

Opgave 5.21. Bestem strukturen af molekylet med bruttoformlen $C_8H_8O_2$ og følgende spektroskopiske data. Navngiv forbindelsen.

IR: $\bar{\nu} / \text{cm}^{-1}$: 3030 (w), 2850 (m), 2730 (m), 1700 (s), 1600 (m), 1580 (m), 1500 (m), 1160 (s), 1020 (s).

MS: EI 70 eV m/z: 136 (67%), 135 (100%), 107 (17%), 92 (18%), 77 (35%), 63 (14%), 50 (11%), 39 (14%).

^1H -NMR: CDCl_3 , ppm: 3.9 (singlet, 3H), 7.0 (doublet, 2H), 7.8 (doublet, 2H), 9.9 (singlet, 1H).

^{13}C -NMR: CDCl_3 , ppm: 55.5 (medium), 114.3 (stor), 130.0 (lille), 131.9 (stor), 164.6 (lille), 190.6 (medium).