Electronic Supplementary Material (ESI) for New Journal of Chemistry.

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## **Supplementary materials**

## **Figure**

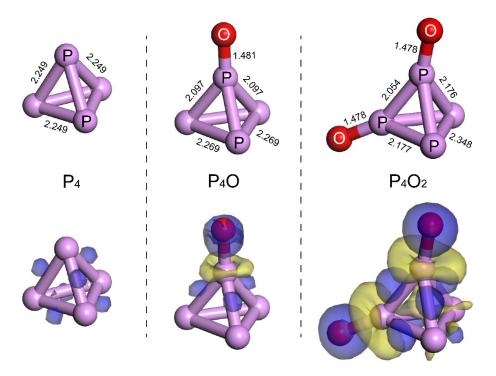
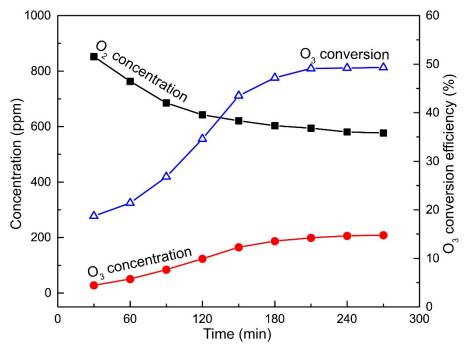


Fig. S1 Bond length and charge density of P<sub>4</sub>, P<sub>4</sub>O and P<sub>4</sub>O<sub>2</sub> (Bond length in Å)



**Fig. S2** Static experiment for  $O_3$  generation over  $P_4$  (Reaction conditions: reaction temperature = 25 °C; gas hourly space velocity = 1000 h<sup>-1</sup>; balanced gas =  $N_2$ , initial  $O_2 = 1000$  ppm)

## **Tables**

**Table S1** Imaginary frequencies of the transition states and bonds corresponding to relative normal vibrations for ozone generation without the involvement of  $\rm H_2O$ 

Transition States	Imaginary frequency	Bonds corresponding to
	(cm <sup>-1</sup> )	relative normal vibrations
TS1	-1429.07	O5-O6
TS2	-1022.86	O6-O7
TS3	-1307.51	O5-P1
TS4	-1148.19	O11-O12
TS5	-989.43	O12-O13

**Table S2** Imaginary frequency of the transition states and bonds corresponding to relative normal vibrations for ozone generation with the involvement of H<sub>2</sub>O

Transition States	Imaginary frequency	Bonds corresponding to
	(cm <sup>-1</sup> )	relative normal vibrations
TS6	-857.35	H8-O7
TS7	-1207.69	H8-O6
TS8	-785.32	O6-O10