

Supporting Information for

Identification of the key oxidative intermediates and the function of
chromium dopants in PKU-8: catalytic dehydrogenation of sec-alcohols with
tert-butylhydroperoxide

Weilu Wang,^a Yang He,^b Junkai He,^c Yanliu Dang,^c Tharindu Kankanmkapuge,^c Wenliang Gao,^{*a}

Rihong Cong,^a Steven L. Suib,^{*c} and Tao Yang^{*a}

^a College of Chemistry and Chemical Engineering, Chongqing University, Chongqing 401331, People's
Republic of China

^b Department of Chemistry and Chemical Engineering, University of Tennessee, Knoxville, TN, 37996,
United States

^c Department of Chemistry, University of Connecticut, Storrs, CT, 06269, United States

*Corresponding authors: gaowl@cqu.edu.cn; steven.suib@uconn.edu; taoyang@cqu.edu.cn.

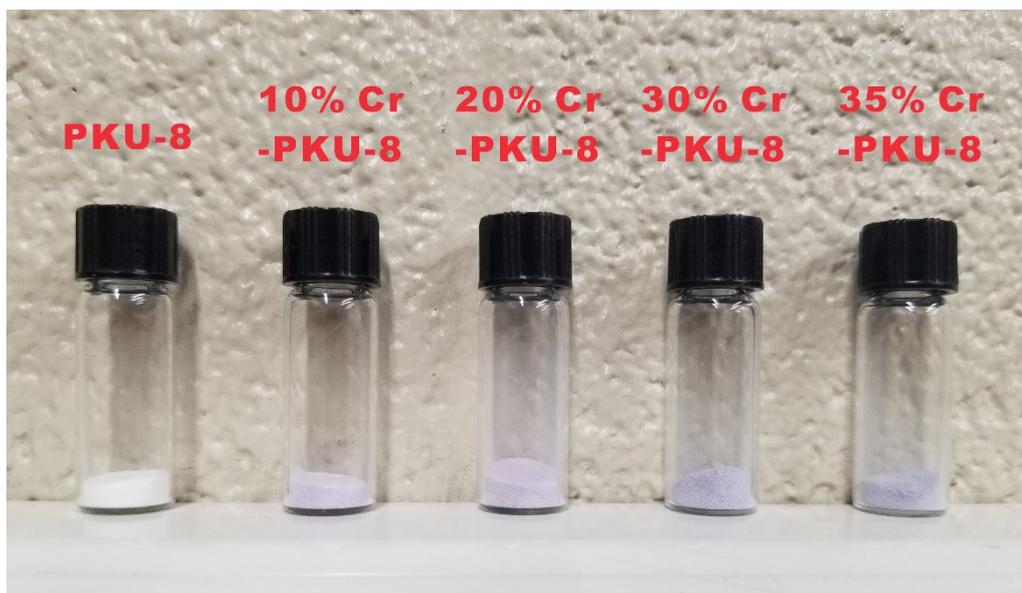


Figure S1. A photograph for as synthesized x Cr-PKU-8 ($x = 0\%$, 10% , 20% , 30% and 35%).

