Direct C–C coupling of acetone at α-position into 2,5-hexanedione induced by photochemical oxidation dehydrogenation

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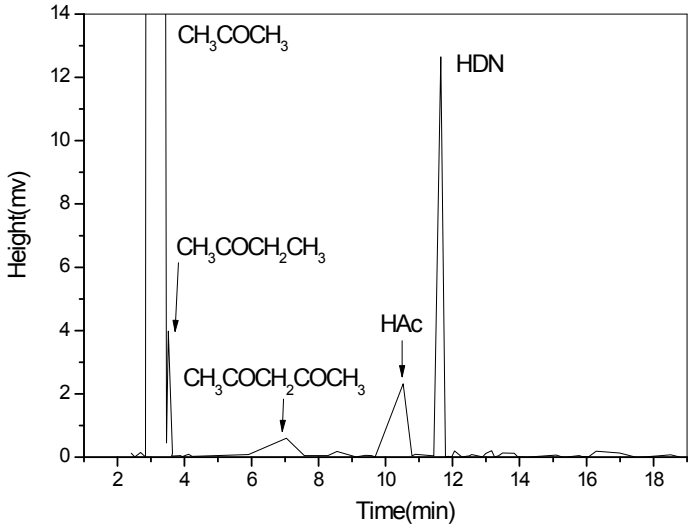

Fig.S1 The GC spectrum for the system(the concentration of H_2O_2 is 0.88 mol/L; the reaction time is 8h; 300W high pressure Hg lamp; the volume is 230mL)

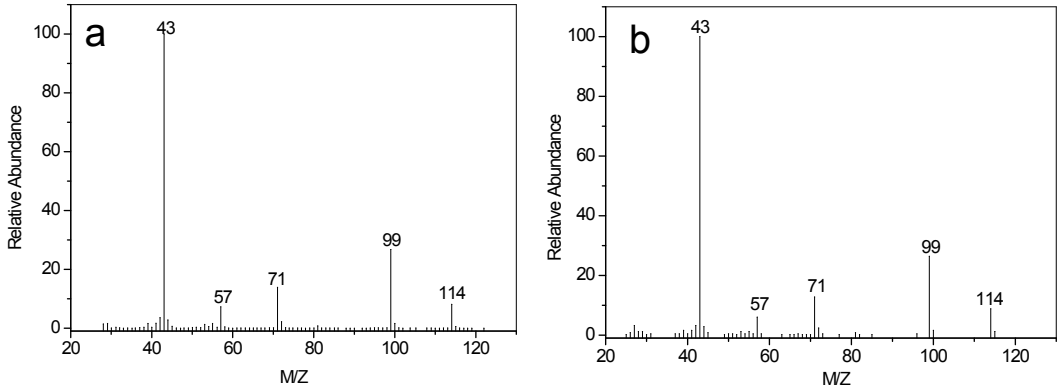

Fig.S2 (a) the mass spectrum of product in the system and (b) the standard mass spectrum of HDN.

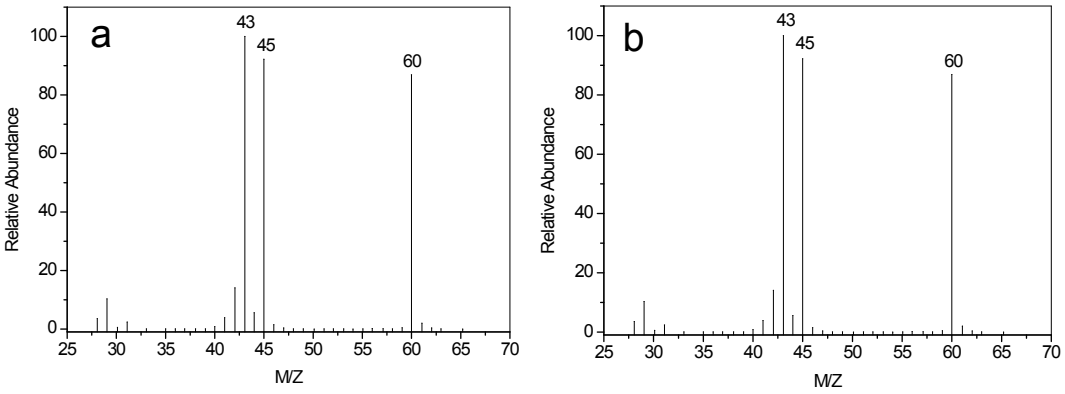

Fig.S3 (a) the mass spectrum of product in the system and (b) the standard mass spectrum of HAc.

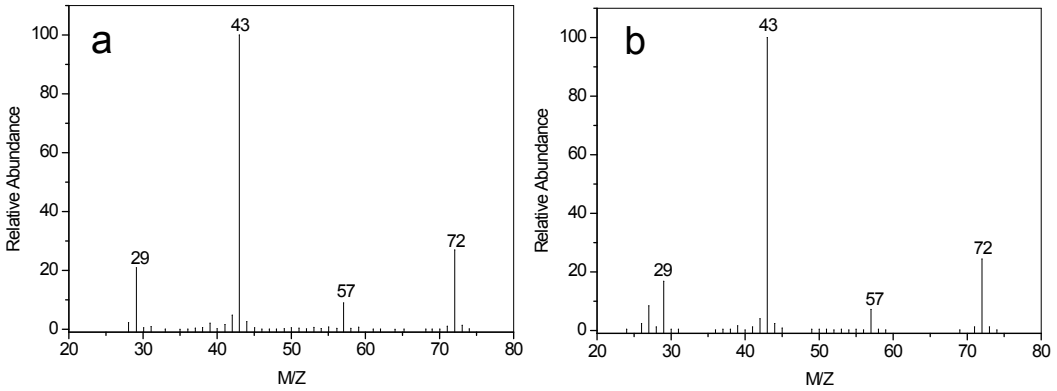

Fig.S4 (a) the mass spectrum of product in the system and (b) the standard mass spectrum $CH_3COCH_2CH_3$

