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Computed and experimental geometries for the ground state of glycine and N-acetylglycine.

Bonds ^a	Theo ^b	Exp ^c	Angles ^a	Theo ^b	Exp ^c	Dihedral angles ^a	Theo ^b	Exp ^c
<i>Glycine</i>								
C ₁ O ₁	1.218	1.207	O ₁ C ₁ C ₂	123.3	125.0	O ₁ C ₁ O ₂ H ₁	0.0	0.0
C ₁ O ₂	1.358	1.357	O ₂ C ₁ C ₂	111.4	111.5	O ₂ C ₁ C ₂ N ₁	180.0	180.0
C ₁ C ₂	1.515	1.532	C ₁ C ₂ N ₁	114.9	113.0	O ₂ C ₁ C ₂ H ₂	122.9	-
C ₂ N ₁	1.451	1.469	C ₁ O ₂ H ₁	105.9	-	C ₁ C ₂ N ₁ H ₃	57.0	-
O ₂ H ₁	0.979	0.966	C ₁ C ₂ H ₂	108.0	-			
C ₂ H ₂	1.095	1.081	C ₂ N ₁ H ₃	108.9	-			
N ₁ H ₃	1.019	1.001						
<i>N-Acetylglycine</i>								
C ₁ O ₁	1.233	-	O ₁ C ₁ C ₂	123.6	-	C ₂ C ₁ N ₁ C ₃	180.0	-
C ₁ C ₂	1.512	-	O ₁ C ₁ N ₁	121.4	-	O ₁ C ₁ N ₁ C ₃	0.0	-
C ₁ N ₁	1.363	-	C ₁ N ₁ C ₃	120.2	-	C ₁ N ₁ C ₃ C ₄	180.0	-
N ₁ C ₃	1.438	-	N ₁ C ₃ C ₄	109.0	-	N ₁ C ₃ C ₄ O ₂	0.0	-
C ₃ C ₄	1.505	-	C ₃ C ₄ O ₂	125.3	-	N ₁ C ₃ C ₄ O ₃	180.0	-
C ₄ O ₂	1.219	-	C ₃ C ₄ O ₃	111.1	-	H ₁ C ₂ C ₁ O ₁	120.0	-
C ₄ O ₃	1.351	-	H ₁ C ₂ C ₁	110.8	-	H ₂ C ₂ C ₁ O ₁	180.0	-
C ₂ H ₁	1.094	-	H ₂ C ₂ C ₁	108.5	-	O ₁ C ₁ N ₁ H ₃	180.0	-
C ₂ H ₂	1.089	-	C ₁ N ₁ H ₃	122.6	-	C ₁ N ₁ C ₃ H ₄	59.3	-
N ₁ H ₃	1.013	-	N ₁ C ₃ H ₄	111.7	-	O ₂ C ₄ O ₃ H ₅	0.0	-
C ₃ H ₄	1.096	-	C ₄ O ₃ H ₅	106.1	-			
O ₃ H ₅	0.980	-						

^a Bonds in Å, angles in degrees. See Figure 1 for atom labeling.

^b MP2/6-31G* level of calculation within the C_s symmetry.

^c Gas-phase electron diffraction and rotational data. Ref. [1]. Uncertainties ± 0.01 Å, $\pm 2^\circ$.

Table 1: Exponents and coefficients^a of the diffuse basis functions used for glycine and N-acetylglycine.

Exponents	<i>Coefficients</i>	
	Glycine 1s	N-Acetylglycine 1s
.024624	.84861256	.56438461
.011253	.30220704	.91088770
.005858	-.01641621	-.55227205
.003346	-.35636724	.19536936
.002048	.32918484	-.52612966
.001324	-.26685488	.47197604
.000893	.14244033	-.25432651
.000624	-.03541903	.06285494
Exponents	1p	1p
.042335	.16745768	.13057398
.019254	.49849059	.38107553
.009988	.31640658	.45842383
.005689	.14017752	.12697083
.003478	-.07994918	-.02216083
.002242	.06974689	.01124448
.001511	-.04163542	-.00827306
.001055	.01154936	.00297586
Exponents	1d	1d
.060540	.04978195	.03632208
.027446	.16899559	.08148195
.014204	.44535551	.42491984
.008077	.27187236	.31609354
.004927	.22697689	.27818879
.003175	-.06605085	-.05627080
.002137	.05433735	.05750428
.001491	-.01554890	-.01653936

^aOptimized as in ref. [2].

References

- [1] Iijima, K.; Tanaka, K.; Onuma, S. *J. Mol. Struct.*, **1991**, *246*, 257.
- [2] Roos, B. O.; Andersson, K.; Fülcher, M. P.; Malmqvist, P.-Å.; Serrano-Andrés, L.; Pierloot, K.; Merchán, M. in *Advances in Chemical Physics: New Methods in Computational Quantum Mechanics, Vol. XCIII:219*, Prigogine, I.; Rice, S. A., Eds. John Wiley & Sons, New York, 1996.