Notes for convert.f90, the Fortran program generating hot CO2 IR line list using AI-3000K data files (01/10/2023)
Use convertLS.f90 to generate line shape parameters along with the line list in HITRAN format
[Prepared for "AI-3000K Infrared Line List for Hot CO2"; contact xhuang@seti.org for questions]

0. Compile the convert.f90 into convert.x, e.g. ifort convert.f90 -o convert.x -mcmodel=large

1. All the files under “code.and.files” should be put under the same working directory. Please decompress the 4 co2.xxx.levels....tgz files first.

2. Select the compressed .tgz files for the range of IR simulation. They are stored in 10 cm-1 bins. Filenames are fort.7000.1xxxx.tgz:
...10001.tgz - 0 - 10 cm-1
...10002.tgz - 10-20 cm-1
...10003.tgz - 20-30 cm-1
…
... 10500.tgz - 4990 - 5000 cm-1
…
… 11000.tgz - 9990 - 10000 cm-1
…
… 11999.tgz - 19980 - 19990 cm-1
…12000.tgz - 19990 - 20000 cm-1
Put the selected .tgz file(s) under the same working directory of the convert.x and the decompressed co2.xxx.levels… and the zpe+part file.

3. Run ./convert.x, it will decompress and convert the fort.7000.xxxxx.tgz files, one by one, into their corresponding list file: co2list.zzzzzcm-1. e.g. fort.7000.11234tgz → co2list.12340cm-1. The convert.f90 is customizable, see below.

4. The line list output format can be adjusted as you need. In convert.f90, lines #151 - #163 explain the data choices

```
! Please choose your own format to write out whatever quantities that fit your needs
! so here is just an example for full length, i.e. including everything I can think of
! iso-isotopologue #, 21-24 for 626/636/628/627
! om2 - transition wavenumber
! a21 - Einstein A21
! si(0:5)*ab(is) - 100% line intensities at user-specified and 5 pre-set temperatures are scaled by their terrestial abundances
! jf, iparf, irf - J, parity, root number for E'
! ji, ipari, iri - J, parity, root number for E"
! jw(1:5) - importance indicator for 5 pre-set temperatures, 0 - to ignore, 1 - to include
! ef, ei - E' and E"
! ie(:,:,:,:,1:3) are the v1v2v3 from vtet, ie(:,:,:,:,6:13) are the p (polyad #),c (wang's sym),n(root# in that polyad) and v1v2l2v3r from CDSD
! if you need wang's symmetry:  mod(j+ipar,2)=0 --> e;  mod(j+ipar,2)=1 --> f
! now the first intensity value after A21 is for the temperature user specified at line #45.

  write(7001,1213)iso,om2,a21,si(0:5)*ab(is),jf,iparf,irf,ji,ipari,iri,jw(1:5), &
                  ef,ei,ie(is,jf,iparf,irf,1:3),ie(is,jf,iparf,irf,6:13),ie(is,ji,ipari,iri,1:3),ie(is,ji,ipari,iri,6:13)
1213    format(i2,f12.5,7es12.5,i4,i2,i6,i4,i2,i6,5i2,2f12.5,3i3,1x,2i3,i5,5i3,2x,3i3,1x,2i3,i5,5i3)
```

A line example is below, note the energies in this example were X01d-PES based, not replaced by CDSD2019 energies yet.

```
22  4999.99970 2.06453E-03 2.30683E-37 2.19914E-45 5.84959E-32 6.98025E-30 1.42623E-29 1.27300E-29  83 1   399  82 2    84 0 1 1 1 1
14713.00637  9713.00667  2 14  0  17  1 -119  7  3  3  0  1    2  3  2  10  1  -35  2  0  0  2  2
```

From '0 1 1 1 1', we can tell this 636 R82 hot band transition is part of 1000K, 2000K, 3000K and 4000K lists, but not for 296K list. Note the first intensity after A21 is at user provided temperature (*T* = 500K here), see #7 below. Its intensity at 2000K is 6.98025E-30 cm/molecule. Terrestrial abundance included in all 6 intensities. E'=14713.10314 cm-1, E"=9713.06930 cm-1, Ames VTET vib quantum numbers are: (v1v2v3)' = 2v1+14v2, (v1v2v3)"= 2v2+3v2+2v3, 399th root of 83e block ← 84th root of 82e block. The CDSD2019 assignment is: 73301e ← 20022e, 119th root of P17 ← 35th root of P10. The minus sign of "-119" and "-35" means the match is probably reliable.

