Level = 2 : At this level of error-checking, in addition: If the arguments
to OPAC or OPAL lie too far outside the opacity matrices, it
is a fatal error and the program halts (normally, such a case
would simply be signalled by a zero returned value of FEDGE).
Also, it is a fatal error if you call SET_ALTMIX_MAIN_FILE and
subsequently use khighz = -2, -3, or -4 (see above), or if any
filename exceeds 255 characters (or an extension exceeds 80).
Level = 3 : At this level of error-checking, in addition: if you have read
the CNO-interpolation opacity files, and you then call the
subroutine OPAL_X_CNO_FU with a metals-composition array xmet
with a size nmet other than 19 elements, it is a fatal error
(you would NOT usually want to use this Level = 3).

*** ASK_ERR_CHECK( LEVEL ) This subroutine returns the error-checking flag
----- value LEVEL of as set by SET_ERR_CHECK above.

```

```

=====
The subroutines that control matrix Z-edge handling:
=====

```

```

*** RESET_Z_LIMITS( vlo, dvlo, vhi, dvhi ) This subroutine can only be called
----- AFTER a set of opacities has been
read in (its effects are nullified during opacity input). WITHOUT affecting
the stored z-values used for Z-interpolation, calling this subroutine resets
the range considered to be "interpolation" (which returns FZEDGE = 1.0) and
the allowed "extrapolation" region (where 0.0 < FZEDGE < 1.0 is returned).
Negative values (actually, below -1.E-6) mean "leave old value unchanged".
All these values should be SINGLE PRECISION REAL.
If vlo is non-negative, then this resets Zlo = vlo .
If dvlo is non-negative, then this resets Zlo_ex = Zlo - dvlo .
If vhi is non-negative, then this resets Zhi = vhi .
If dvhi is non-negative, then this resets Zhi_ex = Zhi + dvhi .
The values of Zlo and Zhi must not lie outside the range of stored z-values
used for Z-interpolation, i.e., cases Zlo < z_low_interpolation_endpoint ,
Zhi > z_high_interpolation_endpoint , and Zlo > Zhi are prohibited. The

```

only constraint on the "extrapolation" region is that $Z_{lo_ex} < Z_{lo}$ and $Z_{hi_ex} > Z_{hi}$ (setting dv_{lo} and dv_{hi} to zero allows extrapolation by up to $\Delta Z = 1.E-6$). Note that FZEDGE is positive (and the opacity is calculated) only for the range $Z_{lo_ex} < Z < Z_{hi_ex}$.

NOTE that if Z_{lo} and/or Z_{hi} is set inside the range covered by the stored z-values, the value of FZEDGE will be less than unity for Z outside the range $[Z_{lo}, Z_{hi}]$, but the actual calculation of opacity values will continue to use interpolation (not extrapolation) as long as Z lies inside the range of stored z-values; however, for $FZEDGE = 0.0$, the opacity will NOT be calculated (even for Z still within the range of stored z-values).

*** ASK_Z_LIMITS(nzmax, zmin, zmax) This subroutine returns the values of
----- the hard-wired Z-interpolation limits,
allowing the user to check what these limiting values actually are.
INTEGER variable nzmax returns NZ: max number of interpolation Z-values.
SINGLE-PRECISION REAL variable zmin returns 0.0 (the lowest allowed Z).
SINGLE-PRECISION REAL variable zmax returns 0.1 (the highest allowed Z).

*** ASK_Z_USE(nzuse, zlo, zmid, zhi, zloex, zhiex) This subroutine returns
----- the current values of
the variables controlling Z-interpolation, allowing the user to check what
the values actually are.
INTEGER variable nzuse returns the number of stored z-values (that will
be used for Z-interpolation); if no opacity files have been read in yet,
then $nzuse = 0$ is returned (and the other five variables will return
meaningless values).
SINGLE-PRECISION REAL variable zlo returns the boundary Z_{lo} below
which a Z value is considered to require extrapolation; note that Z_{lo}
may lie above the lowest stored z-value, but not below it.
SINGLE-PRECISION REAL variable zmid returns the "typical" Z-value (which
has no real significance after the opacities have been read in).
SINGLE-PRECISION REAL variable zhi returns the boundary Z_{hi} above
which a Z value is considered to require extrapolation; note that Z_{hi}
may lie below the highest stored z-value, but not above it.
SINGLE-PRECISION REAL variable zloex returns the boundary Z_{lo_ex} at or
below which Z-extrapolation is considered too extreme to be carried out.
SINGLE-PRECISION REAL variable zhiex returns the boundary Z_{hi_ex} at or
above which Z-extrapolation is considered too extreme to be carried out.

*** ASK_Z_ARRAY(kzstart, karraystart, Zarray, Narray) This subroutine will
----- return (some of) the
stored z-values (that are used for Z-interpolation), in the user-supplied
array variable Zarray (the other inputs to ASK_Z_ARRAY must have values
supplied by the user, and may be constant integers).
kzstart INTEGER: index of the first stored z-value to be returned.
karraystart INTEGER: the index in the user-supplied array Zarray where
the first returned z-value will be placed.
Zarray SINGLE-PRECISION REAL ARRAY: is where the stored z-values are
returned; the array positions Zarray(karraystart) through
Zarray(min{ Narray, karraystart + nzuse - kzstart })
will contain the stored z-values kzstart through nzuse
(where nzuse is the total number of stored z-values); any
subsequent elements of Zarray (up to element Narray)
will be filled with values of -1.0 (note that in no case
will elements beyond Narray be overwritten).
Narray INTEGER: the size of the user-supplied array Zarray, i.e.,
the array is specified as "dimension Zarray(Narray)".

=====

The subroutines that control matrix T,R-edge handling:

=====

*** SET_LOGT6_LIMITS(VLO, DVLO, VHI, DVHI) These subroutines can be called
----- at ANY TIME, and their effects
*** SET_LOGR_LIMITS(VLO, DVLO, VHI, DVHI) will last until they are called
----- again; they are used to set (or
reset) the LogT6 and LogR boundaries. These input boundaries VLO and VHI
must not lie outside the matrix edges, and extrapolation is never allowed
more than one grid-spacing beyond the edge of the matrix. All these input
values should be SINGLE-PRECISION REAL, given in terms of $\log_{10}(T6)$ and
 $\log_{10}(R) = \log_{10}(\rho/T6^{*3})$; values of -90.0 or less mean "leave the present
values unchanged", and are ignored.

If VLO > -90.0, then (for subroutine SET_LOGT6_LIMITS) it is used to set
the lower boundary LogT6_lo (minimum -2.25: $\log T=3.75$), or (for subroutine
SET_LOGR_LIMITS), to set the lower boundary LogR_lo (minimum -8.0).

If VHI > -90.0, then it is used to set the upper boundary LogT6_hi
(maximum +2.70: $\log T=8.70$) or the upper boundary LogR_hi (maximum +1.0).

If DVLO is non-negative, it is used to set the amount of "extrapolation"
dLogT6 or dLogR allowed beyond the lower boundary, except that the extreme
values LogT6_lo - dLogT6 and LogR_lo - dLogR are not allowed to lie more
than one grid spacing beyond the matrix edge; if $-90.0 < DVLO < 0.0$, then
the amount of extrapolation is set to its default (namely, dLogT6 = 0.05 or
dLogR = 0.5); if DVLO < -90.0, then it is ignored.

If DVHI is non-negative, it is used to set the amount of "extrapolation"
dLogT6 or dLogR allowed beyond the upper boundary, except that the extreme
values LogT6_hi + dLogT6 and LogR_hi + dLogR are not allowed to lie more
than one grid spacing beyond the matrix edge; if $-90.0 < DVHI < 0.0$, then
the amount of extrapolation is set to its default (namely, dLogT6 = 0.20 or
dLogR = 0.5); if DVHI < -90.0, then it is ignored.

NOTE that even if the boundaries are set inside the matrix, the opacity
calculation continues to use all available matrix entries: interpolation is
still used (not extrapolation) as long as T6 and R lie inside the edge of
matrix. The boundaries and "extrapolation" distances are used to obtain the
value of FTREDGE to return, and whenever FTREDGE = 0.0 the opacity is NOT
calculated (even if T6 and R lie inside the matrix edges).

*** ASK_LOGT6_LIMITS(VLO, DVLO, VHI, DVHI) These subroutines can be called
----- at any time; they return the
*** ASK_LOGR_LIMITS(VLO, DVLO, VHI, DVHI) current values of the lower and
----- upper LogT6 or LogR boundaries
and the corresponding allowed amounts of "extrapolation" dLogT6 or dLogR
(SINGLE-PRECISION REAL variables must be supplied to hold returned values).

NOTE ALSO that the OPAL arrays have a "cut-out" region where opacity values
are not available at high T6,R values; one grid-spacing of extrapolation is
allowed into this "cut-out" region. The boundary of this "cut-out" lies
roughly at $\log Rho = 4$ for $7.0 < \log T < 7.5$, and at somewhat higher densities
for $\log T > 7.5$ (up to $\log Rho = 6$ at $\log T = 8.7$, the high-T matrix edge).

NOTE ALSO that the X=0.0 and X=0.03 matrices have small "cut-outs" at low T6
and small R. As noted by Rogers and Iglesias, "as a result of the mixing
procedure used to calculate the OPAL opacity data, a few X=0.0 and X=0.03
low T - small R table values fell outside the range of T and R accessible
from the X=0.35 data directly calculated for this purpose. These T-R
locations are filled in with 9.999 (or for diagnostic purposes in some cases
larger values)." In the present program, these regions are treated as a
"cut-out" in the opacity tables (similar to the high T - large R corner),
and one grid spacing of extrapolation is allowed into them, as at any other
edge. For X > 0.1 they have no effect; for $0.03 < X < 0.1$, the corner
($-8.0 < \log R < -7.5$, $3.70 < \log T < 3.95$) [i.e., $T6 < 0.008912509$] is

extrapolated; and for $X < 0.03$, a ragged part of the region ($\log R < -4.5$, $\log T < 4.0$) [i.e., $T_6 < 0.01$] is considered to be outside the opacity grid (i.e., the opacity is not calculated, and $FTREDGE = 0.0$ is returned). Presumably very few users will have applications that take them into these low T - small R regions at low hydrogen abundances X; in any case, they are at temperatures where molecular opacities may become non-negligible.

=====
 The subroutines that control how smoothing is handled:
 =====

*** SET_SMOOTH(initsmooth, lowCOsmooth, interpCOsmooth) This subroutine
 ----- allows the user to
 control how and whether the opacity smoothing is carried out when the OPAL
