



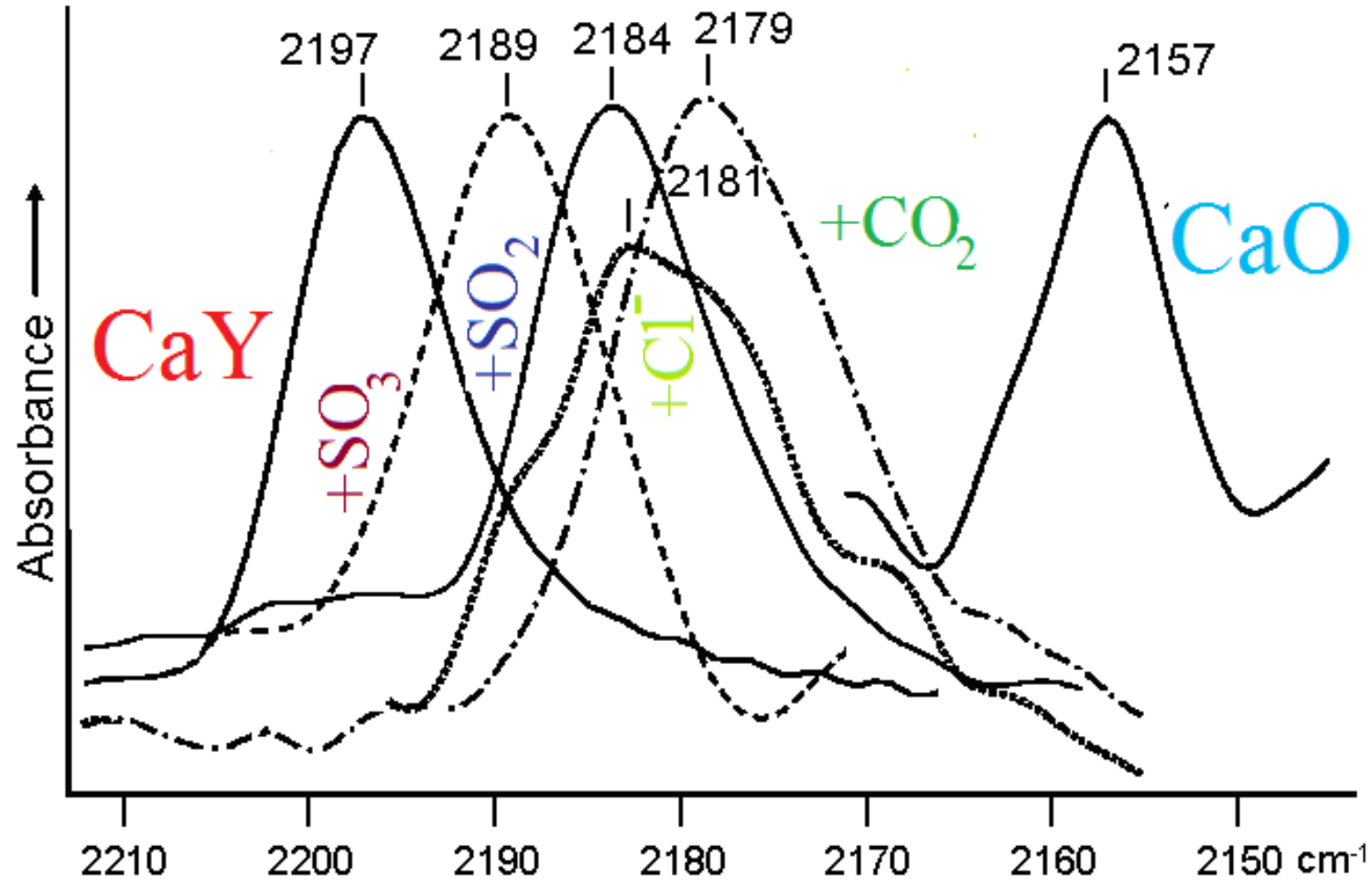
Saint Petersburg
University

Effects of the environment upon the properties of Ca cation. A DFT study

