

## SUPPLEMENTARY MATERIAL

### <sup>17</sup>O NMR study of *ortho* and *alkyl* substituent effects in substituted phenyl and alkyl esters of benzoic acid

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#### 1. EXPERIMENTAL

##### *a. Synthesis of compounds*

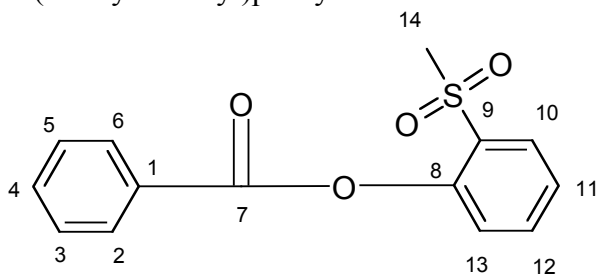
The preparation procedure and characteristics for the most *ortho*-, *meta*-, and *para*-substituted phenyl esters of benzoic acids, C<sub>6</sub>H<sub>5</sub>CO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>-X, and alkyl esters of benzoic acid, C<sub>6</sub>H<sub>5</sub>CO<sub>2</sub>R, have been previously described<sup>9, 51-55</sup>.

The phenyl benzoates, C<sub>6</sub>H<sub>5</sub>CO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>-X, (X = 2-SO<sub>2</sub>CH<sub>3</sub>, 2-COCH<sub>3</sub>, 2-CF<sub>3</sub>, 3-Cl, 4-SO<sub>2</sub>CH<sub>3</sub>, 4-CF<sub>3</sub>) were prepared by the addition of benzoyl chloride to the corresponding substituted phenol in pyridine with stirring at 0 °C (the Einhorn method)<sup>56</sup>. The crude esters were recrystallized from aqueous ethanol. 2-(Methylsulfonyl)phenyl benzoate: yield 42 %, m.p. 172-173 °C. 2-Acetylphenyl benzoate: yield 66 %, m.p. 84-86 °C, Reference<sup>57</sup>, m.p. 87-88 °C. 2-(Trifluoromethyl)phenyl benzoate: yield 56 %, m.p. 39-40 °C, Reference<sup>5</sup>, b.p. 125-126 °C. 3-Chlorophenyl benzoate: yield 73 %, m.p. 70-71 °C, Reference<sup>58</sup>, 70 °C. 4-(Methylsulfonyl)phenyl benzoate: yield 61 %, m.p. 155-156 °C. 4-(Trifluoromethyl)phenyl benzoate: yield 67 %, m.p. 113-114 °C. The phenyl benzoates, C<sub>6</sub>H<sub>5</sub>CO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>-X, (X = 3-Br, 3-N(CH<sub>3</sub>)<sub>2</sub>, 3-CF<sub>3</sub>, 2-Br) and 2,6-dimethylphenyl benzoate, were prepared by addition the benzoyl chloride to the mixture of the corresponding substituted phenol in aqueous 10 % sodium hydroxide (the Schotten-Baumann method). 3-Bromophenyl benzoate: yield 54 %, m.p. 85-86 °C, Reference<sup>27</sup>, m.p. 83-85 °C. 3-(Dimethylamino)phenyl benzoate: yield 55 %, m.p. 92-93 °C, Reference<sup>59</sup>, m.p. 94 °C. 3-(Trifluoromethyl)phenyl benzoate: yield 43 %, b.p. 118-120 °C/1.9 mbar. 2-Bromophenyl benzoate: yield 24 %, b.p. 148-149 °C/1.8 mbar. 2,6-Dimethylphenyl benzoate: yield 49 %, m.p. 41-42 °C, Reference<sup>60</sup>, m.p. 42-42.8 °C. 2,6-Dinitrophenyl benzoate was synthesized by the addition of the thionyl chloride to the mixture of benzoic acid and 2,6-dinitrophenol in pyridine with stirring at 0 °C.<sup>61</sup> 2,6-Dinitrophenyl benzoate: yield 54 %, m.p. 116-117 °C, Reference<sup>62</sup>, m.p. 112 °C. 2,2,2-Trichloroethyl benzoate<sup>12</sup> was purified by distillation, b.p. 108 °C/2.2 mbar.

