Internal rotational barriers by quantum chemical methods. Aromatic carbonyl compounds

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Internal rotational barriers of aromatic carbonl compounds were calculated by means of semi-empirical quantum chemical methods such as AM1 and PM3. Rotational potential barriers in the AM1 approach (VAM1) follow the experimental rotational free energy of activation (?G?) according to the linear relationship ?G? (kJmol-1)= (2-24 ± 0-08) VAM1+(7-79 ± 0-84). A standard deviation of 1-08 kJmol-1 permit leads to a good method for calculations of internal rotational barriers in these aromatic series.