Electronic Supplementary Material (ESI) for Catalysis Science & Technology

Supporting Information

Dependence of cracking activity upon the Brønsted acidity of Y zeolite: DFT study and experimental confirmation

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Table S1. Description of the eleven faujasite systems employed in this study. See also the corresponding figures below which include the protonated octane.

Num.	System[(a)]	Cation Site	Chemical composition of unit cell
1	$H^+(1Al)$		$H_1Al_1Si_{47}O_{96}$
2	$3H^+(3Al)$		$H_3Al_3Si_{45}O_{96}$
3	$H^+Ba^{2+}(3Al)$	I	$Ba_1H_1Al_3Si_{45}O_{96}$
4		II	
5	$H^+Ca^{2+}(3Al)$	I	$Ca_1H_1Al_3Si_{45}O_{96}$
6		II	
7	$H^+La(OH)^{2+}(3Al)$	I'	$La_1H_2Al_3Si_{45}O_{97}$
8	$H^+La^{3+}(4Al)$	I	$La_1H_1Al_4Si_{44}O_{96}$
9		I'	
10	$H^+Al(OH)^{2+}(3Al)$	I'	$H_2Al_4Si_{45}O_{97}$
11		II'	

(a) This notation indicates the protons, the extraframework cations, and the number of framework Al.

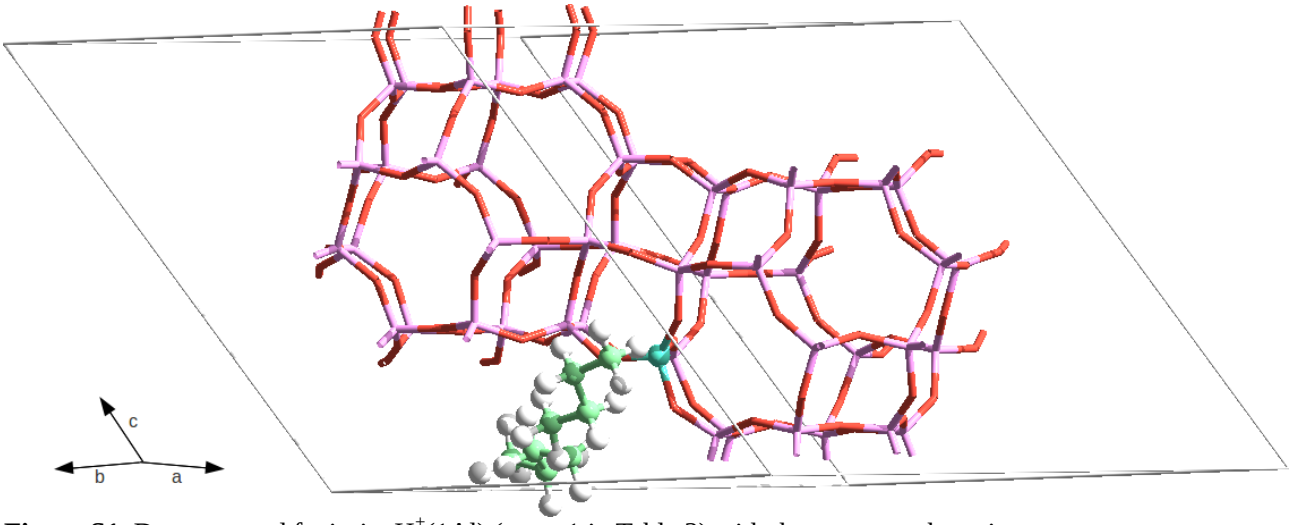

Figure S1. Deprotonated faujasite H^+(1Al) (num. 1 in Table 3) with the octane carbocation.

