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Supporting Information

Direct synthesis of high-density aviation fuel with polycarbonate

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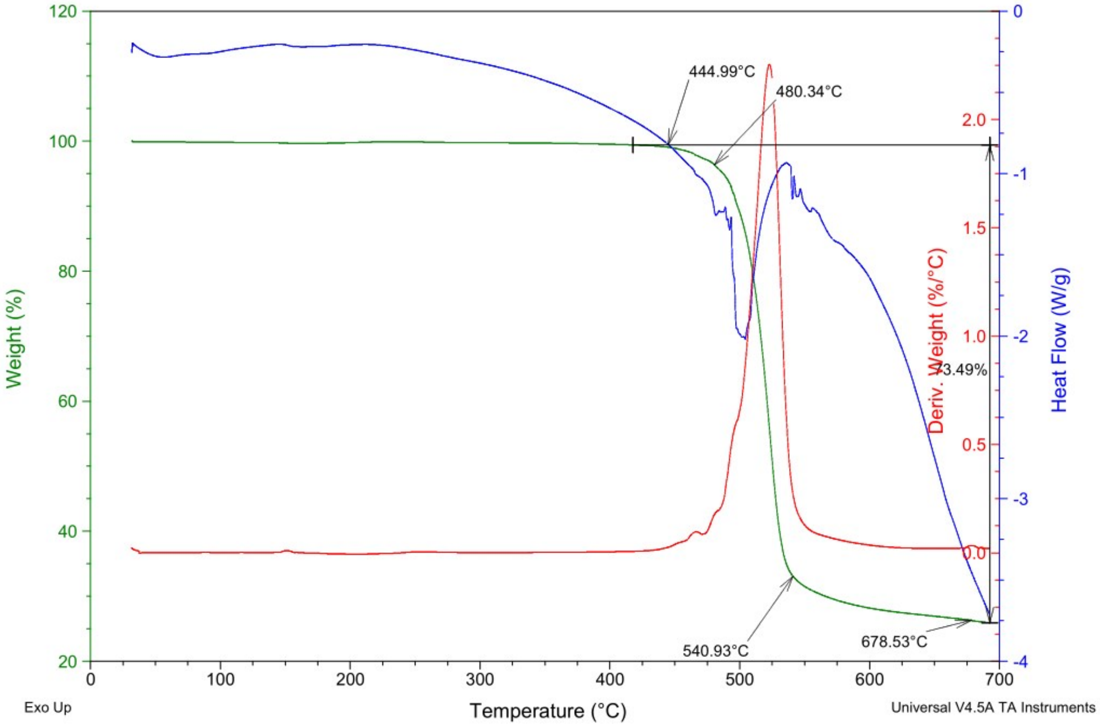

Figure S1. TG-DSC profile of the pure PC pellet used in the activity tests.

The thermogravimetric-differential scanning calorimetry (TG-DSC) analysis of the pure PC pellet was carried out by a SDTQ600 TG. Based on the result illustrated in Figure S1, the decomposition temperature of the pure PC pellet used in the activity test was measured as 718 K. This means that the pure PC pellet itself is stable under the investigated temperature range (443 K-523 K). All PC conversions were achieved under the promotion of catalyst.

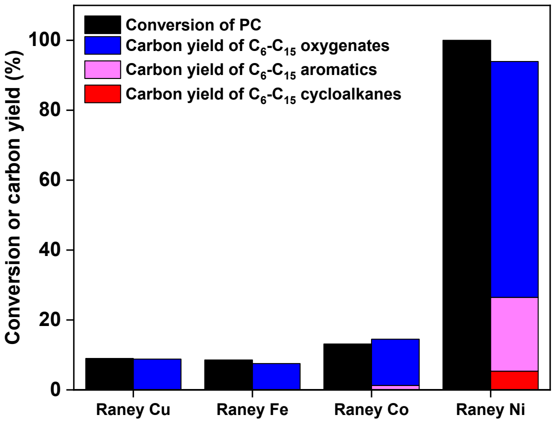

Figure S2. Conversions of PC and the carbon yields of C_6-C_{15} oxygenates and cyclic hydrocarbons over different Raney metal catalysts. Reaction conditions: 463 K, 0.5 h; 2 g pure PC pellets, 0.4 g catalyst and 45 mL isopropanol were used in each test.

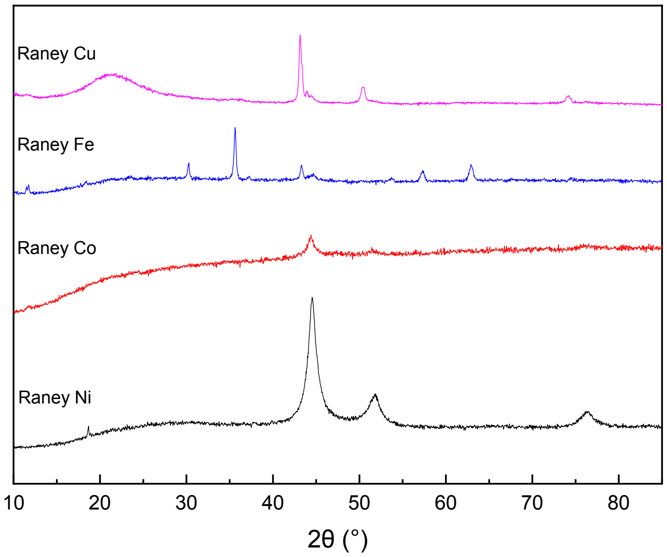

Figure S3. The XRD patterns of the Raney metal catalysts used in this work.

