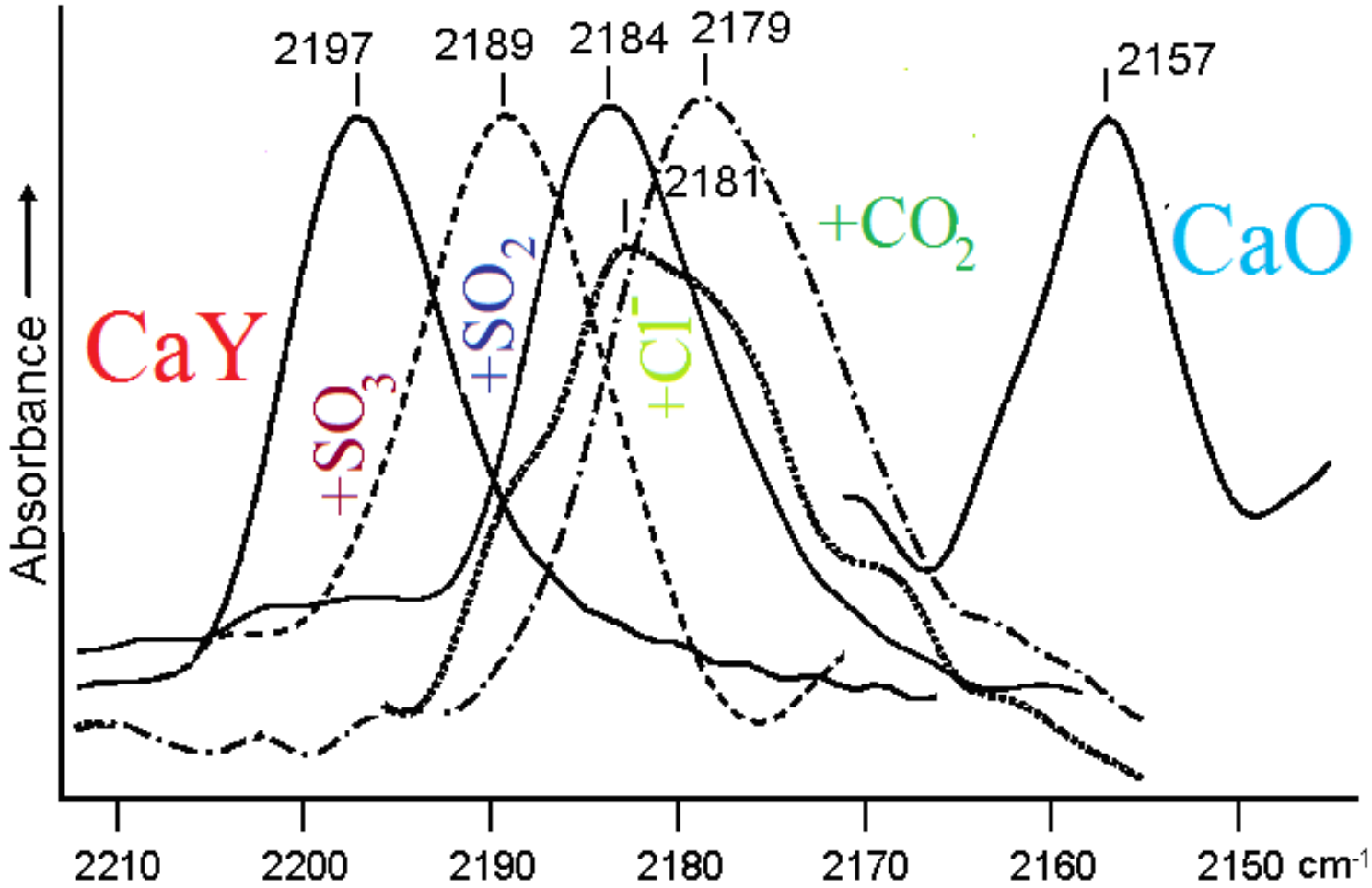
Saint Petersburg University

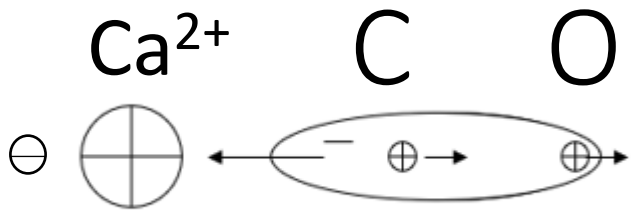
DFT study of the adsorption properties of Ca cation

