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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]
Glycine								
C_1O_1	1.218	1.207	$O_1C_1C_2$	123.3	125.0	$O_1C_1O_2H_1$	0.0	0.0
C_1O_2	1.358	1.357	$O_2C_1C_2$	111.4	111.5	$O_2C_1C_2N_1$	180.0	180.0
C_1C_2	1.515	1.532	$C_1C_2N_1$	114.9	113.0	$O_2C_1C_2H_2$	122.9	-
C_2N_1	1.451	1.469	$C_1O_2H_1$	105.9	-	$C_1C_2N_1H_3$	57.0	-
O_2H_1	0.979	0.966	$C_1C_2H_2$	108.0	-			
C_2H_2	1.095	1.081	$C_2N_1H_3$	108.9	-			
N_1H_3	1.019	1.001						
N-Acetylglycine								
C_1O_1	1.233	-	$O_1C_1C_2$	123.6	-	$C_2C_1N_1C_3$	180.0	-
C_1C_2	1.512	-	$O_1C_1N_1$	121.4	-	$O_1C_1N_1C_3$	0.0	-
C_1N_1	1.363	-	$C_1N_1C_3$	120.2	-	$C_1N_1C_3C_4$	180.0	-
N_1C_3	1.438	-	$N_1C_3C_4$	109.0	-	$N_1C_3C_4O_2$	0.0	-
C_3C_4	1.505	-	$C_3C_4O_2$	125.3	-	$N_1C_3C_4O_3$	180.0	-
C_4O_2	1.219	-	$C_3C_4O_3$	111.1	-	$H_1C_2C_1O_1$	120.0	-
C_4O_3	1.351	-	$H_1C_2C_1$	110.8	-	$H_2C_2C_1O_1$	180.0	-
C_2H_1	1.094	-	$H_2C_2C_1$	108.5	-	$O_1C_1N_1H_3$	180.0	-
C_2H_2	1.089	-	$C_1N_1H_3$	122.6	-	$C_1N_1C_3H_4$	59.3	-
N_1H_3	1.013	-	$N_1C_3H_4$	111.7	-	$O_2C_4O_3H_5$	0.0	-
C_3H_4	1.096	-	$C_4O_3H_5$	106.1	-			
O_3H_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, ± 2°.

Table 1: Exponents and coefficients[a] of the difusse basis functions used for glycine and N-acetylglycine.

	Coefficients	
	Glycine	N-Acetylglycine
Exponents	$1s$	$1s$
.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

[a]Optimized as in ref. [2].

References

[1] Iijima, K.; Tanaka, K.; Onuma, S. *J. Mol. Struct.*, **1991**, *246*, 257.

[2] Roos, B. O.; Andersson, K.; Fülscher, 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.