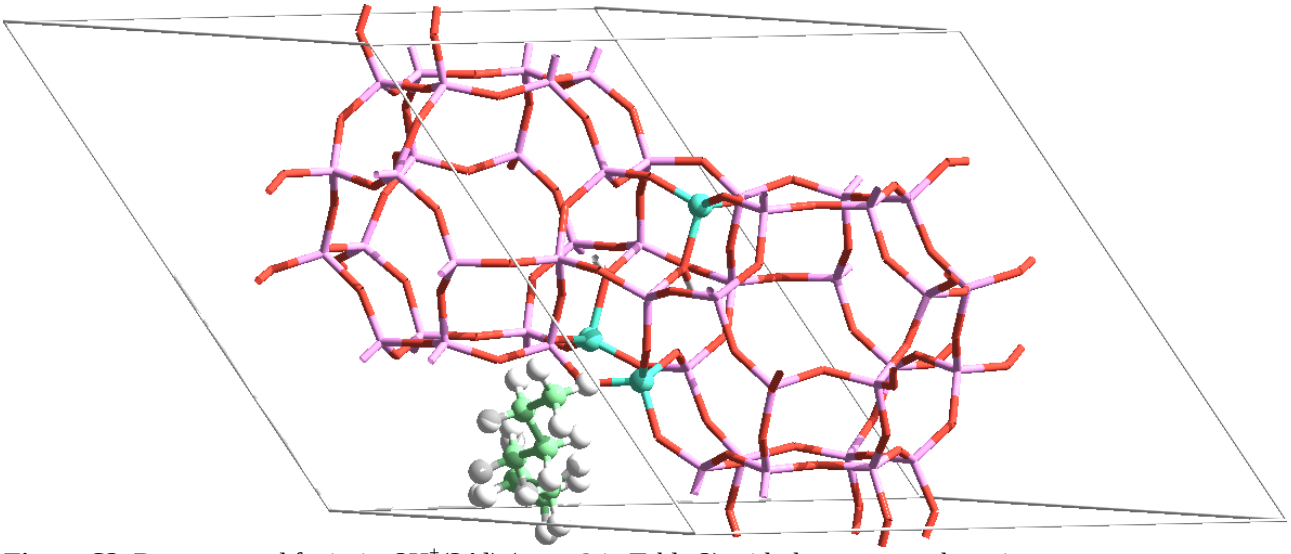

Figure S2. Deprotonated faujasite $3H^+$(3Al) (num. 2 in Table 3) with the octane carbocation.