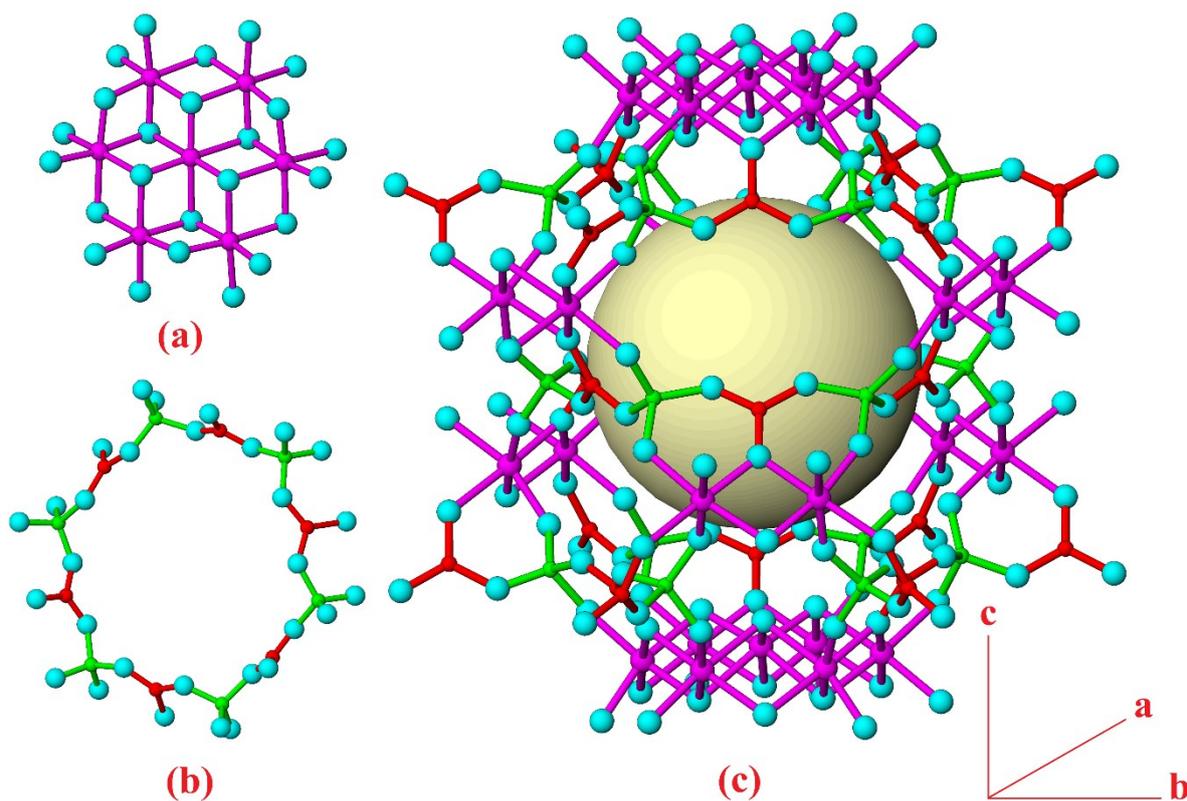


Figure S2. A schematic projection of the structure of PKU-8, (a) octahedral $[Al_7O_{24}]$ clusters; (b) 12-membered borate ring $[B_{12}O_{30}]$; (c) cavity and possible resident species in the structure. Color code: Al, pink; O, cyan; triangular B, red; tetrahedral B, green. The cavity is presented as a large yellow sphere.