 opacities are read in, and which subroutine is used to interpolate in C and
 O when OPAC or OPAL is called. The smoothing and its effects are discussed
 in more detail further below.
 --- IT IS RECOMMENDED THAT THE DEFAULT SMOOTHING VALUES NOT BE CHANGED.

initsmooth INTEGER: if initsmooth = 2 (the default), then the OPAL
 opacities are smoothed by the subroutine OPALTAB when
 they are read in, in order to remove random numerical
 errors; if initsmooth = 0, then this initial smoothing
 will not be carried out. A value initsmooth = 1 means
 that opacities used for CNO-interpolation opacity shifts
 will not be smoothed. A value initsmooth < 0 means
 "do not change the current initial-smoothing setting".

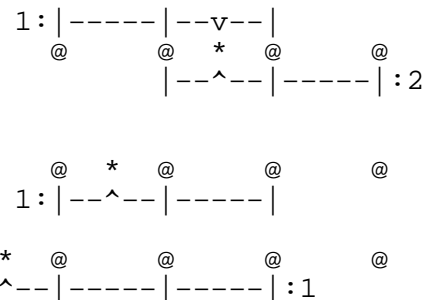
lowCOsmooth INTEGER: if lowCOsmooth = 1 (the default), then the OPAL
 opacities for the three mixes having $\max\{C,O\} = 0.01$ may
 be smoothed in the CO-direction when they are read in;
 this is only done at (T₆,R) points where opacity-changes
 between mixes with C,O = 0.0, 0.03, 0.1 are monotonic
 but the opacity at C,O = 0.01 does not fit the trend;
 the resulting adjustments are small, and only occur at a
 small minority of (T₆,R) points. If lowCOsmooth = 0,
 then this initial CO-direction smoothing is not carried
 out. A value lowCOsmooth < 0 means "do not change the
 current initial-CO-smoothing setting".

interpCOsmooth INTEGER: if interpCOsmooth = 1 (the default), then the
 subroutine COINTSMO is called by OPAC or OPAL in order
 to interpolate in C and/or O. If interpCOsmooth = 0,
 then the older subroutine COINTERP is used instead; this
 yields less smooth interpolation, and it has been less
 thoroughly tested. A value interpCOsmooth < 0 means
 "do not change the current CO-interpolation setting".

*** ASK_SMOOTH(initsmooth, lowCOsmooth, interpCOsmooth) This subroutine
 ----- returns the current
 smoothing settings described above (INTEGER variables must be supplied to
 hold the returned values), allowing the user to check how smoothing is being
 handled.

++++++
 Details of how the opacity interpolation is performed by OPAC or OPAL
 ++++++

In general, a 6-variable interpolation of $\log_{10}(\text{Kappa})$ is performed, using the arguments of OPAC or OPAL, on a subgrid of the stored opacity matrices. In general, 4 stored values ("@" in the diagram at upper right) are used along each interpolation direction. A quadratic fit is performed for each of the 2 sets of 3 adjacent stored values ("1" and "2" at upper right), and then linear interpolation between these overlapping quadratics is used to obtain smoothed results. [For a value near (or beyond) the edge of the matrix, as in the diagrams at lower right, a single quadratic is used.] This procedure produces results that are similar to bicubic spline interpolation, but requires storage of only local information.



--- FIRST, unless excess $C = O = 0.0$, for each $(Z_i, X_j, T6_k, R_n)$ grid value that will be needed, an interpolation is performed in the excess C and O values ("exC" and "exO" in the arguments to OPAC or OPAL). The actual C' and O' values used at each (Z_i, X_j) gridpoint are adjusted by a factor $\text{cmod} = (1 - X_i - Z_j) / (1 - X - Z)$, i.e., C' and O' are set to be proportional to the maximum possible value for their (Z_i, X_j) values, so as to avoid out-of-range C' and O' values (note that X is "xh", Z is "z" in the arguments to the subroutines OPAC or OPAL described above). The above formula for cmod can lead to problems when $(1 - X - Z)$ is small, therefore: as X is increased from 0.7 to 0.8, cmod switches over smoothly to from the above formula to a constant value of unity (note that since the largest grid $\{X_i, Z_j\}$ values are $X=0.7$ and $Z=0.1$ respectively, at $X > 0.8$ a value of $\text{cmod} = 1.0$ will never yield $X_i + Z_j + C' + O' > 1$).

The 2-D bi-quadratic interpolation of $\log(\text{Kappa})$ in $\log(C'+Z_i+0.001)$ and $\log(O'+Z_i+0.001)$ is performed by the subroutine COINTSMO (or by the older subroutine COINTERP, if you so choose: see description of subroutine SET_SMOOTH above). The function QCHK is used to evaluate the quadratic: it checks whether 2 of the 3 grid-points are excessively close together (as may happen near $C + O = 1 - Z - X$ for some values of Z) and, if so, uses more nearly linear interpolation to avoid amplifying small errors in the stored opacity values. For the special case where C or O is slightly negative (slight depletion in C or O), the function QCHK does a linear extrapolation using a combination of the lowest three C or O gridpoints. If C and/or O is zero (to within an accuracy of 1.E-6), then interpolation in that direction is not necessary, and is not performed (unless the user has specified that the old subroutine COINTERP should be used).

--- SECOND, unless Z is within 1.E-6 of a stored z-value (or $Z < 1.E-8$, if the stored value is 0.0), for each $(X_j, T6_k, R_n)$ grid value that will be needed, an interpolation is performed in $\log(Z+0.001)$. If there are only 2 stored z-values ($\text{numz} = 2$), linear interpolation is used; for $\text{numz} = 3$, a quadratic is used, while two overlapping quadratics are used for $\text{numz} > 3$ (unless Z is near the end of the range of stored z-values). The subroutine QZLOG4INT is called to perform this Z-interpolation. Since numerical errors in the stored opacities, or in the CO-interpolation, may be comparable to the opacity differences between adjacent stored z-values, the opacity at Z is not allowed to lie outside the range of the two opacities at the stored z-values bracketing it. (Note that, when opacities are read in for values of Z different from one of those available in the OPAL opacity files, the same type of interpolation with the same constraint is performed by the subroutines READZEXCO, READEXCO, or READCO.)

--- THIRD, a two-variable interpolation is performed in the temperature and density variables T6 and R (note $\text{slt} = \log_{10}(T6)$ and $\text{slr} = \log_{10}(R)$ in the input to OPAL); the 2-D quadratic interpolation in $\log_{10}(T6)$ and $\log_{10}(R)$ uses two overlapping quadratics in each direction, unless T6 or R is within one grid spacing of an edge of the table (in which case a single quadratic is used in the relevant direction). NOTE that the high-T, RHO "cutout" has been filled in (by subroutine REVISE_HITR_FOR_INITSMOOTH) with "reasonable" values, at the time when the opacities were read in; for T or RHO above the actual upper edges of the matrix, switch from extrapolation

with the slope of the quadratic at the edge of the matrix to 2-point linear extrapolation one grid-spacing beyond the edge of the matrix.

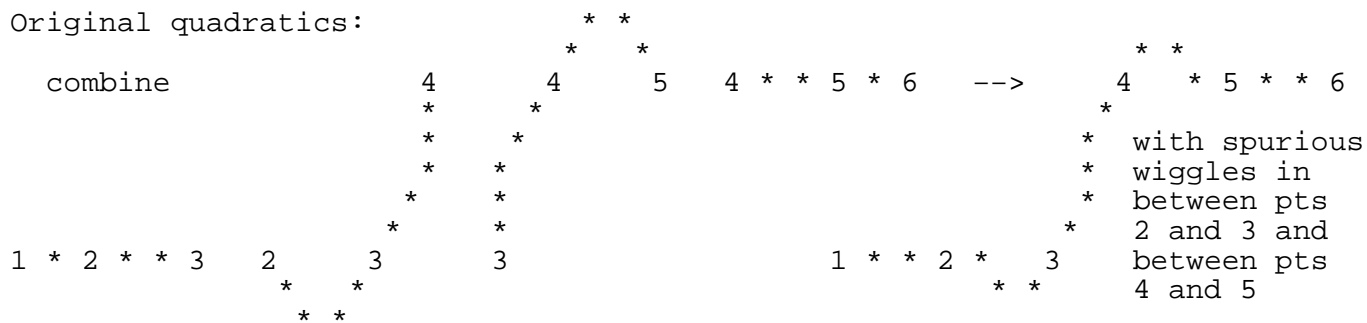
--- FOURTH, unless X is within 1.E-6 of one of the tabulated X-values (X is the input variable xh in OPAC or OPAL), log(Kappa) is interpolated quadratically in log(X+Xdel) , where Xdel = 0.03 is generally used (for 0.03 < X < 0.35, two overlapping quadratics are used). NOTE that pre-1997 versions of the opacity interpolation programs used a value of Xdel = 0.005, which led to non-monotonic behavior of the opacity as a function of X for small X values: for temperatures logT > 5.0 [T6 > 0.1], the interpolated opacity first dropped slightly as X was increased from 0.0 to about 0.005, then increased monotonically thereafter (at least up to X = 0.1). This spurious dip in the opacity for small X values was small (delta log(Kappa) of order 0.03), but it seemed worth getting rid of this dip by setting Xdel to 0.03, in order to obtain qualitatively correct behavior of the opacity for X close to zero. However, at low temperatures (i.e., for logT < 4), the X=0.0 opacities are very small with respect to the X=0.03 and X=0.1 opacities, and a smaller value of Xdel works better near X=0.0. Although such low X values are unlikely to be encountered at such low temperatures, provision was made in the program to reduce the value of Xdel used in such cases to a value that works better (down to a minimum value of 0.001); this was done ONLY for the quadratic that uses opacities at X = 0.0, 0.03, 0.1 (note that for the higher X-values, the value of Xdel used is irrelevant).

--- FIFTH, unless X is within 1.E-6 of one of the tabulated X-values or X < 0.03 or C+O > 0.3 or the "accurate-X" feature was turned off (see the subroutine SET_XHI described above): for the X-values available in 'GN93hz' but not 'Gz???.x??', Z-interpolation and (T6,R)-interpolation is performed in delta-logKappa values, which are then interpolated in X to give opacity corrections. Improvements are small for X < 0.76, but large for X > 0.76 .

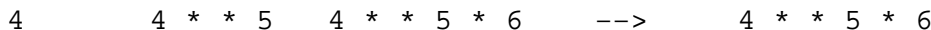
--- SIXTH, if (and only if) CNO- and/or user-interpolation is enabled and the corresponding CNO-interconverted opacity-files (or user-specified files) were available to read in: the delta-logKappa values corresponding to the interconversion of the CNO elements (and/or the user-specified composition shift) are multiplied by the relevant factors FCN, FCON, FCNONE, FU and then interpolated in Z, (T6,R), and X in order to give the corresponding opacity corrections.

NOTE: for the Ferguson et al. (2005) molecular opacity interpolation, MODIFIED quadratics are used for logT < 3.48, where sudden jumps in the opacity can occur between one grid-point and the next in any of the Z-, X-, R-, and/or T-directions. For a large jump, the original quadratics would lead to spurious wiggles on each side of the jump, with opacity errors of order a factor of 2 (occasionally more than an order of magnitude). The MODIFIED 3-pt quadratics switch over (smoothly), for a large jump, to linear interpolation in the flat segment, with a quadratic in the "jump" segment whose slope matches that of the flat segment where the two meet at the middle of the three points (two adjacent such modified 3-pt quadratics are still overlapped in general to get the final interpolated value). This gets rid of almost all the spurious wiggles next to opacity jumps. EXAMPLE:

Original quadratics:



Modified quadratics:




