

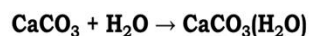
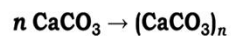


Isabel del Carmen Sáenz-Tavera, Víctor Manuel Rosas-García

Scientific Computation Center, Facultad de Ciencias Químicas, Universidad Autónoma de Nuevo León, Monterrey, N. L. México

E-mail: isabel.saenztv@uanl.edu.mx

Calcium carbonate aggregation is thermodynamically more favourable than solvation, so it is slightly soluble.



$E_{\text{estab./monómero}} = -143.749 \text{ kcal/mol}$

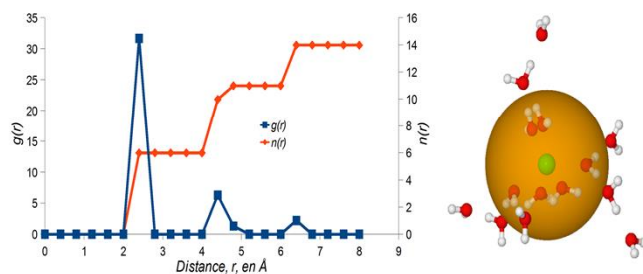
$\Delta E^\circ = -30.92 \text{ kcal/mol}$

Calcium carbonate is the solution for many environmental problems

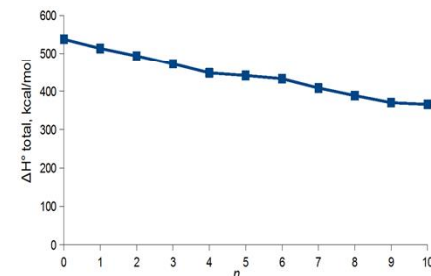
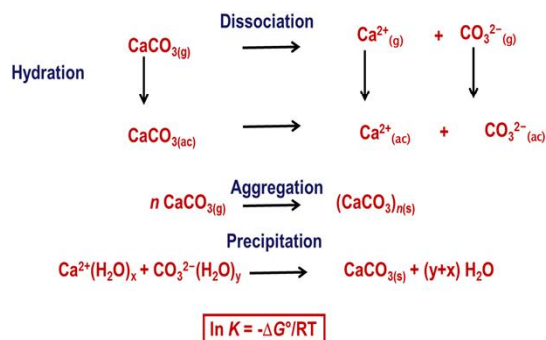
- ❖ Not toxic
- ❖ Desulphurization and defluorination agent for flue gas
- ❖ Lake liming
- ❖ Decrease some excess nutrients, like phosphate

We used an **ab initio Hartree-Fock method at the 6-31G* level and the explicit solvent model** to study calcium carbonate hydration, dissociation and aggregation.

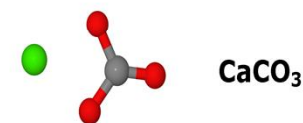
We obtained the first hydration shell structure and estimated thermodynamic properties for the salt and its ions



Radial Distribution Function for $\text{Ca}^{2+}(\text{H}_2\text{O})_{14}$

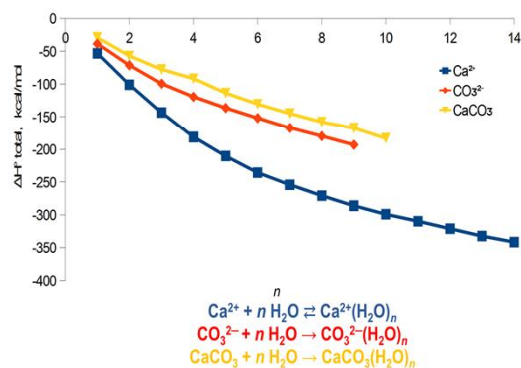


Dissociation total standard enthalpy ($\Delta H^\circ_{\text{total}}$), at 298.15 K, RHF/6-31G



- Calcium ion hydration is more exothermic than that for the anion and the salt
- Dissociation is an endothermic process
- Calcium carbonate clustering is more favorable than hydration

Our lab



Hydration total standard enthalpy ($\Delta H^\circ_{\text{total}}$), at 298.15 K, RHF/6-31G