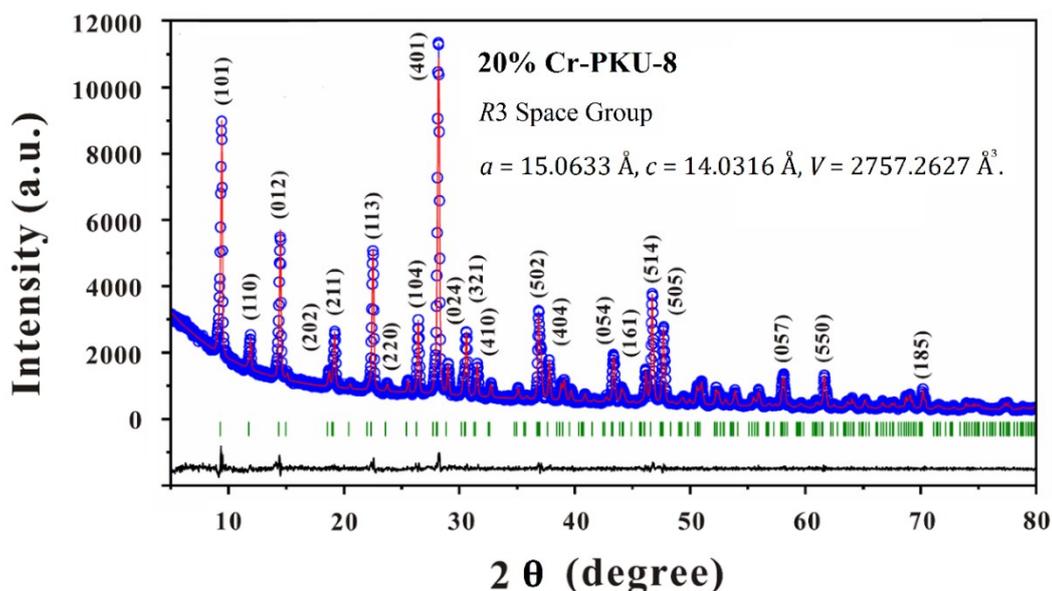


Figure S3. Le Bail fitting to powder XRD pattern for as-synthesized 20% Cr-PKU-8. The blue circles, red and black lines represent the observed, calculated data and the difference between them. The green bars below are the expected reflection positions by the space group $R3$.

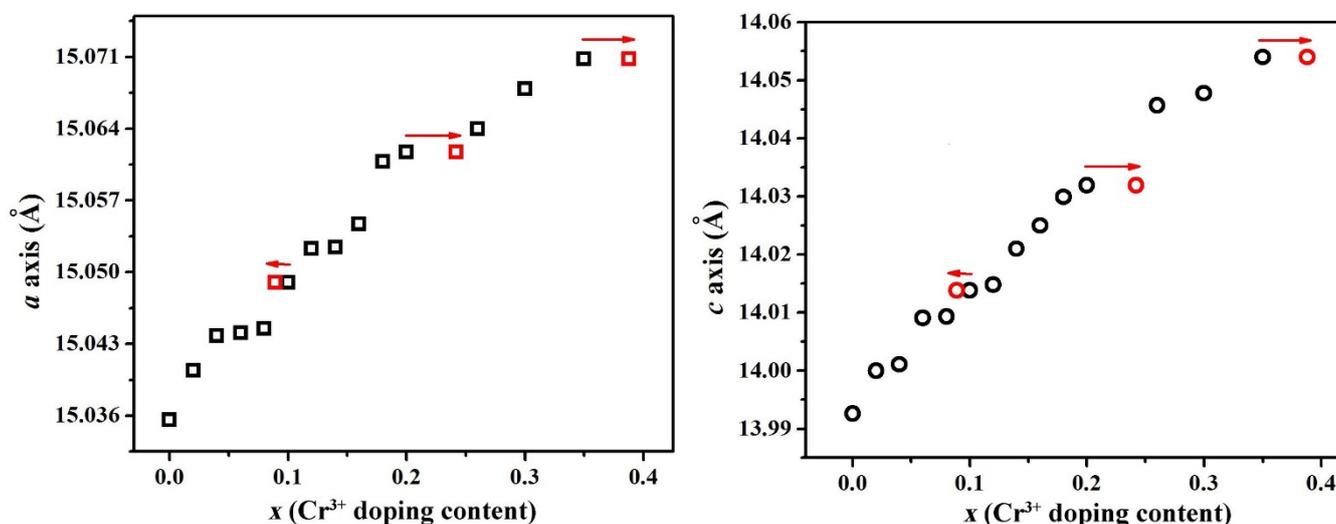


Figure S4. The refined cell lattice patterns (a - and c -axes length) obtained by Le Bail fitting along with the Cr^{3+} doping content. The x values for red ones were obtained from the ICP-AES.