```

combine          *      *
                  *      *
                  *      *
                  *      *
                  *      *
1 * 2 * * 3     2 * * 3     3           1 * 2 * * 3
    
```

The modified quadratic routines QUADSL, QDERSL, and QCHKSL are used only for Ferguson et al. 2005 opacity interpolation at $\log T < 3.48$; they are similar to the functions QUAD, QDER, and QCHK [except that QCHKSL assumes that it is always the case that $x_1 < x_2$ and that x_2 and x_3 are the only pair of points that may coincide (or almost coincide)].

+++++
 Details of the makeup of Z (relative metal abundances), for various mixes
 +++++

Note that the total metallicity Z for the OPAL mixes includes the following 19 elements: {C,N,O,Ne,Na,Mg,Al,Si,P,S,Cl,Ar,K,Ca,Ti,Cr,Mn,Fe,Ni}. Their relative abundances (by mass fraction and/or number fraction) for any mix can be obtained by calling the subroutine ASK_OPAL_Z_MIX, while their atomic weights (and their atomic numbers, i.e., nuclear charges) can be obtained by calling the subroutine ASK_OPAL_MIX_WT (see descriptions further above).

The makeup of Z in the files 'GN93hz', 'Aldr96a2', 'C95hz', and 'W95hz' is shown below, along with the maximum, mean, and spread of opacity differences relative to 'GN93hz' for Z = 0.1 (where the opacity shifts are largest), for $T_6 > 0.01$ ($\log T > 4$), for each X-value. Note that [i/Fe] gives the log of the enhancement of element i relative to Fe, where the solar reference is the 'GN93hz' mix; note that for i = Fe, [i/Fe] = 0.0 by definition. Newer "GS98" and "AGS04" mixes are given further below. NOTE THAT THE CO-RICH OPACITY FILES 'Gz???.x??' HAVE THE SAME COMPOSITION AS THE FILE 'GN93hz'.

NOTE: for this GN93hz mix, Z/X = 0.02448:

	'Gx..z...' and 'GN93hz'		'Aldr96a2'			'C95hz'			'W95hz'		
	[O/Fe] = 0.0		[O/Fe] = 0.3			[O/Fe] = 0.4			[O/Fe] = 0.5		
i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	[i/Fe]	Ni/Nz	Xi/Z	[i/Fe]	Ni/Nz	Xi/Z	[i/Fe]
C	.245518	.173285	.147909	.102693	0.0	.131157	.091924	0.0	.108211	.076451	0.0
N	.064578	.053152	.038904	.031499	0.0	.034498	.028196	0.0	.028462	.023450	0.0
O	.512966	.482273	.616594	.570253	.30	.688325	.642620	.40	.714945	.672836	.50
Ne	.083210	.098668	.100010	.116656	.30	.044451	.052341	0.0	.071502	.084869	.29
Na	.001479	.001999	.001778	.002363	.30	.000790	.001060	0.0	.000652	.000882	0.0
Mg	.026308	.037573	.031622	.044428	.30	.035301	.050066	.40	.029125	.041639	.40
Al	.002042	.003238	.000617	.000962	-.3	.001091	.001718	0.0	.000900	.001428	0.0
Si	.024552	.040520	.029512	.047912	.30	.032945	.053992	.40	.021591	.035669	.30
P	.000195	.000355	.000234	.000420	.30	.000104	.000188	0.0	.000086	.000157	0.0
S	.011222	.021142	.013490	.024999	.30	.015059	.028172	.40	.010575	.019942	.33
Cl	.000219	.000456	.000263	.000539	.30	.000117	.000242	0.0	.000096	.000201	0.0
Ar	.002291	.005379	.002754	.006360	.30	.001224	.002853	0.0	.001010	.002373	0.0
K	.000091	.000210	.000055	.000124	0.0	.000122	.000279	.40	.000040	.000092	0.0
Ca	.001586	.003734	.001906	.004415	.30	.002127	.004975	.40	.002210	.005209	.50
Ti	.000075	.000211	.000089	.000245	.29	.000099	.000275	.39	.000137	.000387	.62
Cr	.000329	.001005	.000198	.000595	0.0	.000176	.000533	0.0	.000145	.000443	0.0
Mn	.000170	.000548	.000072	.00023	-.15	.000036	.000116	-.4	.000075	.000242	0.0
Fe	.021877	.071794	.013177	.042538	0.0	.011687	.038085	0.0	.009642	.031675	0.0
Ni	.001293	.004459	.000816	.002769	.02	.000691	.002365	0.0	.000595	.002056	.02

h>.093729 .192623 .096583 .178899 .101569 .184919 .076879 .142395
=====

where h> is the sum of everything heavier than Ne

opacity-shifts	'Aldr96a2'			'C95hz'			'W95hz'		
dLogKappa	-----			-----			-----		
for T6 > .01	[O/Fe] = 0.3			[O/Fe] = 0.4			[O/Fe] = 0.5		
for Z = 0.1,	=====			=====			=====		
relative	max	mean	sigma	max	mean	sigma	max	mean	sigma
to 'GN93hz'	-----			-----			-----		
X=0:	-.1512	-.0270	.0321	-.1844	-.0351	.0371	-.2669	-.0537	.0514
X=.03:	-.1457	-.0258	.0303	-.1835	-.0343	.0364	-.2270	-.0514	.0487
X=.10:	-.1464	-.0249	.0297	-.1849	-.0334	.0361	-.2286	-.0498	.0477
X=.35:	-.1490	-.0236	.0292	-.1886	-.0321	.0359	-.2334	-.0474	.0471
X=.70:	-.1539	-.0227	.0297	-.1952	-.0311	.0367	-.2416	-.0458	.0480

NOTE: if you are using 'Aldr96a2' having [O/Fe] = 0.3 (khighz = 2), then your mix Al abundance will go negative if you extrapolate [O/Fe] > 0.476 ; the Mn abundance will go negative if you extrapolate [O/Fe] > 0.644 .
--- If you are using 'C95hz' having [O/Fe] = 0.4 (khighz = 3), then your mix Mn abundance will go negative if you extrapolate [O/Fe] > 0.546 .
--- If you are using 'W95hz' having [O/Fe] = 0.5 (khighz = 4), then your mix Ti abundance will go negative if you extrapolate [O/Fe] < -0.501 .

By default, the CNO-interpolation files for the "GN93" mix are 'GN93hz' , 'GN93hz.CtON' , 'GN93hz.COtoN' , 'GN93hz.CNOtoNe' , and 'GN93hz.user' ; for other mixes, the default filenames are obtained by appending '.CtoN' , '.COtoN' , '.CNOtoNe' , and '.user' to the main mix filename ('GS98hz' or 'AGS04hz'). If such non-GN93 files are not found, CNO-interpolation opacity differences are obtained from the "GN93" files instead (if these are found).

Opacities for the "GS98" solar/meteoritic abundances (N. Grevesse & A.J. Sauval 1998, Space Sci. Rev. 85, 161) are contained in the file 'GS98hz' ; three other files were created with opacities for [O/Fe] enhancements (and alpha-element enhancements) RELATIVE TO THE "GS98" MIX, patterned after the corresponding three cases above. These files and compositions are:

NOTE: for this GS98hz mix, Z/X = 0.02300:

	GS98hz		GS98hz_OFe.3_Aldr96a2			GS98hz_OFe.4_C95			GS98hz_OFe.5_W95		
	[O/Fe] = 0.0		[O/Fe] = 0.3			[O/Fe] = 0.4			[O/Fe] = 0.5		
	=====		=====			=====			=====		
i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	[i/Fe]	Ni/Nz	Xi/Z	[i/Fe]	Ni/Nz	Xi/Z	[i/Fe]
C	.245825	.171836	.148069	.101930	0.0	.131883	.091638	0.0	.108877	.076359	0.0
N	.061748	.050335	.037193	.029858	0.0	.033128	.026843	0.0	.027349	.022368	0.0
O	.501922	.467356	.603216	.553139	.30	.676395	.626052	.40	.702986	.656744	.50
Ne	.089265	.104831	.107280	.124072	.30	.047890	.055905	0.0	.077089	.090832	.29
Na	.001562	.002090	.001877	.002473	.30	.000838	.001114	0.0	.000692	.000929	0.0
Mg	.028224	.039924	.033921	.047252	.30	.038036	.053480	.40	.031401	.044563	.40
Al	.002294	.003603	.000693	.001071	-.3	.001231	.001921	0.0	.001016	.001601	0.0
Si	.026954	.044057	.032394	.052144	.30	.036324	.059017	.40	.023820	.039063	.30
P	.000235	.000423	.000282	.000501	.30	.000126	.000226	0.0	.000104	.000188	0.0
S	.012602	.023513	.015145	.027829	.30	.016982	.031497	.40	.011933	.022339	.33
Cl	.000141	.000292	.000170	.000346	.30	.000076	.000156	0.0	.000063	.000130	0.0
Ar	.001865	.004335	.002241	.005131	.30	.001000	.002312	0.0	.000826	.001927	0.0
K	.000100	.000228	.000060	.000135	0.0	.000135	.000305	.40	.000044	.000101	0.0
Ca	.001670	.003896	.002007	.004611	.30	.002251	.005218	.40	.002339	.005474	.50

Ti.000070	.000195	.000082	.000226	.29	.000092	.000256	.39	.000129	.000362	.62
Cr.000369	.001117	.000222	.000663	0.0	.000198	.000596	0.0	.000163	.000496	0.0
Mn.000244	.000779	.000104	.000327	-.15	.000052	.000165	-.4	.000108	.000346	0.0
Fe.023517	.076433	.014165	.045339	0.0	.012616	.040761	0.0	.010416	.033965	0.0
Ni.001393	.004757	.000878	.002955	.02	.000747	.002537	0.0	.000646	.002214	.02

h>.101240	.205642	.104241	.191003		.110704	.199561		.083700	.153698	

where h> is the sum of everything heavier than Ne

Opacities can be read in for the newer "AGS04" solar/meteoritic abundances (M. Asplund, N. Grevesse, & A.J. Sauval 2004, astro-ph/0410214 [v2];

ALSO: M. Asplund, N. Grevesse, & A.J. Sauval 2005, Cosmic Abundances as Records of Stellar Evolution and Nucleosynthesis [eds. F.N. Bush & T.G. Barnes], ASP Conf. Series, Vol. 336, p. 25;

ALSO: M. Asplund, N. Grevesse, & A.J. Sauval 2006, Nucl. Phys. A 777, 1).

NOTE: for this AGS04hz mix, Z/X = 0.016555973

	AGS04hz			AGS04hz_OFe.3_Aldr96a2			AGS04hz_OFe.4_C95			AGS04hz_OFe.5_W95		
	[O/Fe] = 0.0			[O/Fe] = 0.3			[O/Fe] = 0.4			[O/Fe] = 0.5		
i	Ni/Nz	Xi/Z		Ni/Nz	Xi/Z	[i/Fe]	Ni/Nz	Xi/Z	[i/Fe]	Ni/Nz	Xi/Z	[i/Fe]
C	.257854	.176688		.157301	.106433	0.0	.138833	.094547	0.0	.116312	.080363	0.0
N	.063296	.050578		.038613	.030467	0.0	.034080	.027065	0.0	.028551	.023004	0.0
O	.480145	.438260		.584425	.526743	.30	.649367	.589077	.40	.684888	.630346	.50
Ne	.072700	.083693		.088481	.100581	.30	.039143	.044785	0.0	.063935	.074215	.29
Na	.001956	.002565		.002381	.003084	.30	.001053	.001373	0.0	.000882	.001166	0.0
Mg	.035594	.049354		.043324	.059318	.30	.048138	.066338	.40	.040329	.056385	.40
Al	.002827	.004352		.000865	.001315	-.3	.001522	.002328	0.0	.001275	.001979	0.0
Si	.033992	.054464		.041375	.065461	.30	.045972	.073207	.40	.030593	.049426	.30
P	.000264	.000466		.000321	.000560	.30	.000142	.000249	0.0	.000119	.000212	0.0
S	.015184	.027771		.018483	.033381	.30	.020536	.037330	.40	.014644	.027007	.33
Cl	.000178	.000361		.000216	.000431	.30	.000096	.000193	0.0	.000080	.000163	0.0
Ar	.001590	.003623		.001935	.004355	.30	.000856	.001939	0.0	.000717	.001648	0.0
K	.000121	.000269		.000074	.000163	0.0	.000163	.000361	.40	.000054	.000121	0.0
Ca	.002050	.004686		.002495	.005633	.30	.002771	.006297	.40	.002924	.006742	.50
Ti	.000082	.000223		.000099	.000267	.29	.000109	.000296	.39	.000153	.000422	.62
Cr	.000458	.001358		.000279	.000817	0.0	.000247	.000728	0.0	.000207	.000619	0.0
Mn	.000310	.000972		.000133	.000412	-.15	.000066	.000206	-.4	.000140	.000442	0.0
Fe	.029696	.094613		.018112	.056981	0.0	.015989	.050629	0.0	.013395	.043032	0.0
Ni	.001703	.005704		.001088	.003598	.02	.000917	.003052	0.0	.000802	.002708	.02

h>.126005	.250781	.131180		.235776			.138577	.244526		.106314	.192072	

where h> is the sum of everything heavier than Ne

Unlike earlier papers, "AGS04" above gives meteoritic H, He, C, N, O, Ne, Ar abundances. There are almost no noble gases (He, Ne, Ar ...), less C, N, O (relative to Si or Fe) than in the solar mix, and almost no hydrogen. [For other elements, meteoritic abundances were used in the above "AGS04" mix, instead of the less-accurate solar-surface observations.] The actual values for the meteoritic mix are given below [with many digits, to show the actual abundances of He, Ne, Ar; note that Ab_i = log10(N_i/N_H_sun) + 12.0]:

	Complete "AGS04" meteoritic abundances				Meteoritic mix (components of Z)	
i	Ab_i	Ni	Xi		Ni/Nz	Xi/Z
H	8.25	.312727500321341	.020944433890450			[Z=.979055556989581]

He	1.29	.000000034289886	.000000009119969		
C	7.40	.044173943244219	.035255788483962	.064274280534767	.036009997831346
N	6.25	.003127275003213	.002910629954482	.004550269595690	.002972895596887
O	8.39	.431684461811492	.458939274347532	.628112551500661	.468757131371265
Ne	-1.06	.00000000153167	.00000000205377	.00000000222863	.00000000209770
Na	6.27	.003274596717318	.005002390294590	.004764626668792	.005109403913677
Mg	7.53	.059588954783339	.096237981691629	.086703538675350	.098296752420816
Al	6.43	.004732763251461	.008485288886437	.006886298360263	.008666810403005
Si	7.51	.056906999803204	.106202066768971	.082801221741094	.108473994157720
P	5.40	.000441970109086	.000909645014595	.000643078446095	.000929104592789
S	7.16	.025419977789240	.054153160875713	.036986754263261	.055311632204228
Cl	5.23	.000297994997793	.000702016082572	.000433590770473	.000717033959472
Ar	-0.45	.00000000623973	.000000001656328	.00000000907898	.000000001691761
K	5.06	.000202569633331	.000526280567971	.000294744287793	.000537539023413
Ca	6.29	.003431964862220	.009140199460691	.004993601570053	.009335731149717
Ti	4.89	.000137278594489	.000436941664783	.000199744062802	.000446288938011
Cr	5.63	.000766751174096	.002649167869084	.001115643667846	.002705840184626
Mn	5.47	.000518980052336	.001894561100742	.000755129993520	.001935090493299
Fe	7.45	.049714940755353	.184489597541457	.072336581572827	.188436290692971
Ni	6.19	.002851042029444	.011120564522665	.004148343157951	.011358461165226

h> .208286785176682 .481949863998228 .303062898146020 .492259974990732

where h> is the sum of everything heavier than Ne

Meteoritic mixes as obtained from solar abundances by reducing C,N,O,Ne,Ar as per the AGS04 meteoritic abundances, and "antimeteor" Z-mixes that yield solar abundances when added to 50% and 20% as much meteoritic Z-material:

i	GN93hz.meteor		GN93hz.5antimeteor		GN93hz.2antimeteor	
	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
C	.062096387323045	.034055950767625	.3096329	.2428995	.2728055	.2011308
