

C₁–C₂ 燃料燃烧机理的框架简化

李树豪¹ 李 瑞¹ 郭俊江² 谈宁馨² 王 繁^{3,*}

李象远²

(¹ 四川大学空天科学与工程学院, 成都 610065; ² 四川大学化学与工程学院, 成都 610065;

³ 四川大学原子与分子物理研究所, 成都 610065)

Skeletal Kinetic Model Generation for the Combustion of C₁–C₂ Fuels

LI Shu-Hao¹ LI Rui¹ GUO Jun-Jiang² TAN Ning-Xin² WANG Fan^{3,*}

LI Xiang-Yuan²

(¹ *School of Aeronautics & Astronautics, Sichuan University, Chengdu 610065, P. R. China;*

² *School of Chemical Engineering, Sichuan University, Chengdu 610065, P. R. China;*

³ *Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, P. R. China)*

*Corresponding author. Email: wangf44@gmail.com; Tel: +86-28-85403537.

Table S1 Retained species in the corresponding skeletal mechanisms with the predicted errors of ignition delay time controlled within 10%

Method	Number	Species in skeletal mechanism
DRG	171	HCOH, CH3COCH3, CH3COCH2, CH3COCH2O2, C3KET21, C2H3CO, C2H5CHO, C2H5CO, C3H5-T, C3H4-A, C3H3, C3H6OOH2-1, C3H6OOH2-1O2, C3H6OOH2-2, IC3H7O2H, IC3H7O2, IC3H7O, C3H6O1-2, C3H6O1-3, C3KET12, C3H51-2,3OOH, C3H52-1,3OOH, CH3CHCO, AC3H5OOH, C4H8-1, C4H8-2, PC4H9, SC4H9, C4H71-2, C4H71-3, C4H71-4, SC4H9O2H, PC4H9O2, SC4H9O2, PC4H9O, SC4H9O, C4H7O, C4H8O1-3, PC4H8OH, SC4H8OH, C4H8OH-1O2, C4H8OH-2O2, C4H8OOH1-3, C4H8OOH2-4, C4H8OOH1-3O2, C4H8OOH2-4O2, NC4KET13, NC4KET24, IC4H10, IC4H9, TC4H9, IC4H8, IC4H7, TC4H9O2, IC4H9O2, TC4H8O2H-I, IC4H8O2H-I, IC4H8O2H-T, IC4H8O, CC4H8O, IC4H9O, TC4H9O, IC4H9O2H, TC4H9O2H, IC4H7O, IC3H7CHO, TC3H6CHO, IC3H7CO, IC3H6CHO, IC4H7OH, IC4H6OH, IC3H5CHO, IC3H5CO, TC3H6OCHO, IC3H6CO, TC3H6OH, IC3H5OH, CH2CCCH2OH, C4H4, C4H3-I, C4H3-N, C4H612, C4H5-I, C4H5-N, CH3CHCHCO, CH2CHCHCHO, C2H3CHOCH2, C4H5-2, C4H6-2, H2C4O, H, H2, O, O2, OH, OH*, H2O, N2, HO2, H2O2, AR, CO, CO2, CH2O, HCO, HO2CHO, O2CHO, HOCHO, OCHO, HOCH2O, CH3OH, CH2OH, CH3O, CH3O2H, CH3O2, CH4, CH3, CH2, CH2(S), CH, C2H6, C2H5, C2H4, C2H3, C2H2, C2H, CH3CHO, C2H3OH, C2H2OH, CH3CO, CH2CHO, CH2CO, HCCO, CH3CO3H, CH3CO3, CH3CO2, C2H5OH, C2H5O, PC2H4OH, SC2H4OH, O2C2H4OH, C2H5O2H, C2H5O2, C2H4O2H, C2H4O1-2, C2H3O1-2, C2H3CHO, CH3OCO, HE, C3H8, IC3H7, NC3H7, C3H6, C3H5-A, C3H5-S, C3H4-P, C3H5O, C3H6OOH1-2, C3H6OOH1-3, C3H6OOH1-2O2, C3H6OOH1-3O2, NC3H7O2H, NC3H7O2, NC3H7O, C3KET13, H2CC, C4H10, C4H6, C4H2, C4H6O23, CH3CHCHCHO
DRGEP	119	HCOH, HOCH2O2H, HOCH2O2, OCH2O2H, C, HCCOH, CH3COCH3, CH3COCH2C2H3CO, C2H5CHO, CH3OCH3, CH3OCH2OCH3OCHO, C3H5-T, C3H4-A, C3H3C3H6OOH2-1, IC3H7O2, IC3H7O, CH3CHCOC4H8-1, PC4H9, SC4H9, C4H71-3C4H71-4, C4H7O, IC4H10, C4H4, C4H3-I, C4H3-N, C4H612, C4H5-IC4H5-N, CH3CHCHCO, CH2CHCHCHO, C4H5-2, C4H6-2, H2C4O, H, H2, O, O2, OH, OH*, H2O, N2, HO2, H2O2, AR, CO, CO2, CH2O, HCO, HO2CHO, O2CHO, HOCHO, OCHO, HOCH2O, CH3OH, CH2OH, CH3O, CH3O2H, CH3O2, CH4, CH3, CH2, CH2(S), CH, C2H6, C2H5, C2H4, C2H3, C2H2, C2H, CH3CHO, C2H3OH, C2H2OH, CH3CO, CH2CHO, CH2CO, HCCO, CH3CO3H, CH3CO3, CH3CO2, C2H5OH, C2H5O, PC2H4OH, SC2H4OH, O2C2H4OH, C2H5O2H, C2H5O2, C2H4O2H, C2H4O1-2, C2H3O1-2, C2H3CHO, CH3OCO, HE, C3H8, IC3H7, NC3H7, C3H6, C3H5-A, C3H5-S, C3H4-P, C3H5O, C3H6OOH1-2, C3H6OOH1-3, C3H6OOH1-2O2, C3H6OOH1-3O2, NC3H7O2H, NC3H7O2, NC3H7O, C3KET13, H2CC, C4H10, C4H6, C4H2, C4H6O23, CH3CHCHCHO
r-DRG	131	C, HCCOH, CH3COCH3, CH3COCH2, C3KET21, C2H3CO, C2H5CHO, C2H5CO, C3H5-T, C3H4-A, C3H3, C3H6OOH2-1, C3H6OOH2-1O2, IC3H7O2H, IC3H7O2, IC3H7O, C3H6O1-3, C3KET12, C3H51-2,3OOH, C3H52-1,3OOH, CH3CHCO, AC3H5OOH, C4H8-1, C4H8-2, PC4H9, SC4H9, C4H71-2, C4H71-3, C4H71-4, PC4H9O2, PC4H9O, C4H7O, C4H8O1-3, PC4H8OH, C4H8OH-1O2, C4H8OOH1-3, IC4H10, IC4H9, C4H4, C4H3-I, C4H3-N, C4H612, C4H5-I, C4H5-N, CH3CHCHCO, CH2CHCHCHO, C2H3CHOCH2, C4H5-2, C4H6-2, H2C4O, H,