Ya. Shergin

st054872@student.spbu.ru

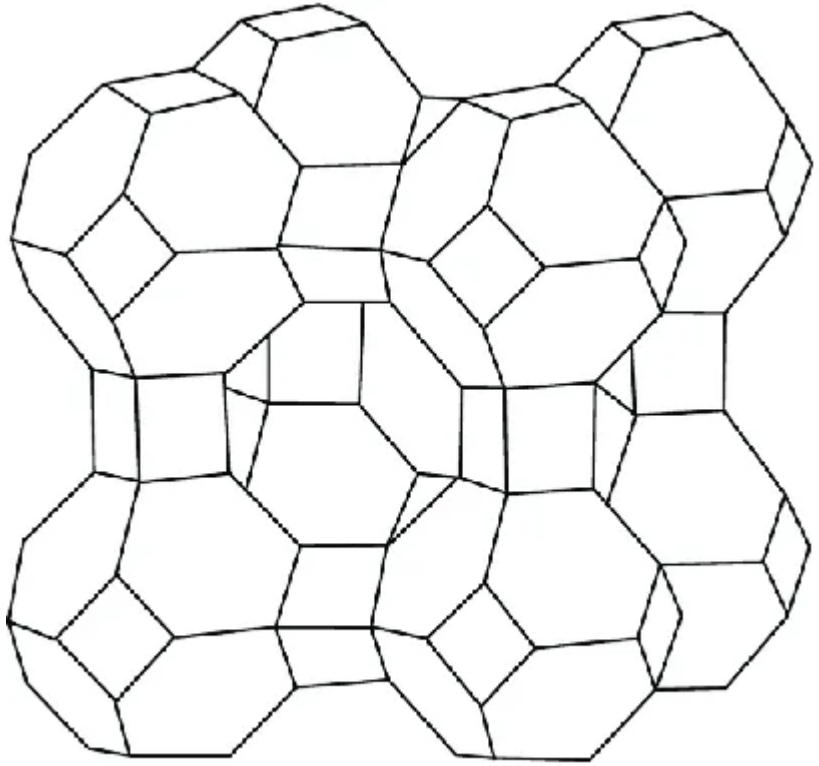
Blue shift



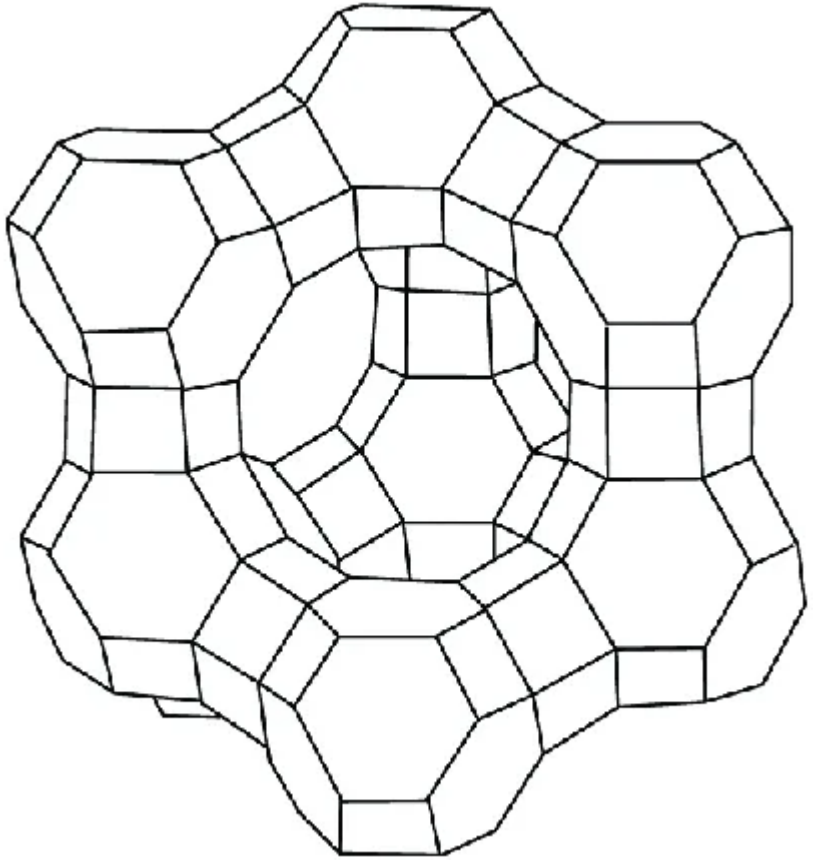


[1] K.V.Voronina, A.A.Tsyganenko. 2-nd Memorial Symp. “Molecular Photonics” St. Petersburg, 2009. abstr. p. 163.