Table S1. The average particle sizes, metal dispersions, the amounts of active sites and TOFs of PC over the investigated Raney metal catalysts.

Catalyst	Average particle size (nm)[a]	Metal dispersion (%)[b]	Active sites (mmol g^{-1})[c]	TOF (kg_{PC} mol^{-1} h^{-1})[d]
Raney Ni	11.8	8.55	1.46	6.80
Raney Co	17.1	5.86	0.993	1.34
Raney Fe	31.4	3.70	0.663	1.29
Raney Cu	27.4	3.78	0.594	1.51

a: Calculated according to XRD results (see Figure S3). *b*: Estimated according to the average particle size of metal particles. *c*: Calculated according to the metal dispersion and atomic weight. *d*: Calculated according to the results of activity tests at 0.5 h.

To compare the activities of Raney metal catalysts, we characterized them by XRD (see Figure S3). Based on the strongest peaks, we estimated the average sizes of metal particles by Debye-Scherrer equation. Subsequently, we calculated the metal dispersion and the numbers of active sizes according to the method described in a textbook (pages 439-442, **Handbook of Heterogeneous Catalysis** Edited by G. Ertl, H. Knozinger, J. Weitkamp, ISBN 3-527-29212-8; https://onlinelibrary.wiley.com/doi/book/10.1002/9783527619474). Finally, we calculated the TOFs over different Raney metal catalysts based on the conversions of PC at a reaction time of 0.5 h and the numbers of active sizes. From Table S2, we can see that Raney Ni demonstrated higher TOF for PC conversion than those of other Raney metal catalysts. That is the reason why we chose this catalyst for further investigation.

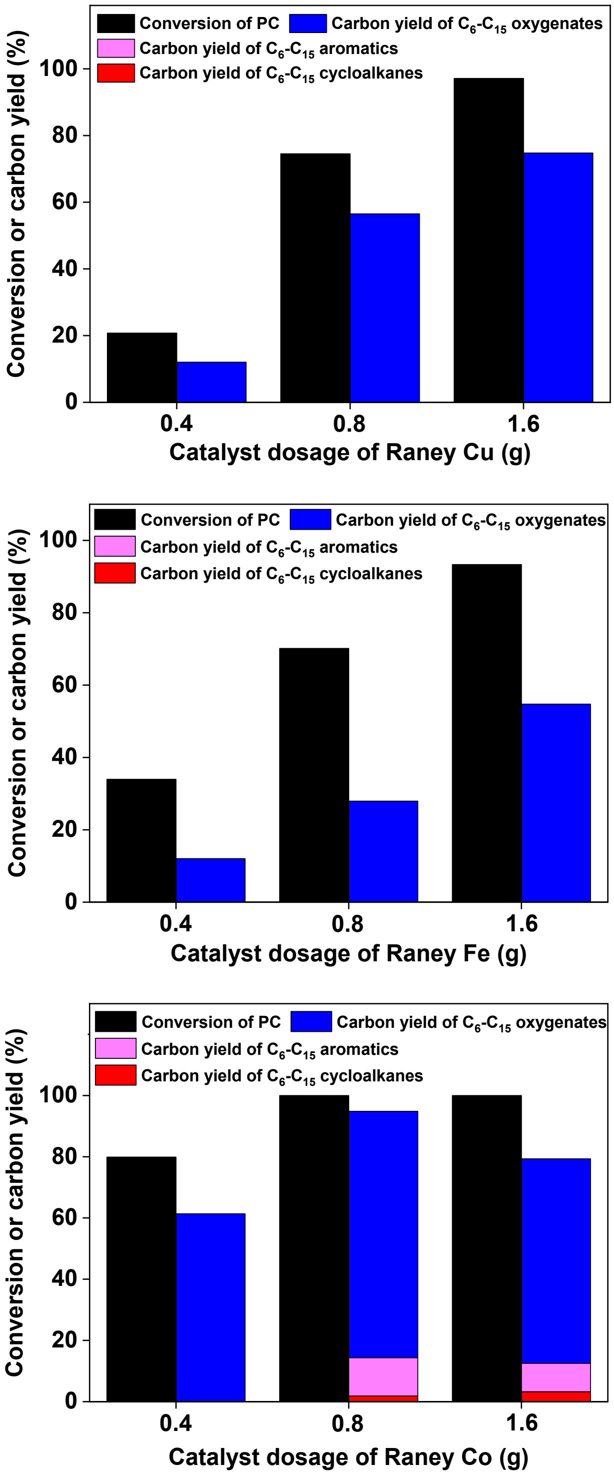

Figure S4. Conversions of PC and the carbon yields of C_6-C_{15} oxygenates and cyclic hydrocarbons over different Raney metal catalysts. Reaction conditions: 463 K, 1 h; 2 g pure PC pellets and 45 mL isopropanol were used in each test.