N	.004396103132102	.002811584920288	.0856148	.0783222	.0735314	.0632201
O	.606837084080657	.443326132928943	.4801523	.5017450	.4989998	.4900612
Ne	.00000000215357	.00000000198429	.1122968	.1480020	.0955898	.1184016
Na	.005283859474681	.005546683967014	.0001500	.0002252	.0009138	.0012895
Mg	.093987679773822	.104307149947153	.0026495	.0042059	.0162384	.0242262
Al	.007295227181013	.008987793491910	.0002060	.0003631	.0012607	.0020880
Si	.087714215091835	.112486310445815	.0024732	.0045368	.0151550	.0261267
P	.000696654916553	.000985278857158	.0000197	.0000399	.0001204	.0002289
S	.040091598026506	.058690042443895	.0011309	.0023680	.0069273	.0136324
Cl	.000782397036934	.001266565623746	.0000219	.0000507	.0001351	.0002939
Ar	.000000000877017	.000000001599745	.0030924	.0080685	.0026323	.0064548
K	.000325105632923	.000580403334678	.0000097	.0000248	.0000566	.0001359
Ca	.005666126529857	.010369588461345	.0001590	.0004162	.0009783	.0024069
Ti	.000267944210671	.000586040222841	.0000075	.0000235	.0000463	.0001360
Cr	.001175381889649	.002790592585741	.0000330	.0001122	.0002030	.0006479
Mn	.000607340179662	.001523534791034	.0000168	.0000602	.0001046	.0003529
Fe	.078157536632930	.199305017419850	.0022038	.0080385	.0135039	.0462918
Ni	.004619357794785	.012381327992788	.0001298	.0004978	.0007978	.0028745
h>	.326670425248838	.519806331184714	.0123032	.0290313	.0590735	.1271863

(NOTE: some abundances would go negative beyond GN93hz.561743antimeteor)

i	GS98hz.meteor		GS98hz.5antimeteor		GS98hz.2antimeteor	
	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z

C	.061833419528987	.033847976603222	.3108195	.2408300	.2734442	.1994336
N	.004377442231746	.002794386850040	.0820144	.0741053	.0703603	.0598431
O	.604274480285562	.440624098408040	.4657653	.4807222	.4865568	.4727025
Ne	.000000000214427	.000000000197201	.1207976	.1572465	.1026646	.1257972
Na	.005179390157206	.005426796827570	.0002843	.0004216	.0010191	.0014226
Mg	.093587138052187	.103667372071604	.0051357	.0080523	.0184132	.0271753
Al	.007606607490520	.009353799223261	.0004180	.0007276	.0014971	.0024528
Si	.089375982574740	.114401914525715	.0049037	.0088845	.0175839	.0299880
P	.000779229621820	.001099992396139	.0000423	.0000845	.0001529	.0002876
S	.041786601600009	.061056356041069	.0022925	.0047413	.0082210	.0160043
Cl	.000467537763442	.000755439983010	.0000264	.0000603	.0000926	.0001993
Ar	.000000000873527	.000000001590383	.0025233	.0065025	.0021445	.0052020
K	.000331587065415	.000590861589288	.0000185	.0000466	.0000655	.0001554
Ca	.005537504221631	.010115144589889	.0003042	.0007864	.0010898	.0026522
Ti	.000232110957854	.000506712319369	.0000127	.0000391	.0000456	.0001327
Cr	.001223556258112	.002899506965060	.0000673	.0002257	.0002409	.0007605
Mn	.000809072444438	.002025771911462	.0000439	.0001556	.0001588	.0005296
Fe	.077979330676706	.198476752244634	.0042777	.0154111	.0153411	.0520243
Ni	.004619007981672	.012357115663043	.0002527	.0009569	.0009081	.0032370
h>	.329514657739278	.522733537941497	.0206032	.0470960	.0669741	.1422236

(NOTE: some abundances would go negative beyond GS98hz.624814antimeteor)

i	AGS04hz.meteor		AGS04hz.5antimeteor		AGS04hz.2antimeteor	
	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
C	.064274208429525	.036009888957169	.3303785	.2470271	.2883952	.2048236
N	.004550290959465	.002972903901491	.0853040	.0743805	.0725636	.0600990
O	.628110449385059	.468754671183736	.4247136	.4230127	.4568036	.4321613
Ne	.000000000222945	.000000000209847	.0999372	.1255395	.0841701	.1004316
Na	.004764660515098	.005109430493010	.0009033	.0012928	.0015125	.0020561
Mg	.086704154588141	.098297263764627	.0164453	.0248824	.0275300	.0395653
Al	.006886347278212	.008666855488115	.0013066	.0021946	.0021869	.0034890
Si	.082801809933137	.108474558443967	.0157052	.0274587	.0262910	.0436619
P	.000643083014308	.000929109426030	.0001216	.0002344	.0002039	.0003734
S	.036987017004729	.055311919937648	.0070150	.0140005	.0117437	.0222628
Cl	.000433593850556	.000717037689513	.0000829	.0001830	.0001382	.0002898
Ar	.000000000907947	.000000001691848	.0021853	.0054345	.0018405	.0043476
K	.000294746381558	.000537541819713	.0000553	.0001347	.0000931	.0002153
Ca	.004993637042920	.009335779714580	.0009463	.0023611	.0015848	.0037560
Ti	.000199745481717	.000446291259625	.0000374	.0001114	.0000630	.0001783
Cr	.001115651593004	.002705854260520	.0002113	.0006841	.0003540	.0010884
Mn	.000755135357710	.001935100559721	.0001434	.0004904	.0002399	.0007794
Fe	.072337095427584	.188437270946424	.0137206	.0477009	.0229685	.0758481
Ni	.004148372626387	.011358520252416	.0007872	.0028767	.0013175	.0045731
h>	.303065051003006	.492262535747757	.0596667	.1300402	.0980675	.2024845

(NOTE: some abundances would go negative beyond AGS04hz.998696antimeteor)

Since the solar C, N, and O abundances have been reduced more-or-less in concert from one abundance paper to the next, it is not unreasonable to consider them NOT to be independent, and to vary all of them together by their quoted uncertainties (or by double this amount) to get mixes with shifted C, N, and O that can still be considered "reasonable" (note that Ne and Ar should be shifted by the same amount as O, since it is their ratios Ne/O and Ar/O that are measured). The shifted-CNO mixes would have the same meteoritic abundances as "AGS04" above, but different "anti-meteor" mixes:

Z/X = 0.01809864 AGS04hiCNO_{Ne}_OFe.5_W95 AGS04hiCNO_{Ne}.2antimeteor
 AGS04hiCNO_{Ne} || AGS04hiCNO_{Ne}.5antimeteor ||

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=====
i d:Ab_i  Ni/Nz  Xi/Z  Ni/Nz  Xi/Z  Ni/Nz  Xi/Z  Ni/Nz  Xi/Z
-----
C +0.05 .261002 .181349 .117585 .082019 .3333123 .2540186 .2915434 .2104168
N +0.06 .065561 .053122 .029536 .024025 .0879866 .0781965 .0750329 .0631518
O +0.05 .486005 .449821 .692380 .643323 .4337738 .4403542 .4639452 .4460345
Ne +0.05 .073584 .085897 .064632 .075741 .1006317 .1288455 .0850084 .1030764
Na 0.00 .001765 .002347 .000795 .001061 .0006621 .0009658 .0012990 .0017945
Mg 0.00 .032110 .045147 .036336 .051288 .0120428 .0185719 .0236341 .0345169
Al 0.00 .002551 .003981 .001149 .001800 .0009568 .0016381 .0018774 .0030438
Si 0.00 .030665 .049822 .027564 .044958 .0115013 .0204957 .0225709 .0380915
P 0.00 .000238 .000427 .000107 .000192 .0000895 .0001759 .0001755 .0003266
S 0.00 .013698 .025404 .013194 .024565 .0051371 .0104500 .0100819 .0194224
Cl 0.00 .000161 .000330 .000072 .000148 .0000607 .0001365 .0001186 .0002526
Ar +0.05 .001609 .003719 .000725 .001682 .0022008 .0055785 .0018591 .0044628
K 0.00 .000109 .000246 .000049 .000111 .0000404 .0001002 .0000799 .0001877
Ca 0.00 .001849 .004287 .002634 .006131 .0006931 .0017626 .0013607 .0032772
Ti 0.00 .000074 .000204 .000138 .000384 .0000273 .0000829 .0000540 .0001555
Cr 0.00 .000413 .001242 .000186 .000562 .0001546 .0005101 .0003038 .0009492
Mn 0.00 .000280 .000889 .000126 .000402 .0001050 .0003659 .0002059 .0006798
Fe 0.00 .026789 .086548 .012069 .039143 .0100475 .0356034 .0197181 .0661701
Ni 0.00 .001537 .005218 .000723 .002465 .0005766 .0021477 .0011312 .0039899
-----
h> .113848 .229811 .095867 .174892 .0442956 .0985852 .0844701 .1773205
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(NOTE: some abundances would go negative beyond AGS04hiCNO_{Ne.841962}amet)

Z/X = 0.01983278 AGS04vhCNO_{Ne_OFe.5_W95} AGS04vhCNO_{Ne.2antimeteor}
 AGS04vhCNO_{Ne} || AGS04vhCNO_{Ne.5antimeteor} ||

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i d:Ab_i  Ni/Nz  Xi/Z  Ni/Nz  Xi/Z  Ni/Nz  Xi/Z  Ni/Nz  Xi/Z
-----
C +0.10 .263820 .185686 .118732 .083546 .3358885 .2605241 .2943424 .2156212
N +0.12 .067812 .055659 .030518 .025042 .0906599 .0820020 .0774886 .0661962
O +0.10 .491254 .460576 .699138 .655310 .4418255 .4564867 .4703199 .4589405
Ne +0.10 .074376 .087948 .065260 .077148 .1012381 .1319220 .0857528 .1055376
Na 0.00 .001590 .002142 .000716 .000964 .0004434 .0006583 .0011044 .0015485
Mg 0.00 .028927 .041200 .032700 .046561 .0080606 .0126514 .0200899 .0297805
Al 0.00 .002298 .003633 .001034 .001634 .0006406 .0011161 .0015959 .0026262
Si 0.00 .027625 .045465 .024806 .040815 .0076973 .0139602 .0191852 .0328631
P 0.00 .000214 .000389 .000096 .000174 .0000594 .0001189 .0001487 .0002810
S 0.00 .012340 .023183 .011874 .022302 .0034384 .0071185 .0085700 .0167572
Cl 0.00 .000145 .000301 .000065 .000135 .0000406 .0000930 .0001007 .0002178
Ar +0.10 .001627 .003808 .000732 .001713 .0022142 .0057120 .0018755 .0045696
K 0.00 .000098 .000225 .000044 .000101 .0000272 .0000687 .0000681 .0001625
Ca 0.00 .001666 .003912 .002370 .005565 .0004637 .0012001 .0011566 .0028272
Ti 0.00 .000066 .000186 .000123 .000345 .0000181 .0000559 .0000458 .0001339
Cr 0.00 .000372 .001133 .000167 .000509 .0001032 .0003466 .0002581 .0008184
Mn 0.00 .000252 .000811 .000114 .000367 .0000702 .0002489 .0001749 .0005862
Fe 0.00 .024134 .078981 .010861 .035534 .0067250 .0242529 .0167609 .0570897
Ni 0.00 .001384 .004762 .000650 .002235 .0003861 .0014637 .0009616 .0034427
-----
h> .102738 .210131 .086352 .158954 .0303880 .0690652 .0720963 .1537045
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(NOTE: some abundances would go negative beyond AGS04vhCNO_{Ne.714584}amet)

The components of the metallicity for the CNO-varied mixes are given below. Note that burning C to N increases Z slightly, burning O to N decreases Z slightly, and burning CNO to Ne increases Z significantly; thus, although the mass fraction <Xheavy> of elements heavier than Ne does not change, the ratio <h> = <Xheavy>/Z differs between these CNO-varied mixes:

	'GN93hz'			'GN93hz.CtOaN'		'GN93hz.COtoN'		'GN93hz.CNOtoNe'	
	solar CNO			most C --> N		most C,O --> N		all C,N,O --> Ne	
i	Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
C	8.55	.245518	.173285	.000246	.000169	.000246	.000179	.000000	.000000
N	7.97	.064578	.053152	.309850	.247897	.817686	.694328	.000000	.000000
O	8.87	.512966	.482273	.512966	.468789	.005130	.004976	.000000	.000000
Ne	8.08	.083210	.098668	.083210	.095909	.083210	.101793	.906272	.847998
Na	6.33	.001479	.001999	.001479	.001942	.001479	.002061	.001479	.001577
Mg	7.58	.026308	.037573	.026308	.036523	.026308	.038764	.026308	.029650
Al	6.47	.002042	.003238	.002042	.003147	.002042	.003340	.002042	.002555
Si	7.55	.024552	.040520	.024552	.039387	.024552	.041803	.024552	.031975
P	5.45	.000195	.000355	.000195	.000345	.000195	.000366	.000195	.000280
S	7.21	.011222	.021142	.011222	.020550	.011222	.021811	.011222	.016683
Cl	5.50	.000219	.000456	.000219	.000443	.000219	.000471	.000219	.000360
Ar	6.52	.002291	.005379	.002291	.005228	.002291	.005548	.002291	.004244
K	5.12	.000091	.000210	.000091	.000203	.000091	.000216	.000091	.000165
Ca	6.36	.001586	.003734	.001586	.003631	.001586	.003854	.001586	.002948
Ti	5.03	.000075	.000211	.000075	.000205	.000075	.000218	.000075	.000167
Cr	5.68	.000329	.001005	.000329	.000977	.000329	.001037	.000329	.000793
Mn	5.39	.000170	.000548	.000170	.000533	.000170	.000566	.000170	.000433
Fe	7.50	.021877	.071794	.021877	.069787	.021877	.074068	.021877	.056653
Ni	6.25	.001293	.004459	.001293	.004335	.001293	.004601	.001293	.003519
<h>		.093729	.192623	.093729	.187236	.093729	.198724	.093729	.152002

where <h> is the sum of everything heavier than Ne.

For the GS98 mix, the corresponding CNO-varied metallicity components are:

	'GS98hz'			'GS98hz.CtOaN'		'GS98hz.COtoN'		'GS98hz.CNOtoNe'	
	solar CNO			most C --> N		most C,O --> N		all C,N,O --> Ne	
i	Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
C	8.52	.245825	.171836	.000246	.000167	.000246	.000177	.000000	.000000
N	7.92	.061748	.050335	.307327	.243574	.804230	.675229	.000000	.000000
O	8.83	.501922	.467356	.501922	.454393	.005019	.004813	.000000	.000000
Ne	8.08	.089265	.104831	.089265	.101924	.089265	.107973	.898760	.836936
Na	6.32	.001562	.002090	.001562	.002032	.001562	.002153	.001562	.001657
Mg	7.58	.028224	.039924	.028224	.038816	.028224	.041120	.028224	.031657
Al	6.49	.002294	.003603	.002294	.003502	.002294	.003710	.002294	.002856
Si	7.56	.026954	.044057	.026954	.042835	.026954	.045377	.026954	.034935
P	5.56	.000235	.000423	.000235	.000412	.000235	.000436	.000235	.000336
S	7.20	.012602	.023513	.012602	.022861	.012602	.024218	.012602	.018645
Cl	5.28	.000141	.000292	.000141	.000283	.000141	.000300	.000141	.000231
Ar	6.40	.001865	.004335	.001865	.004216	.001865	.004466	.001865	.003438
K	5.13	.000100	.000228	.000100	.000221	.000100	.000234	.000100	.000180
Ca	6.35	.001670	.003896	.001670	.003787	.001670	.004012	.001670	.003089
Ti	4.94	.000070	.000195	.000070	.000190	.000070	.000201	.000070	.000155
