Suo Yang <suo-yang@umn.edu>

Error in thermo.dat file

5 messages

Praveen Prakash <praka069@umn.edu> Mon, Feb 22, 2021 at 5:53 PM
To: Suo Yang <suo-yang@umn.edu>
Cc: Sai Ranjeet Narayanan <naray202@umn.edu>, Taaresh Sanjeev Taneja <tanej013@umn.edu>, joh19246@umn.edu

Dear all,

The thermo datafile (thermo.dat) placed in /g/m-y-crfel2/COMMON/Xu_Flames (also attached below) has an error in A1CH3CH3 species. All atoms (N,C,O,H) are represented as 0 and I get the error "molecular weight is not appropriate for species A1CH3CH3."

Thank you.
Regards.

thermo.dat
61K

Praise Noah Johnson <joh19246@umn.edu> Mon, Feb 22, 2021 at 8:14 PM
To: Praveen Prakash <praka069@umn.edu>
Cc: Suo Yang <suo-yang@umn.edu>, Sai Ranjeet Narayanan <naray202@umn.edu>, Taaresh Sanjeev Taneja <tanej013@umn.edu>

Praveen,

The elemental composition for A1CH3CH3 is C10H8. You can correct it as H 10C 8O 0N 0G in the thermo file.

Suo Yang <suo-yang@umn.edu> Wed, Feb 24, 2021 at 11:47 PM
To: Praise Noah Johnson <joh19246@umn.edu>
Cc: Praveen Prakash <praka069@umn.edu>, Sai Ranjeet Narayanan <naray202@umn.edu>, Taaresh Sanjeev Taneja <tanej013@umn.edu>, Shufan Zou <zou00066@umn.edu>, Dezhi Zhou <zhou0195@umn.edu>, Dezhi Zhou <dezhi.zhou@sjtu.edu.cn>

Praise and All,

If this is indeed an error, **we need to fix the Stanford Mechanism for all future simulations**. I just checked the folder, but found one weird thing:

While thermo.dat is wrong as this email thread mentioned, the TheSoot.chthermo file looks correct:

A1CH3CH3 000000N 0H 10O 0C 8AR 0G 300 5000 1000 1
-1.95577967E+00 7.09552723E-02-4.19975432E-05 1.18372259E-08-1.28339716E-12 2
-6.91883225E+01 3.59161008E+01-3.46066830E+00 7.17789316E-02-2.55611032E-05 3
-1.74870775E-08 1.22856956E-11 1.62314629E+02 4.36521185E+01 4

So two questions for everyone:

(1) Which one does the .pre file actually use during its generation? This determines whether our .pre file is also wrong for this part.
(2) TheSoot.chthermo file looks older, so does it generate the thermo.dat file? If yes, why this mistake can happen?

Best wishes

Suo Yang
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Dezhi Zhou <dezhi.zhou@sjtu.edu.cn> Thu, Feb 25, 2021 at 12:35 AM
To: Suo Yang <suo-yang@umn.edu>, Praise Noah Johnson <joh19246@umn.edu>
Cc: Praveen Prakash <praka069@umn.edu>, Sai Ranjeet Narayanan <naray202@umn.edu>, Taaresh Sanjeev Taneja <tanej013@umn.edu>, Shufan Zou <zou00066@umn.edu>, Dezhi Zhou <zhou0195@umn.edu>

Dear All,

I remember TheSoot.chthermo is generated when we are converting CK format to FM format. If it is different from the original CK thermos file, I guess the converting tool did some corrections?

Dezhi Zhou

[Quoted text hidden]

Suo Yang <suo-yang@umn.edu> Thu, Feb 25, 2021 at 12:43 AM
To: Dezhi Zhou <dezhi.zhou@sjtu.edu.cn>
Cc: Praise Noah Johnson <joh19246@umn.edu>, Praveen Prakash <praka069@umn.edu>, Sai Ranjeet Narayanan <naray202@umn.edu>, Taaresh Sanjeev Taneja <tanej013@umn.edu>, Shufan Zou <zou00066@umn.edu>, Dezhi Zhou <zhou0195@umn.edu>

Thanks Dezhi.

Could someone double confirm what Dezhi said? If it is true, then our .pre file for FM and NGA is safe and our previous simulations should be correct, but we still need to fix it for Chemkin, Converge, and OF.

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