Zeolites

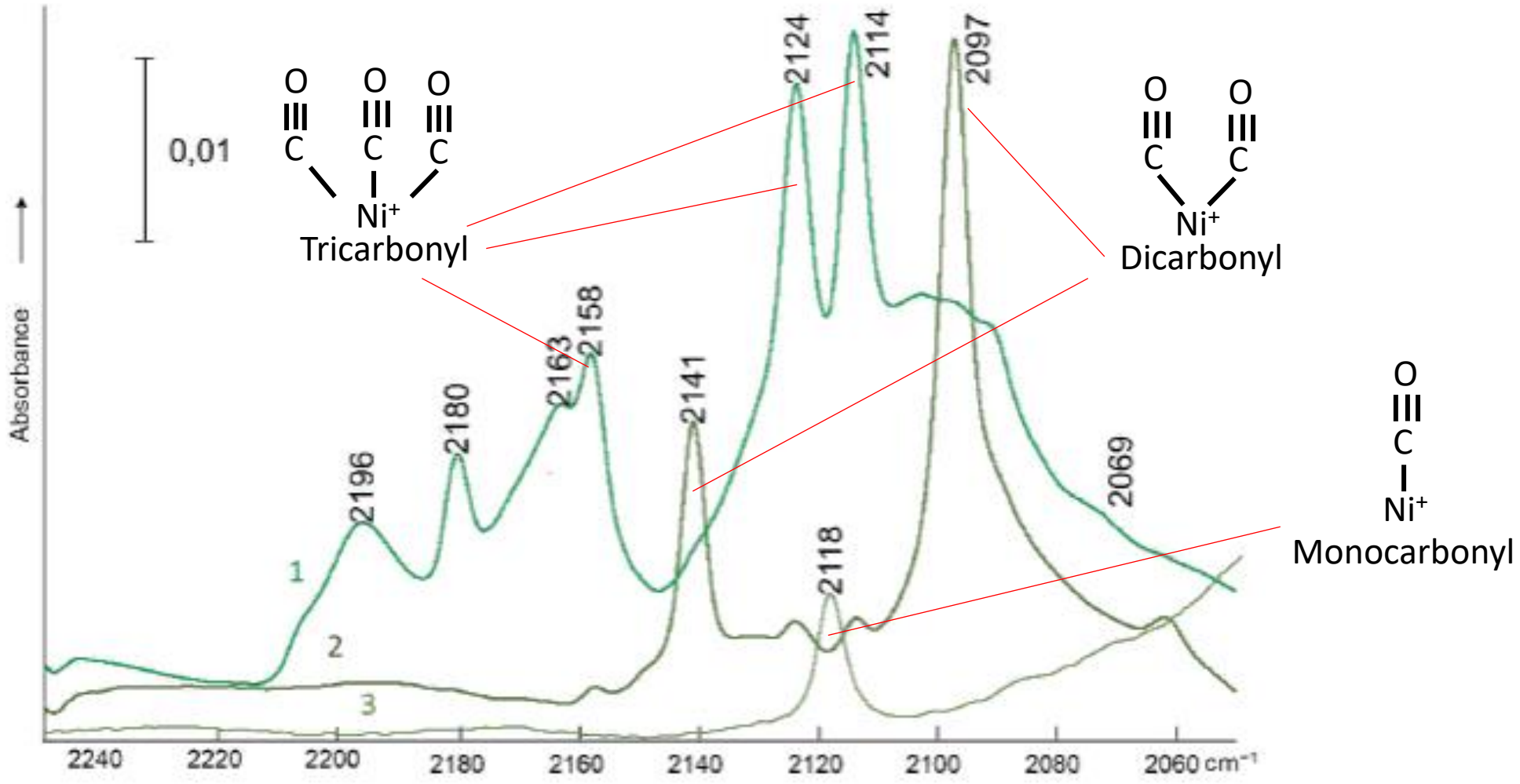


Structure of A and B zeolites



Structure of X and Y zeolites

CO adsorbed on Ni-USY zeolite