Cr	5.69	.000369	.001117	.000369	.001086	.000369	.001150	.000369	.000885
Mn	5.53	.000244	.000779	.000244	.000759	.000244	.000804	.000244	.000619
Fe	7.50	.023517	.076433	.023517	.074315	.023517	.078726	.023517	.060608
Ni	6.25	.001393	.004757	.001393	.004627	.001393	.004901	.001393	.003773
<h>		.101240	.205642	.101240	.199942	.101240	.211808	.101240	.163064

where <h> is the sum of everything heavier than Ne.

For the AGS04 mix, the corresponding CNO-varied metallicity components are:

	'AGS04hz'			'AGS04hz.Ct0N'		'AGS04hz.COtoN'		'AGS04hz.CNotoNe'	
	solar CNO			most C --> N		most C,O --> N		all C,N,O --> Ne	
i	Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
C	8.39	.257854	.176688	.002579	.001717	.002579	.001812	.000000	.000000
N	7.78	.063296	.050578	.318571	.247373	.793915	.650653	.000000	.000000
O	8.66	.480145	.438260	.480145	.425880	.004801	.004494	.000000	.000000
Ne	7.84	.072700	.083693	.072700	.081329	.072700	.085836	.873995	.800479
Na	6.27	.001956	.002565	.001956	.002493	.001956	.002631	.001956	.002041
Mg	7.53	.035594	.049354	.035594	.047960	.035594	.050618	.035594	.039266
Al	6.43	.002827	.004352	.002827	.004229	.002827	.004463	.002827	.003462
Si	7.51	.033992	.054464	.033992	.052926	.033992	.055859	.033992	.043331
P	5.40	.000264	.000466	.000264	.000453	.000264	.000478	.000264	.000371
S	7.16	.015184	.027771	.015184	.026987	.015184	.028483	.015184	.022095
Cl	5.23	.000178	.000361	.000178	.000350	.000178	.000369	.000178	.000286
Ar	6.18	.001590	.003623	.001590	.003521	.001590	.003716	.001590	.002883
K	5.06	.000121	.000269	.000121	.000262	.000121	.000277	.000121	.000215
Ca	6.29	.002050	.004686	.002050	.004555	.002050	.004807	.002050	.003729
Ti	4.89	.000082	.000223	.000082	.000218	.000082	.000230	.000082	.000178
Cr	5.63	.000458	.001358	.000458	.001320	.000458	.001393	.000458	.001081
Mn	5.47	.000310	.000972	.000310	.000944	.000310	.000996	.000310	.000773
Fe	7.45	.029696	.094613	.029696	.091941	.029696	.097036	.029696	.075273
Ni	6.19	.001703	.005704	.001703	.005542	.001703	.005849	.001703	.004537
<h>		.126005	.250781	.126005	.243701	.126005	.257205	.126005	.199521

where <h> is the sum of everything heavier than Ne.

For the high-C,N,O,Ne version of the "AGS04" mix:

	'AGS04hiCNONE'			'AGS04hiCNONE.Ct0N'		'AGS04hiCNONE.COtoN'		'AGS04hiCNONE.CNotoNe'	
	solar CNO			most C --> N		most C,O --> N		all C,N,O --> Ne	
i	Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
C	8.44	.261002	.181349	.002610	.001761	.002610	.001861	.000000	.000000
N	7.84	.065561	.053122	.323953	.254885	.805098	.669508	.000000	.000000
O	8.71	.486005	.449821	.486005	.436791	.004860	.004616	.000000	.000000
Ne	7.89	.073584	.085897	.073584	.083408	.073584	.088156	.886152	.818221
Na	6.27	.001765	.002347	.001765	.002279	.001765	.002409	.001765	.001857
Mg	7.53	.032110	.045147	.032110	.043839	.032110	.046335	.032110	.035711
Al	6.43	.002551	.003981	.002551	.003866	.002551	.004086	.002551	.003149
Si	7.51	.030665	.049822	.030665	.048378	.030665	.051132	.030665	.039408
P	5.40	.000238	.000427	.000238	.000414	.000238	.000438	.000238	.000337
S	7.16	.013698	.025404	.013698	.024669	.013698	.026073	.013698	.020095
Cl	5.23	.000161	.000330	.000161	.000321	.000161	.000339	.000161	.000261
Ar	6.23	.001609	.003719	.001609	.003611	.001609	.003816	.001609	.002941
K	5.06	.000109	.000246	.000109	.000239	.000109	.000253	.000109	.000195
Ca	6.29	.001849	.004287	.001849	.004163	.001849	.004400	.001849	.003391
Ti	4.89	.000074	.000204	.000074	.000199	.000074	.000210	.000074	.000162
Cr	5.63	.000413	.001242	.000413	.001206	.000413	.001275	.000413	.000983
Mn	5.47	.000280	.000889	.000280	.000864	.000280	.000913	.000280	.000704
Fe	7.45	.026789	.086548	.026789	.084039	.026789	.088823	.026789	.068457
Ni	6.19	.001537	.005218	.001537	.005068	.001537	.005357	.001537	.004128
<h>		.113848	.229811	.113848	.223155	.113848	.235859	.113848	.181779

where <h> is the sum of everything heavier than Ne.

For the very-high-C,N,O,Ne version of the "AGS04" mix:

i	'AGS04vhCNO'Ne'					'AGS04vhCNO'Ne.COtoN'				'AGS04vhCNO'Ne.CNOtoNe'	
	Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
---	---	---	---	---	---	---	---	---	---	---	---
C	8.49	.263820	.185686	.002638	.001802	.002638	.001907	.000000	.000000	.000000	.000000
N	7.90	.067812	.055659	.328994	.262029	.815335	.687252	.000000	.000000	.000000	.000000
O	8.76	.491254	.460576	.491254	.446925	.004913	.004730	.000000	.000000	.000000	.000000
Ne	7.94	.074376	.087948	.074376	.085341	.074376	.090318	.897262	.834689	.897262	.834689
Na	6.27	.001590	.002142	.001590	.002079	.001590	.002200	.001590	.001685	.001590	.001685
Mg	7.53	.028927	.041200	.028927	.039978	.028927	.042310	.028927	.032412	.028927	.032412
Al	6.43	.002298	.003633	.002298	.003526	.002298	.003731	.002298	.002858	.002298	.002858
Si	7.51	.027625	.045465	.027625	.044117	.027625	.046690	.027625	.035768	.027625	.035768
P	5.40	.000214	.000389	.000214	.000377	.000214	.000399	.000214	.000306	.000214	.000306
S	7.16	.012340	.023183	.012340	.022496	.012340	.023808	.012340	.018238	.012340	.018238
Cl	5.23	.000145	.000301	.000145	.000292	.000145	.000309	.000145	.000237	.000145	.000237
Ar	6.28	.001627	.003808	.001627	.003696	.001627	.003911	.001627	.002996	.001627	.002996
K	5.06	.000098	.000225	.000098	.000218	.000098	.000231	.000098	.000177	.000098	.000177
Ca	6.29	.001666	.003912	.001666	.003797	.001666	.004018	.001666	.003078	.001666	.003078
Ti	4.89	.000066	.000186	.000066	.000180	.000066	.000190	.000066	.000146	.000066	.000146
Cr	5.63	.000372	.001133	.000372	.001100	.000372	.001164	.000372	.000892	.000372	.000892
Mn	5.47	.000252	.000811	.000252	.000787	.000252	.000833	.000252	.000638	.000252	.000638
Fe	7.45	.024134	.078981	.024134	.076640	.024134	.081110	.024134	.062135	.024134	.062135
Ni	6.19	.001384	.004762	.001384	.004620	.001384	.004889	.001384	.003745	.001384	.003745
---	---	---	---	---	---	---	---	---	---	---	---
<h>	.102738	.210131	.102738	.203903	.102738	.215793	.102738	.165311	.102738	.165311	.102738
=====	=====	=====	=====	=====	=====	=====	=====	=====	=====	=====	=====

where <h> is the sum of everything heavier than Ne.

There are indications that Ne might have an abundance up to 3 times that inferred from the observed Solar coronal Ne/O ratios, although there are arguments against this too; at the very least, the Ne abundance may be quite uncertain, so here are AGS04 mixes with Ne * 1.5, 2.0, 2.5, and 3.0:

Z/X = 0.01724878		AGS04x15Ne_OFe.5_W95									
		AGS04x15Ne					AGS04x15Ne.5amet		AGS04x15Ne.2amet		
i	d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
---	---	---	---	---	---	---	---	---	---	---	---
C	0.000	.248810	.169591	.112709	.077488	.3184504	.2363816	.2781026	.1963072	.2781026	.1963072
N	0.000	.061076	.048547	.027666	.022181	.0824077	.0713340	.0700487	.0576618	.0700487	.0576618
O	0.000	.463305	.420657	.663672	.607789	.4011116	.3966082	.4371453	.4110377	.4371453	.4110377
Ne	+1.76	.105225	.120496	.092932	.107340	.1449344	.1807440	.1219276	.1445952	.1219276	.1445952
Na	0.000	.001887	.002462	.000855	.001125	.0008012	.0011383	.0014303	.0019325	.0014303	.0019325
Mg	0.000	.034345	.047372	.039079	.054367	.0145862	.0219094	.0260341	.0371869	.0260341	.0371869
Al	0.000	.002728	.004177	.001236	.001909	.0011587	.0019321	.0020679	.0032790	.0020679	.0032790
Si	0.000	.032800	.052277	.029646	.047659	.0139299	.0241782	.0248626	.0410375	.0248626	.0410375
P	0.000	.000255	.000448	.000116	.000206	.0001083	.0002074	.0001933	.0003518	.0001933	.0003518
S	0.000	.014651	.026656	.014190	.026040	.0062221	.0123280	.0111057	.0209248	.0111057	.0209248
Cl	0.000	.000172	.000346	.000077	.000156	.0000733	.0001605	.0001305	.0002718	.0001305	.0002718
Ar	0.000	.001534	.003478	.000695	.001589	.0021132	.0052170	.0017777	.0041736	.0017777	.0041736
K	0.000	.000116	.000258	.000052	.000116	.0000489	.0001182	.0000880	.0002021	.0000880	.0002021
Ca	0.000	.001978	.004498	.002833	.006499	.0008394	.0020791	.0014988	.0035304	.0014988	.0035304
Ti	0.000	.000079	.000214	.000148	.000406	.0000331	.0000979	.0000595	.0001675	.0000595	.0001675
Cr	0.000	.000442	.001303	.000200	.000595	.0001872	.0006016	.0003346	.0010224	.0003346	.0010224

Mn	0.000	.000299	.000933	.000136	.000428	.0001272	.0004319	.0002269	.0007326
Fe	0.000	.028654	.090812	.012980	.041493	.0121689	.0419994	.0217199	.0712869
Ni	0.000	.001644	.005475	.000778	.002614	.0006983	.0025332	.0012460	.0042983
h>		.121584	.240709	.103021	.185202	.0530959	.1149322	.0927758	.1903981

(NOTE: some abundances would go negative beyond AGS04x15Ne.921257amet)

Z/X = 0.01794158 AGS04x2Ne_OFe.5_W95

		AGS04x2Ne				AGS04x2Ne.5amet		AGS04x2Ne.2amet	
i d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	
C	0.000	.240379	.163043	.109323	.074812	.3072900	.2265596	.2684938	.1884496
N	0.000	.059006	.046672	.026835	.021415	.0796959	.0685215	.0676994	.0554118
O	0.000	.447605	.404412	.643730	.586793	.3790228	.3722407	.4187884	.3915437
Ne	+ .301	.135546	.154458	.120186	.138176	.1870455	.2316870	.1571847	.1853496
Na	0.000	.001823	.002367	.000829	.001086	.0007056	.0009958	.0013536	.0018185
Mg	0.000	.033182	.045543	.037906	.052491	.0128463	.0191659	.0246373	.0349921
Al	0.000	.002636	.004016	.001199	.001843	.0010207	.0016906	.0019571	.0030858
Si	0.000	.031688	.050258	.028755	.046012	.0122678	.0211497	.0235282	.0386147
P	0.000	.000246	.000430	.000112	.000198	.0000949	.0001804	.0001824	.0003302
S	0.000	.014155	.025626	.013764	.025141	.0054793	.0107830	.0105093	.0196888
Cl	0.000	.000166	.000333	.000075	.000151	.0000648	.0001410	.0001237	.0002562
Ar	0.000	.001482	.003344	.000674	.001534	.0020455	.0050160	.0017190	.0040128
K	0.000	.000112	.000248	.000051	.000114	.0000430	.0001032	.0000832	.0001901
Ca	0.000	.001911	.004324	.002748	.006275	.0007390	.0018181	.0014182	.0033216
Ti	0.000	.000076	.000206	.000143	.000390	.0000292	.0000859	.0000564	.0001579
Cr	0.000	.000427	.001253	.000194	.000575	.0001650	.0005266	.0003167	.0009624
Mn	0.000	.000289	.000897	.000132	.000413	.0001121	.0003779	.0002147	.0006894
Fe	0.000	.027683	.087306	.012590	.040059	.0107174	.0367404	.0205546	.0670797
Ni	0.000	.001588	.005264	.000754	.002522	.0006152	.0022167	.0011793	.0040451
h>		.117464	.231415	.099926	.178804	.0469458	.1009912	.0878337	.1792453

(NOTE: some abundances would go negative beyond AGS04x2Ne.856526amet)

Z/X = 0.01863439 AGS04x25Ne_OFe.5_W95

		AGS04x25Ne				AGS04x25Ne.5amet		AGS04x25Ne.2amet	
i d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	
C	0.000	.232500	.156981	.106134	.072313	.2968211	.2174666	.2594992	.1811752
N	0.000	.057072	.044937	.026052	.020700	.0771536	.0659190	.0655014	.0533298
O	0.000	.432932	.389378	.624950	.567196	.3583114	.3496897	.4016121	.3735029
Ne	+ .398	.163879	.185894	.145851	.166953	.2265366	.2788410	.1901794	.2230728
Na	0.000	.001764	.002279	.000805	.001050	.0006160	.0008638	.0012818	.0017129
Mg	0.000	.032094	.043849	.036800	.050737	.0112136	.0166249	.0233291	.0329593
Al	0.000	.002549	.003867	.001164	.001782	.0008914	.0014671	.0018535	.0029070
Si	0.000	.030650	.048389	.027916	.044475	.0107089	.0183462	.0222792	.0363719
P	0.000	.000238	.000414	.000109	.000192	.0000828	.0001564	.0001727	.0003110
S	0.000	.013691	.024674	.013362	.024301	.0047837	.0093550	.0099520	.0185464
Cl	0.000	.000161	.000321	.000073	.000147	.0000569	.0001230	.0001173	.0002418
Ar	0.000	.001434	.003219	.000655	.001484	.0019815	.0048285	.0016635	.0038628
K	0.000	.000109	.000239	.000050	.000111	.0000376	.0000897	.0000789	.0001793
Ca	0.000	.001848	.004164	.002667	.006064	.0006455	.0015781	.0013433	.0031296
Ti	0.000	.000074	.000198	.000140	.000380	.0000253	.0000739	.0000533	.0001483
Cr	0.000	.000413	.001206	.000189	.000557	.0001438	.0004561	.0002998	.0009060
Mn	0.000	.000280	.000863	.000128	.000399	.0000975	.0003269	.0002031	.0006486
Fe	0.000	.026776	.084060	.012223	.038722	.0093558	.0318714	.0194638	.0631845
Ni	0.000	.001536	.005068	.000732	.002437	.0005370	.0019227	.0011166	.0038099
h>		.113617	.222810	.097013	.172838	.0411773	.0880837	.0832079	.1689193

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 (NOTE: some abundances would go negative beyond AGS04x25Ne.797451amet)

Z/X = 0.01932720 AGS04x3Ne_ofe.5_W95

		AGS04x3Ne				AGS04x3Ne.5amet		AGS04x3Ne.2amet	
i	d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
C	0.000	.225122	.151354	.103126	.069977	.2869847	.2090261	.2510645	.1744228
N	0.000	.055261	.043326	.025314	.020031	.0747640	.0635025	.0634395	.0513966
O	0.000	.419197	.375420	.607243	.548880	.3388465	.3287527	.3855011	.3567533
Ne	+.477	.190413	.215077	.170059	.193870	.2636471	.3226155	.2211244	.2580924