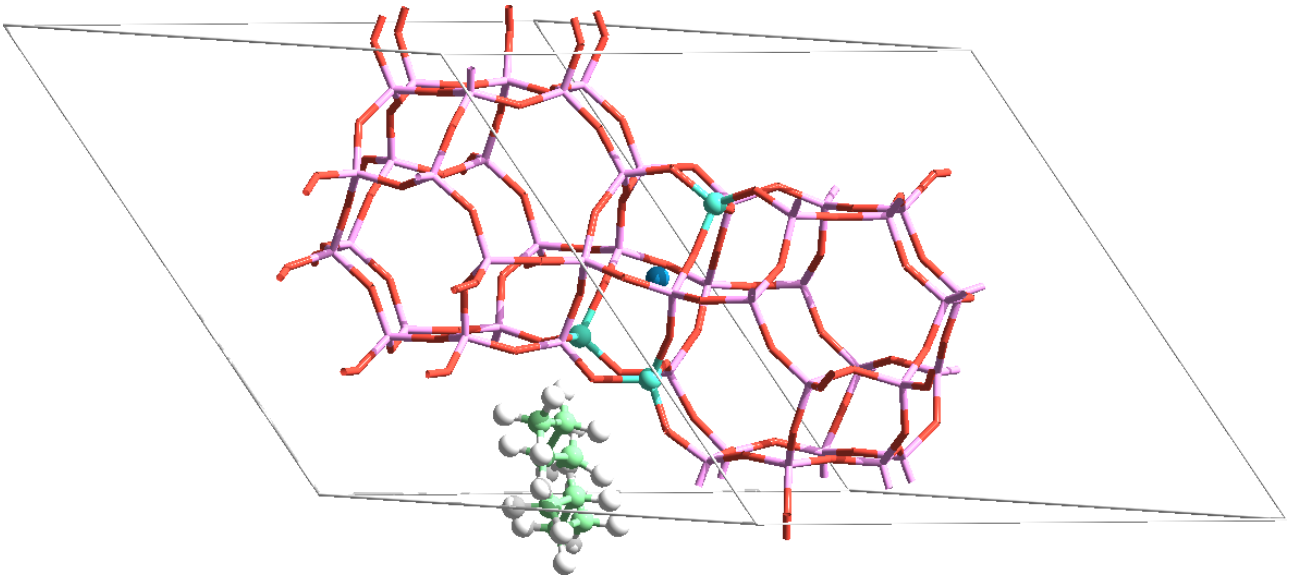

Figure S3. Deprotonated faujasite H^+Ba^{2+}(3Al) (num. 3 in Table 3) with the octane carbocation.

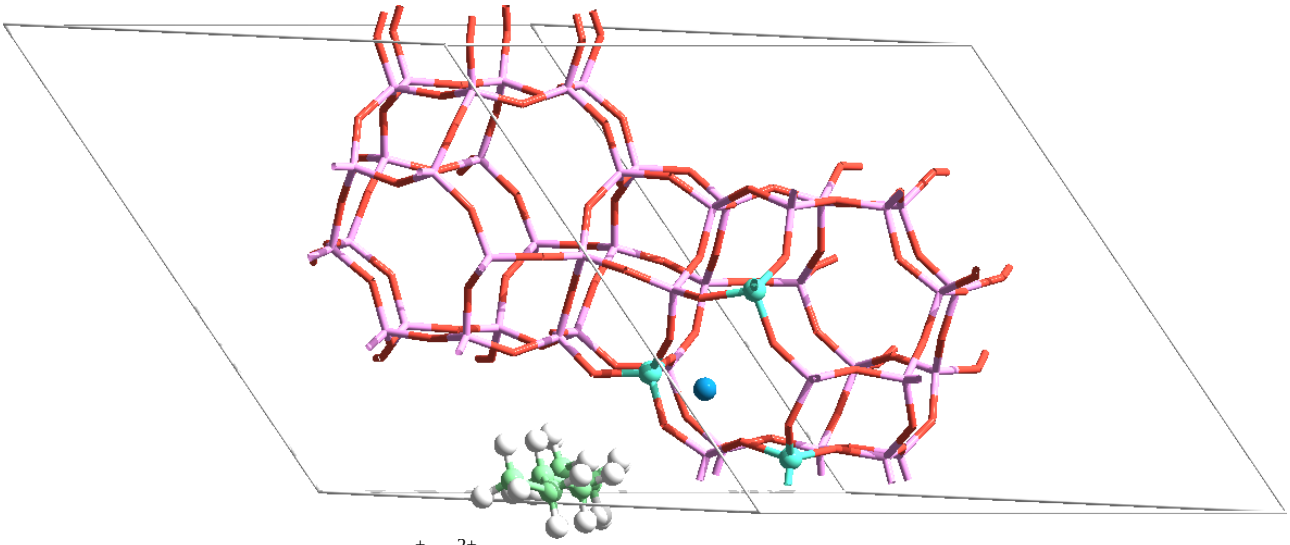

Figure S4. Deprotonated faujasite $H^{+}Ba^{2+}$(3Al) (num. 4 in Table 3) with the octane carbocation.