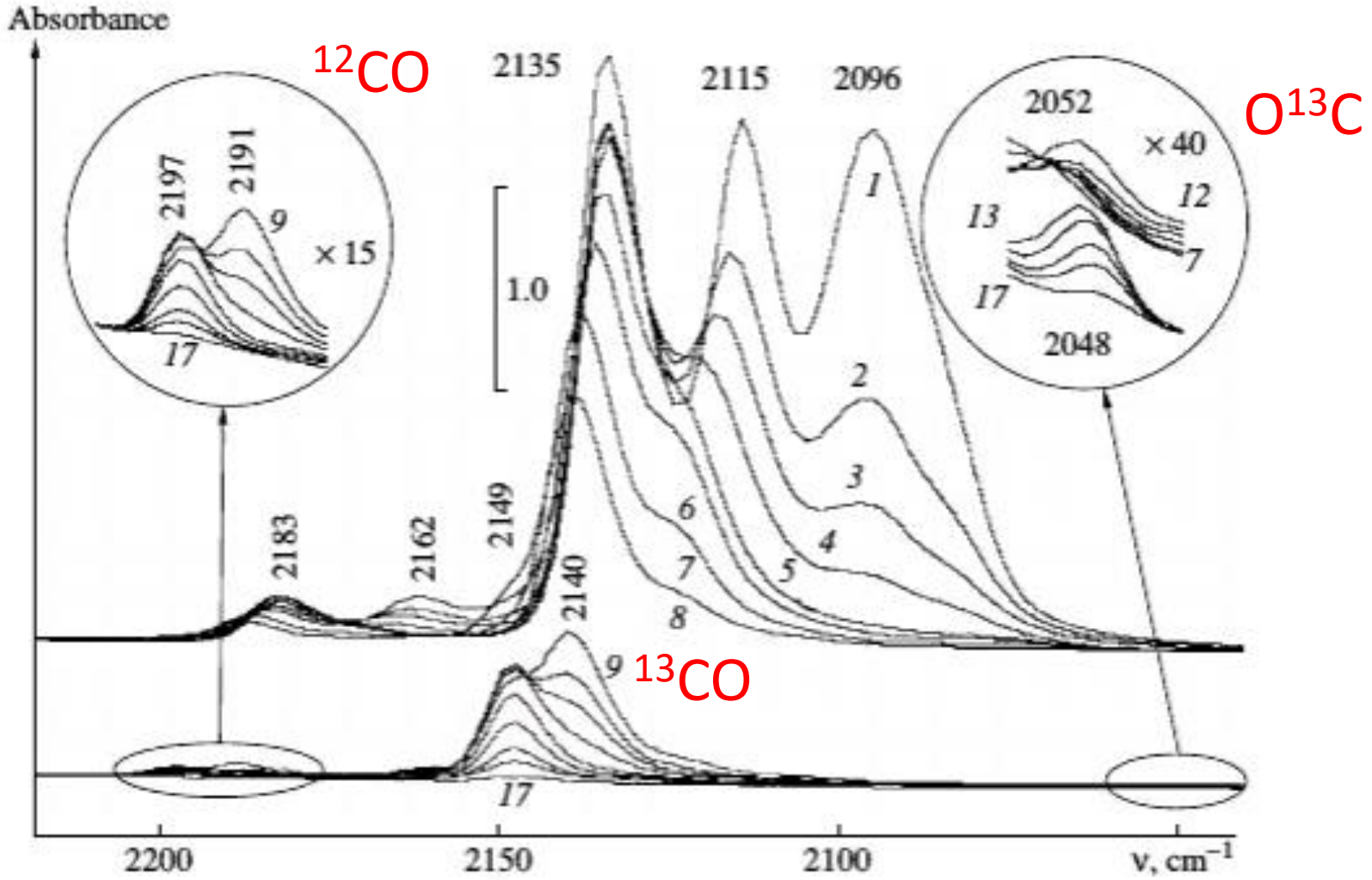


[2] R.Belykh, F.Mauge, A.Tsyganenko. Applied Catalysis A. 583 (2019) 117140.