b.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of phenyl benzoates

Purity of synthesized phenyl benzoates,  $\text{C}_6\text{H}_5\text{CO}_2\text{C}_6\text{H}_4\text{X}$  ( $\text{X} = 2\text{-SO}_2\text{CH}_3$ ,  $2\text{-COCH}_3$ ,  $2\text{-CF}_3$ ,  $2\text{-Br}$ ,  $2,6\text{-(CH}_3)_2$ ,  $2,6\text{-(NO}_2)_2$ ,  $3\text{-Cl}$ ,  $3\text{-Br}$ ,  $3\text{-N(CH}_3)_2$ ,  $3\text{-CF}_3$ ,  $4\text{-SO}_2\text{CH}_3$ ,  $4\text{-CF}_3$ ) and 2,2,2-trichloroethyl benzoate was confirmed by  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy in deuterated chloroform at  $25^\circ\text{C}$ .

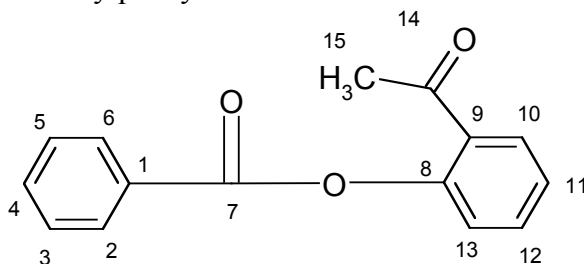
## 2-(Methylsulfonyl)phenyl benzoate



$^1\text{H}$  NMR: 8.24 m, 2H (H-2,6); 7.55 t, 2H (H-3,5)  $^3J_{av} = 7.6$ ; 7.65-7.78 m, 2H (H-4,12); 8.10 m, 1H (H-10); 7.44-7.51 m, 2H (H-11,13), 3.16 s, 3H (H-14).

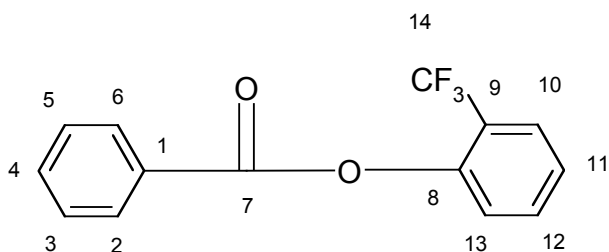
$^{13}\text{C}$  NMR: 129.00 (C-1); 130.47 (C-2,6); 128.90 (C-3,5); 134.13 (C-4); 164.37 (C-7); 148.99 (C-8); 133.12 (C-9); 130.07 (C-10); 126.50 (C-11); 135.03 (C-12); 124.80 (C-13); 44.01 (C-14).

## 2-Acetylphenyl benzoate



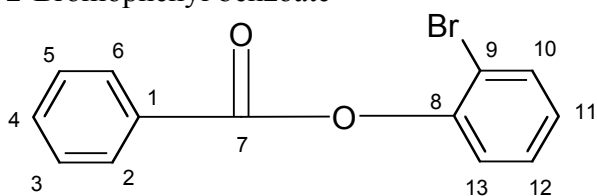
$^1\text{H}$  NMR: 8.21 m, 2H (H-2,6); 7.46-7.68 m, 4H (H-3,4,5,12); 7.85 dd, 1H (H-10),  $^3J = 7.8$ ,  $^4J = 1.8$ ; 7.34 dt, 1H (H-11),  $^3J_{av} = 7.6$ ,  $^4J = 1.3$ ; 7.22 dd, 1H (H-13) 2.53 s, 3H (H-15).  $^{13}\text{C}$  NMR: 129.33 (C-1); 130.28 (C-2,6); 128.69 (C-3,5); 133.78 (C-4); 165.10 (C-7); 149.38 (C-8); 131.38 (C-9); 130.23 (C-10); 126.14 (C-11); 133.33 (C-12); 123.90 (C-13); 197.40 (C-14); 29.70 (C-15).