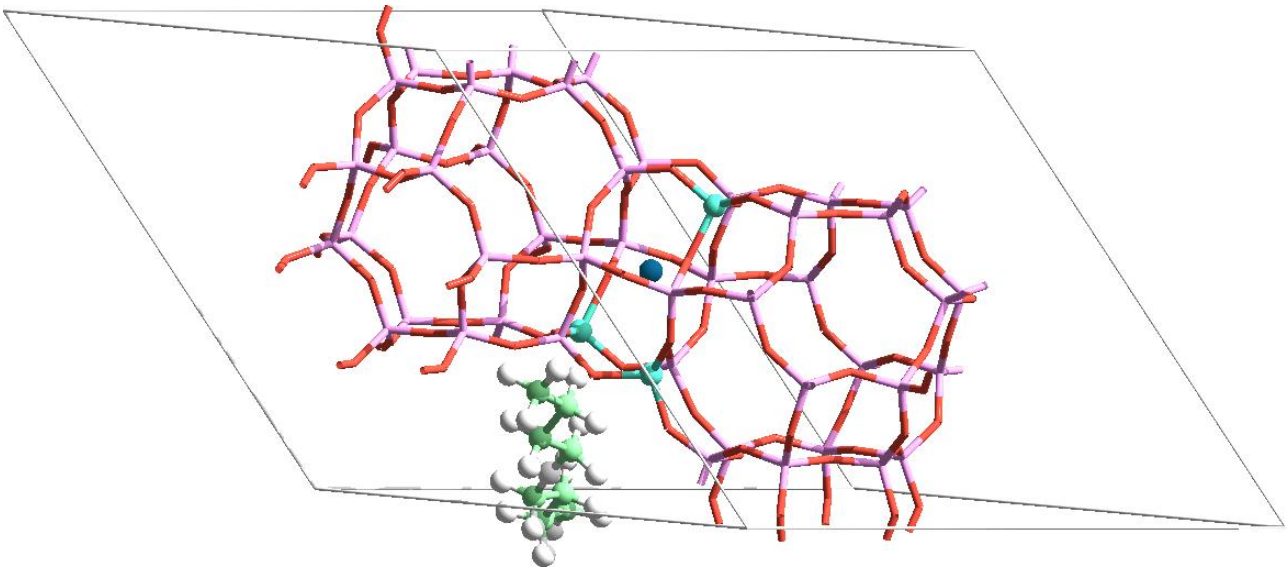

Figure S5. Deprotonated faujasite $H^{+}Ca^{2+}$(3Al) (num. 5 in Table 3) with the octane carbocation.