Table S2. Specific densities of the cyclic hydrocarbons obtained in this work.

	Density ($g\ mL^{-1}$)	Temperature for density measurement (K)	Reference
Isopropylbenzene	0.86	298.15	[1]
Isopropylcyclohexane	0.80	293.15	[2]
2,2-Diphenylpropane	1.00	293.15	[3]
2-Phenyl-2-(1-piperidinyl)propane	0.95	293.15	[3]
Propane-2,2-diyldicyclohexane	0.91	293.15	[3]

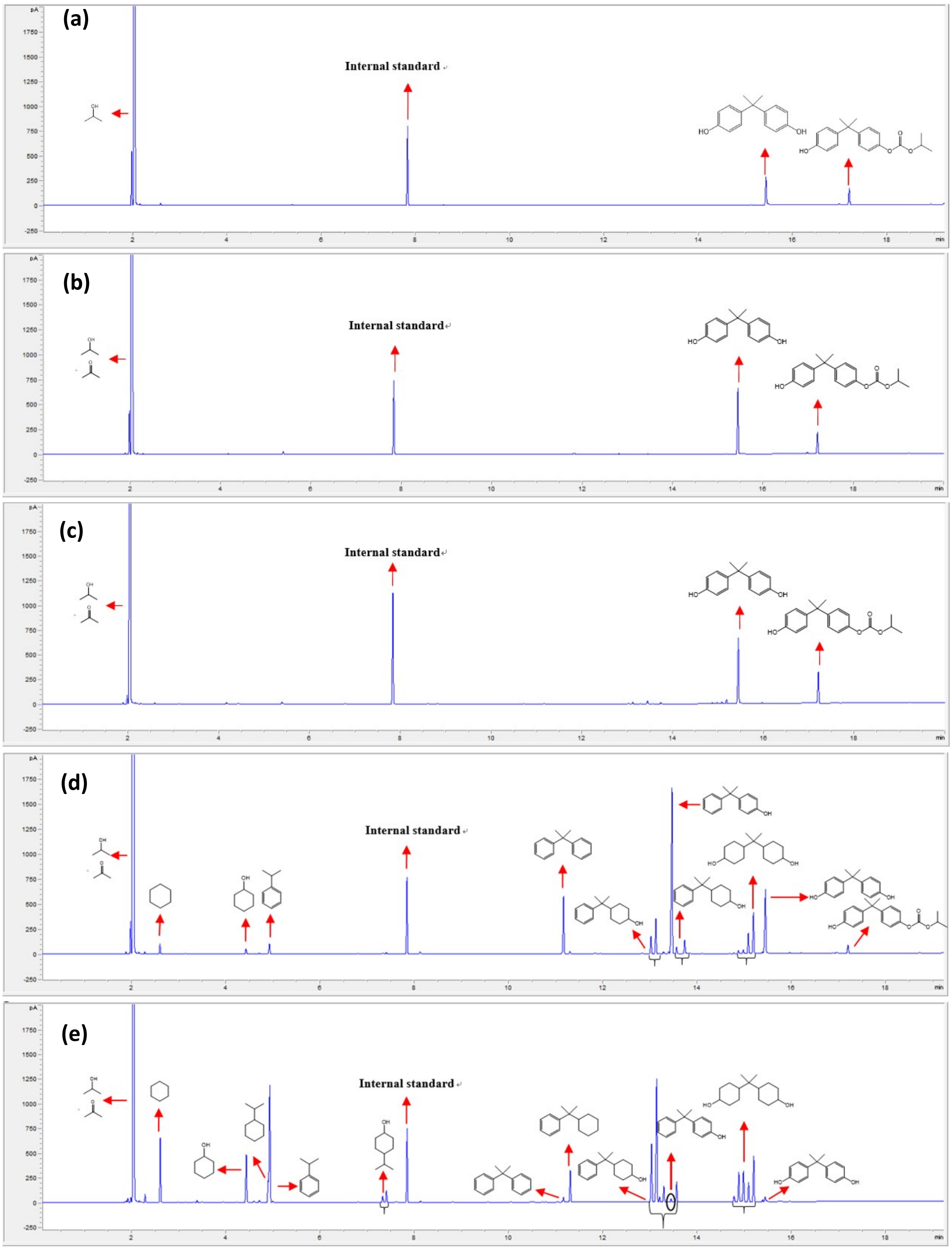

Figure S5. GC chromatograms of the products obtained in blank experiment (a) or from the reaction of pure PC pellets over the Raney Cu (b), Raney Fe (c) Raney Co (d) and Raney Ni (e) catalysts. Reaction conditions: 463 K, 1 h; 2 g pure PC pellets, 0 or 0.4 g Raney metal catalyst and 45 mL isopropanol were used in the tests.