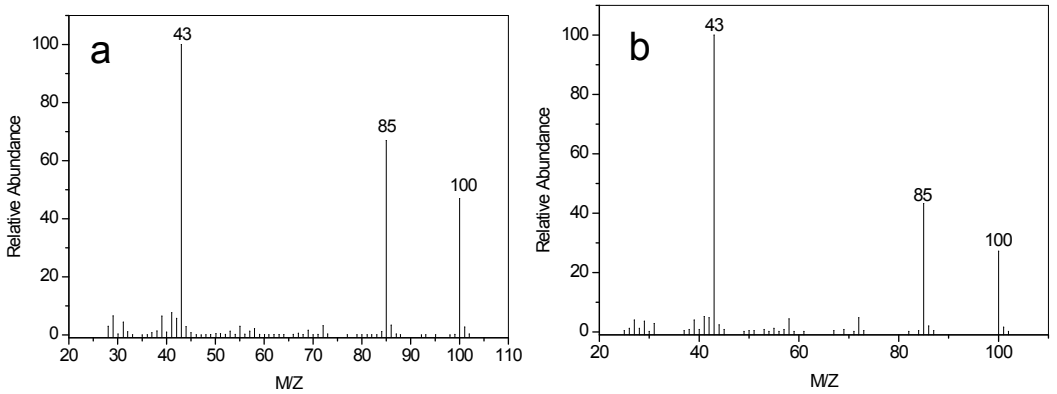

Fig.S5 (a) the mass spectrum of product in the system and (b) the standard mass spectrum of $CH_3COCH_2COCH_3$

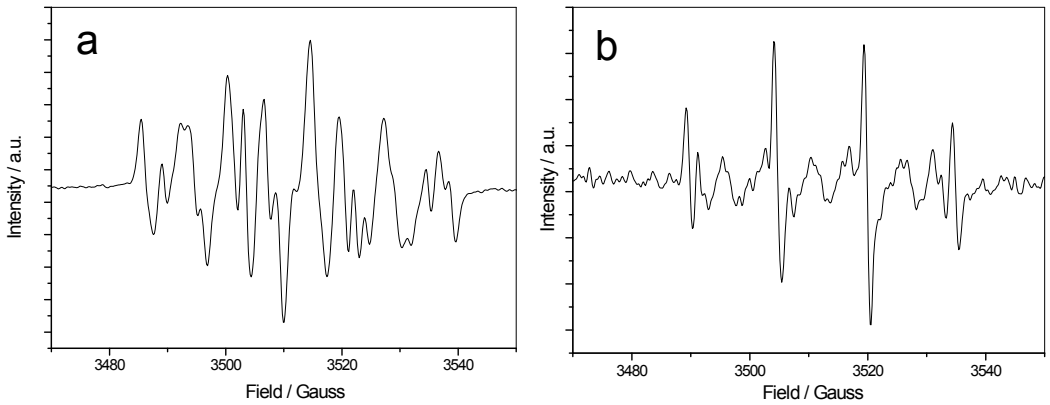

Fig.S6 Experimental EPR spectrums of the CH_3COCH_3-DMPO (a) and H_2O_2-DMPO (b) system after 7 min illumination.

Table S1 Effect of initial concentration of H_2O_2 on the selectivity of products.

c(H_2O_2) (mol/L)	**Selectivity (%)**						
	HDN	CH_3COOH	$CH_3COCH_2CH_3$	$CH_3COCH_2COCH_3$	CH_4	CO	CO_2
3.27	16.6	62.2	2.8	1.9	9.3	4.5	2.7
2.23	34.8	45.1	4.1	3.1	7.6	3.4	1.9
1.65	44.7	36.0	5.0	4.1	6.3	2.6	1.3
1.31	49.1	32.1	5.7	4.7	5.4	2.1	0.9
1.09	51.7	29.9	6.1	5.1	4.8	1.7	0.7
0.87	52.9	28.6	6.6	5.7	4.3	1.4	0.5

Table S2 Effect of the feed rate (instantaneous concentration) of H_2O_2 after 3 h on the selectivity of products.

R(H_2O_2) (mmol/h)	**Selectivity(%)**						
	HDN	CH_3COOH	$CH_3COCH_2CH_3$	$CH_3COCH_2COCH_3$	CH_4	CO	CO_2
16	73.1	7.4	8.3	8.4	1.9	0.8	0.1
24	70.2	10.4	8.3	8.2	2.0	0.8	0.1
32	67.4	13	8.1	8.2	2.1	1	0.2
40	64.9	15.4	8.0	8.1	2.3	1.1	0.2
48	62.5	18	7.8	7.8	2.5	1.2	0.2
64	59	21.8	7.4	7.5	2.7	1.3	0.3

Analysis method of selectivity:

$$HDN\ Selectivity = \frac{6 * n(HDN)}{6 * n(HDN) + 2 * n(CH3COOH) + 4 * n(CH3COCH2CH3) + 5 * n(CH3COCH2COCH3) + n(CO) +}$$