Na	0.000	.001708	.002198	.000783	.001017	.0005325	.0007423	.0012150	.0016157
Mg	0.000	.031075	.042278	.035756	.049097	.0096809	.0142684	.0221037	.0310741
Al	0.000	.002468	.003728	.001131	.001724	.0007692	.0012586	.0017558	.0027402
Si	0.000	.029677	.046655	.027125	.043039	.0092449	.0157452	.0211086	.0342911
P	0.000	.000230	.000399	.000105	.000184	.0000713	.0001339	.0001635	.0002930
S	0.000	.013256	.023789	.012983	.023515	.0041291	.0080275	.0094286	.0174844
Cl	0.000	.000156	.000309	.000071	.000142	.0000488	.0001050	.0001109	.0002274
Ar	0.000	.001388	.003104	.000636	.001435	.0019220	.0046560	.0016120	.0037248
K	0.000	.000105	.000230	.000048	.000106	.0000321	.0000762	.0000745	.0001685
Ca	0.000	.001789	.004014	.002591	.005867	.0005567	.0013531	.0012723	.0029496
Ti	0.000	.000071	.000191	.000135	.000365	.0000218	.0000634	.0000505	.0001399
Cr	0.000	.000400	.001163	.000183	.000538	.0001242	.0003916	.0002841	.0008544
Mn	0.000	.000271	.000832	.000124	.000385	.0000842	.0002804	.0001924	.0006114
Fe	0.000	.025926	.081047	.011876	.037470	.0080765	.0273519	.0184408	.0595689
Ni	0.000	.001487	.004886	.000711	.002358	.0004635	.0016497	.0010578	.0035915
h>		.110007	.214823	.094258	.167242	.0357577	.0761032	.0788705	.1593349

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 (NOTE: some abundances would go negative beyond AGS04x3Ne.747866amet)

Z/X = 0.01887595 AGS04hiCNOx15Ne_ofe.5_W95

		AGS04hiCNOx15Ne				AGS04hiCNOx15Ne.5amet				AGS04hiCNOx15Ne.2amet	
i	d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z
C	+.050	.251740	.173881	.113904	.079026	.3212059	.2428166	.2810428	.2014552		
N	+.060	.063234	.050934	.028611	.023148	.0849795	.0749145	.0724070	.0605262		
O	+.050	.468761	.431300	.670709	.619856	.4097142	.4125727	.4438537	.4238093		
Ne	+.226	.106459	.123540	.093912	.109465	.1459095	.1853100	.1231012	.1482480		
Na	0.000	.001702	.002250	.000770	.001023	.0005669	.0008203	.0012231	.0016781		
Mg	0.000	.030971	.043288	.035199	.049417	.0103179	.0157834	.0222584	.0322861		
Al	0.000	.002460	.003817	.001113	.001735	.0008198	.0013921	.0017680	.0028470		
Si	0.000	.029577	.047770	.026702	.043319	.0098536	.0174177	.0212567	.0356291		
P	0.000	.000230	.000409	.000104	.000186	.0000764	.0001489	.0001650	.0003050		
S	0.000	.013211	.024358	.012780	.023667	.0044013	.0088810	.0094951	.0181672		
Cl	0.000	.000155	.000316	.000070	.000143	.0000518	.0001155	.0001114	.0002358		
Ar	+.050	.001552	.003566	.000702	.001620	.0021275	.0053490	.0017949	.0042792		
K	0.000	.000105	.000236	.000047	.000106	.0000346	.0000852	.0000753	.0001757		
Ca	0.000	.001783	.004110	.002551	.005906	.0005935	.0014971	.0012813	.0030648		
Ti	0.000	.000071	.000195	.000133	.000368	.0000230	.0000694	.0000506	.0001447		
Cr	0.000	.000398	.001191	.000180	.000541	.0001325	.0004336	.0002862	.0008880		
Mn	0.000	.000270	.000852	.000122	.000387	.0000898	.0003104	.0001938	.0006354		
Fe	0.000	.025839	.082984	.011691	.037714	.0086083	.0302574	.0185702	.0618933		
Ni	0.000	.001482	.005003	.000700	.002373	.0004940	.0018252	.0010653	.0037319		
h>		.109806	.220345	.092864	.168505	.0381909	.0843862	.0795953	.1659613		

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 (NOTE: some abundances would go negative beyond AGS04hiCNOx15Ne.775992amet)

Z/X = 0.01965326 AGS04hiCNOx2Ne_ofe.5_W95

		AGS04hiCNOx2Ne				AGS04hiCNOx2Ne.5amet				AGS04hiCNOx2Ne.2amet	
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i d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	
C	+ .050	.243112	.167004	.110446	.076243	.3098835	.2325011	.2712458	.1932028
N	+ .060	.061067	.048920	.027742	.022333	.0821687	.0718935	.0699583	.0581094
O	+ .050	.452697	.414238	.650349	.598029	.3872014	.3869797	.4250999	.4033349
Ne	+ .351	.137081	.158205	.121416	.140815	.1882627	.2373075	.1586465	.1898460
Na	0.000	.001644	.002161	.000747	.000987	.0004782	.0006868	.0011525	.0015713
Mg	0.000	.029909	.041576	.034130	.047677	.0087044	.0132154	.0209747	.0302317
Al	0.000	.002376	.003666	.001079	.001673	.0006916	.0011656	.0016661	.0026658
Si	0.000	.028563	.045881	.025891	.041793	.0083129	.0145842	.0200310	.0333623
P	0.000	.000222	.000393	.000101	.000180	.0000646	.0001249	.0001556	.0002858
S	0.000	.012759	.023394	.012393	.022836	.0037125	.0074350	.0089470	.0170104
Cl	0.000	.000150	.000304	.000068	.000139	.0000440	.0000975	.0001053	.0002214
Ar	+ .050	.001499	.003425	.000681	.001564	.0020588	.0051375	.0017349	.0041100
K	0.000	.000101	.000227	.000046	.000103	.0000294	.0000717	.0000711	.0001649
Ca	0.000	.001722	.003948	.002473	.005697	.0005009	.0012541	.0012077	.0028704
Ti	0.000	.000069	.000188	.000130	.000358	.0000197	.0000589	.0000480	.0001363
Cr	0.000	.000385	.001144	.000175	.000523	.0001118	.0003631	.0002697	.0008316
Mn	0.000	.000260	.000819	.000118	.000373	.0000760	.0002609	.0001829	.0005958
Fe	0.000	.024953	.079702	.011336	.036386	.0072621	.0253344	.0174992	.0579549
Ni	0.000	.001431	.004805	.000679	.002291	.0004168	.0015282	.0010038	.0034943
h>		.106043	.211633	.090047	.162580	.0324837	.0713182	.0750495	.1555069

(NOTE: some abundances would go negative beyond AGS04hiCNOx2Ne.727860amet)

Z/X = 0.02043057 AGS04hiCNOx25Ne_ofe.5_W95 AGS04hiCNOx25Ne.2amet
 AGS04hiCNOx25Ne || AGS04hiCNOx25Ne.5amet ||

i d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	
C	+ .050	.235057	.160650	.107192	.073650	.2992678	.2229701	.2620815	.1855780
N	+ .060	.059044	.047059	.026925	.021574	.0795330	.0691020	.0676675	.0558762
O	+ .050	.437697	.398479	.631190	.577693	.3661031	.3633412	.4075643	.3844241
Ne	+ .448	.165674	.190232	.147299	.170033	.2279647	.2853480	.1918908	.2282784
Na	0.000	.001589	.002079	.000725	.000953	.0003954	.0005638	.0010867	.0014729
Mg	0.000	.028918	.039994	.033124	.046055	.0071915	.0108424	.0197738	.0283333
Al	0.000	.002297	.003527	.001047	.001616	.0005719	.0009571	.0015710	.0024990
Si	0.000	.027617	.044135	.025128	.040371	.0068680	.0119652	.0188840	.0312671
P	0.000	.000214	.000378	.000098	.000174	.0000533	.0001024	.0001467	.0002678
S	0.000	.012336	.022504	.012028	.022059	.0030673	.0061000	.0084349	.0159424
Cl	0.000	.000145	.000292	.000066	.000134	.0000361	.0000795	.0000990	.0002070
Ar	+ .050	.001449	.003295	.000661	.001511	.0019945	.0049425	.0016789	.0039540
K	0.000	.000098	.000218	.000045	.000101	.0000240	.0000582	.0000669	.0001541
Ca	0.000	.001665	.003798	.002401	.005505	.0004139	.0010291	.0011386	.0026904
Ti	0.000	.000066	.000181	.000125	.000343	.0000163	.0000484	.0000453	.0001279
Cr	0.000	.000372	.001100	.000170	.000506	.0000921	.0002971	.0002541	.0007788
Mn	0.000	.000252	.000787	.000115	.000361	.0000625	.0002129	.0001721	.0005574
Fe	0.000	.024126	.076670	.011002	.035148	.0060003	.0207864	.0164976	.0543165
Ni	0.000	.001384	.004622	.000659	.002213	.0003443	.0012537	.0009463	.0032747
h>		.102528	.203580	.087394	.157050	.0271314	.0592387	.0707959	.1458433

(NOTE: some abundances would go negative beyond AGS04hiCNOx25Ne.682227amet)

Z/X = 0.02120788 AGS04hiCNOx3Ne_ofe.5_W95 AGS04hiCNOx3Ne.2amet
 AGS04hiCNOx3Ne || AGS04hiCNOx3Ne.5amet ||

i d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	
C	+ .050	.227518	.154762	.104125	.071229	.2892973	.2141381	.2534926	.1785124
N	+ .060	.057150	.045334	.026155	.020865	.0770566	.0665145	.0655198	.0538062

O	+.050	.423658	.383873	.613128	.558696	.3462824	.3414322	.3911257	.3668969
Ne	+.527	.192433	.219912	.171701	.197330	.2652590	.3298680	.2230522	.2638944
Na	0.000	.001538	.002003	.000704	.000922	.0003175	.0004498	.0010251	.0013817
Mg	0.000	.027991	.038528	.032177	.044541	.0057706	.0086434	.0186483	.0265741
Al	0.000	.002223	.003397	.001017	.001563	.0004583	.0007621	.0014811	.0023430
Si	0.000	.026731	.042518	.024409	.039044	.0055117	.0095397	.0178097	.0293267
P	0.000	.000207	.000364	.000095	.000168	.0000426	.0000814	.0001382	.0002510
S	0.000	.011940	.021679	.011683	.021332	.0024611	.0048625	.0079547	.0149524
Cl	0.000	.000140	.000282	.000064	.000129	.0000295	.0000645	.0000938	.0001950
Ar	+.050	.001403	.003174	.000642	.001461	.0019339	.0047610	.0016262	.0038088
K	0.000	.000095	.000210	.000043	.000096	.0000192	.0000462	.0000630	.0001445
Ca	0.000	.001612	.003658	.002332	.005323	.0003316	.0008191	.0010734	.0025224
Ti	0.000	.000064	.000174	.000121	.000330	.0000128	.0000379	.0000426	.0001195
Cr	0.000	.000360	.001060	.000165	.000489	.0000740	.0002371	.0002397	.0007308
Mn	0.000	.000244	.000759	.000112	.000350	.0000505	.0001709	.0001626	.0005238
Fe	0.000	.023353	.073860	.010687	.033992	.0048149	.0165714	.0155587	.0509445
Ni	0.000	.001340	.004453	.000640	.002140	.0002765	.0010002	.0008926	.0030719

h> .099241 .196119 .084891 .151880 .0221047 .0480472 .0668097 .1368901

(NOTE: some abundances would go negative beyond AGS04hiCNOx3Ne.639022amet)

Z/X = 0.02070490 AGS04vhCNOx15Ne_ofe.5_W95 AGS04vhCNOx15Ne.2amet
 AGS04vhCNOx15Ne || AGS04vhCNOx15Ne.5amet ||

i d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	
C	+.100	.254360	.177864	.114980	.080443	.3236246	.2487911	.2836549	.2062348
N	+.120	.065381	.053315	.029554	.024112	.0875472	.0784860	.0747562	.0633834
O	+.100	.473639	.441177	.677043	.630963	.4173540	.4273882	.4498350	.4356617
Ne	+.276	.107564	.126365	.094797	.111424	.1467589	.1895475	.1241412	.1516380
Na	0.000	.001533	.002051	.000693	.000928	.0003546	.0005218	.0010342	.0014393
Mg	0.000	.027890	.039464	.031667	.044832	.0064587	.0100474	.0188256	.0276973
Al	0.000	.002215	.003480	.001001	.001573	.0005134	.0008866	.0014955	.0024426
Si	0.000	.026635	.043550	.024023	.039300	.0061680	.0110877	.0179784	.0305651
P	0.000	.000207	.000373	.000094	.000170	.0000479	.0000949	.0001396	.0002618
S	0.000	.011897	.022206	.011498	.021472	.0027549	.0056530	.0080305	.0155848
Cl	0.000	.000140	.000289	.000063	.000130	.0000331	.0000750	.0000948	.0002034
Ar	+.100	.001568	.003648	.000709	.001650	.0021401	.0054720	.0018103	.0043776
K	0.000	.000095	.000215	.000043	.000098	.0000215	.0000537	.0000636	.0001505
Ca	0.000	.001606	.003747	.002295	.005358	.0003713	.0009526	.0010837	.0026292
Ti	0.000	.000064	.000178	.000120	.000335	.0000143	.0000439	.0000429	.0001243
Cr	0.000	.000359	.001086	.000162	.000491	.0000830	.0002761	.0002421	.0007620
Mn	0.000	.000243	.000777	.000110	.000352	.0000563	.0001979	.0001640	.0005454
Fe	0.000	.023269	.075654	.010518	.034215	.0053889	.0192624	.0157065	.0530973
Ni	0.000	.001335	.004561	.000630	.002154	.0003093	.0011622	.0009010	.0032015

h> .099056 .201279 .083626 .153058 .0247153 .0557872 .0676127 .1430821

(NOTE: some abundances would go negative beyond AGS04vhCNOx15Ne.663458amet)

Z/X = 0.02157703 AGS04vhCNOx2Ne_ofe.5_W95 AGS04vhCNOx2Ne.2amet
 AGS04vhCNOx2Ne || AGS04vhCNOx2Ne.5amet ||

i d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	
C	+.100	.245556	.170675	.111458	.077562	.3121591	.2380076	.2736893	.1976080
N	+.120	.063118	.051160	.028649	.023249	.0846360	.0752535	.0722074	.0607974
O	+.100	.457245	.423344	.656303	.608366	.3944695	.4006387	.4307287	.4142621
Ne	+.401	.138454	.161677	.122524	.143245	.1893233	.2425155	.1599419	.1940124
Na	0.000	.001480	.001968	.000672	.000895	.0002722	.0003973	.0009694	.0013397
Mg	0.000	.026925	.037869	.030698	.043228	.0049614	.0076549	.0176472	.0257833
Al	0.000	.002139	.003339	.000971	.001518	.0003942	.0006751	.0014017	.0022734

Si	0.000	.025713	.041790	.023287	.037893	.0047383	.0084477	.0168531	.0284531
P	0.000	.000200	.000358	.000091	.000163	.0000368	.0000724	.0001309	.0002438
S	0.000	.011486	.021309	.011147	.020705	.0021165	.0043075	.0075282	.0145084
Cl	0.000	.000135	.000277	.000061	.000125	.0000253	.0000570	.0000887	.0001890
Ar	+ .100	.001514	.003500	.000687	.001590	.0020703	.0052500	.0017490	.0042000
K	0.000	.000091	.000206	.000041	.000093	.0000162	.0000402	.0000594	.0001397
Ca	0.000	.001550	.003596	.002224	.005164	.0002854	.0007261	.0010161	.0024480
Ti	0.000	.000062	.000171	.000117	.000325	.0000110	.0000334	.0000403	.0001159
Cr	0.000	.000346	.001042	.000157	.000473	.0000637	.0002101	.0002269	.0007092
Mn	0.000	.000235	.000746	.000107	.000341	.0000434	.0001514	.0001539	.0005082
Fe	0.000	.022463	.072596	.010196	.032990	.0041396	.0146754	.0147232	.0494277
Ni	0.000	.001288	.004377	.000610	.002075	.0002378	.0008862	.0008447	.0029807

h> .095627 .193144 .081066 .147578 .0194121 .0435847 .0634327 .1333201

(NOTE: some abundances would go negative beyond AGS04vhCNOx2Ne.621160amet)

Z/X = 0.02244915 AGS04vhCNOx25Ne_ofe.5_W95 AGS04vhCNOx25Ne.2amet

AGS04vhCNOx25Ne || AGS04vhCNOx25Ne.5amet ||

i d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	
C	+ .100	.237341	.164045	.108145	.074880	.3014154	.2280626	.2643742	.1896520
N	+ .120	.061006	.049172	.027797	.022445	.0819071	.0722715	.0698241	.0584118