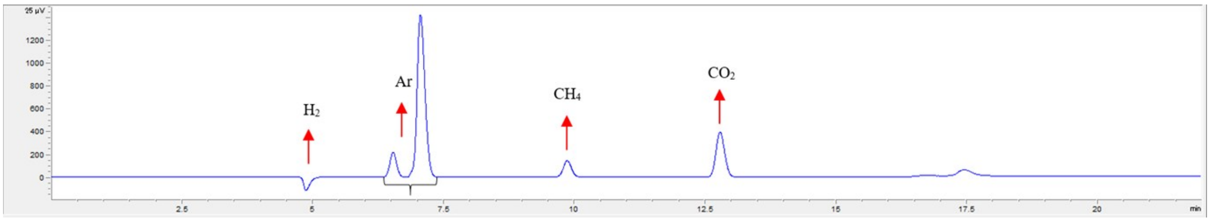

Figure S6. GC chromatogram of the gas phase products from the transfer hydrodeoxygenation of pure PC pellets. Reaction conditions: 463 K, 1 h; 2 g pure PC pellets, 0.4 g Raney Ni and 45 mL isopropanol were used in the test (Ar was used as the shielding gas).

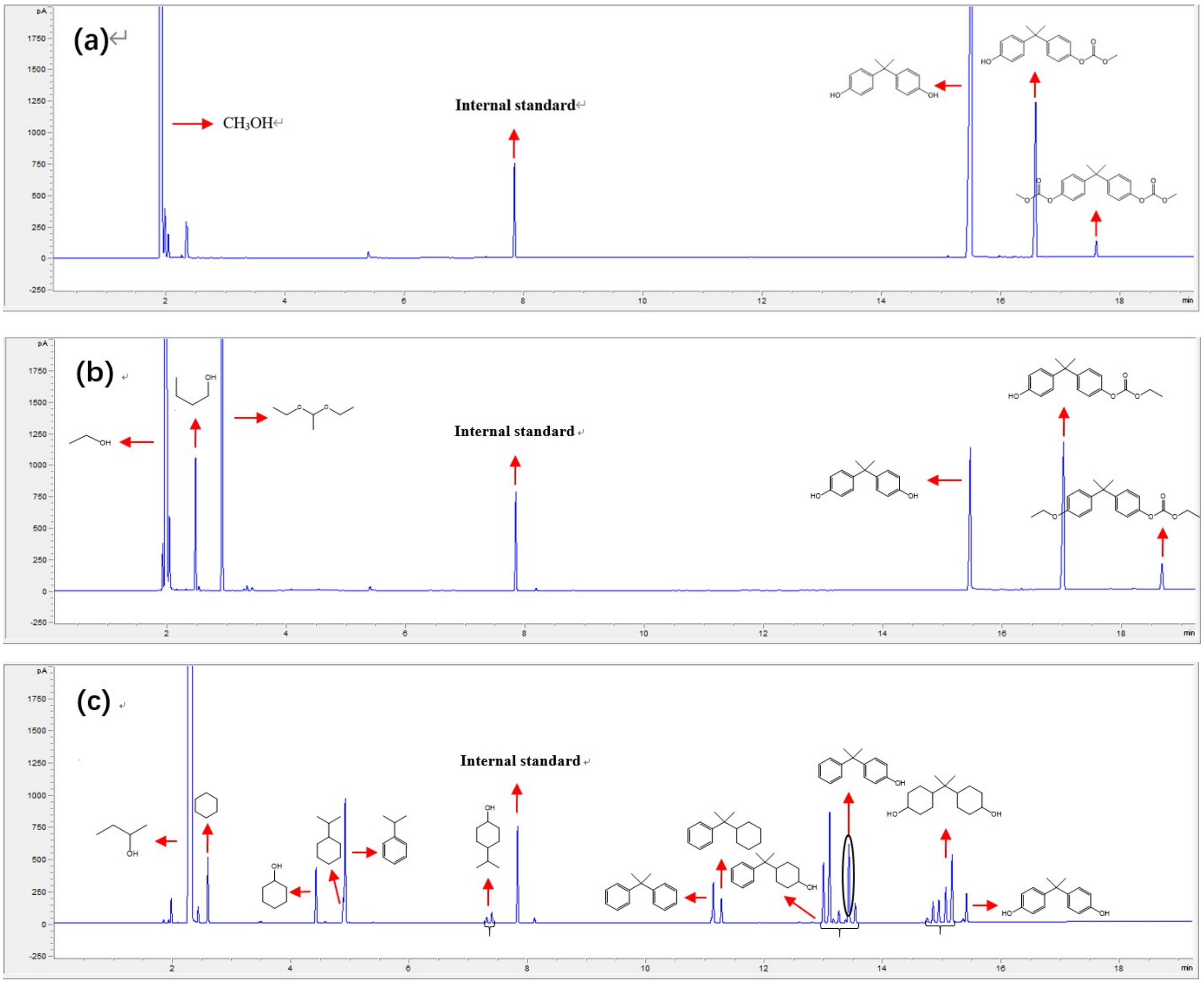

Figure S7. GC chromatograms of the products from the transfer hydrodeoxygenation of pure PC pellets in methanol (a), ethanol (b), 2-butanol (c). Reaction conditions: 463 K, 1 h; 2 g pure PC pellets, 0.4 g Raney Ni and 45 mL alcohol were used in the tests.