## 2-(Trifluoromethyl)phenyl benzoate



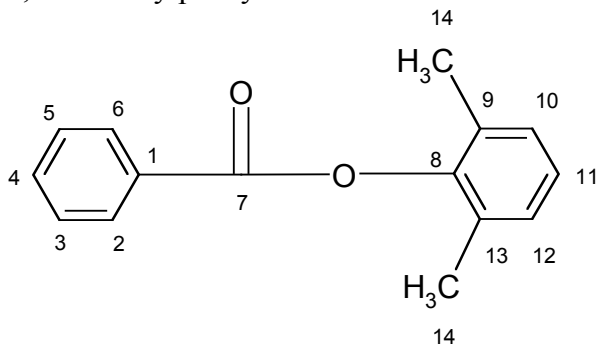
$^1\text{H}$  NMR: 7.2-7.7 m, 7H (H-3,4,5,10,11,12,13); 8.21 m, 2H (H-2,6).  $^{13}\text{C}$  NMR: 129.10 (C-1); 130.46 (C-2,6); 128.76 (C-3,5); 133.93 (C-4); 164.52 (C-7); 148.70 q (C-8),  $^3J_{\text{C-F}}=2.0$ ; 123.20 q (C-9),  $^2J_{\text{C-F}}=31.2$ ; 127.00 q (C-10),  $^3J_{\text{C-F}}=5.0$ ; 125.92 (C-11); 133.05 (C-12); 124.55 (C-13); 123.30 q (C-14),  $^1J_{\text{C-F}}=273.0$ .

### 2-Bromophenyl benzoate



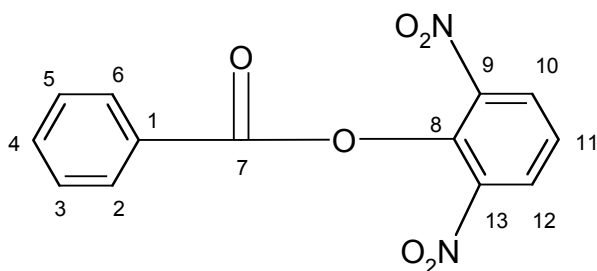
$^1\text{H}$  NMR: 8.23 m, 2H (H-2,6); 7.47 m, 2H (H-3,5); 7.56-7.64 m, 2H (H-4, 10); 7.10 ddd, 1H (H-11),  $^3J=7.9$ ,  $^3J=7.0$ ,  $^4J=2.0$ ; 7.31 ddd, 1H (H-12),  $^3J=8.0$ ,  $^3J=7.0$ ,  $^4J=1.5$ ; 7.25 ddd, 1H (H-13),  $^3J=8.0$ ,  $^4J=2.0$ ,  $^5J=0.5$ .  $^{13}\text{C}$  NMR: 129.10 (C-1); 130.33 (C-2,6,10); 128.61 (C-3,5); 133.36 (C-4); 164.13 (C-7); 148.53 (C-8); 116.27 (C-9); 133.75 (C-10); 127.26 (C-11); 128.43 (C-12); 123.92 (C-13).

### 2,6-Dimethylphenyl benzoate



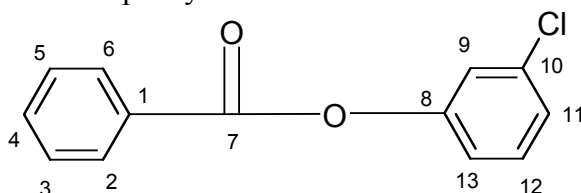
$^1\text{H}$  NMR: 8.25 m, 2H (H-2,6); 7.50 m, 2H (H-3,5); 7.62 m, 1H (H-4),  $^3J=7.3$ ; 7.09 br s, 2H (H-10, 12) 7.08 br s, 1H (H-11).  $^{13}\text{C}$  NMR: 129.59 (C-1); 130.18 (C-2,6); 128.65 (C-3,5,10,12); 133.51 (C-4); 164.31 (C-7); 148.54 (C-8); 130.43 (C-9,13); 125.90 (C-11); 16.34 (C-14).

### 2,6-Dinitrophenyl benzoate



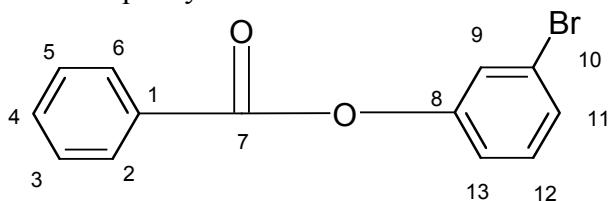
$^1\text{H NMR}$ : 7.50-7.74 m, 4H (H-3,4,5,11); 8.17 m, 2H (H-2,6); 8.34 d, 2H (H-10,12),  $^3J = 8.2$ .  $^{13}\text{C NMR}$ : 127.39 (C-1); 129.94 (C-2,6); 128.91 (C-3,5); 134.77 (C-4); 163.21 (C-7); 139.03 (C-8); 144.03 (C-9,13); 130.86 (C-10,12); 126.61 (C-11).

