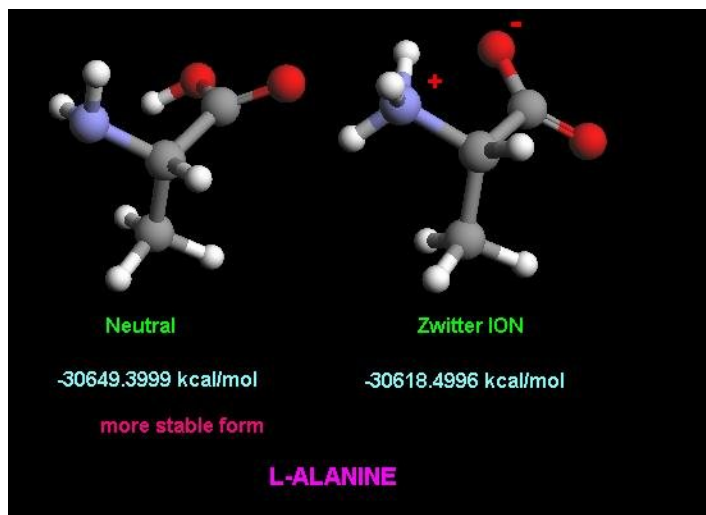


<http://www.ugc-inno-nehu.com/ToxicHE.html>

	NO Solvent	6H2O	12H2O	24H2O
<b>L-Alanine_neut</b>	-30649.3999 kcal/mol	-78913.5039 kcal/mol	-127191.4901 kcal/mol	-223743.5204 kcal/mol
<b>L-Alanine_ZI</b>	-30618.4996 kcal/mol	-78901.9898 kcal/mol	-127195.3701 kcal/mol	-223746.0048 kcal/mol
<b>Remarks On Stability of neutral form vs ZI form</b>	NEUT is more Stable than ZI Neut-ZI= <b>-30.9003</b>	NEUT is more Stable than ZI Neut-ZI= <b>-11.5141</b>	ZI is more stable than NEUT Neut-ZI= <b>+3.88</b>	ZI is more stable than NEUT= Neut-ZI= <b>+2.4844</b>
	<b>NOTE the reversal in Stability trend as compared to the previous two columns for No Solvent &amp; 6H2O</b>			
<b>singlept</b>	In the solvated ZI structure the Aminoacid is deleted and the Water system was subjected to single point energy calculation	-48234.4488 kcal/mol	-96500.8360 kcal/mol	-193048.9025 kcal/mol
<b>G.O.</b>	After Calculating the single point energy, the same was subjected to Optimization	-48262.7168 kcal/mol	-96543.5626 kcal/mol	-193107.6346 kcal/mol
<b>One H2O G.O.</b>	Single h2o optimized -8036.9395 kcal/mol	6 x -8036.9395= -48221.637 kcal/mol	12 x -8036.9395= -96443.274 kcal/mol	24 x -8036.0395= 192886.548 kcal/mol

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Results on Alanine using a relatively speedy method: the AM1 semiempirical method. **Conclusion:** *Nonionic form is more stable than the Zwitterionic form for the isolated molecule in the absence of surrounding water molecules*

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[http://www.ugc-inno-nehu.com/the\\_gamess.html](http://www.ugc-inno-nehu.com/the_gamess.html)

How to ascertain the role of neighboring water molecules for the detailing after conclusions as above? **“This question is nothing new!”**

[http://www.ugc-inno-nehu.com/crsi\\_13nsc\\_nmrs2007.html](http://www.ugc-inno-nehu.com/crsi_13nsc_nmrs2007.html)