		H2, O, O2, OH, OH*, H2O, N2, HO2, H2O2, AR, CO, CO2, CH2O, HCO, HO2CHO, O2CHO, HOCHO, OCHO, HOCH2O, CH3OH, CH2OH, CH3O, CH3O2H, CH3O2, CH4, CH3, CH2, CH2(S), CH, C2H6, C2H5, C2H4, C2H3, C2H2, C2H, CH3CHO, C2H3OH, C2H2OH, CH3CO, CH2CHO, CH2CO, HCCO, CH3CO3H, CH3CO3, CH3CO2, C2H5OH, C2H5O, PC2H4OH, SC2H4OH, O2C2H4OH, C2H5O2H, C2H5O2, C2H4O2H, C2H4O1-2, C2H3O1-2, C2H3CHO, CH3OCO, HE, C3H8, IC3H7, NC3H7, C3H6, C3H5-A, C3H5-S, C3H4-P, C3H5O, C3H6OOH1-2, C3H6OOH1-3, C3H6OOH1-2O2, C3H6OOH1-3O2, NC3H7O2H, NC3H7O2, NC3H7O, C3KET13, H2CC, C4H10, C4H6, C4H2, C4H6O23, CH3CHCHCHO
(r-DRG)EP	85	HOCH2O2H, HOCH2O2, OCH2O2H, C3H6O1-3, H, H2, O, O2, OH, OH*, H2O, N2, HO2, H2O2, AR, CO, CO2, CH2O, HCO, HO2CHO, O2CHO, HOCHO, OCHO, HOCH2O, CH3OH, CH2OH, CH3O, CH3O2H, CH3O2, CH4, CH3, CH2, CH2(S), CH, C2H6, C2H5, C2H4, C2H3, C2H2, C2H, CH3CHO, C2H3OH, C2H2OH, CH3CO, CH2CHO, CH2CO, HCCO, CH3CO3H, CH3CO3, CH3CO2, C2H5OH, C2H5O, PC2H4OH, SC2H4OH, O2C2H4OH, C2H5O2H, C2H5O2, C2H4O2H, C2H4O1-2, C2H3O1-2, C2H3CHO, CH3OCO, HE, C3H8, IC3H7, NC3H7, C3H6, C3H5-A, C3H5-S, C3H4-P, C3H5O, C3H6OOH1-2, C3H6OOH1-3, C3H6OOH1-2O2, C3H6OOH1-3O2, NC3H7O2H, NC3H7O2, NC3H7O, C3KET13, H2CC, C4H10, C4H6, C4H2, C4H6O23, CH3CHCHCHO
PFA	176	C, CH3COCH3, CH3COCH2, CH3COCH2O2, C3KET21, C2H3CO, C2H5CHO, C2H5CO, C3H5-T, C3H4-A, C3H3, C3H6OOH2-1, C3H6OOH2-1O2, C3H6OOH2-2, IC3H7O2H, IC3H7O2, IC3H7O, C3H6O1-2, C3H6O1-3, C3KET12, C3H51-2,3OOH, C3H52-1,3OOH, CH3CHCO, AC3H5OOH, C4H8-1, C4H8-2, PC4H9, SC4H9, C4H71-2, C4H71-3, C4H71-4, PC4H9O2H, SC4H9O2H, PC4H9O2, SC4H9O2, PC4H9O, SC4H9O, C4H7O, C4H8O1-3, C4H8O1-4, C4H8O2-3, PC4H8OH, SC4H8OH, C4H8OH-1O2, C4H8OH-2O2, C4H8OOH1-3, C4H8OOH1-4, C4H8OOH2-3, C4H8OOH2-4, C4H8OOH1-3O2, C4H8OOH2-4O2, NC4KET13, NC4KET24, IC4H