### 3-Chlorophenyl benzoate



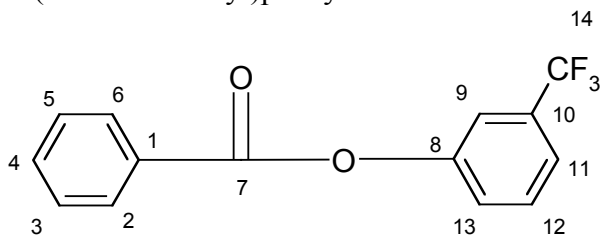
$^1\text{H NMR}$ : 8.18 m, 2H (H-2,6); 7.50 m, 2H (H-3,5); 7.64 m, 1H (H-4); 7.22-7.29 m, 2H (H-9,11); 7.35 m, 1H (H-12); 7.13 ddd, 1H (H-13),  $^3J = 7.9$   $^4J = 1.5$   $^4J = 2.1$ .  $^{13}\text{C NMR}$ : 129.32 (C-1); 130.24 (C-2,6); 128.67 (C-3,5); 133.79 (C-4); 164.71 (C-7); 151.63 (C-8); 122.46 (C-9); 134.85 (C-10); 126.16 (C-11); 130.24 (C-12); 120.15.

### 3-Bromophenyl benzoate



$^1\text{H NMR}$ : 8.17 m, 2H (H-2,6); 7.49 m, 2H (H-3,5); 7.63 m, 1H (H-4)  $^3J = 7.3$ ; 7.37-7.42 m, 2H (H-9,11); 7.28 t, 1H (H-12),  $^3J_{av} = 8.2$ ; 7.16 ddd, 1H (H-13),  $^3J = 8.1$ ,  $^4J = 1.5$ ,  $^4J = 2.0$ .  $^{13}\text{C NMR}$ : 129.27 (C-1); 130.22 (C-2,6); 128.65 (C-3,5); 133.78 (C-4); 164.66 (C-7); 151.64 (C-8); 125.29 (C-9); 122.46 (C-10); 129.05 (C-11); 130.48 (C-12); 120.61 (C-13).

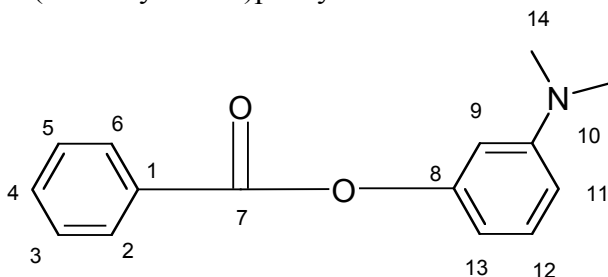
### 3-(Trifluoromethyl)phenyl benzoate



$^1\text{H NMR}$ : 8.18 m, 2H (H-2,6); 7.37-7.51 m, 6H (H-3,5,9,11,12,13); 7.62 m, 1H (H-4)  $^3J = 7.3$ .

$^{13}\text{C}$  NMR: 129.30 (C-1); 130.34 (C-2,6); 128.79 (C-3,5); 133.98 (C-4); 164.78 (C-7); 151.40 (C-8); 119.18 (C-9),  $^3J_{F-C}=3.9$ ; 132.25 (C-10),  $^2J_{F-C}=33.2$ ; 122.72 (C-11),  $^3J_{F-C}=3.8$ ; 130.14 (C-12); 125.57 (C-13),  $^5J_{F-C}=1.2$ ; 123.81 (C-14),  $^1J_{F-C}=272.4$ .

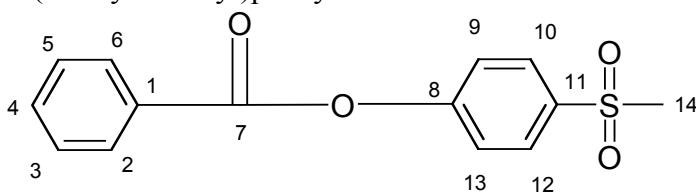
### 3-(Dimethylamino)phenyl benzoate



$^1\text{H}$  NMR: 8.20 m, 2H (H-2,6); 7.48 m, 2H (H-3,5); 7.61 m, 1H (H-4)  $^3J=7.3$ ; 6.51-6.64 m, 3H (H-9,11,13); 7.26 t, 1H (H-12),  $^3J_{av}=8.0$ ; 2.94 s, 6H (H-14).