O	+ .100	.441949	.406897	.636799	.587335	.3730252	.3759682	.4128692	.3945257
Ne	+ .498	.167278	.194245	.148603	.172865	.2292092	.2913675	.1934070	.2330940
Na	0.000	.001430	.001892	.000652	.000864	.0001956	.0002833	.0009093	.0012485
Mg	0.000	.026024	.036398	.029785	.041732	.0035585	.0054484	.0165456	.0240181
Al	0.000	.002067	.003210	.000942	.001465	.0002833	.0004816	.0013147	.0021186
Si	0.000	.024853	.040167	.022595	.036583	.0033987	.0060132	.0158014	.0265055
P	0.000	.000193	.000344	.000088	.000157	.0000263	.0000514	.0001227	.0002270
S	0.000	.011101	.020481	.010815	.019988	.0015178	.0030655	.0070581	.0135148
Cl	0.000	.000130	.000266	.000059	.000121	.0000181	.0000405	.0000830	.0001758
Ar	+ .100	.001463	.003364	.000667	.001536	.0020051	.0050460	.0016919	.0040368
K	0.000	.000088	.000198	.000040	.000090	.0000114	.0000282	.0000557	.0001301
Ca	0.000	.001498	.003456	.002158	.004986	.0002044	.0005161	.0009525	.0022800
Ti	0.000	.000060	.000164	.000113	.000312	.0000076	.0000229	.0000376	.0001075
Cr	0.000	.000335	.001001	.000153	.000459	.0000454	.0001486	.0002125	.0006600
Mn	0.000	.000227	.000717	.000104	.000329	.0000312	.0001079	.0001443	.0004734
Fe	0.000	.021712	.069776	.009893	.031850	.0029690	.0104454	.0138042	.0460437
Ni	0.000	.001245	.004207	.000592	.002003	.0001707	.0006312	.0007920	.0027767

h> .092426 .185641 .078656 .142475 .0144431 .0323302 .0595255 .1243165

(NOTE: some abundances would go negative beyond AGS04vhCNOx25Ne.580960amet)

Z/X = 0.02332128 AGS04vhCNOx3Ne_ofe.5_W95 AGS04vhCNOx3Ne.2amet

AGS04vhCNOx3Ne || AGS04vhCNOx3Ne.5amet ||

i d:Ab_i	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	Ni/Nz	Xi/Z	
C	+ .100	.229658	.157910	.105024	.072378	.2913253	.2188601	.2556460	.1822900
N	+ .120	.059031	.047333	.026995	.021695	.0793452	.0695130	.0675919	.0562050
O	+ .100	.427642	.391682	.618420	.567711	.3528913	.3531457	.3961398	.3762677
Ne	+ .577	.194235	.224377	.173177	.200507	.2666617	.3365655	.2247580	.2692524
Na	0.000	.001384	.001821	.000633	.000835	.0001230	.0001768	.0008523	.0011633
Mg	0.000	.025181	.035037	.028925	.040337	.0022411	.0034069	.0155137	.0223849
Al	0.000	.002000	.003090	.000915	.001417	.0001787	.0003016	.0012327	.0019746
Si	0.000	.024048	.038665	.021942	.035359	.0021405	.0037602	.0148158	.0247031
P	0.000	.000187	.000331	.000086	.000153	.0000165	.0000319	.0001150	.0002114
S	0.000	.010742	.019715	.010503	.019320	.0009557	.0019165	.0066178	.0125956
Cl	0.000	.000126	.000256	.000057	.000116	.0000115	.0000255	.0000778	.0001638
Ar	+ .100	.001416	.003238	.000648	.001485	.0019439	.0048570	.0016384	.0038856

K	0.000	.000085	.000191	.000039	.000087	.0000072	.0000177	.0000524	.0001217
Ca	0.000	.001450	.003327	.002096	.004820	.0001287	.0003226	.0008932	.0021252
Ti	0.000	.000058	.000158	.000110	.000302	.0000046	.0000139	.0000353	.0001003
Cr	0.000	.000324	.000964	.000148	.000442	.0000286	.0000931	.0001994	.0006156
Mn	0.000	.000219	.000690	.000100	.000315	.0000196	.0000674	.0001352	.0004410
Fe	0.000	.021009	.067166	.009607	.030784	.0018695	.0065304	.0129429	.0429117
Ni	0.000	.001205	.004049	.000575	.001937	.0001074	.0003942	.0007424	.0025871

h> .089434 .178698 .076384 .137709 .0097765 .0219157 .0558643 .1159849

(NOTE: some abundances would go negative beyond AGS04vhCNOx3Ne.548057amet)

OPAL ATOMIC MASSES: We list the OPAL atomic masses (atomic weights) used to convert number fractions (Ni) to mass fractions (X, Y, Z, Xi).

Element	Mass (a.u.)	Element	Mass (a.u.)	Element	Mass (a.u.)
1 H	1.00790	12 Mg	24.30500	19 K	39.09830
2 He	4.00260	13 Al	26.98154	20 Ca	40.08000
6 C	12.01100	14 Si	28.08550	22 Ti	47.90000
7 N	14.00670	15 P	30.97376	24 Cr	51.99600
8 O	15.99940	16 S	32.06000	25 Mn	54.93800
10 Ne	20.17900	17 Cl	35.45300	26 Fe	55.84700
11 Na	22.98977	18 Ar	39.94800	28 Ni	58.70000

+++++
 Details of the accuracy of the X-, Z-, and CO-interpolation
 +++++

Z-interpolation errors if 'GN93hz' file not used:

For the non-CO-rich mixes (C=O=0.0), one can check the accuracy of the Z-interpolation among the 'Gz???.x??' files when opacities are read in, by looking at the 'GN93hz' opacities. Where the Z values are in both files, the opacities are identical. When only 'GN93hz' (or only the 'Gz???.x??' files) contains the Z value, errors in interpolation among 'Gz???.x??' files are shown below; the largest, the mean, and the rms error in logKappa are given (at T6 of 0.01 or higher, and all log R values). Note that the 'Gz???.x??' files contain Z = 0.05, but 'GN93hz' does not; for this case, interpolation in 'GN93hz' is tested, rather than interpolation among 'Gz???.x??' files. Note that the Z-interpolation errors tend to be quite small, with an rms error of less than 4% even in the worst case; applying the 'GN93hz' opacity-shifts (as is the default) when interpolating in Z should significantly reduce these errors (note: T6 < 0.01 omitted):

Z-interpolation errors if 'GN93hz' file not used (if khighz=0 in READZEXCO):

Z	dLogKappa(X=0.00)			dLogKappa(X=0.10)			dLogKappa(X=0.35)			dLogKappa(X=0.70)		
	max	mean	rms	max	mean	rms	max	mean	rms	max	mean	rms
.0001	.128	.0078	.0169	.042	.0047	.0084	.040	.0041	.0077	.039	.0040	.0078
.0003	.112	.0072	.0151	.045	.0046	.0084	.043	.0041	.0079	.046	.0040	.0081
.002	-.036	-.0018	.0038	-.012	-.0012	.0023	-.012	-.0011	.0022	-.013	-.0010	.0025
.04	-.003	.0000	.0003	-.001	.0000	.0002	.001	.0000	.0002	.001	.0000	.0002
.05 *	-.003	.0000	.0003	.001	.0000	.0002	.001	.0000	.0002	.001	.0000	.0002
.06	-.004	.0000	.0004	-.001	.0000	.0003	.001	.0000	.0003	-.001	.0000	.0003
.08	-.003	.0000	.0004	-.001	.0000	.0003	.001	.0000	.0003	-.001	.0000	.0003

It is clear from the following table that X-interpolation errors in the file 'GN93hz' (to get X=0.03) would be much larger than any Z-interpolation error in the files Gz???.x03 ; thus any opacity shifts for X=0.03 are interpolated from the X=0, X=0.1, and X=0.35 opacity shifts (unless only a single mix is being read in, which is NOT the default case). The size of the error in these X-interpolated opacity shifts is presumably somewhat smaller than the opacity shifts themselves, which in turn are smaller than the errors shown below that would result if the 'GN93hz' opacities were interpolated in X to get the X=0.03 opacities.

X-interpolation errors at X=0.03 if ONLY the 'GN93hz' file were used:
 =====

X interpolation errors, for X = 0.03, interpolating in X = 0.0, 0.1, 0.2 in the file 'GN93hz' (note that a value of Xdel = 0.005 was used for this interpolation, and all T6 < 0.01 opacities were omitted):

X-interpolation errors that would occur if 'Gz???.x??' files were not used:

Z:	0.	0.001	0.004	0.01	0.02	0.03	0.1	(at X=0.03)
max	-.3514	-.2971	-.2454	-.1913	-.1396	-.1062	-.0614	(dLogKappa)
mean	-.0159	-.0149	-.0141	-.0132	-.0124	-.0118	-.0103	
rms	.0399	.0350	.0305	.0259	.0219	.0196	.0158	

X-interpolation/extrapolation errors if 'GN93hz' file not used:
 =====

The file 'GN93hz' contains (non-CO-rich) opacities at X-values not available from the 'Gz???.x??' files, namely, X = 0.2, 0.5, 0.8, 0.9, 0.95, and 1-Z. If one sets khighz = 0 in the call to READZEXCO that reads the opacities, then the 'GN93hz' file is not read in and X-interpolation is less accurate [or alternatively, if one turns off "accurate-X" by calling SET_XHI(0)]. For X < 0.75 or so, the errors are comparable to or smaller than the errors from the original OPAL opacity computation; but for extrapolation to larger X-values, the error grows very rapidly, and can become as large as an order of magnitude as X approaches 1-Z:

X-interpolation/extrapolation errors if 'GN93hz' file not used (khighz=0):

***Interpolation (dLogKappa):

Z:	0.	0.0001	0.001	0.004	0.01	0.02	0.03	0.05	0.08	0.1
X=0.2:										
max	-.0146	.0375	-.0153	-.0147	-.0139	-.0137	-.0142	-.0129	-.0124	-.0126
mean	-.0023	-.0017	-.0021	-.0018	-.0016	-.0014	-.0013	-.0012	-.0010	-.0010
rms	.0044	.0051	.0040	.0036	.0033	.0031	.0029	.0027	.0025	.0024
X=0.5:										
max	.0291	.0291	.0284	.0269	.0260	.0249	.0244	.0243	.0234	.0234
mean	.0028	.0027	.0023	.0019	.0016	.0013	.0011	.0010	.0008	.0008
rms	.0076	.0073	.0066	.0059	.0053	.0048	.0045	.0042	.0039	.0038

***Extrapolation (dLogKappa):

Z:	0.	0.0001	0.001	0.004	0.01	0.02	0.03	0.05	0.08	0.1
X=0.8:										
max	-.0732	-.0721	-.0706	-.0680	-.0637	-.0620	-.0597	-.0578	-.0557	-.0565
mean	-.0071	-.0068	-.0059	-.0049	-.0041	-.0035	-.0031	-.0027	-.0024	-.0023
rms	.0178	.0172	.0153	.0134	.0119	.0107	.0100	.0092	.0086	.0084
X=0.9:										

max	-.2415	-.2405	-.2328	-.2220	-.2063	-.1980	-.1914	-.1854	-.1828	-.1860
mean	-.0226	-.0216	-.0186	-.0154	-.0129	-.0110	-.0099	-.0088	-.0082	-.0085
rms	.0565	.0544	.0480	.0416	.0366	.0328	.0306	.0284	.0273	.0281
X=0.95:	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
max	-.4256	-.4189	-.4025	-.3805	-.3555	-.3321	-.3264	-.3213		
mean	-.0377	-.0360	-.0307	-.0253	-.0212	-.0181	-.0165	-.0154		
rms	.0950	.0910	.0797	.0684	.0600	.0537	.0505	.0486		
X=1-Z:	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----
max	-.9901	-.9632	-.8694	-.7293	-.6045	-.4773	-.4059	-.3213	-.2219	-.1860
mean	-.0818	-.0758	-.0609	-.0468	-.0370	-.0306	-.0279	-.0154	-.0175	-.0085
rms	.2079	.1941	.1592	.1249	.0982	.0769	.0645	.0486	.0356	.0281

CO-interpolation errors:

=====

Note that there are six cases (at three different metallicities) where mixes on the line $C+O = 1-X-Z$, with identical compositions, are interpolated in two different ways when being read into two different positions in the matrix CO; since these cases all have $X > 0$, they do not correspond to mixes that are likely to be encountered by investigators, but they do give another estimate of interpolation errors for some CO-rich mixes. (Note that there are several other cases where mixes with identical compositions appear at two different places in the matrix CO, but these occur at tabulated Z-values and thus have identical opacity values.) Differences for the CO-rich cases with identical compositions (note that $T6 < 0.01$ were omitted):

Differences for CO-rich mixes interpolated in two different ways:

case:	Z=0.04	X=0.35	Z=0.07	X=0.7	Z=0.09	X=0.7	
	=====	=====	=====	=====	=====	=====	
C & O:	.01 .6	.6 .01	.03 .2	.2 .03	.01 .2	.2 .01	
	-----	-----	-----	-----	-----	-----	
max	-.0333	-.0026	-.0491	-.0110	-.0422	-.0084	(dLogKappa)
mean	-.0029	-.0002	-.0046	-.0014	-.0041	-.0011	
rms	.0061	.0008	.0091	.0029	.0081	.0023	

These errors are still quite small, with an rms of 1% or less, smaller than the estimated error in the opacity computations quoted above or than the largest of the Z-interpolation errors at $C=O=0.0$ (though larger than the errors for the $C=O=0.0$ mix for the same metallicity Z). The maximum error is less than 12% (note that the maximum errors tend to lie at fairly low temperatures, where CO-rich opacities are less likely to be needed).

The above tables of errors were obtained by considering Z-interpolation as the opacities were read in. One may also compare opacities where the only Z-interpolation was performed on input (i.e., $N_{zin} = 1$ in READZEXCO) with opacities interpolated in Z by the call to OPAC or OPAL (i.e., which had had $Z > 4$ in READZEXCO). These are interpolated among somewhat different grid points, and thus give some idea of the Z-interpolation and CO-interpolation errors. NOTE THAT USE OF COINTERP WILL LEAD TO SIGNIFICANTLY LARGER ERRORS, as discussed further below. For several Z-values, the number of points compared and the maximum and rms differences in $\log_{10}(Kappa)$ are given below both at and between (X,T6,R,C,O) gridpoints, for low ($4 < \log T < 6$) and high ($\log T > 6$) temperatures ($T6 < 0.01$ are omitted; table Z-values are also omitted, since opacity differences are zero there, as expected). Note that rms differences are always small, less than 0.3%, but this may be misleading as many comparison points will interpolate between the same gridpoints, just in a different order, and thus will have identical interpolated $\log_{10}(Kappa)$ values. For $C = O = 0.0$, the maximum differences are small, less than 1%; however, the CO-interpolation can induce somewhat larger errors in opacities

of CO-rich mixes at low metallicity: for $\log T > 6$ at $X = 0.0$ (where CO-rich opacities are likely to be needed), the maximum differences do not exceed 1% for $Z > 0.001$, but they can be as high as 8% for $0.0001 < Z < 0.001$, and can reach 11% for $Z < 0.0001$.

"max" gives some indications of combined Z- and CO-interpolation errors:

