

## Application of *ab initio* Calculations on the Study of the Tanning Process

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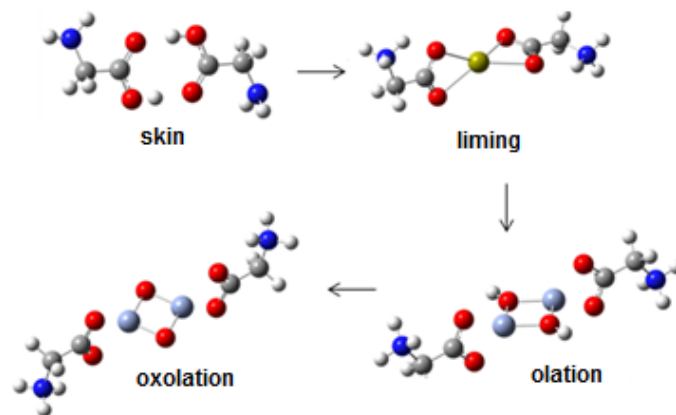
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In 2010, the Brazilian leather production was 44.5 million pieces, signifying 14.2% of world production. Regarding the destinations of Brazilian exports of leathers and skins, these have usually been the American, European and Asian continents. As a result, in 2011, 75.5% of the Brazilian production was directed to Italy, China, United States and Germany [1]. However, despite the importance of leather for the Brazil and the world, and the long period that elapses from the beginning of the development of tanning process, even in 1998 little was known about their molecular bases or the reaction mechanism involved [2] and this scenario has not undergone great evolution to the present day. In the same sense, on calculations involving chemical and molecular aspects of the tanning process, at our knowledge, only one work found in the literature suggests a model for the molecular complex of chromium and formic acid [3]. So, inspired on the literature [3], we would like to present molecular models that simulate the collagenous material (skin), the liming step, the olation and the oxolation (wet-blue) steps. These models were obtained using the B3LYP/6-31+G(d) on Gaussian 09W. Some aspects such as heat of formation, bond lengths and bond angles are discussed.

Structure \ Property	Heat of formation (Hartree)*
(a)	-568.72377052
(b)	-1245.88357209
(c)	-1612.04216633
(d)	-2807.46543783

\* 1 Hartree = 627,51 kcal mol<sup>-1</sup>



### References

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