$^{13}\text{C}$  NMR: 130.18 (C-1); 130.17 (C-2,6); 128.52 (C-3,5); 133.34 (C-4); 165.24 (C-7); 152.27 (C-8); 105.75 (C-9); 151.92 (C-10); 110.09 (C-11); 129.69 (C-12); 109.47 (C-13); 40.44 (C-14).

### 4-(Methylsulfonyl)phenyl benzoate

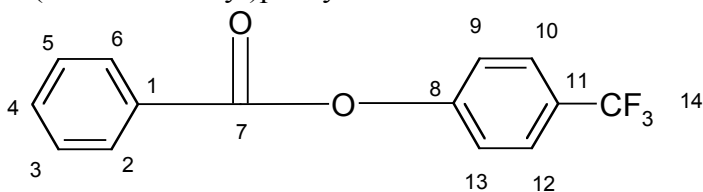


$\text{CD}_3\text{CN}$ ,  $40^\circ\text{C}$ , shifts relative to the solvent residual peak

$^1\text{H}$  NMR: 8.20 m, 2H (H-2,6); 7.50-7.63 m, 4H (H-3,5,9,13); 7.73 m, 1H (H-4),  $^3J=7.7$ ,  $^4J=1.3$ ; 8.03 d, 2H (H-10,12),  $^3J=8.7$ ; 3.10 s, 3H (H-14).

$^{13}\text{C}$  NMR: 130.36 (C-1); 131.21 (C-2,6); 130.04 (C-3,5); 135.25 (C-4); 165.72 (C-7); 156.29 (C-8); 124.09 (C-9,13); 130.22 (C-10,12); 139.88 (C-11); 44.92 (C-14).

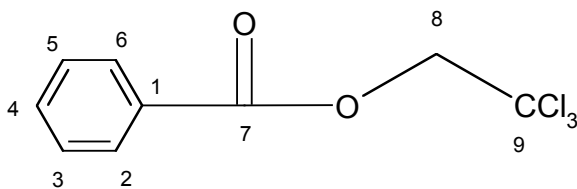
### 4-(Trifluoromethyl)phenyl benzoate



$^1\text{H}$  NMR: 8.20 m, 2H (H-2,6); 7.51 m, 2H (H-3,5); 7.61-7.71 m, 3H (H-4,10,12); 7.34 d, 2H (H-9,13),  $^3J=8.5$ .

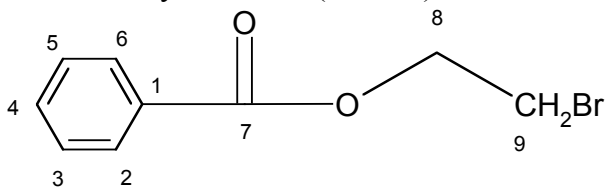
$^{13}\text{C}$  NMR: 129.28 (C-1); 130.35 (C-2,6); 128.77 (C-3,5); 133.97 (C-4); 164.66 (C-7); 153.76 (C-8),  $^5J_{F-C}=1.5$ ; 122.32 (C-9,13); 126.91 (C-10,12),  $^3J_{F-C}=3.7$ ; 128.34 (C-11),  $^2J_{F-C}=32.8$ ; 124.07 (C-14),  $^1J_{F-C}=272.2$ .

### 2,2,2-Trichloroethyl benzoate



$^1\text{H}$  NMR: 8.12 m, 2H (H-2,6); 7.44 m, 2H (H-3,5); 7.58 m, 1H (H-4); 4.95 s, 2H (H-8).  $^{13}\text{C}$  NMR: 128.72 (C-1); 130.00 (C-2,6); 128.54 (C-3,5); 133.69 (C-4); 164.68 (C-7); 74.36 (C-8); 95.12 (C-9).