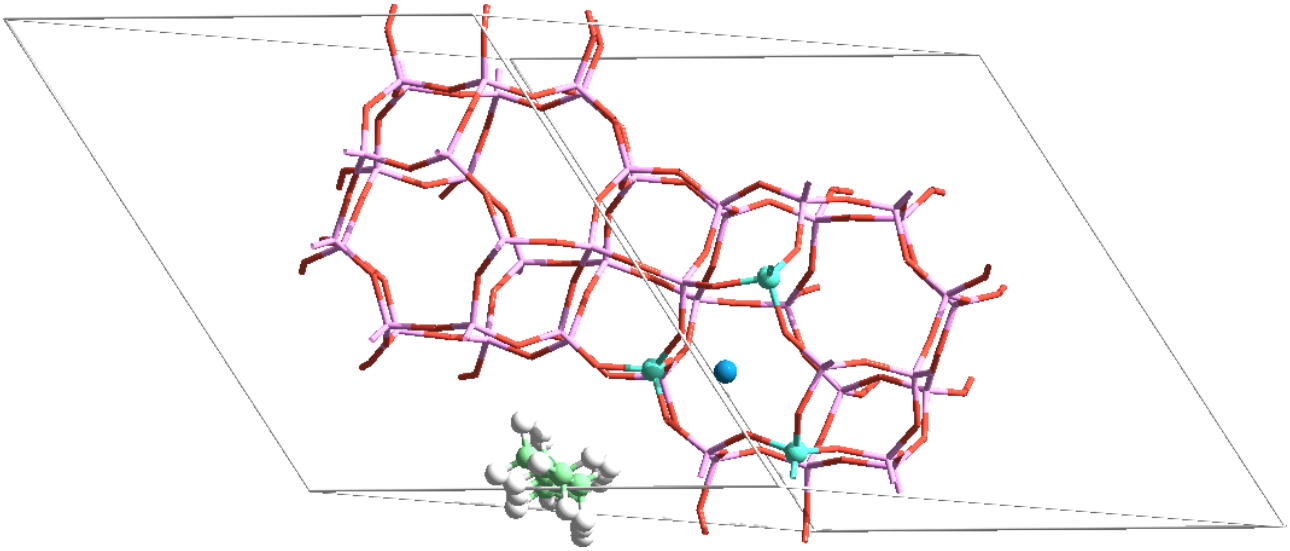

Figure S6. Deprotonated faujasite $H^{+}Ca^{2+}$(3Al) (num. 6 in Table 3) with the octane carbocation.

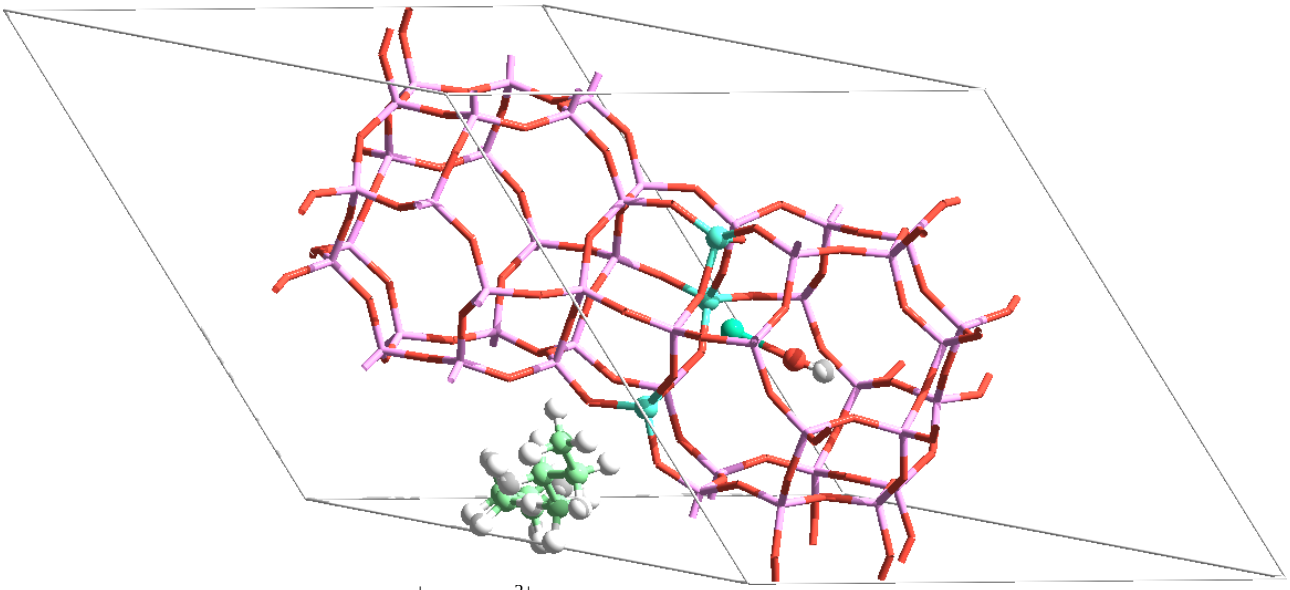

Figure S7. Deprotonated faujasite $H^{+}La(OH)^{2+}$(3Al) (num. 7 in Table 3) with octane carbocation.