10, IC4H9, TC4H9, IC4H8, IC4H7, TC4H9O2, IC4H9O2, TC4H8O2H-I, IC4H8O2H-I, IC4H8O2H-T, IC4H8O, CC4H8O, IC4H9O, TC4H9O, IC4H9O2H, TC4H9O2H, IC4H7O, IC3H7CHO, TC3H6CHO, IC3H7CO, IC3H6CHO, IC4H7OH, IC4H6OH, IC3H5CHO, IC3H5CO, TC3H6OCHO, IC3H6CO, TC3H6OH, IC3H5OH, CH2CCH2OH, C4H4, C4H3-I, C4H3-N, C4H612, C4H5-I, C4H5-N, CH3CHCHCO, CH2CHCHCHO, C2H3CHOCH2, C4H5-2, C4H6-2, H2C4O, H, H2, O, O2, OH, OH*, H2O, N2, HO2, H2O2, AR, CO, CO2, CH2O, HCO, HO2CHO, O2CHO, HOCHO, OCHO, HOCH2O, CH3OH, CH2OH, CH3O, CH3O2H, CH3O2, CH4, CH3, CH2, CH2(S), CH, C2H6, C2H5, C2H4, C2H3, C2H2, C2H, CH3CHO, C2H3OH, C2H2OH, CH3CO, CH2CHO, CH2CO, HCCO, CH3CO3H, CH3CO3, CH3CO2, C2H5OH, C2H5O, PC2H4OH, SC2H4OH, O2C2H4OH, C2H5O2H, C2H5O2, C2H4O2H, C2H4O1-2, C2H3O1-2, C2H3CHO, CH3OCO, HE, C3H8, IC3H7, NC3H7, C3H6, C3H5-A, C3H5-S, C3H4-P, C3H5O, C3H6OOH1-2, C3H6OOH1-3, C3H6OOH1-2O2, C3H6OOH1-3O2, NC3H7O2H, NC3H7O2, NC3H7O, C3KET13, H2CC, C4H10, C4H6, C4H2, C4H6O23, CH3CHCHCHO
PFAEP	105	HCOH, HOCH2O2H, HOCH2O2, OCH2O2H, C, HCCOH, CH3COCH2, C2H3CO, CH3OCH2O, CH3OCHO, C3H5-T, C3H4-A, C3H3, C3H6O1-3, CH3CHCO, C4H8-1, PC4H9, SC4H9, C4H7O, C4H4, C4H3-I, C4H3-N, C4H5-I, CH2CHCHCHO, H, H2, O, O2, OH, OH*, H2O, N2, HO2, H2O2, AR, CO, CO2, CH2O, HCO, HO2CHO, O2CHO, HOCHO, OCHO, HOCH2O, CH3OH, CH2OH, CH3O, CH3O2H, CH3O2, CH4, CH3, CH2, CH2(S), CH, C2H6, C2H5, C2H4, C2H3, C2H2, C2H, CH3CHO, C2H3OH, C2H2OH, CH3CO, CH2CHO, CH2CO, HCCO, CH3CO3H, CH3CO3, CH3CO2, C2H5OH, C2H5O, PC2H4OH, SC2H4OH, O2C2H4OH, C2H5O2H, C2H5O2, C2H4O2H, C2H4O1-2, C2H3O1-2, C2H3CHO, CH3OCO, HE, C3H8, IC3H7, NC3H7, C3H6, C3H5-A, C3H5-S, C3H4-P, C3H5O, C3H6OOH1-2, C3H6OOH1-3, C3H6OOH1-2O2, C3H6OOH1-3O2, NC3H7O2H, NC3H7O2, NC3H7O, C3KET13, H2CC, C4H10, C4H6, C4H2, C4H6O23, CH3CHCHCHO