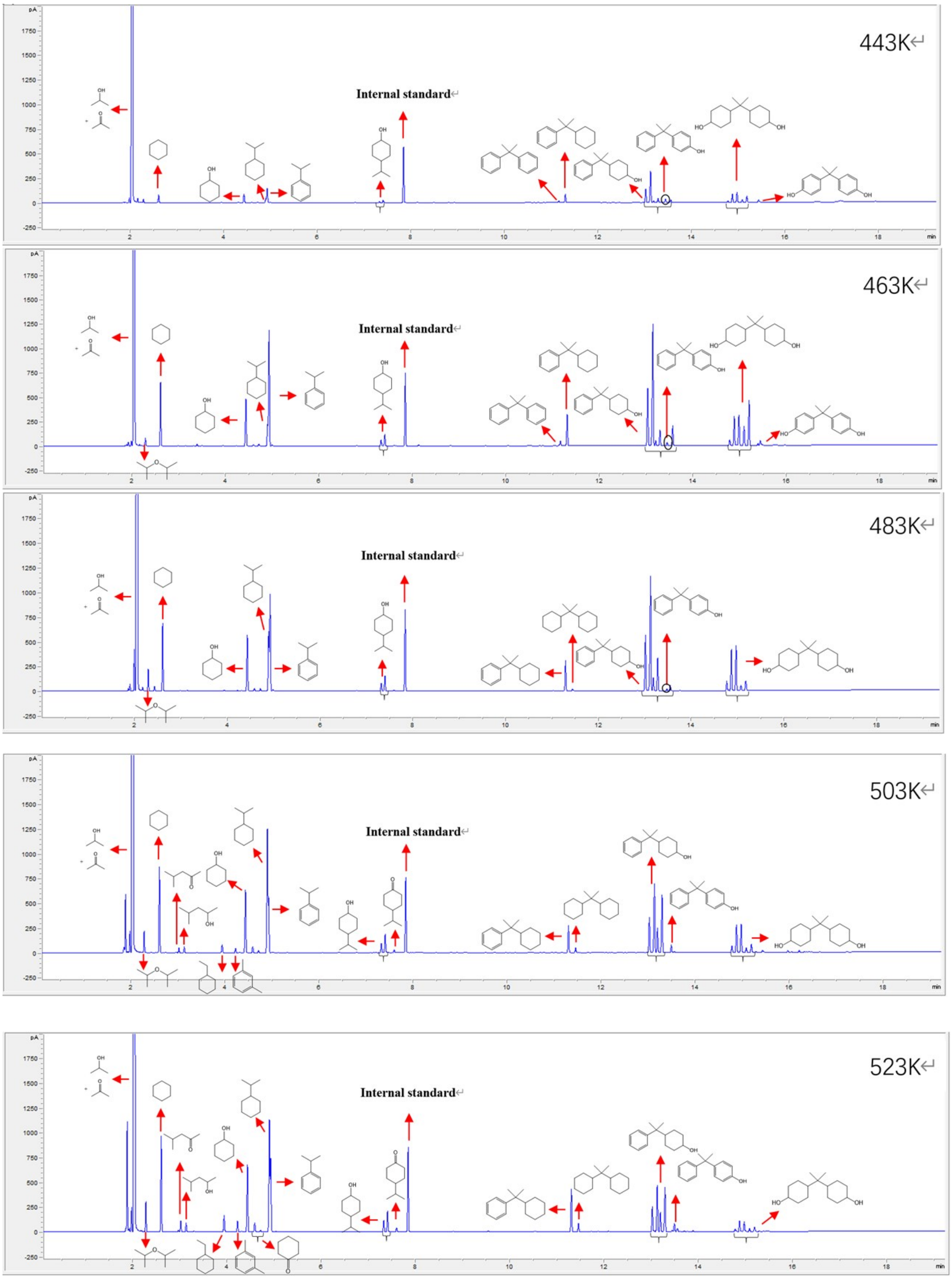

Figure S8. GC chromatograms of the products from the transfer hydrodeoxygenation of pure PC pellets over the Raney Ni catalyst at different reaction temperatures. Reaction conditions: 1 h; 2 g pure PC pellets, 0.4 g Raney Ni and 45 mL isopropanol were used in the tests. The 4-methyl-2-pentanone and methyl isobutyl carbinol might be produced by the self-aldol condensation/hydrogenation of the acetone generated from the dehydrogenation of isopropanol.

