

**Job 65189: C2H5O2N-GLY-6W**

Totally it required about 550 iterations to complete the optimization

35 Jobs of 1.02 mins

initial input

Job 65189:  
This first job was by AMI method  
All the remaining jobs were by abinitio STO3G basis set calculations

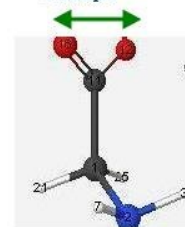
0	-0.537170833643	16	-0.755485852305
1	-0.591502230788	17	-0.756787204761
2	-0.641238384671	18	-0.751302225637
3	-0.674695332086	19	-0.7558510114731
4	-0.718337142199	20	-0.7566942157633
5	-0.735326689308	21	-0.752171400538
6	-0.729878743890	22	-0.756960128264
7	-0.741857129057	23	-0.757290496163
8	-0.699738691087	24	-0.7556802228908
9	-0.742733383882	25	-0.755351902685
10	-0.746375422029	26	-0.757263150024
11	-0.751136401934	27	-0.757437122859
12	-0.751594088937	28	-0.7571356893812
13	-0.747331530162	29	-0.757437160674
14	-0.752678368650	30	-0.757678750810
15	-0.743123588528	31	-0.758120883176
32	-0.758783244361		
33	-0.758959858996		
34	-0.759740509961		
35	-0.760725707336		
36	-0.761330425924		
37	-0.762130398611		
38	-0.763138475461		
39	-0.764114801047		
40	-0.764933712048		
41	-0.765496582529		
42	-0.766365710367		
43	-0.764710784382		
44	-0.767040483838		
45	-0.767836357353		
46	-0.768589718852		
47	-0.766915617639		
48	-0.769821235164		
49	-0.770076188668		
50	-0.771228048032		
51	-0.767555441792		
52	-0.771512477286		
53	-0.772106008326		
54	-0.772395339197		
55	-0.772736368707		

**Job 65237: C2H5O2N-GLY-6W G.O. Completed**

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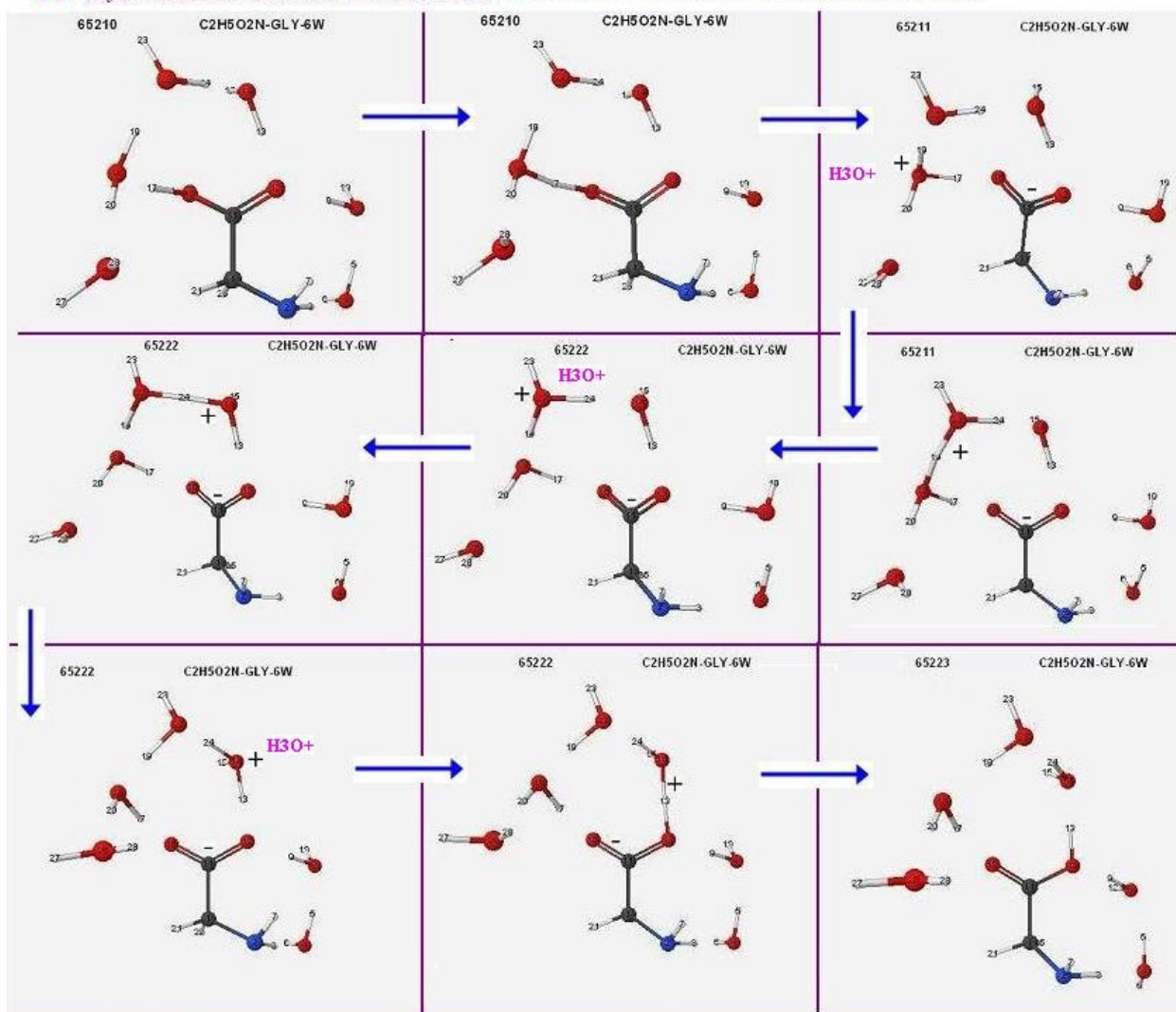
0	-729.048642201
1	-729.048641872
2	-729.048637150
3	-729.048638415
4	-729.048638913
5	-729.048642281
6	-729.048642090
7	-729.048642473
8	-729.048642333
9	-729.048642500

This is an intramolecular proton transfer from O10 to O12. Such processes are amenable for studies by NMR technique



Is this intra molecular or inter molecular? The combination of both seems to be not to be well discerned in terms of individual components !

**H3O+** Hydronium ION mediated Proton Transfer between the two oxygens within carboxyl functional



GLYCINE Hydronium ION mediated Proton Transfer 04 Sept 2010