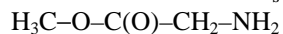


1333  $\text{C}_3\text{H}_7\text{NO}_2$ 

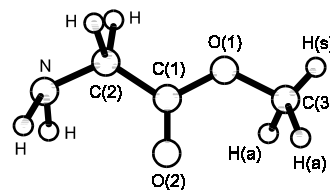
Glycine methyl ester

 $\text{C}_s$ ED, *ab initio*

calculations (HF/4-21G)

$r_g$	$\text{\AA}^a$	$\theta^b$	$\text{deg}^a$
C–N	1.447(7)	C–C–N	113.1(17)
C–C	1.507(7)	C–C=O(2)	125.8(17)
C(1)=O(2)	1.205(3)	C(2)–C(1)–O(1)	110.4(17)
C(3)–O(1)	1.344(7)	O(1)–C(1)=O(2)	123.1(20)
C(1)–O(1)	1.448(7)	C(1)–O(1)–C(3)	117.6(17)
N–H	1.035(22)	H–N–C	110(14)
C(2)–H	1.114(22)	H–C–C	106(14)
C(3)–H(s)	1.108(22)	O–C(3)–H(s)	103(14)
C(3)–H(a)	1.111(22)	O–C(3)–H(a)	108(14)
		C–C–N–H	–63(12)
		O(2)=C–C–H	–122(12)
		H(a)–C–O–C	–60(12)

The nozzle temperature was 75 °C.

<sup>a</sup>) Three times the estimated standard errors.<sup>b</sup>) Unidentified, possibly  $\theta_a$ .

Klimkowski, V.J., Ewbank, J.D., van Alsenoy, C., Scarsdale, J.N., Schäfer, L.: J. Am. Chem. Soc. **104** (1982) 1476.