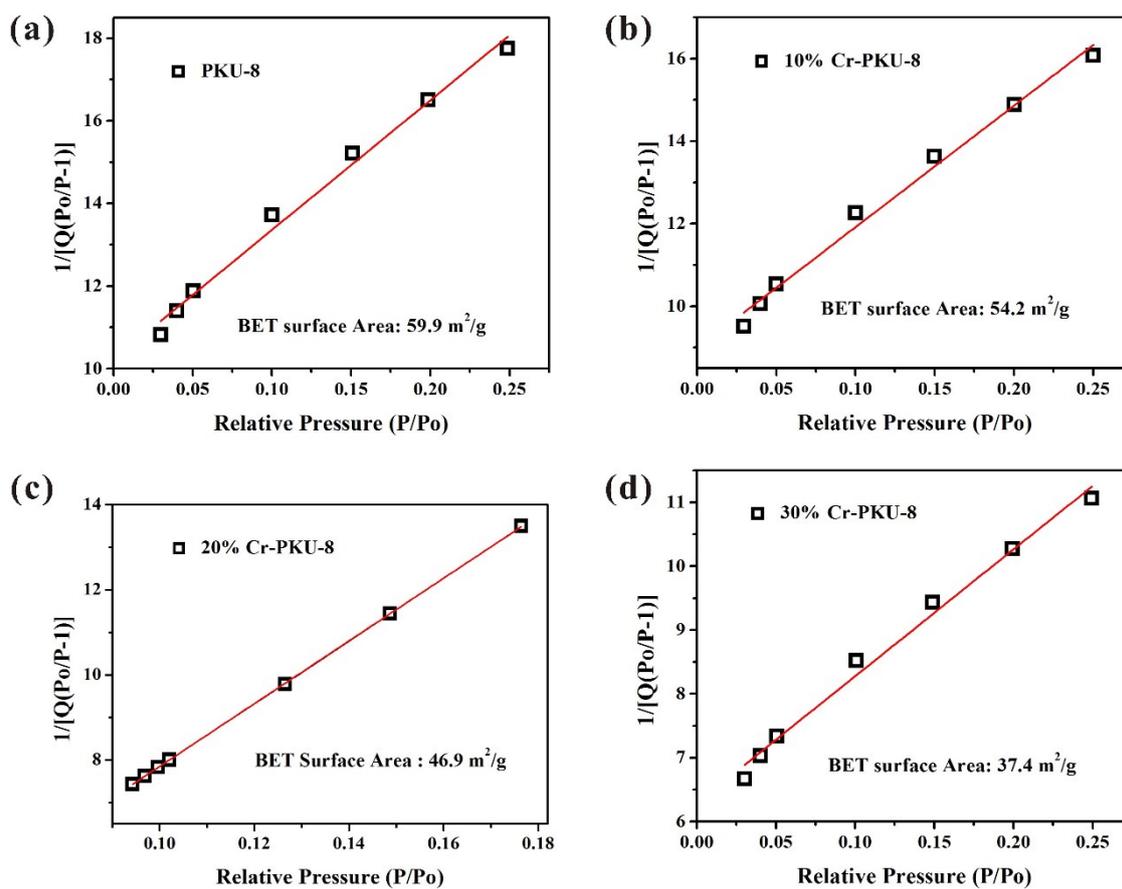


Figure S5. The BET specific surface area determined by N_2 adsorption-desorption method: (a) PKU-8, (b) 10% Cr-PKU-8, (c) 20% Cr-PKU-8 and (d) 30% Cr-PKU-8.

