Supplemental Material 1 for Phys. Chem. Chem. Phys.

Neural network potential energy surface assisted molecular dynamics study on pyrolysis behaviors of two spiro-hydrocarbons

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Table **S1**. Several key parameters set for training potential energy surfaces.

dp_version	2.1.5	Learning rate	
descriptor		type	exp
type	se_a	start_lr	0.001
sel	[52, 40] (Fuel**1**)	decay_steps	400
	[56, 36] (Fuel**2**)	training	
rcut_smth	1 Å	stop_batch	400000
rcut	6 Å	dp_compress	TRUE
neuron	[25, 50, 100]	model_devi_dt	0.0001
resnet_dt	FALSE	model_devi_skip	100
axis_neuron	12	model_devi_f_trust_lo	0.15
fitting net		model_devi_f_trust_hi	0.45
neuron	[240, 240, 240]	use_cluster	TRUE
resnet_dt	TRUE	cluster_cutoff	3.5 Å

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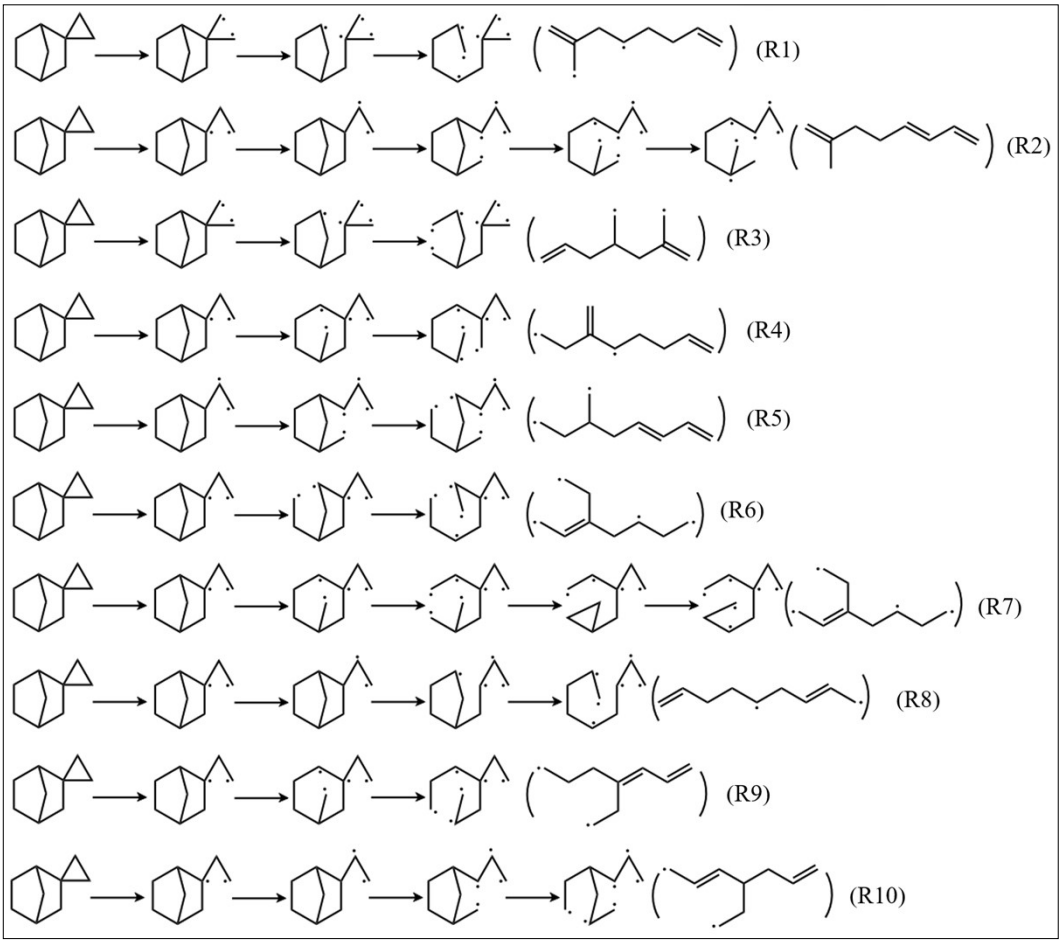
Table **S2**. Temperature, time, and "Accuracy" for each iteration of training for two fuels.