UNDERSTANDING THE FRIENDLY CALCIUM CARBONATE

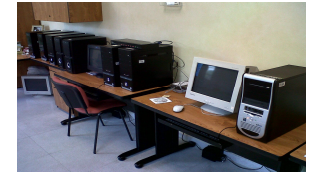
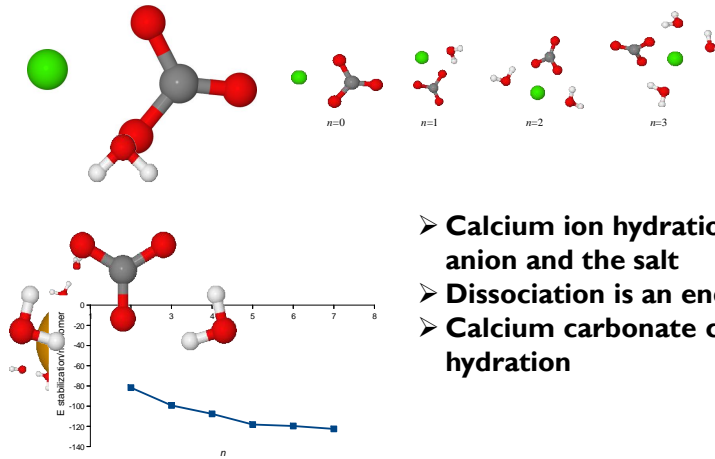
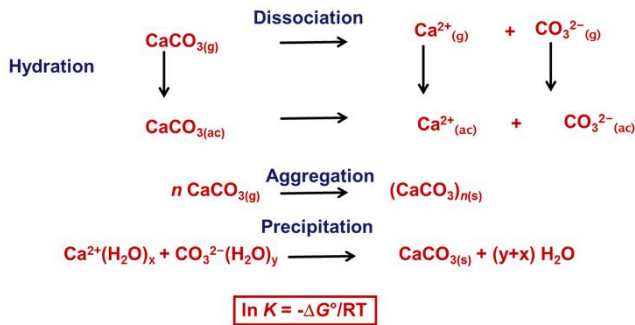
Isabel del Carmen Sáenz-Tavera, Víctor Manuel Rosas-García

Scientific Computation Center, Facultad de Ciencias Químicas, Universidad Autónoma de Nuevo León, Monterrey, N. L. México

E-mail: isabel.saenztv@uanl.edu.mx

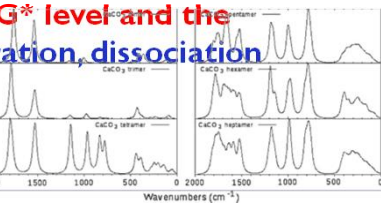
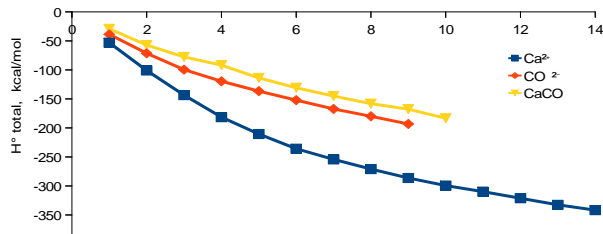
Calcium carbonate is the solution for many environmental problems

- ❖ Not toxic
- ❖ Desulphurization and defluorination agent for flue gas
- ❖ Lake liming
- ❖ Decrease some excess nutrients, like phosphate

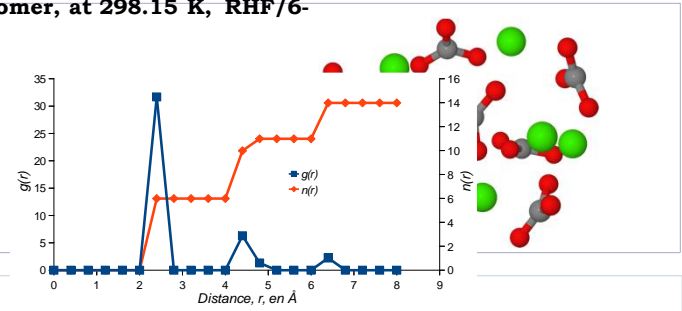
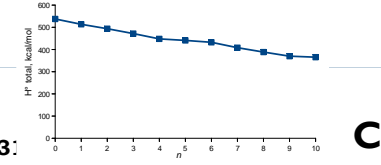


- Calcium ion hydration is more exothermic than that for the anion and the salt
- Dissociation is an endothermic process
- Calcium carbonate clustering is more favorable than hydration

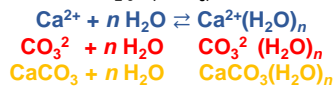
We used an **ab initio Hartree-Fock method at the 6-31G* level and the explicit solvent model** to study calcium carbonate hydration, dissociation and aggregation.



Calculated IR spectra for $(\text{CaCO}_3)_n$, $n=2-7$, HF/6-31G*



Calcium carbonate aggregation is thermodynamically more favourable than solvation, so it is slightly soluble.



Dissociation total standard enthalpy (ΔH°_d), at 298.15 K, RHF/6-31G*