### 2-Bromoethyl benzoate (Aldrich)



$^1\text{H}$  NMR: 8.05 m, 2H (H-2,6); 7.41 m, 2H (H-3,5); 7.54 m, 1H (H-4); 4.58 t, 2H (H-8),  $^3J = 6.1$ ; 3.60 t, 2H (H-9),  $^3J = 6.1$ .  $^{13}\text{C}$  NMR: 129.75 (C-1); 129.70 (C-2,6); 128.40 (C-3,5); 133.17 (C-4); 165.87 (C-7); 64.19 (C-8); 28.83 (C-9).

## 2. DATA PROCESSING

The values of chemical shifts,  $\delta(^{17}\text{O})$ , for the carbonyl oxygen and the single-bonded oxygen in the *ortho*-, *para*- and *meta*-substituted phenyl esters of benzoic acid,  $\text{C}_6\text{H}_5\text{CO}_2\text{C}_6\text{H}_4\text{-X}$ , given in Table I were treated according to the Taft and Charton equations using the Taft's  $\sigma^\circ$ <sup>63,64</sup>, inductive  $\sigma_{\text{I}}$ <sup>64,65</sup>, and the resonance  $\sigma^\circ_{\text{R}}$  ( $\sigma^\circ_{\text{R}} = \sigma^\circ_{\text{p}} - \sigma_{\text{I}}$ )<sup>64,66</sup> substituent constants:

$$\delta(^{17}\text{O})_{\text{para(meta)}} = \delta(^{17}\text{O})_{\text{H}} + (\rho)_{\text{para(meta)}}\sigma^\circ \quad (1)$$

$$\delta(^{17}\text{O})_{\text{para(meta)}} = \delta(^{17}\text{O})_{\text{H}} + (\rho_{\text{I}})_{\text{para(meta)}}\sigma_{\text{I}} + (\rho_{\text{R}})_{\text{para(meta)}}\sigma^\circ_{\text{R}} \quad (2)$$

In the case of *ortho* derivatives the significance of the inductive, resonance and steric effects to the substituent-induced chemical shift,  $\delta(^{17}\text{O})$ , was estimated using the following Charton equations<sup>50</sup> (3) and (4):

$$\delta(^{17}\text{O})_{\text{ortho}} = \delta(^{17}\text{O})_{\text{H}} + (\rho_{\text{I}})_{\text{ortho}}\sigma_{\text{I}} + (\rho_{\text{R}})_{\text{ortho}}\sigma^\circ_{\text{R}} + \delta_{\text{ortho}}E_{\text{s}}^{\text{B}} \quad (3)$$

$$\delta(^{17}\text{O})_{\text{ortho}} = \delta(^{17}\text{O})_{\text{H}} + (\rho_{\text{I}})_{\text{ortho}}\sigma_{\text{I}} + (\rho_{\text{R}})_{\text{ortho}}\sigma^\circ_{\text{R}} + \delta_{\text{ortho}}\nu \quad (4)$$

Eqs (11) and (12) were used separately for *ortho*-substituted derivatives containing the *ortho* electron-donating +R substituents (X = H, OCH<sub>3</sub>, CH<sub>3</sub>, (CH<sub>3</sub>)<sub>2</sub>, C(CH<sub>3</sub>)<sub>3</sub>, F, Cl, Br)

and derivatives with the *ortho* electron-withdrawing  $-R$  substituents ( $X = \text{H}, \text{NO}_2, \text{CN}, \text{CF}_3, \text{SO}_2\text{CH}_3, \text{CO}_2\text{CH}_3, \text{COCH}_3, 2,6\text{-(NO}_2)_2$ ).

To compare of the substituent effects on the carbonyl oxygen chemical shifts,  $\delta(^{17}\text{O})$ , for *ortho*-, *para*-, and *meta*-substituted phenyl and *alkyl* esters of benzoic acid ( $\text{C}_6\text{H}_5\text{CO}_2\text{C}_6\text{H}_4\text{-X}$ ,  $\text{C}_6\text{H}_5\text{CO}_2\text{R}$ ) with those in the corresponding carbonyl carbon  $^{13}\text{C}$  NMR chemical shifts,  $\delta_{\text{CO}}$ , the infrared stretching frequencies of the carbonyl group,  $\nu_{\text{CO}}$ , and the  $\Delta \log k$  values of the alkaline hydrolysis following relationships were used:

$$\delta(^{17}\text{O})_{\text{ortho}} = \delta(^{17}\text{O})_{\text{H}} + a_{1(\text{ortho})}((\Delta\delta_{\text{CO}})_{\text{X}}(\Delta\nu_{\text{CO}})_{\text{X}}(\Delta \log k)_{\text{X}}) + a_{2(\text{ortho})}\sigma_{\text{R}}^{\circ} + a_{3(\text{ortho})}E_{\text{s}}^{\text{B}} \quad (6)$$