Fuel **1**				Fuel **2**			
Iteration	T/K	Time/ps	Accuracy	Iteration	T/K	Time/ps	Accuracy
0	2500	0.2	83.86%	0	2500, 2800	0.2	67.06%
1	2500	0.2	98.75%	1	2500, 2800	0.2	94.64%
2	2500	0.2	98.96%	2	2500, 2800	0.2	96.91%
3_check	2500	0.2	99.02%	3	2500, 2800	0.2	98.62%
3	2500	0.4	99.01%	4_check	2500, 2800	0.2	99.08%
4	2500	0.8	98.84%	4	2500, 2800	0.4	98.87%
5	2500	0.8	98.42%	5	2500, 2800	0.4	98.41%
6	2500	0.8	98.91%	6_check	2500, 2800	0.4	99.07%
7	2500	0.8	98.86%	6	2500, 2800	0.8	98.89%
8	2500	0.8	98.62%	7	2500, 2800	0.8	98.76%
9_check	2500	0.8	99.21%	8	2500, 2800	0.8	98.78%
9	2500	1.6	99.03%	9_check	2500, 2800	0.8	99.02%
10	2500	1.6	97.93%	9	2500, 2800	1.6	98.75%
11_check	2500	1.6	99.20%	10_check	2500, 2800	1.6	99.04%
11	2500	3.2	98.87%	10	2500, 2800	3.2	98.88%
12	2500	3.2	95.42%	11_check	2500, 2800	3.2	99.03%
13	2500	3.2	98.15%	11	2500, 2800	6.4	98.72%
14	2500	3.2	97.96%	12	2500, 2800	6.4	98.27%
15	2500	3.2	98.40%	13	2500, 2800	6.4	98.64%
16	2500	3.2	98.36%	14	2500, 2800	6.4	98.09%
17	2500	3.2	98.01%	15_check	2500, 2800	6.4	99.04%
18_check	2500	3.2	99.47%	15	2500, 2800	12.8	98.80%
18	2500	6.4	99.36%	16	2500, 2800	12.8	98.82%
19	2500	6.4	98.95%	17	2500, 2800	12.8	97.94%
20_check	2500	6.4	99.34%	18	2500, 2800	12.8	98.70%
20	2500	12.8	99.07%	19_check	2500, 2800	12.8	99.06%
21	2500	12.8	98.07%	19	2500, 2800	25.6	99.01%
22	2500	12.8	96.57%	20	2500, 2800	25.6	98.93%
23	2500	12.8	97.64%	21_check	2500, 2800	25.6	99.38%
24	2500	12.8	98.66%	21	2500, 2800	51.2	98.93%
25_check	2500	12.8	99.22%	22	2500, 2800	51.2	97.82%
25	2500	25.6	99.00%	23	2500, 2800	51.2	98.30%
26	2500	25.6	98.54%	24_check	2500, 2800	51.2	99.39%
27_check	2500	25.6	99.29%	24	2500, 2800	102.4	99.38%
27	2500	51.2	99.25%	25	2500, 2800	102.4	98.98%
27_check	2500	51.2	99.17%	26	2500, 2800	102.4	98.97%
28	2500	102.4	98.80%	27	2500, 2800	102.4	99.11%
29	2500	102.4	93.76%				
30	2500	102.4	99.03%				

31_check	2500	102.4	99.20%				

Continue with Table **S2**

31	2800	102.4	98.72%				
32	2800	102.4	95.91%				
33_check	2800	102.4	99.21%				



Scheme **S1**. Primary pathways of all structures of initial pyrolysis products of Fuel **2** at 2500K and 2800K. R1 and R2 are for structure a), R3 is for structure b), R4 and R5 are for structure c), R6 and R7 are for structure d), R8 is for structure e), R9 and R10 are for structure f).