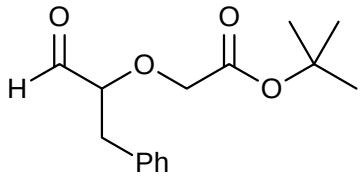
Problem R-96J ($C_{15}H_{20}O_4$)
300 MHz ^{1}H NMR spectrum in $CDCl_3$
Source: Brian Austad/Burke 11/26 g



PLT EX-2-1996-g.PLT

Problem R-96J ($C_{15}H_{20}O_4$). Determine the structure of **R-96J** from the 300 MHz proton NMR spectrum provided. **The compound contains a Ph and a $CO_2C(CH_3)_3$ group**.

(a) Analyze each of the proton signals, report multiplicity and coupling constants, and report any part structures you derived from the data.

δ 1.4

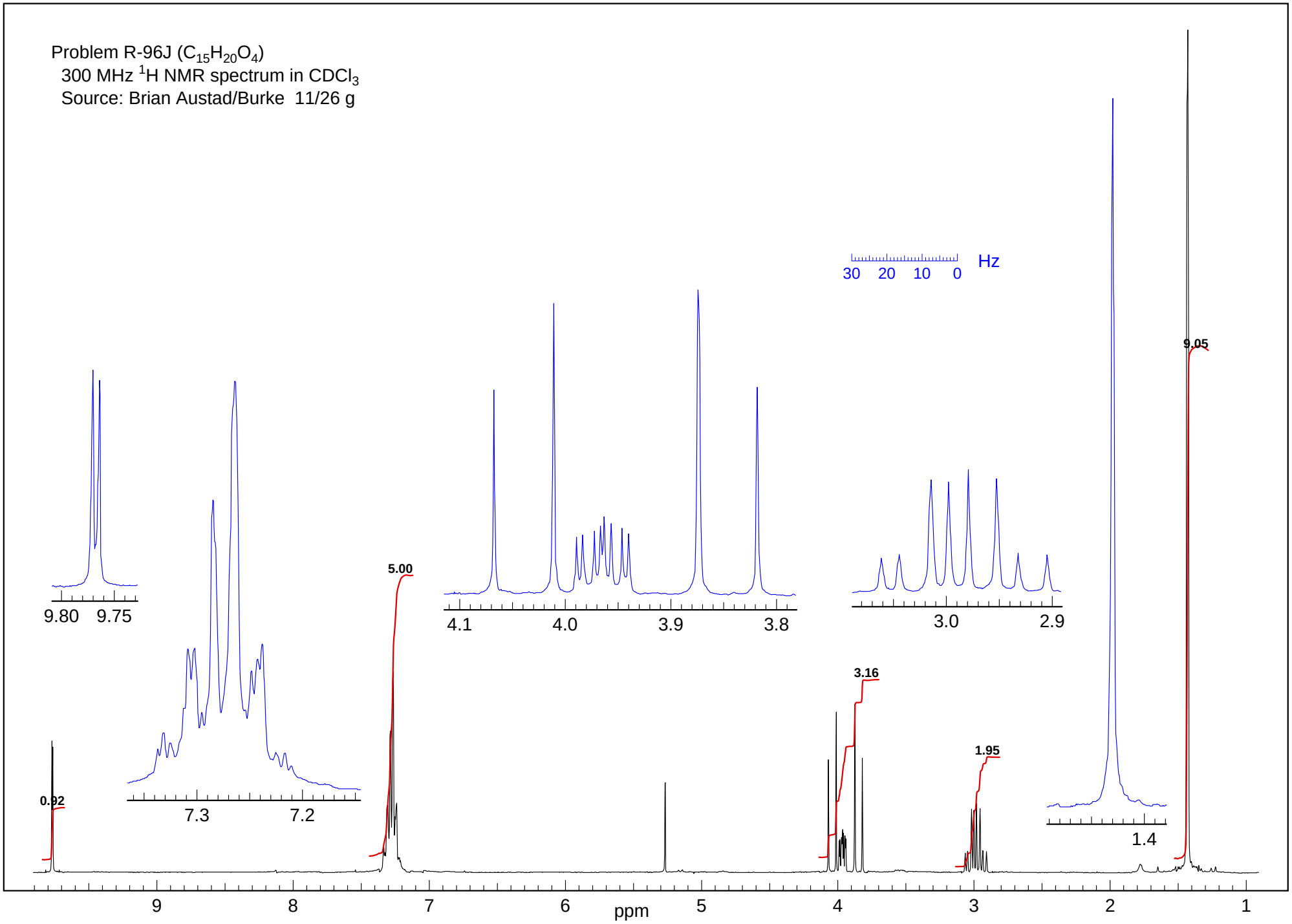
δ 3.0

δ 3.9

δ 7.3

δ 9.7

(b) Draw a structure for **R-96J**. If more than one structure is possible, show them, but circle the one you prefer, and give reasons for your preference.



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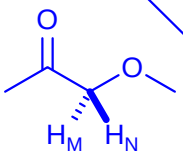
δ 1.4 s, 9H, $C(CH_3)_3$

δ 3.0 AB of **AB**XY, J_{AB} = 14 Hz, J_{AX} = 5 Hz, J_{BX} = 8 Hz

δ 3.9 3.85 and 4.05, MN quartet, J_{MN} = 16 Hz

Diastereotopic CH_2
- the large *J* suggest α-carbonyl or maybe α-Ph
- the δ suggests α to O:



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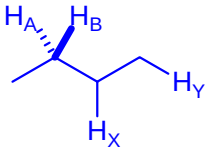
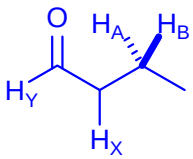
3.95, ddd, *J* = 8, 5, 2 H, 1H, X of AB**X**Y



δ 7.3 5H, Ph

δ 9.7 d, *J* = 2 Hz, 1H (Y of ABX**Y**)

Must be aldehyde proton



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2 The known groups are H-C(=O)-CH-CH_2-, O-CH_2-, Ph, CO_2-t-Bu. Quite a few ways of putting these together, some can be distinguished by chemical shift considerations

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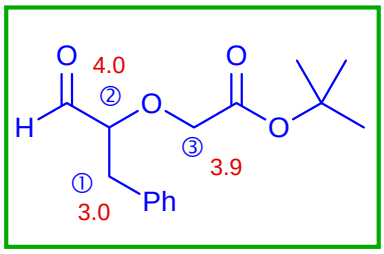

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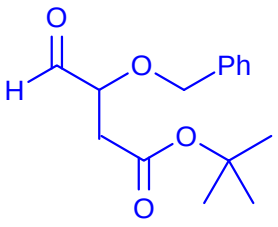

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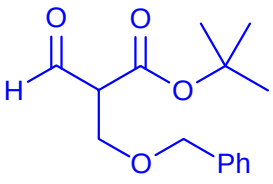

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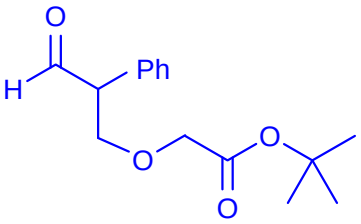

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	①	②	③	①	②	③	①	②	③	①	②	③
Calc δ	3.10	4.50	4.60	2.67	4.95	4.60	4.12	4.95	3.45	4.45	4.50	3.45
Δδ (error)	0.1	0.6	0.6	0.3	1.0	0.6	1.1	1.0	0.5	1.4	0.6	0.5
Sum Δδ:		1.3			1.9			2.6			2.5	

Correct structure, and smallest error

These structures can probably be ruled out on the basis of the large shift error