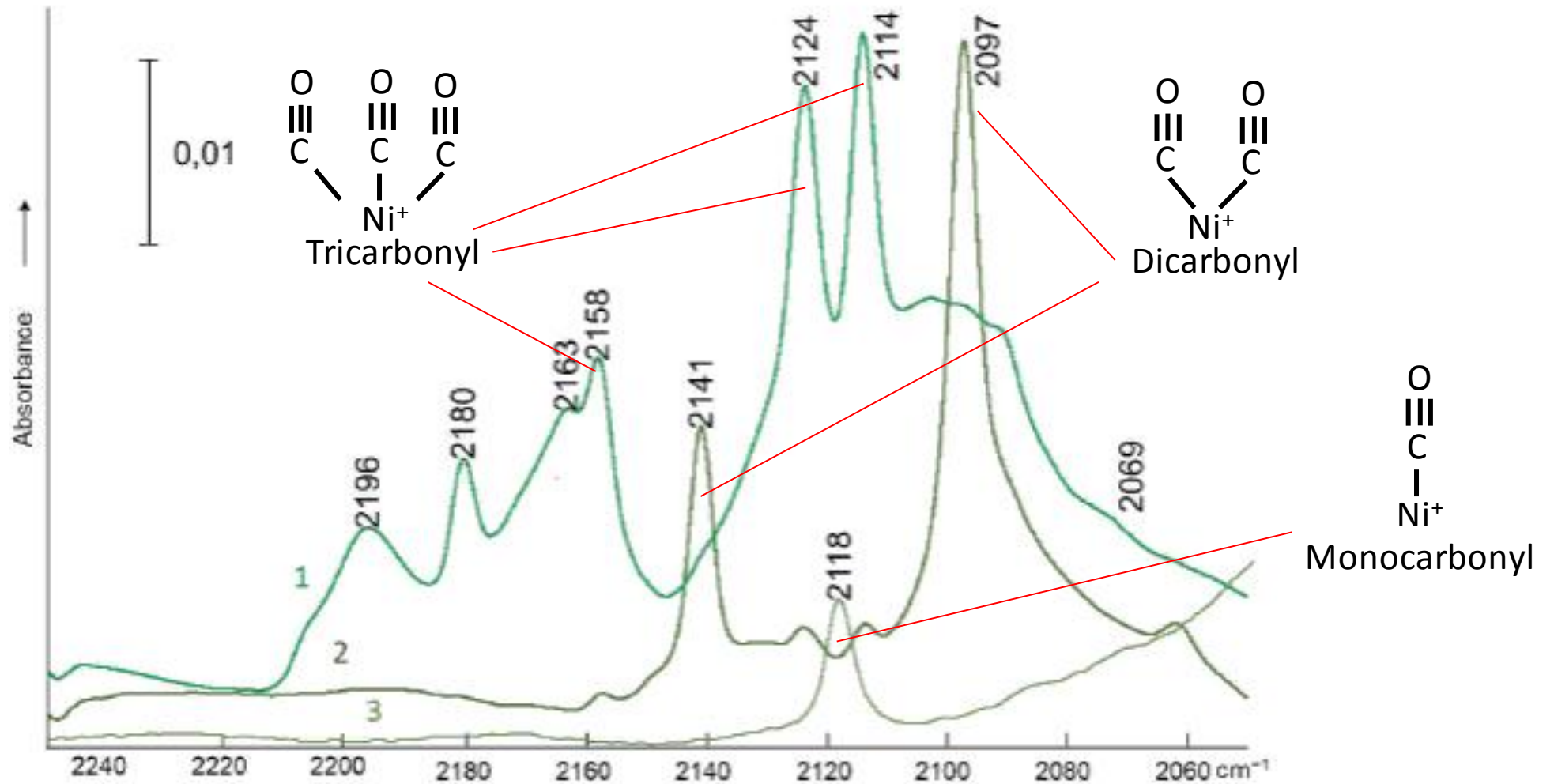
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Induced Lewis acidity