Note: the CDSD2019 levels are available up to 24,000 cm-1 and J=150. AI-3000K list has J up to 250 (200) and E' up to 40,000 (36,000) cm-1 for 626 (636, 628, 627).

Example: to write out om2, A21, E", J' and Ames vtet based vib quanta differences v1v2v3' - v1v2v3" -- we know sometimes it could be badly off

```
      write(7001,1213)om2,a21*ab(is),ei,jf,ie(is,jf,iparf,irf,1:3)-ie(is,ji,ipari,iri,1:3)
1213  format(f12.5,es12.5,f12.5,i4,3i3)
```

5. Convert.f90 lines #99-#117, explain the two sets of line positions: Ames X01d PES based vs. CDSD2019 replaced. This is a 1-to-1 replacement.

```
! You can choose Ames-X01d PES based energies OR CDSD energies (when available, J=0-150, 0-24000 cm-1)
! the .tgz data were sorted by Ames-X01d based wavenumbers. You may re-sort them after using CDSD energies.
! to use Ames original:
! ef=e(is,jf,iparf,irf,1); ei=e(is,ji,ipari,iri,1)
! by default to use CDSD levels when available + Ames original for remains
  ef=e(is,jf,iparf,irf,1)+e(is,jf,iparf,irf,3)
  ei=e(is,ji,ipari,iri,1)+e(is,ji,ipari,iri,3)

! 2021-04-13 update: We tried to match part of X01d-PES levels with CDSD2019 (J<150, E'<15,000 cm-1)
!      if the 8th parameter in the ie() array was set to negative, which indicates the match was probably reliable (no guarantee though)
!      It is interesting to find out how much impact the inevitable inconsistency caused by such replacements will have at certain temperature
!   for high-T test, suggest to start with CDSD energy replacement for ALL J<=150 and E<15000 cm-1 levels.
!   if runs into some problems, we can enforce the filter below, i.e. to use the ie(,8)<0 & E<15000 cm-1 filter.
!   for potential fixes, we just need to update the energy level list files in future.
!   but for now, not sure how much difference they will make
        !if(ie(is,jf,iparf,irf,8).gt.0)ef=e(is,jf,iparf,irf,1)
  !if(ie(is,ji,ipari,iri,8).gt.0)ei=e(is,ji,ipari,iri,1)
        !if(ef.gt.15000.d0)ef=e(is,jf,iparf,irf,1)
        !if(ei.gt.15000.d0)ei=e(is,ji,ipari,iri,1)
```

6. Convert.f90 lines #119-#121, this serves as the filters on isotopologue & E' / E" thresholds. 'ef' / 'ei' for E' / E" in cm-1.

```
! Your E' cutoff for co2 626 (and other iso) can be put here, I suggest to try E'=37500 cm-1 and E=40000 cm-1
!       if(is.eq.1.and.ef.gt.36000.d0)goto 301
! by default it will go up to 40,000 cm-1 for 626.  (other 3 isos always up to 36000 cm-1)
```

7. How to generate a line list at user-specified temperature, other than 296K, 1000K, 2000K, 3000K, or 4000K.

User can specify a target temperature at line #45, as t(0). Accordingly, the partition function values of 4 isos are computed at line #54, and write out in line #58. The intensity at t(0) is computed from line #134 to line #140, saved as si(0), then output by line #163 - #165.

The convert.f90 is updated (old version saved as convert.f90.20210415). The screenshot on page 1 of this google.doc is also updated.

8. calculate the total number of lines for whole list generation vs for each 10 cm-1

Current convert.f90 has “nab=0” at line #66, for #lines in each 10 cm-1.

If one needs to get the total number of lines from each isotopologue in a wide (or full) range line list generation, the nab(4) should be defined as integer*8, and do not reset nab=0 for each .tgz list file.