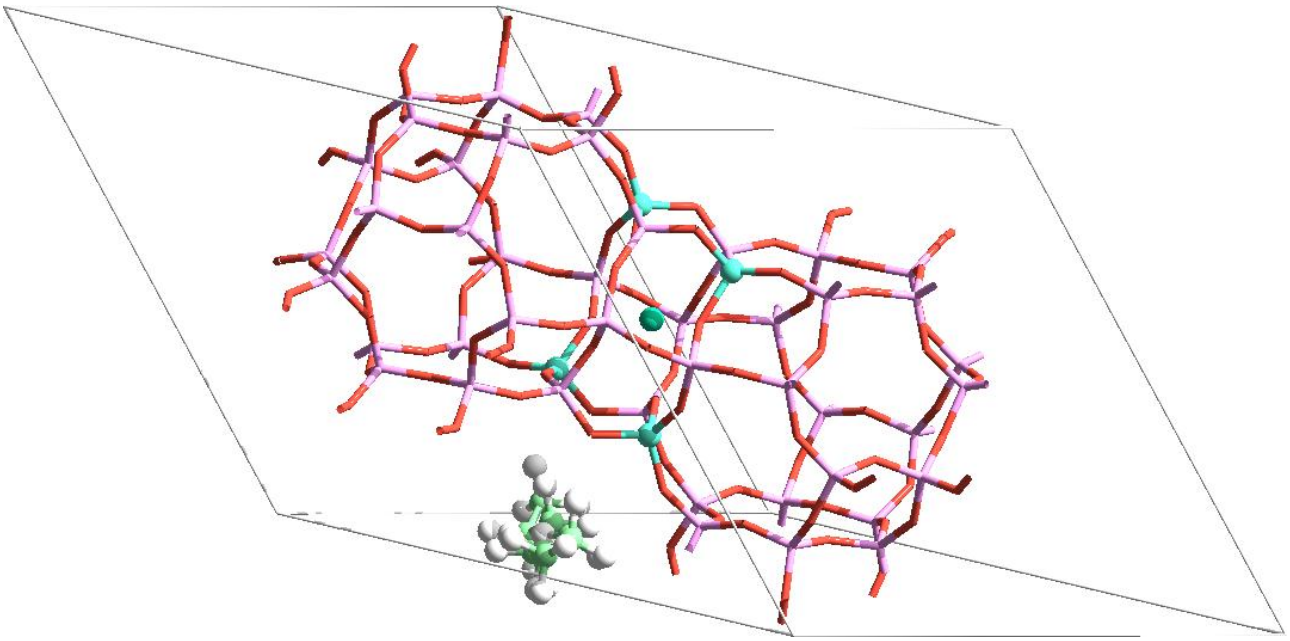

Figure S8. Deprotonated faujasite $H^{+}La^{3+}$(4Al) (num. 8 in Table 3) with the octane carbocation.