CO adsorbed on Ni-USY zeolite

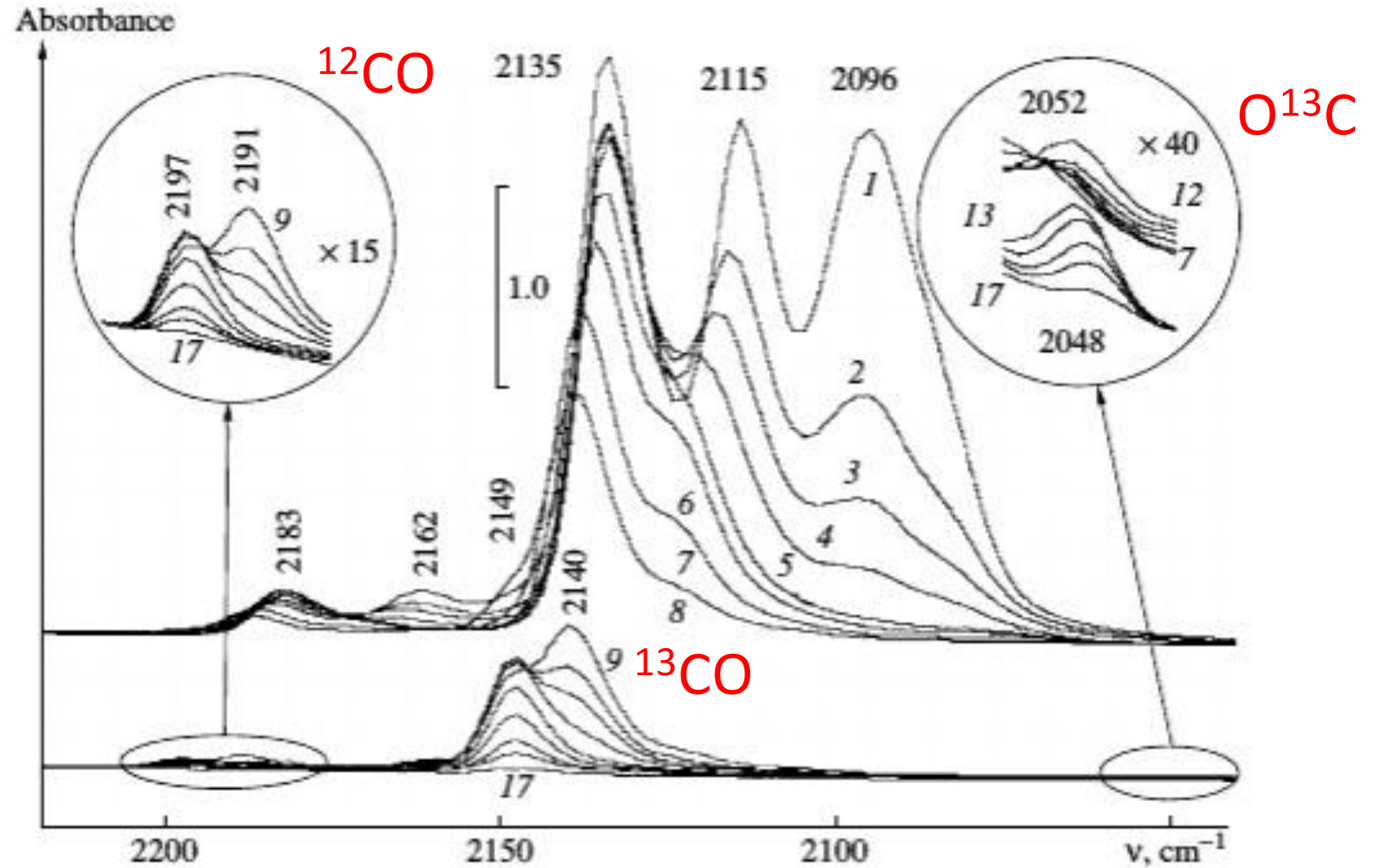


[2] R. Belykh, F. Mauge, A. Tsyganenko. Applied Catalysis A. 583 (2019) 117140.

