

ZipFile Updates Since Original Posting

Last Update - 110726

The original files were posted on the web on June 24, 2011. Since the posting, the following modifications have been made to the posted files.

110714 - A potential problem was corrected in the chem.inp file and the manuscript model listing. Earlier we neglected to include the "E" in the activation energy parameters for the following reaction:

Troe, Combust. Flame, 158:594-601 (2011)

! Rate constant is for Ar

H2O2(+M) = OH+OH(+M) 2.00E+12 0.90 4.8749E+04

LOW/2.49E+24 -2.30 4.8749E+04/

TROE/0.43 1E-30 1E+30/

H2O/7.5/ CO2/1.6/

N2/1.5/ O2/1.2/

HE/0.65/ H2O2/7.7/

! Efficiencies for H2 and CO taken from Li et al., Int. J. Chem. Kinet. 36:566-575 (2004)

H2/3.7/ CO/2.8/

This can cause errors in some system software installations and is corrected in downloads after July 14, 2011. Our systems are transparent to this type of omission and there are no resulting modifications in the reported information in the paper and supplemental materials.

110726 — A typo error in a commented-out reaction listing in the manuscript and chem.inp was noted for

! Fernandez-Ramos and Varandas, J. Phys. Chem. A 106:4077-4083 (2002)

!HO2+O = O2+OH 4.750E+11 1.00 -7.2393E+02

!Scaled by 0.60

HO2+O = O2+OH 2.850E+10 1.00 -7.2393E+02

The typo was corrected in the manuscript and chem.inp file to

! Fernandez-Ramos and Varandas, J. Phys. Chem. A 106:4077-4083 (2002)

!HO2+O = O2+OH 4.750E+10 1.00 -7.2393E+02

!Scaled by 0.60

HO2+O = O2+OH 2.850E+10 1.00 -7.2393E+02

This correction has no effect on reported information in the manuscript and supplemental materials.