CO adsorbed on CaY zeolite

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

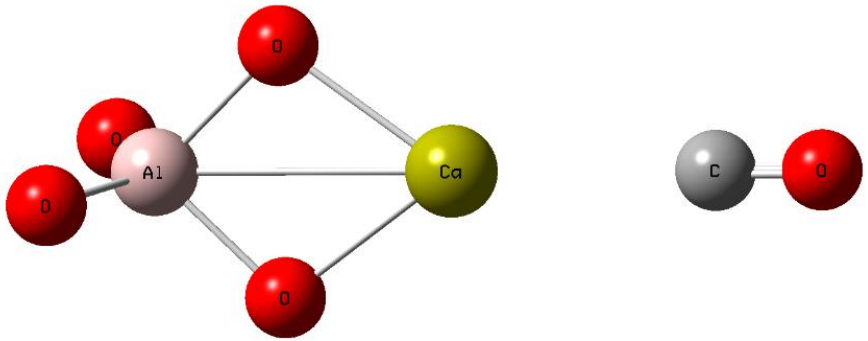
	$^{12}CO^{12}CO$
exp. cm^{-1}	2197; 2191
calc. cm^{-1}	2197,5; 2188,9



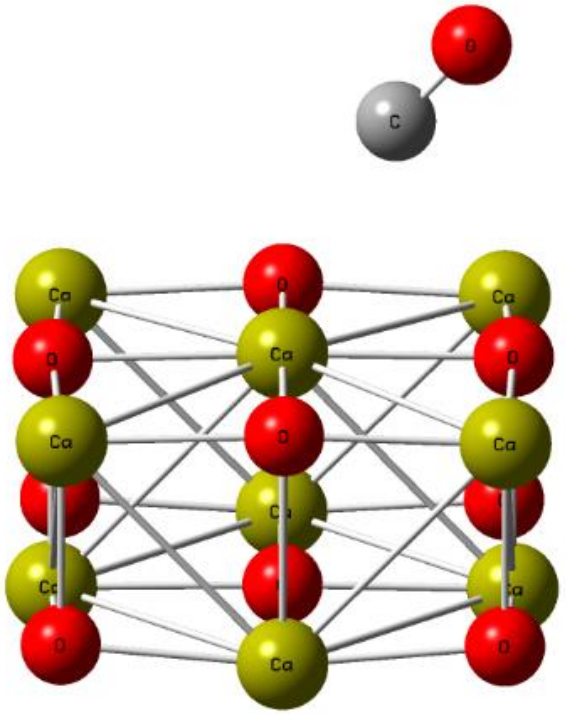
[3] A.Tsyganenko, P.Storozhev, C.Otero Areán. Kinet. Catalysis, 45 (2004) 530.