CO adsorbed on CaY zeolite

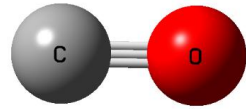
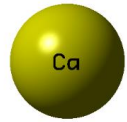
	^{12}CO
exp. cm^{-1}	2197
calc. cm^{-1}	2198,5

	$^{12}\text{CO}^{12}\text{CO}$
exp. cm^{-1}	2197; 2191
calc. cm^{-1}	2197,5; 2188,9

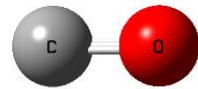
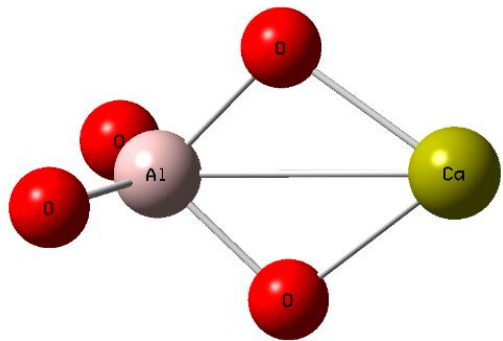


[3] A. Tsyganenko, P. Storozhev, C. Otero Areán. Kinet. Catalysis, 45 (2004) 530.

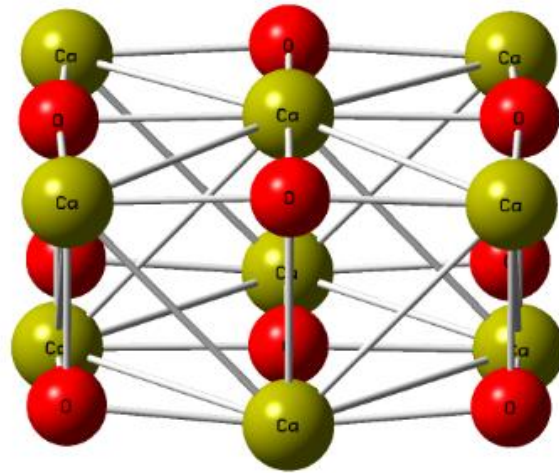
Models



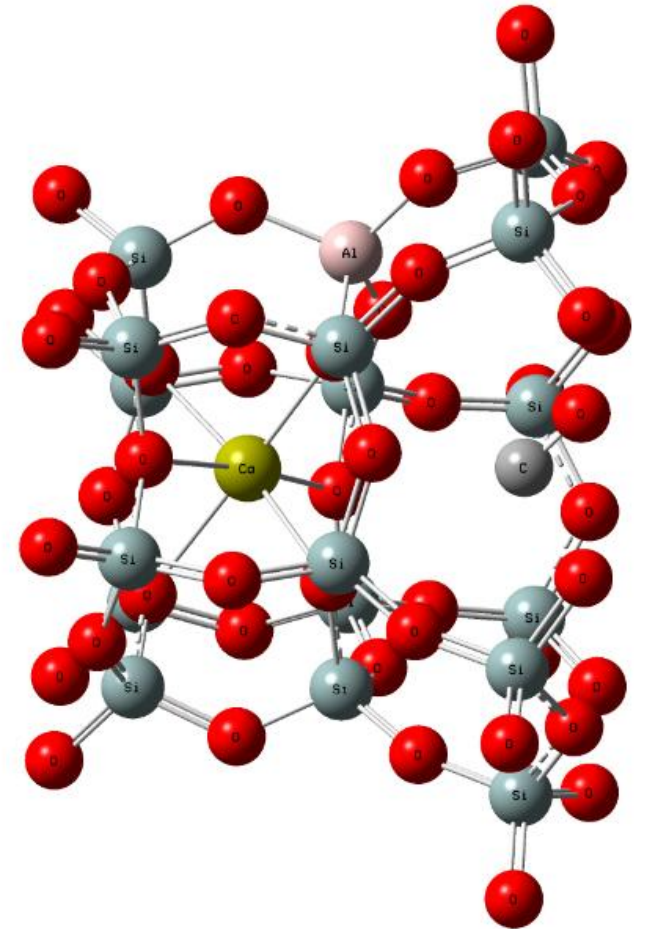