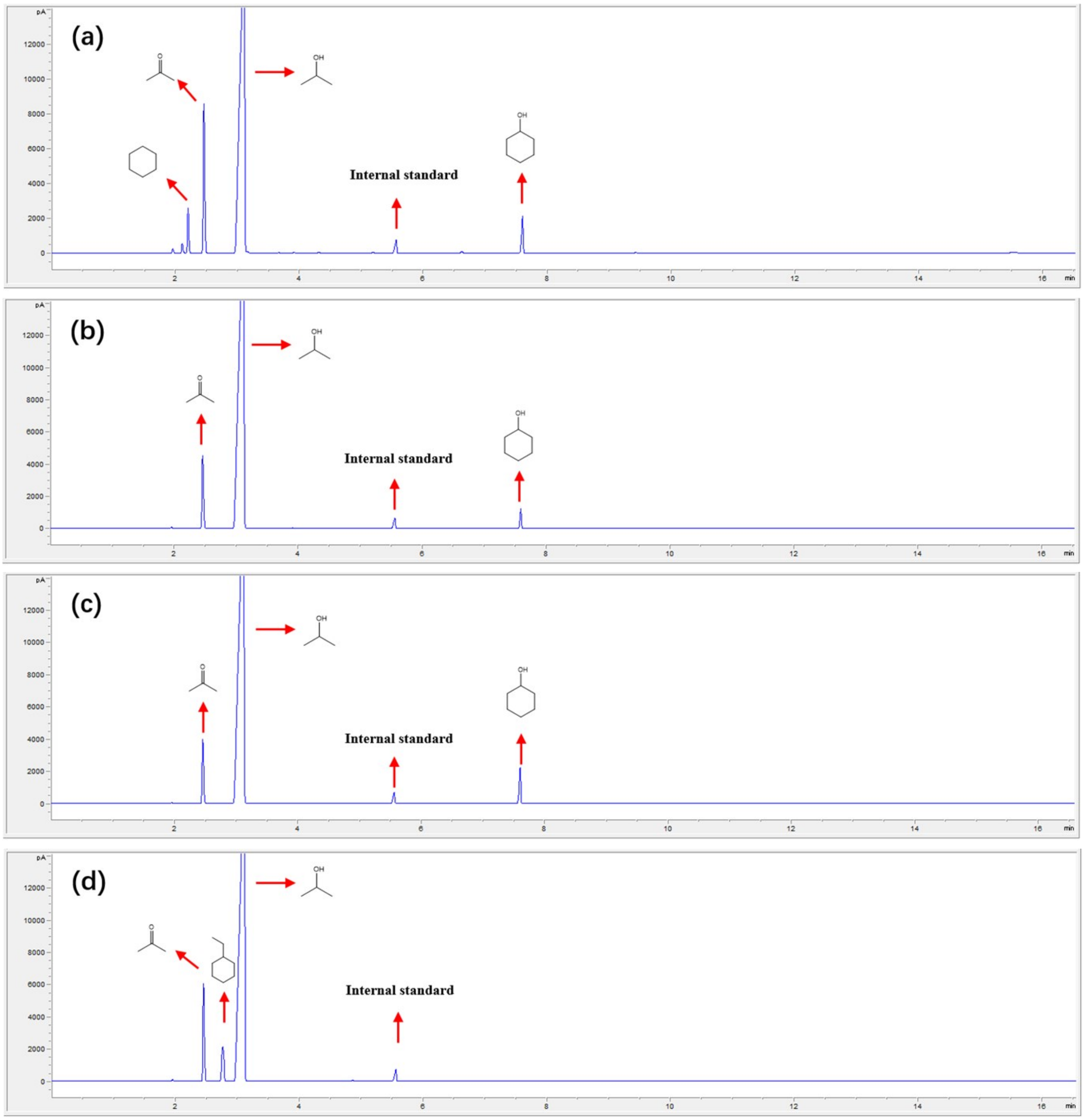

Figure S9. GC chromatograms of the products from transfer hydrodeoxygenation (or transfer hydrogenation) of diphenyl carbonate (a), phenol (b), cyclohexanol (c), ethylbenzene (d). Reaction conditions: 463 K, 1 h; 8 mmol model compound, 0.4 g Raney Ni and 45 mL isopropanol were used in the tests. The products were analyzed by a FFAF column.