```

-----
dLogKappa for: <----- max{C,O} > 0.0 ----->
<----- C = 0 = 0.0 , all X -----> <-----On-Grid-----> <-----Off-Grid---->
<-----On-Grid-----> <-----Off-Grid----> all X X = 0.0 all X X = 0.0
Z 4<logT<6 logT>6 4<logT<6 logT>6 logT>4 logT>6 logT>4 logT>6
=====
.00001:N= 3895 2075 27695 15375 273426 21580 7185558 315535
max -.000038 .000067 -.000069 .000121 -.066377 .009322 -.093110 .012053
rms .000003 .000004 .000004 .000004 .000178 .000103 .000174 .000074
-----
.00005:N= 3895 2075 27695 15375 279396 21995 7228628 314790
max -.000080 .000171 -.000156 .000310 .046540 .039973 -.118741 .046853
rms .000008 .000009 .000010 .000010 .000401 .000363 .000352 .000230
.0002:-----
max -.000214 .000447 -.000404 .000828 -.041788 .028401 -.058897 -.035296
rms .000010 .000015 .000012 .000016 .000365 .000267 .000317 .000197
.0005:-----
max -.000316 -.000304 -.000512 .000854 -.044971 .017734 -.061407 .020958
rms .000025 .000025 .000032 .000030 .000357 .000155 .000271 .000121
.0015:-----
max .001481 -.000494 .002325 .001390 -.019924 .001625 -.025380 .001904
rms .000086 .000033 .000111 .000042 .000202 .000062 .000165 .000059
.0030:-----
max -.001855 -.000593 -.002934 -.001971 -.006332 -.001797 .006585 -.002046
rms .000107 .000032 .000138 .000049 .000181 .000076 .000158 .000072
-----
.0070: N= 3895 2075 27695 15375 279396 21995 7218820 314790
max .000882 .000475 .001406 -.001663 -.005493 .001000 -.008853 .001083
rms .000054 .000026 .000070 .000041 .000098 .000044 .000111 .000043
-----
.0150: N= 3895 2075 27695 15375 279396 21995 7199204 314790
max -.000052 -.000111 -.000136 -.000213 -.009724 -.000550 .038904 -.001056
rms .000002 .000010 .000003 .000009 .000087 .000019 .000482 .000019
-----
.0250: N= 3895 2075 27695 15375 277008 21995 7137840 314790
max .000087 -.000088 .000233 -.000140 -.003307 .000414 .036001 -.000738
rms .000006 .000009 .000009 .000009 .000049 .000025 .000439 .000023
-----
.0350: N= 3895 2075 27695 15375 277008 21995 7059376 314790
max -.000253 -.000406 .002127 .000610 -.005123 -.000655 -.041995 -.000777
rms .000024 .000031 .000032 .000033 .000099 .000046 .000626 .000050
-----
.0450: N= 3895 2075 27695 15375 274620 21995 7022532 314790
max .000980 .000782 .001798 .003339 .009452 .000765 .054504 .001237
rms .000061 .000076 .000069 .000090 .000149 .000065 .000921 .000080
-----
.0550: N= 3895 2075 27695 15375 268650 21995 6940230 311300
max .000457 -.000596 .001611 -.001637 .004770 -.000654 .006170 .001523
rms .000043 .000055 .000047 .000060 .000081 .000045 .000108 .000041
-----
.0700: N= 3895 2075 27695 15375 266262 21995 6844538 311300
max -.000404 -.000476 .001360 -.001767 .007161 -.000599 .042980 -.001666
rms .000027 .000038 .000032 .000046 .000175 .000036 .000708 .000097
-----
.0900: N= 3895 2075 27695 15375 263874 21995 6665478 311300
max -.000236 .000500 -.001106 .002409 .008298 .000866 -.045470 .004078
-----

```

rms .000022 .000042 .000034 .000066 .000221 .000029 .000966 .000140

Z-interpolation errors when one uses linear Z-interpolation (Nzin = 2):

=====

If, for example, diffusion leads to relatively small Z-variations in a star (say, of order 10%), then one might wish to use linear interpolation in logZ by setting nZin = 2 in READZEXCO. (Note that opacity interpolation with nZin = 2 will usually be significantly faster than nZin = 3, which will in general be faster than nZin = 4; however, all values of nZin > 4 take the same amount of time as the nZin = 4 case, except for the slight added start-up time to read in the extra opacity files). The size of the errors introduced by nZin = 2 linear interpolation are easily estimated, e.g., by comparing { nZin = 2, Zlo = .019, Zhi = .021 } opacities at Z = 0.02 with the Z=0.02 opacity tables themselves. Such errors for the nZin = 2 case are tabulated below for several values of Z, for two different cases with Z-ranges of +/- 10% and of +/- 20%, respectively (referred to as cases "1" and "2" in the table headings on the left). The mean errors are given as well as the maximum and rms errors, since it is not unreasonable to expect a systematic tendency from linear interpolation of a curve; however, they turn out to be negligible (always < 0.04%) for a Z-range of +/- 10%. The rms error in the Z-interpolation is likewise negligible (always < 0.2%) for a Z-range of +/- 10%; the maximum errors are less than 1% for C = O = 0.0, and also for Z > 0.001 at logT > 6 with X = 0.0, max{C,O} > 0.0, although for Z < 0.001 the CO-interpolation can result in errors up to 9% in a few places for CO-rich mixes. Even for a Z-range of +/- 20%, the mean errors are always < 0.14%; the C = O = 0.0 case has rms errors < 0.2% and maximum errors < 1.7%, while { Z > 0.001, logT > 6, X = 0.0, max{C,O} > 0.0 } has rms errors < 0.21% and maximum errors < 1.4% (up to 9% for Z < 0.001).

Errors if linear Z-interpolation is used, with Z-ranges +/-10% and +/-20%:

	Z= 0.0001	0.001	0.004	0.01	0.02	0.03	0.05	0.08
Zlo1=	0.00009	0.0009	0.0036	0.009	0.018	0.027	0.045	0.072
Zhi1=	0.00011	0.0011	0.0044	0.011	0.022	0.033	0.055	0.088
Zlo2=	0.00008	0.0008	0.0032	0.008	0.016	0.024	0.040	0.064
Zhi2=	0.00012	0.0012	0.0048	0.012	0.024	0.036	0.060	0.096
C=O=0.0, OnGrid, logT>4 dLogKappa:								
max1	-.000703	.001008	.001107	.000764	.000989	.000925	-.001984	.001149
mean1	-.000026	.000017	.000065	.000103	.000133	.000145	.000150	.000149
rms1	.000056	.000064	.000109	.000146	.000183	.000199	.000241	.000214
max2	-.002772	.001246	-.002859	.003076	.003924	.003731	.004402	.004059
mean2	-.000103	.000043	.000238	.000416	.000537	.000583	.000612	.000609
rms2	.000219	.000145	.000375	.000587	.000733	.000793	.000857	.000853
C=O=0.0, OffGrid, logT>4 dLogKappa:								
max1	-.000707	-.002721	.003203	.001427	.002620	.002294	.003412	.002120
mean1	-.000024	.000015	.000065	.000100	.000130	.000143	.000149	.000149
rms1	.000051	.000076	.000119	.000141	.000178	.000197	.000245	.000213
max2	-.002806	-.002473	-.005426	.005459	.005472	.003856	.006457	.007094
mean2	-.000095	.000041	.000232	.000405	.000524	.000573	.000606	.000605
rms2	.000198	.000153	.000367	.000568	.000713	.000780	.000848	.000849
max{C,O}>0.0, X=0.0, OnGrid, logT>6 dLogKappa:								
max1	-.032688	.000776	.000689	-.000687	.000569	.000581	-.001612	.000677

mean1	-.000003	.000007	.000030	.000065	.000098	.000115	.000148	.000147
rms1	.000221	.000024	.000063	.000117	.000163	.000190	.000248	.000219

max2	-.032967	.000873	.001402	.001871	.002107	.002235	.002763	.002591
mean2	-.000005	.000027	.000122	.000262	.000395	.000464	.000589	.000593
rms2	.000223	.000071	.000247	.000468	.000651	.000749	.000905	.000875
=====								
max{C,O}>0.0, X=0.0, OffGrid, logT>6 dLogKappa:								
max1	-.038349	.001053	.000879	-.001188	-.000875	-.001059	-.002342	-.002052
mean1	-.000002	.000007	.000029	.000064	.000097	.000114	.000148	.000148
rms1	.000140	.000023	.000060	.000114	.000160	.000187	.000244	.000222

max2	-.038750	-.001171	.001398	.002108	.002854	-.003313	-.004253	-.006058
mean2	-.000004	.000027	.000118	.000257	.000390	.000458	.000586	.000594
rms2	.000156	.000071	.000239	.000458	.000641	.000740	.000898	.000881
=====								
max{C,O}>0.0, all-X, OnGrid, logT>4 dLogKappa:								
max1	-.032688	-.025873	-.001446	.001413	-.003337	.003056	-.009148	.001397
mean1	-.000017	.000015	.000039	.000078	.000106	.000121	.000134	.000137
rms1	.000111	.000135	.000075	.000118	.000159	.000179	.000261	.000198

max2	-.036713	-.025350	.005615	.005444	.007725	-.008038	-.007972	.007035
mean2	-.000058	.000047	.000154	.000320	.000439	.000495	.000567	.000569
rms2	.000237	.000228	.000250	.000463	.000615	.000697	.000813	.000804
=====								
max{C,O}>0.0, all-X, OffGrid, logT>4 dLogKappa:								
max1	-.038349	-.034450	-.004328	-.004072	-.028706	-.028234	-.047400	.041999
mean1	-.000015	.000016	.000039	.000078	.000102	.000116	.000119	.000143
rms1	.000073	.000101	.000075	.000116	.000377	.000375	.000776	.000729

max2	-.050575	-.032346	.005371	.008759	-.027245	.052397	-.045954	.042481
mean2	-.000056	.000050	.000152	.000318	.000432	.000494	.000546	.000576
rms2	.000193	.000174	.000245	.000461	.000692	.000952	.001109	.001302
=====								

++++
 Details of opacity shifts from initial smoothing when opacities are read in
 +++++

The opacity tables to be interpolated among (i.e., the OPAL files) are known to have somewhat random numerical errors of a few percent. Consequently, adjusting the data prior to performing the interpolation is justified at this level. The code first reads the original (unsmoothed) tabular data; this data is then passed through a smoothing filter, using a set of routines developed by Mike Seaton (see M.J. Seaton, MNRAS 265, L25, 1993). It is the adjusted data that is actually used in carrying out the interpolations in OPAC or OPAL. The initial adjustment step helps improve the smoothness of the OPAC output, particularly at the smallest values of R. The medium to large R output is only slightly affected by this step. It takes only a few seconds to carry out the initial data smoothing step, but this initial smoothing can be skipped by calling the subroutine SET_SMOOTH (described further above) with a value of initsmooth = 0.

In addition, a few opacities in the mixes adjacent to the C=O=0.0 mix (i.e., in the three mixes with C or O = 0.01, and C+O no more than 0.02) are smoothed in the C-O direction, if opacity changes between mixes with C,O = 0.0, 0.03, 0.1 are monotonic but the opacity at C,O = 0.01 does not fit the trend; the resulting adjustments are small, and only occur at a small minority of the (T6,R) points, but this smoothing can also be skipped, by calling SET_SMOOTH (described further above) with lowCOsmooth = 0.

Maximum and rms differences between smoothed and unsmoothed opacity tables for selected metallicities Z, for non-CO-rich mixes ("CO=0") and CO-rich

mixes ("CO>0") of each hydrogen abundance X, at intermediate temperatures ("4<logT<6") and high temperatures ("logT>6"); note: T6 < 0.01 was omitted:

Opacity shifts resulting from initial smoothing when they are read in:

```

-----
dLogKappa for:
  X =      0.00      0.03      0.10      0.35      0.70
-----
      max  rms      max  rms      max  rms      max  rms      max  rms
Z=0.0: CO=0: =====
  4<logT<6 .0288 .0062 .0492 .0082 .0534 .0072 .0278 .0044 .0168 .0026
  logT>6   .0172 .0023 .0175 .0022 .0160 .0021 .0125 .0016 -.0038 .0006
CO>0: -----
  4<logT<6 -.0512 .0077 .0761 .0075 .0763 .0064 .0800 .0050 .0874 .0037
  logT>6   .0767 .0025 .0771 .0026 .0776 .0026 .0782 .0027 .0757 .0017
Z=.001:CO=0: =====
  4<logT<6 -.0416 .0064 .0469 .0079 .0524 .0069 .0255 .0043 .0154 .0027
  logT>6   -.0149 .0022 -.0148 .0021 -.0145 .0020 -.0124 .0016 .0059 .0011
CO>0: -----
  4<logT<6 .0792 .0072 .0689 .0072 .0528 .0061 -.0517 .0047 .0458 .0033
  logT>6   -.0324 .0023 -.0341 .0023 -.0362 .0024 -.0369 .0024 -.0153 .0015
Z=.02: CO=0: =====
  4<logT<6 -.0570 .0069 .0483 .0076 .0517 .0066 .0200 .0043 -.0128 .0031
  logT>6   -.0108 .0021 -.0113 .0021 -.0110 .0021 -.0107 .0020 -.0083 .0017
CO>0: -----
  4<logT<6 .0785 .0071 .0675 .0069 .0521 .0057 -.0493 .0044 -.0375 .0033
  logT>6   -.0303 .0023 -.0320 .0023 -.0345 .0024 -.0343 .0024 -.0140 .0016
Z=.10: CO=0: =====
  4<logT<6 -.0397 .0073 .0564 .0078 .0496 .0066 .0182 .0047 -.0137 .0038
  logT>6   -.0093 .0021 -.0096 .0021 -.0097 .0021 -.0096 .0021 -.0087 .0018
CO>0: -----
  4<logT<6 .0765 .0074 .0664 .0070 .0497 .0058 -.0404 .0046 -.0259 .0038
  logT>6   -.0246 .0023 -.0262 .0023 -.0273 .0024 -.0259 .0023 -.0095 .0017
    
```

For T6 > 0.01, the rms effect of the smoothing is always less than 2%, i.e., comparable to the Z-interpolation errors found for the CO-rich mixes above, and smaller than the estimated opacity computation errors.

```

+++++
Details of differences in CO-rich opacities from COINTSMO vs. COINTERP
+++++
    
```

Use of the smoother CO-interpolation routine COINTSMO (rather than the old routine COINTERP) yields opacities that differ at only a few grid-points (those which COINTERP ignores when interpolating opacities), but that differ over a significant area of the CO-plane between grid-points. Opacities were compared at points chosen randomly in log T, log RHO, C, and O (always with C+O > 0, and with some excess probability of having either C=0, O=0, or C+O=1-X-Z). Opacity differences are tabulated below for selected metallicities Z, for X = 0 and for two ranges of non-zero X, at intermediate temperatures ("4<logT<6") and high temperatures ("logT>6"); note that very low temperatures (T6 < 0.01) were omitted:

CO-interpolation differences: from using subroutines COINTSMO vs. COINTERP:

```

-----
dLogKappa for:
  X = 0.0      0.0 < X < 0.35      0.35 < X < 0.8
-----
      N  max  rms      N  max  rms      N  max  rms
Z=0.0: =====
  4<logT<6 209131 -.0495 .0021  91697 -.0540 .0042 117239 -.0939 .0061
    
```

	logT>6	252334	-.0198	.0009	109760	-.0575	.0045	142313	.1272	.0062
Z=0.001:	===== 4<logT<6	208824	-.0376	.0019	91547	-.0525	.0040	117033	.0872	.0056
	logT>6	251965	-.0195	.0008	109603	-.0568	.0045	142087	.1259	.0061
Z=0.02:	===== 4<logT<6	208225	-.0275	.0014	91265	.0388	.0032	116669	.0975	.0042
	logT>6	251235	-.0161	.0006	109266	.0538	.0039	141670	.1031	.0051
Z=0.1:	===== 4<logT<6	207954	-.0189	.0010	91162	.0318	.0024	116518	.0591	.0031
	logT>6	250923	-.0104	.0003	109122	.0452	.0029	141482	.0812	.0039

The routine COINTERP may have opacity discontinuities of the same order as the opacity differences (up to 5%, for X=0 and logT > 6; larger elsewhere), at those points where it switches over from interpolation in one direction to interpolation in another direction, interpolating among a different set of gridpoints (this generally occurs somewhere in the region $0 = C \pm 0.2$).

 Details of the individual OPAL opacity tables and program storage space

Each of the individual tables in a file Gz???.x?? covers 70 temperatures in the range logT=3.75 [T6=0.0056341325] (referred to as temperature 1) to logT=8.7 [T6=501.187] (note that the logT step size is 0.05 below logT=6.0, 0.10 below logT=8.1, and 0.20 above that), and covers 19 values of log R in the range logR=-8.0 (referred to as 1) to logR=+1.0, at half-integer steps. (NOTE: earlier tables were explicitly in terms of T6. For convenience the present tables tabulate log Kappa vs logT. The interpolation however still uses logT6 for the temperature variable, not logT.) Values of Z from 0.0 to 0.1 are available (at up to 14 values of Z). Type 2 OPAL tables have 8 Z-values from Z = 0.0 to Z = 0.1 and 5 X-values from X = 0.0 to X = 0.7 (plus 8 each of excess-C and excess-O values from 0.0 to 1 - X - Z), while Type 1 OPAL tables have 13 Z-values from Z = 0.0 to Z = 0.1 and 10 X-values from X = 0.0 to X = 1 - Z (but with less-good X-interpolation at low X); combining these tables allows accurate X-interpolation at all X, and more accurate Z-interpolation among 14 Z-values.

The sizes of the matrices (holding the input opacities) are set by the constant values in parameter statements. The number NZ of available Z-storage values was mentioned above (in the discussion of the inputs to the subroutine READZEXCO); its value in the parameter statements can be changed to any value between 1 and 14 (provided that it is the same everywhere!) and the program recompiled. Smaller values of NZ yield smaller ranges where Z can be interpolated (or less accurate interpolation over a wide range), but also save storage space; NZ = 5 is a reasonable compromise. Low values (NZ = 2 or 3) yield less accurate interpolation, but reduce both the storage space and the typical amount of CPU-time per opacity interpolation, since fewer Z-grid values need to be computed in general. For NZ = 1, only a constant Z can be accommodated. Other than NZ, no size parameter of the OPAL matrices should be changed.

The molecular and conductive opacity matrix sizes are independent of NZ, taking up about 1 Mb; their sizes should never be changed. The Ferguson et al. (2005) molecular opacity tables have the same range in logR as the OPAL tables, but with $2.7 < \log T < 4.5$ (or possibly $2.8 < \log T < 4.5$ for some cases); they are available at 16 Z-values from Z = 0.0 to Z = 0.1, and at 10 X-values from X = 0.0 to X = 1 - Z. For low X, their X-interpolation is less accurate (but at low temperatures where molecular opacities are needed one seldom will encounter X values close to zero).

Roughly (1.1 Mb) + NZ * (1.63 Mb) of storage space is required in total.