Free Calcium cation



Simple zeolite model

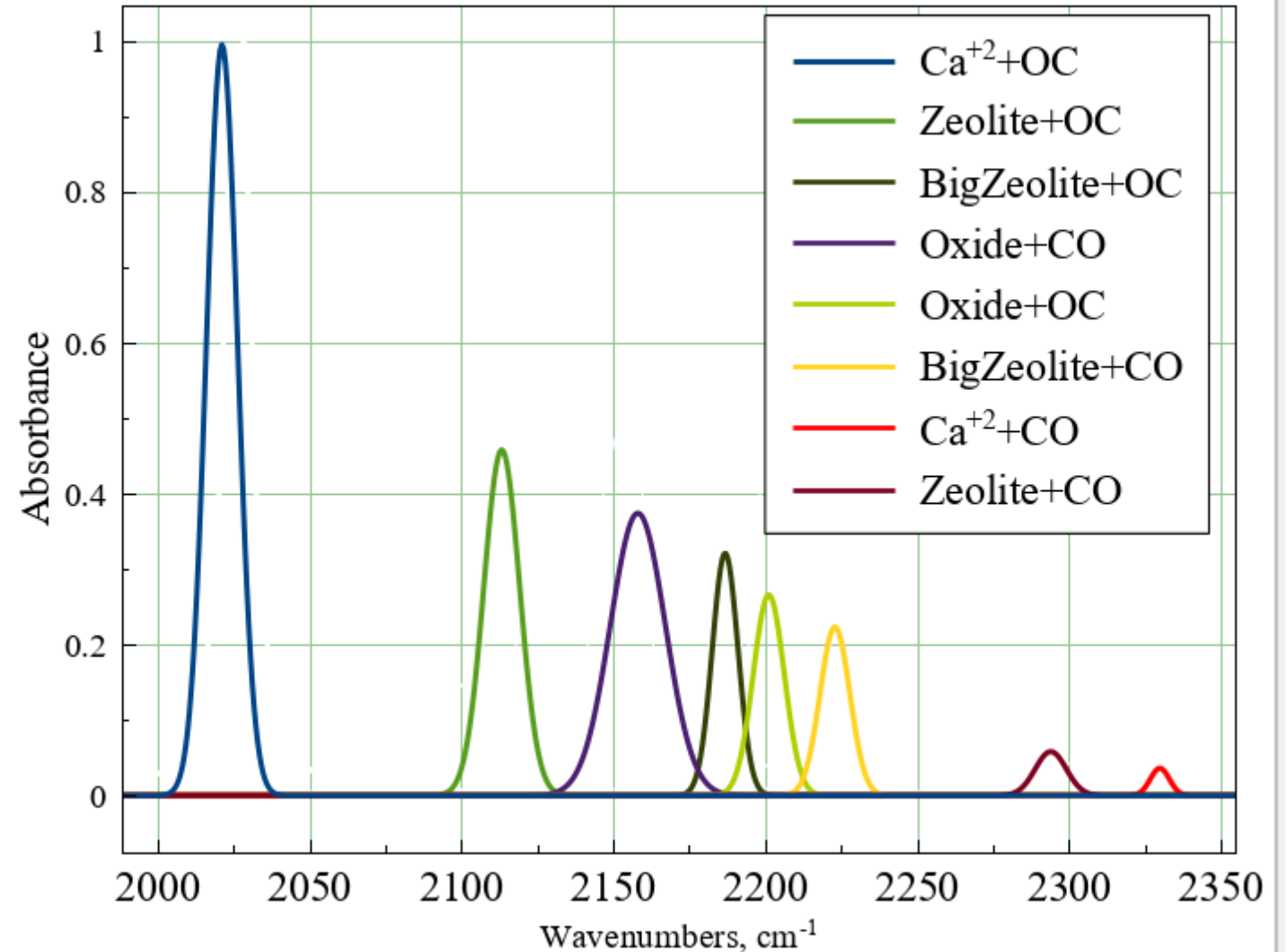
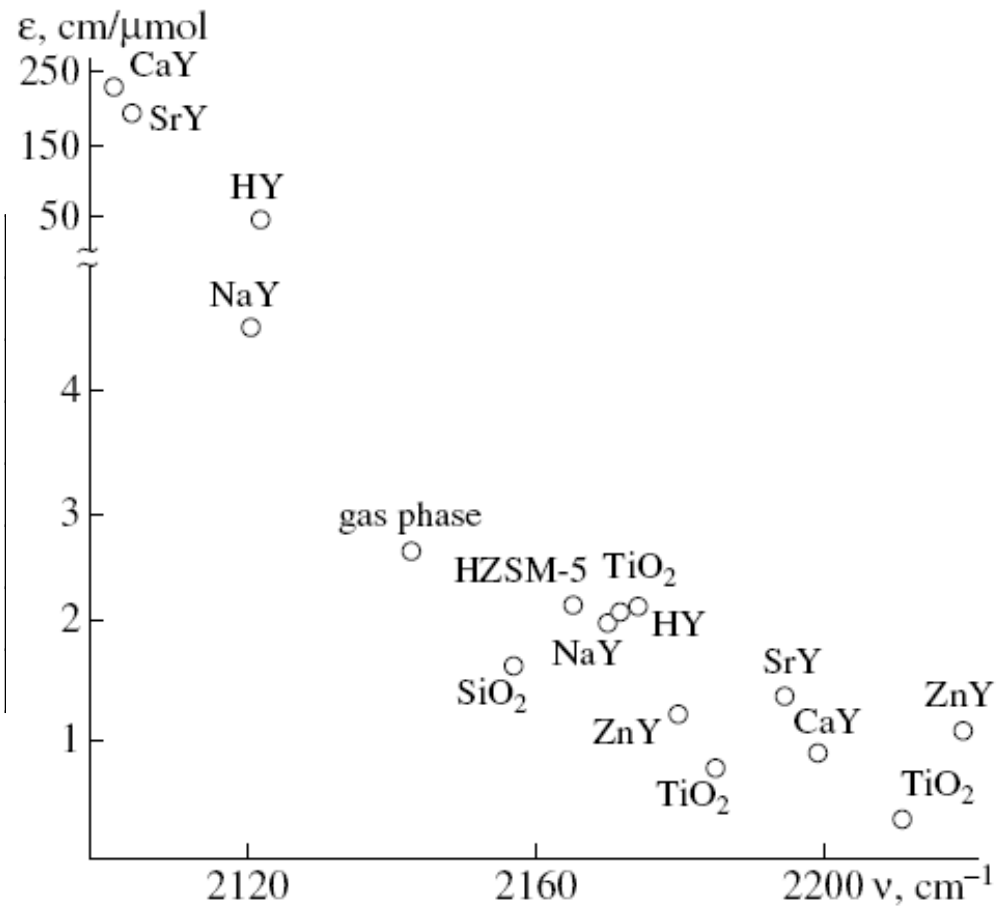


Oxide model



Big zeolite model

Effect of adsorption upon frequency and intensity of CO



Thanks for your attention