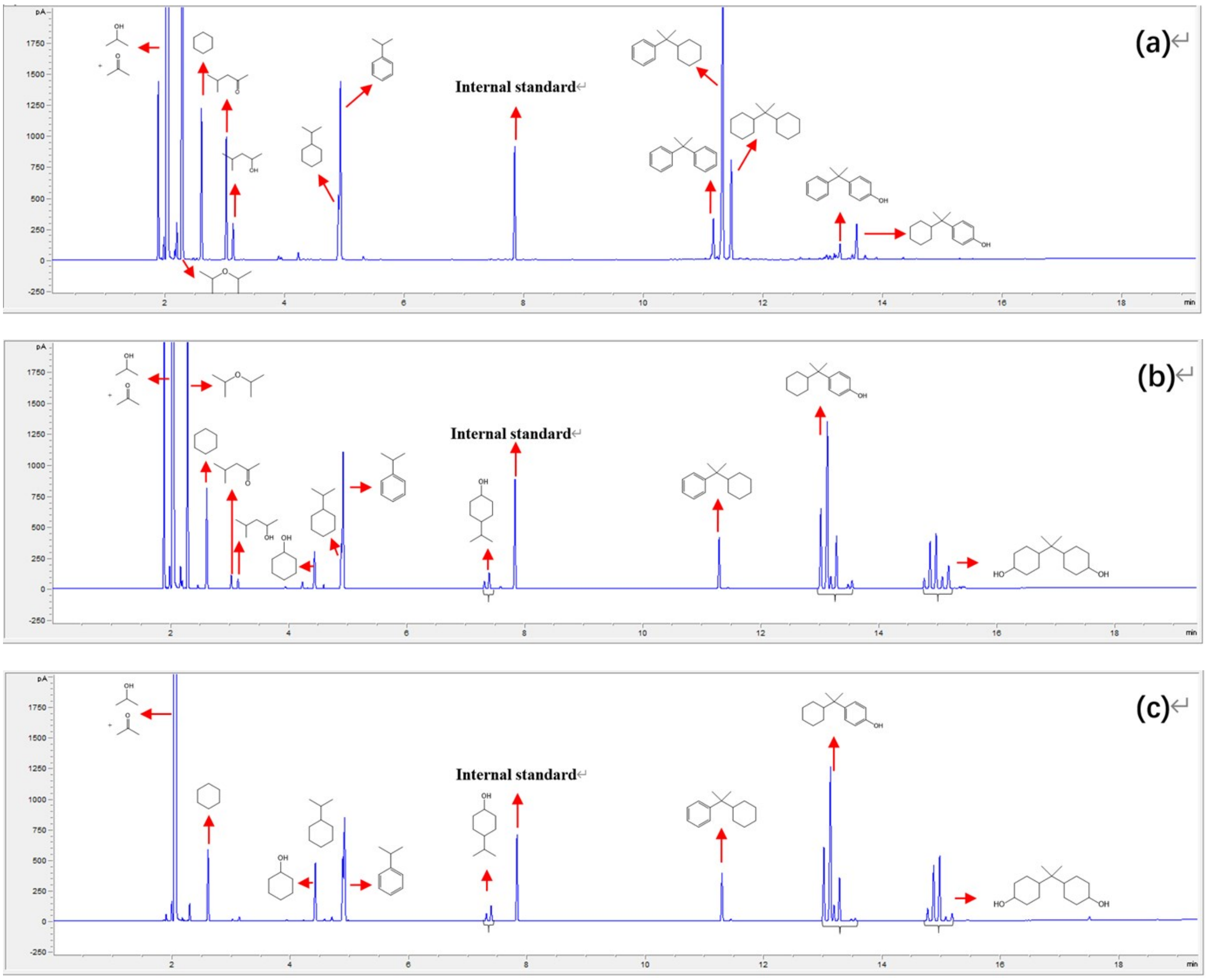

Figure S10. GC chromatograms of the products from the one-pot transfer hydrodeoxygention of pure PC pellets under the co-catalysis of Raney Ni and USY (a), H-ZSM-5 (b) and Al_2O_3 (c) catalysts. Reaction conditions: 463 K, 1 h; 2 g pure PC pellets, 0.4 g Raney Ni and 0.2 g zeolite or Al_2O_3 were used in the tests.

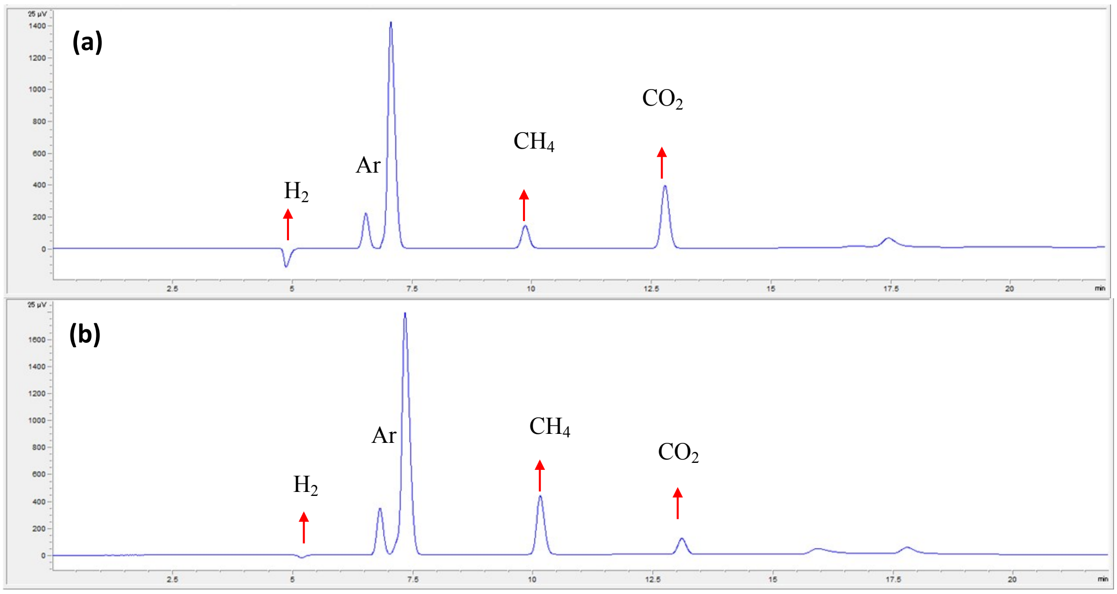

Figure S11. GC chromatograms of the gas phase products from the first step (a) and the second step (b) of the one-pot transfer hydrodeoxygenation of pure PC pellets Reaction conditions: 463 K, 1 h; 2 g pure PC pellets, 0.4 g Raney Ni and 45 mL isopropanol were used in the first test. After cooling down the reaction system to room temperature, 0.2 g USY was introduced into the reaction system, the reaction was conducted at 463 K for another 1 h. Ar was used as the shielding gas.