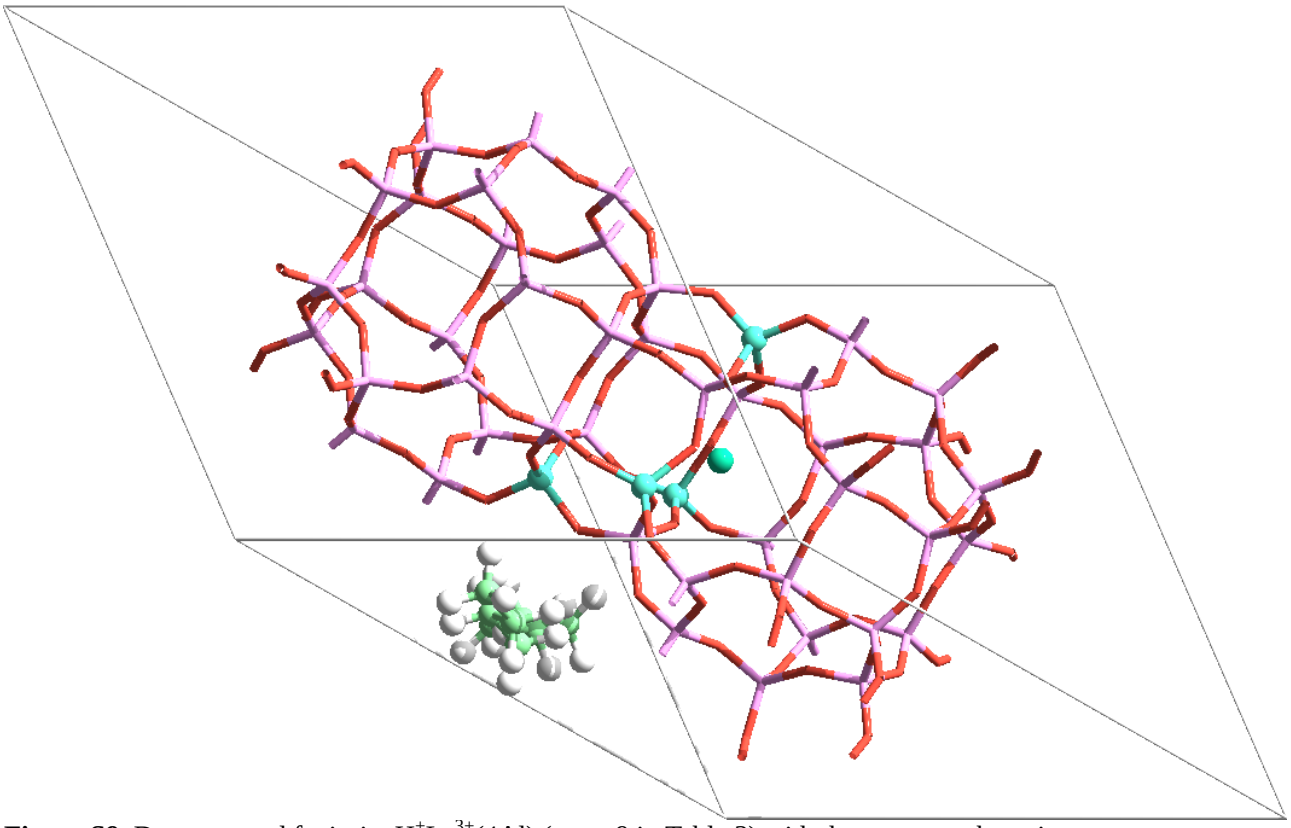

Figure S9. Deprotonated faujasite $H^{+}La^{3+}$(4Al) (num. 9 in Table 3) with the octane carbocation.