		CH3CO3H, CH3CO3, CH3CO2, C2H5OH, C2H5O, PC2H4OH, SC2H4OH , O2C2H4OH, C2H5O2H, C2H5O2, C2H4O2H, C2H4O1-2 ,C2H3O1-2, C2H3CHO, CH3OCO, HE, C3H8, IC3H7, NC3H7, C3H6, C3H5-A, C3H5-S, C3H4-P, C3H5O, C3H6OOH1-2, C3H6OOH1-3, C3H6OOH1-2O2, C3H6OOH1-3O2, NC3H7O2H, NC3H7O2, NC3H7O, C3KET13, H2CC, C4H10, C4H6, C4H2 , C4H6O23 , CH3CHCHCHO
Intersection	81	H, H2, O, O2, OH, OH*, H2O, N2, HO2, H2O2, AR, CO, CO2, CH2O, HCO, HO2CHO, O2CHO, HOCHO, OCHO, HOCH2O, CH3OH, CH2OH, CH3O, CH3O2H, CH3O2, CH4, CH3, CH2, CH2(S), CH, C2H6, C2H5, C2H4, C2H3, C2H2, C2H, CH3CHO, C2H3OH, C2H2OH, CH3CO , CH2CHO, CH2CO, HCCO, CH3CO3H, CH3CO3, CH3CO2, C2H5OH, C2H5O, PC2H4OH, SC2H4OH , O2C2H4OH, C2H5O2H, C2H5O2, C2H4O2H, C2H4O1-2 ,C2H3O1-2, C2H3CHO, CH3OCO, HE, C3H8, IC3H7, NC3H7, C3H6, C3H5-A, C3H5-S, C3H4-P, C3H5O, C3H6OOH1-2, C3H6OOH1-3, C3H6OOH1-2O2, C3H6OOH1-3O2, NC3H7O2H, NC3H7O2, NC3H7O, C3KET13, H2CC, C4H10, C4H6, C4H2 , C4H6O23 , CH3CHCHCHO