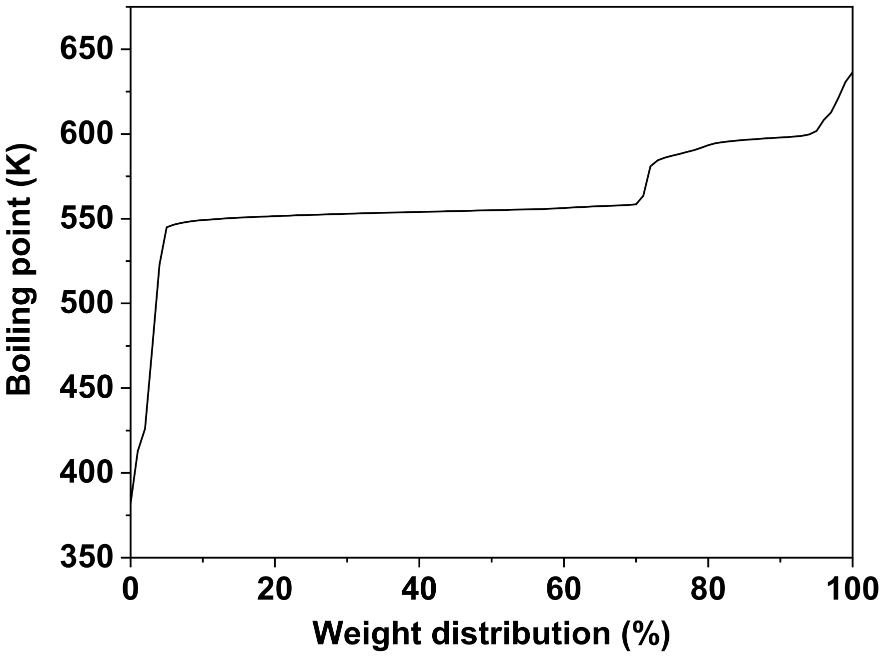

Figure S12. Boiling point distribution of the cyclic hydrocarbon mixture obtained from the transfer hydrodeoxygenation of the chopped DVD disk.

From Figure S12, we can see that the boiling point distribution of the cyclic hydrocarbon mixture obtained from the transfer hydrodeoxygenation of the chopped DVD disk is similar as those of conventional aviation fuels.[4]

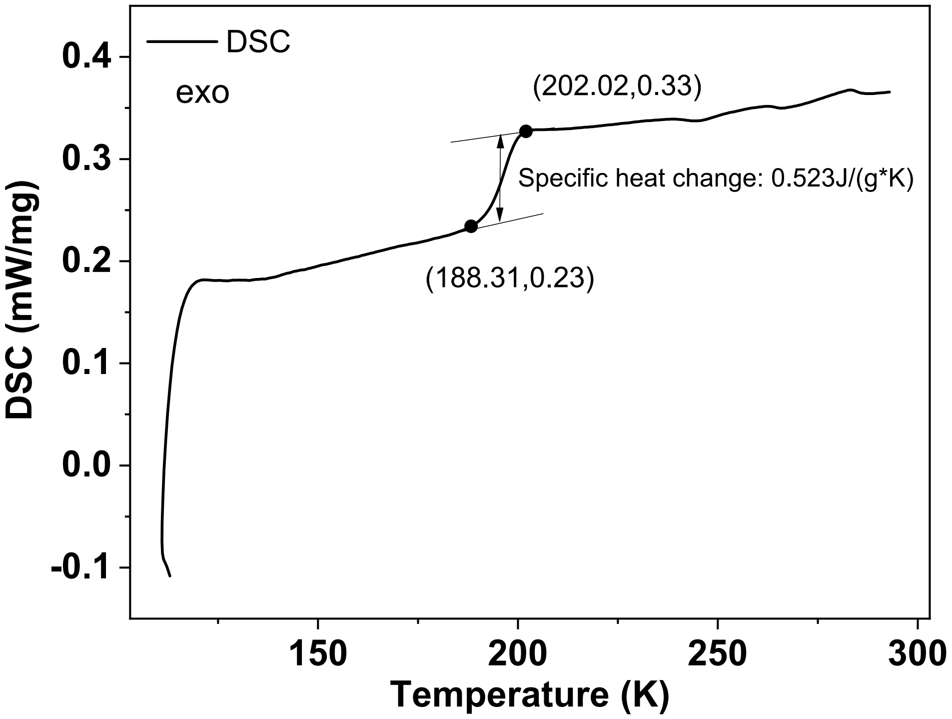

Figure S13. DSC profile of the cyclic hydrocarbon mixture obtained from the transfer hydrodeoxygenation of the chopped DVD disk.

The freezing point of the cyclic hydrocarbon mixture obtained from the one-pot transfer hydrodeoxygenation of chopped DVD disk was measured by a NETZSCH DSC 200F3. Based on Figure S13, the freezing point of the cyclic hydrocarbon mixture was estimated as 202~188 K.

References

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