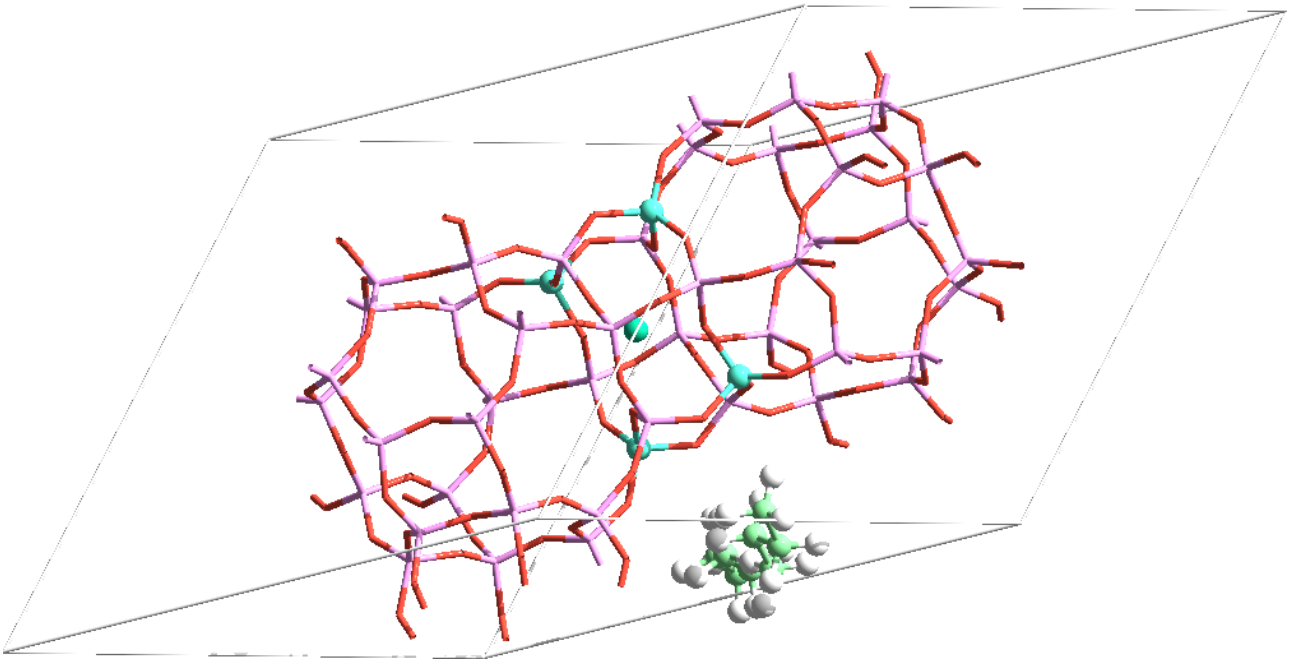

Figure S10. Deprotonated faujasite $H^{+}La^{3+}$(4Al) (num. 10 in Table 3) with the octane carbocation.

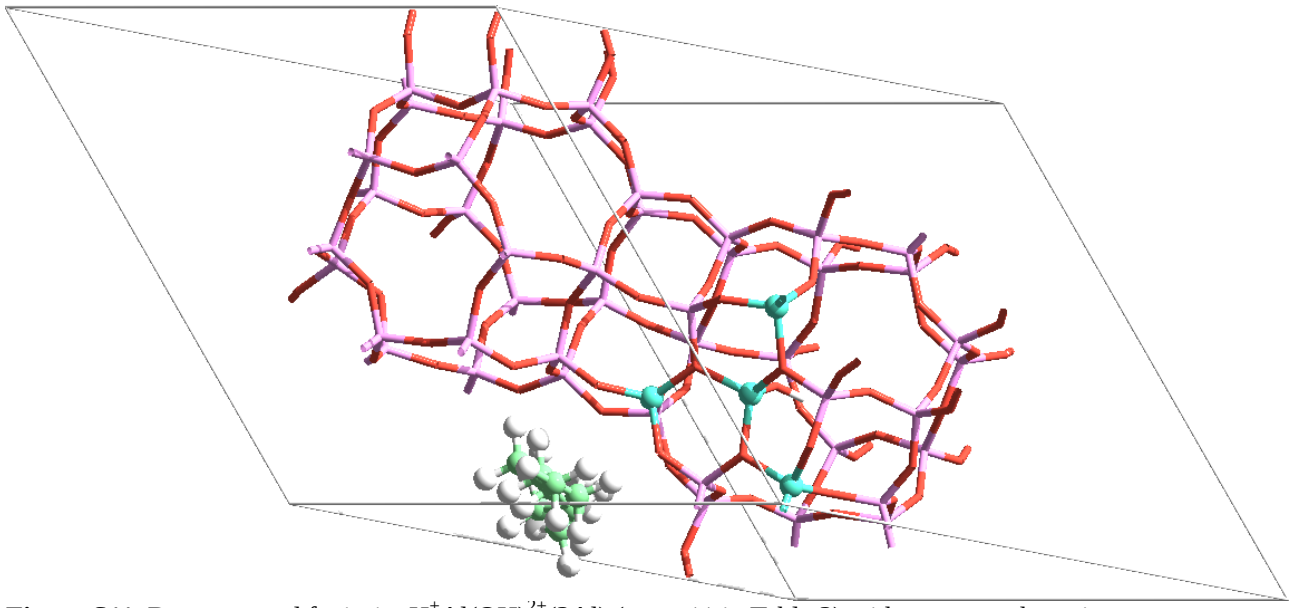

Figure S11. Deprotonated faujasite $H^{+}Al(OH)^{2+}$(3Al) (num. 11 in Table 3) with octane carbocation.