Models

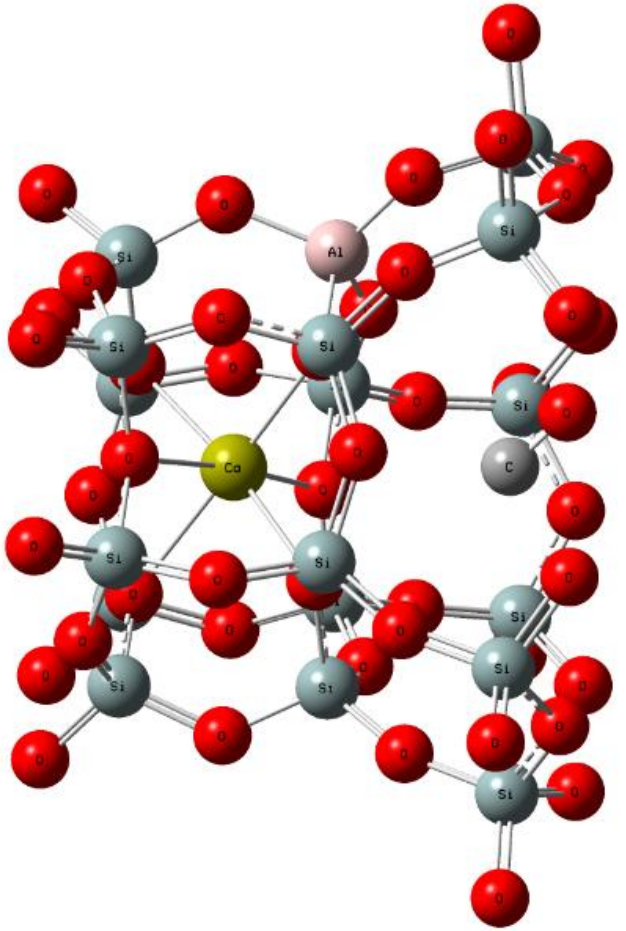
Free Calcium cation



Simple zeolite model

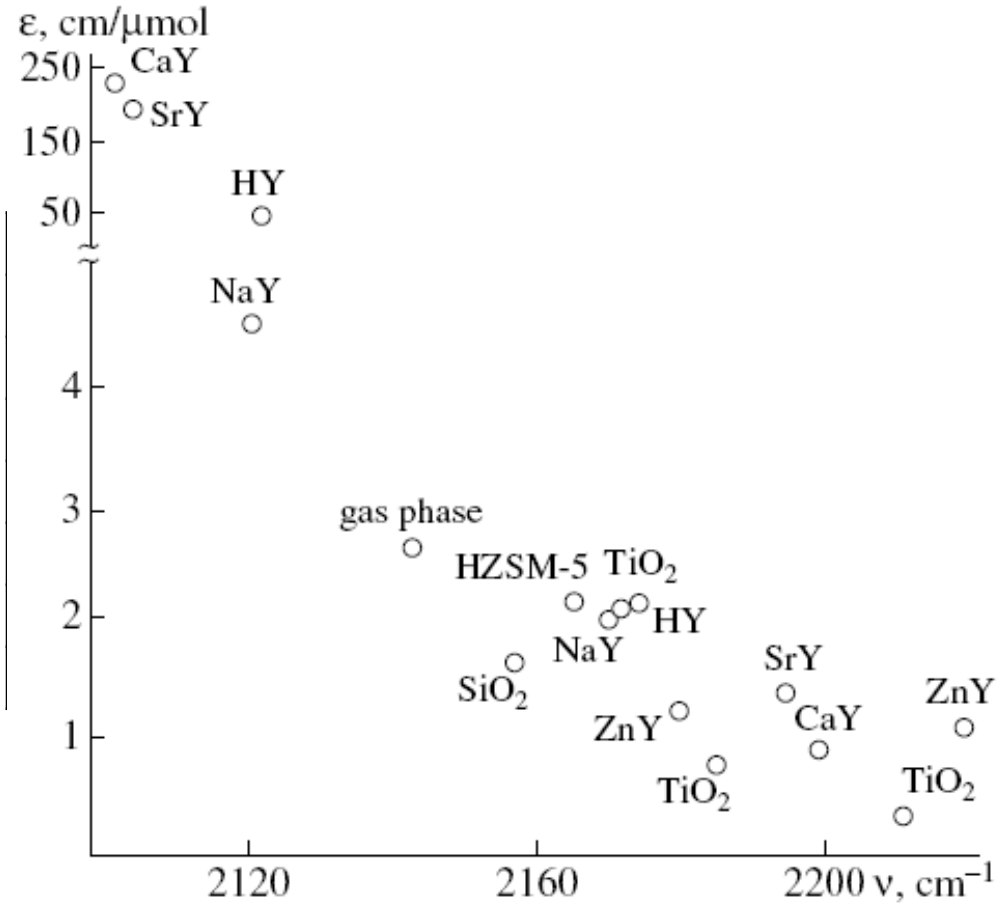


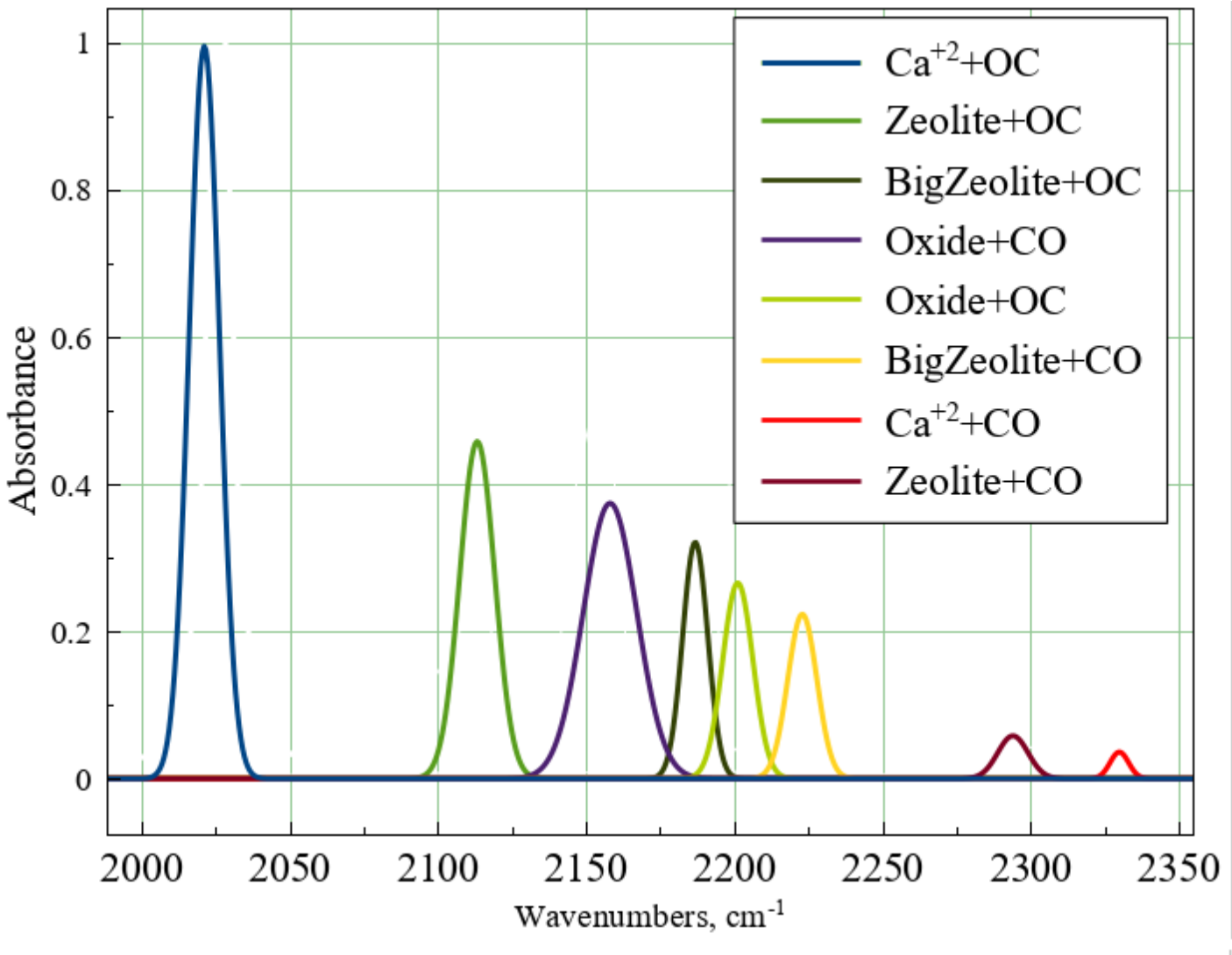
Oxide model



Big zeolite model

Effect of adsorption upon frequency and intensity of CO





[4] E.V.Kondratieva, O.V.Manoilova, A.A.Tsyganenko. Kinet. Catal., 49 (2008) 451.

Conclusions

- The DFT method was used to calculate CO adsorption on models

- It was shown why the splitting of the dicarbonyl band does not occur in the spectrum of CO adsorbed on CaY zeolite.

- Models of CaY zeolite reveal linkage isomerism. When CO is adsorbed by oxygen, the frequency decreases by approximately the same value by which it increases when adsorbed by carbon.

- The greater is the size of the surrounding anions, the higher is the frequency of CO adsorbed on Ca^{2+}

-The increase of CO vibrational frequency is accompanied by the decrease of absorbance, in a fair agreement with the experiment

Thanks for your attention