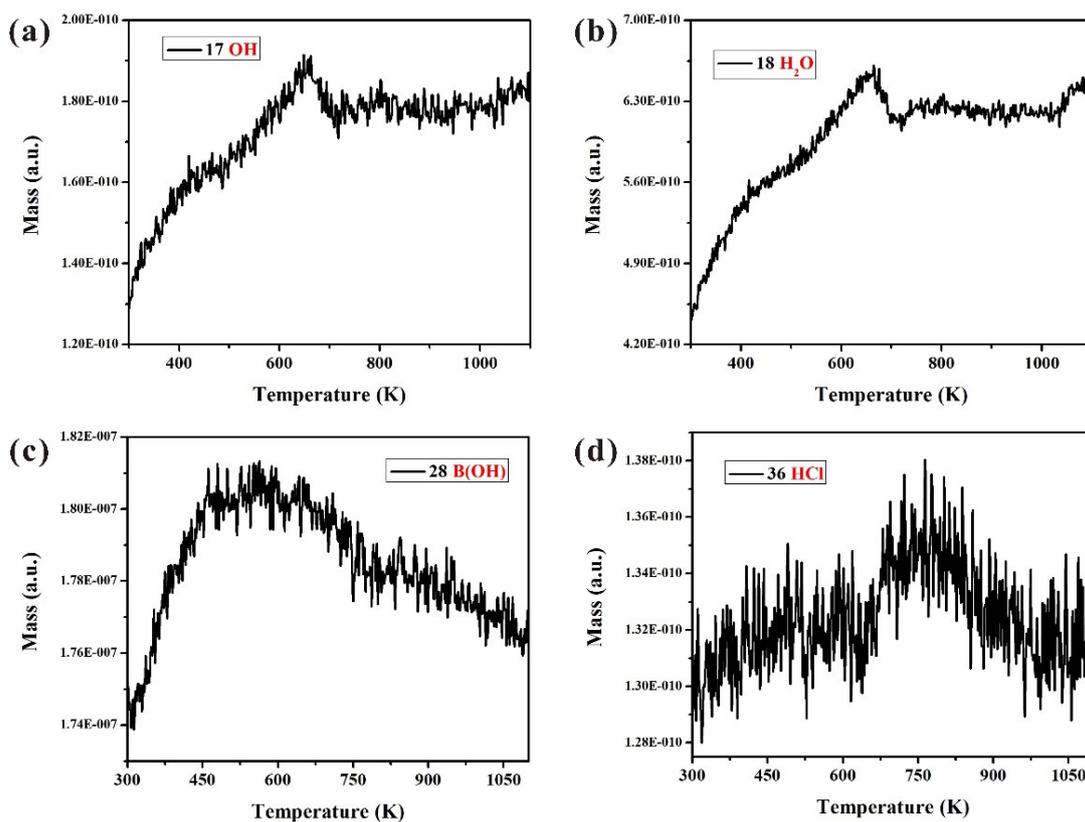


Figure S6. TG-MS analysis for 20% Cr-PKU-8: (a) OH (b) H₂O (c) B(OH), and (d) HCl.

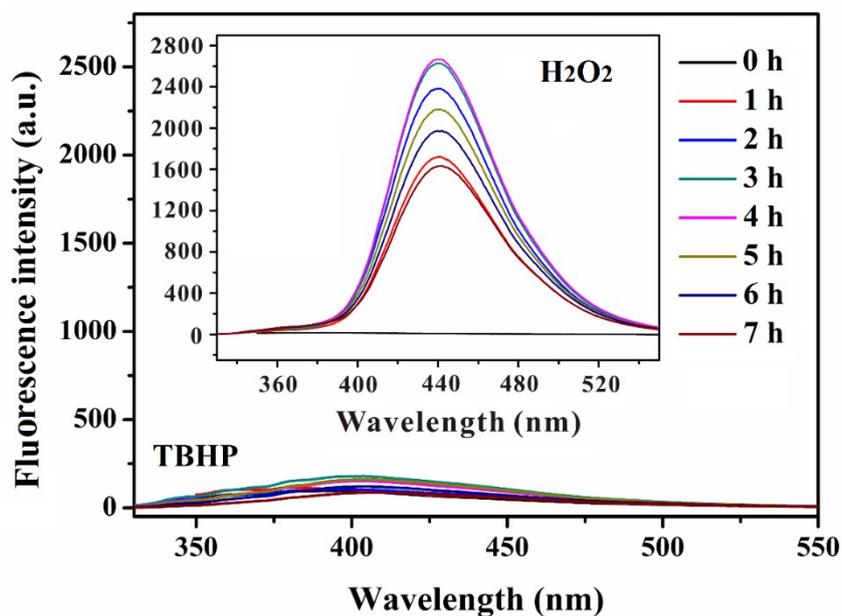


Figure S7. OH* active species evidenced by fluorescent TA method using different oxidants: 70% TBHP and 30% H₂O₂ (inset).

