XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

Study of the interaction between resins and albite by MM/QM methods.

Kelly F.Pessôa, Fernanda B. da Silva, Júlio C.G.Correia[a], Alexandre N.M.Carauta[a,b]

Address: [a]Centro de Tecnologia Mineral – CETEM/MCTI. Rio de Janeiro-RJ. Brasil
[b]Fundação Técnico-Educacional Souza Marques. Rio de Janeiro-RJ. Brasil

Abstract: The resin process of ornamental stones is crucial in the treatment of this type of stone, because, besides conferring an esthetic beauty, it protects against the action of physical, chemical and biological inclement weather increasing the mineral durability. However, the epoxy resin, which is the most used in this process, it presents toxicity, besides of not being biodegradable, thus creating an important environmental liability and contributes to the interest in finding alternatives in renewable sources[1]. The present work studies, through molecular modeling techniques, the interaction of epoxy resin and two possible active principles of biodegradable resins, cardanol [2] and ricinoleic acid [3], with the mineral albite which is representative of granitic stone, in order to better understand the adsorption process and the energies involved, in order to investigate a renewable alternative to the epoxy resin. A conformational analysis, using mechanical and molecular dynamics techniques, with the COMPASS force field, it was carried out for each of the representative molecules of the resins. The most stable structures obtained were submitted to a geometric optimization with frequency calculation by semi-empirical PM6-DH + [3] methodology, in order to obtain the minimum energy structure and ensure that they were in the ground state. Obtained the minimum structure, geometric optimization calculations with the PM6-DH+ method [4] were performed for successive approximations and in different orientations of each resin in relation to the albite structure constructed from crystallographic data. The maximum distance between the resin and the albite so that the method used admits that there is an interaction was 5Å. Above this value, the optimizations did not evolve into an interaction and the two structures have separated. In all cases, the resins assumed a position very close of the albite indicating the formation of chemical bonds. This seems to indicate that phenomena of chemisorption are expected. The figure 1 shows the results for the adsorption energy of the three systems studied and it indicates that the interaction with ricinoleic acid is the strongest, followed by the epoxy and finally by the resin the cardanol.

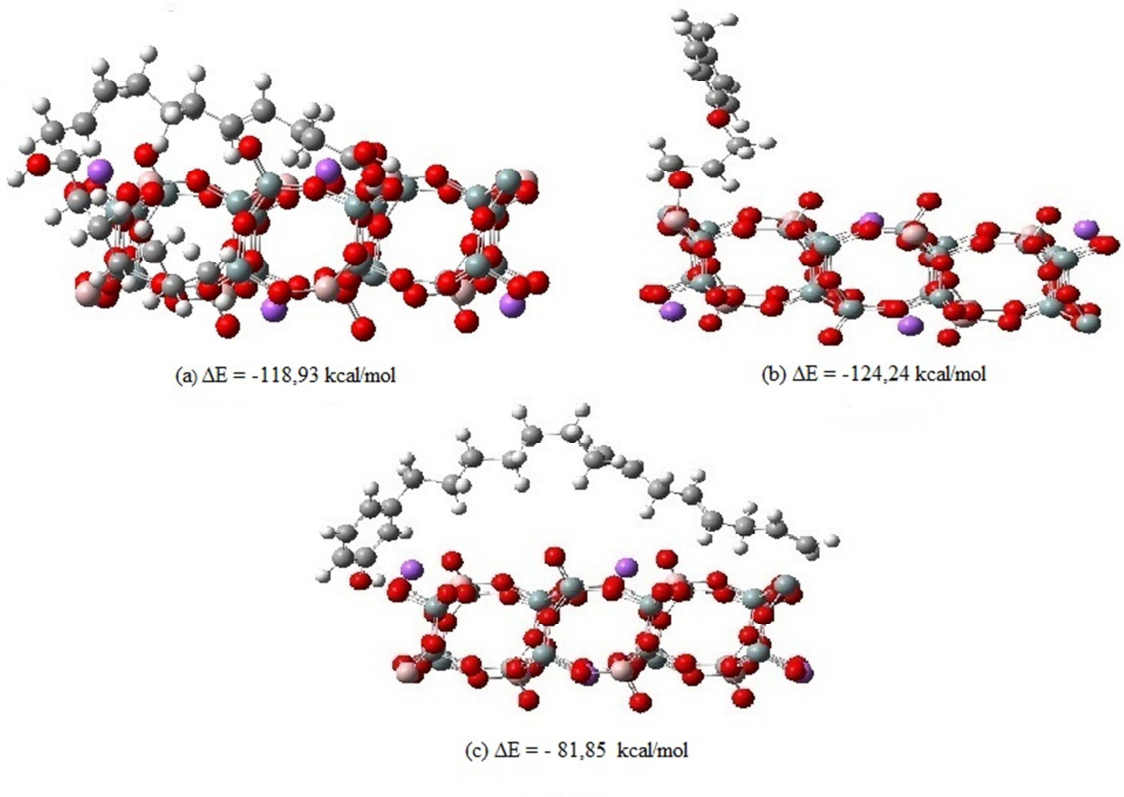

Figure 1 – Resin-Albite structures and respective adsorption energies: (a) Ricinoleic Acid-Albite; (b) Epoxy-Albite; (c) Cardanol-Albite.

Key-words: Ornamental Stones, Resins, Compass force field, PM6-DH+

Support: The authors acknowledge support from CNPq and PCI/CETEM and LABMOL collaborators. The authors thanks Prof. Prof. Peter Seidl by the Accelerys Inc. package license.

References:

[1] Silva, B. B. R.; Santana, R. M. C., Forte, M, M. C., International Journal of Adhesion & Adhesives, 2010, 30, pp 559–565.
[2] Mazzetto, S. E.; Lomonaco, D.; Mele, G., Química Nova, 2009, 32 (3), pp 732-741.
[3] Dalen, M. B.; Ibrahim, A. Q.; Adamu, H. M., British Journal of Applied Science & Technology 4(18): 2661-2683, 2014
[4] M. Korth, J. Chem. Theory Comput., 2010, 6 (12), pp 3808–3816.