

Supporting Information

Observation of Dihydrated Glycine

Table S1. Cartesian coordinates for the observed conformer of dihydrated glycine from MP2/6-311++G(d,p) calculations.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	3.025614	0.738135	0.031747
2	6	0	2.235664	-0.477418	-0.003856
3	6	0	0.725273	-0.290621	-0.017653
4	8	0	0.187216	0.807104	-0.062498
5	8	0	0.086351	-1.453181	0.014749
6	1	0	-0.896300	-1.310644	-0.013413
7	1	0	2.775829	1.329994	-0.754118
8	1	0	2.797494	1.270697	0.865123
9	1	0	2.495961	-1.062198	-0.892160
10	8	0	-2.504106	1.568481	0.108392
11	1	0	-1.536176	1.497924	0.049231
12	1	0	-2.741203	2.274758	-0.496261
13	8	0	-2.568162	-1.135868	-0.087802
14	1	0	-2.783369	-0.184334	-0.038482
15	1	0	-3.149381	-1.560589	0.547274
16	1	0	2.481845	-1.106606	0.856906

Rotational constants (GHZ): 3.6930617 1.0952084 0.8555568

Dipole moment (field-independent basis, Debye):
X= -1.6521 Y= 0.6804 Z= 0.0926 Tot= 1.7891

Complete reference 15.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; AlLaham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; González, C.; Pople, J. A. Gaussian 03, Revision B.04; Gaussian, Inc.: Pittsburgh, PA, 2003.