$$\delta(^{17}\text{O})_{\text{para}} = \delta(^{17}\text{O})_{\text{H}} + a_{1(\text{para})}((\Delta\delta_{\text{CO}})_{\text{X}}(\Delta\nu_{\text{CO}})_{\text{X}}(\Delta \log k)_{\text{X}}) + a_{2(\text{para})}\sigma_{\text{R}}^{\circ} \quad (7)$$

$$\delta(^{17}\text{O})_{\text{meta}} = \delta(^{17}\text{O})_{\text{H}} + a_{1(\text{meta})}((\Delta\delta_{\text{CO}})_{\text{X}}(\Delta\nu_{\text{CO}})_{\text{X}}(\Delta \log k)_{\text{X}}) + a_{2(\text{meta})}\sigma_{\text{R}}^{\circ} \quad (8)$$

$$\delta(^{17}\text{O})_{\text{Alk}} = \delta(^{17}\text{O})_{\text{CH}_3} + a_{1(\text{Alk})}((\Delta\delta_{\text{CO}})_{\text{R}}(\Delta\nu_{\text{CO}})_{\text{R}}(\Delta \log k)_{\text{R}}) + a_{2}E_{\text{s}}^{\text{B}} \quad (9)$$

In Eqs (6)-(9)  $(\Delta\delta_{\text{CO}})_{\text{X}} = (\delta_{\text{CO}})_{\text{X}} - (\delta_{\text{CO}})_{\text{H}}$ ,  $(\Delta\nu_{\text{CO}})_{\text{X}} = (\nu_{\text{CO}})_{\text{X}} - (\delta_{\text{CO}})_{\text{H}}$ , and  $\Delta \log k_{\text{X}} = \log k_{\text{H}} - \log k_{\text{X}}$ . In correlations with Eqs (6)-(9) the carbonyl carbon  $^{13}\text{C}$  NMR chemical shifts,  $\delta_{\text{CO}}$ , given in Reference<sup>12</sup>, the IR stretching frequencies of the carbonyl group,  $\nu_{\text{CO}}$ , in Reference<sup>13</sup> and the  $\log k$  values for alkaline hydrolysis in water and aqueous 0.5 M  $\text{Bu}_4\text{NNBr}$  for phenyl benzoates,  $\text{C}_6\text{H}_5\text{CO}_2\text{C}_6\text{H}_4\text{-X}$ , and alkylbenzoates,  $\text{C}_6\text{H}_5\text{CO}_2\text{R}$ , in Reference<sup>5,10,11,51,52</sup> were used.

The slope  $a_1$  in Eqs (6)-(9) is the ratio of the inductive effects in the  $^{17}\text{O}$  NMR chemical shifts and in the corresponding process compared. In Eqs (6)-(9)  $a_1 = \rho_{\text{I}}(^{17}\text{O})/\rho_{\text{I}}(\delta_{\text{CO}})$ ,  $\rho_{\text{I}}(\delta(^{17}\text{O}))/\rho_{\text{I}}(\nu_{\text{CO}})$ ,  $\rho_{\text{I}}(^{17}\text{O})/\rho_{\text{I}}(\text{AH})$ ,  $a_2 = \rho_{\text{R}}(\delta^{17}\text{O}) - a_1\rho_{\text{R}}(\delta_{\text{CO}})$ ,  $\rho_{\text{R}}(\delta^{17}\text{O}) - a_1\rho_{\text{R}}(\nu_{\text{CO}})$ ,  $\rho_{\text{R}}(\delta^{17}\text{O}) - a_1\rho_{\text{R}}(\text{AH})$  and  $a_3 = \delta_{\text{S}}(\delta^{17}\text{O}) - a_1\delta_{\text{S}}(\delta_{\text{CO}})$ ,  $\delta_{\text{S}}(\delta^{17}\text{O}) - a_1\delta_{\text{S}}(\nu_{\text{CO}})$ ,  $\delta_{\text{S}}(\delta^{17}\text{O}) - a_1\delta_{\text{S}}(\text{AH})$ . In relations shown the carbonyl carbon  $^{13}\text{C}$  chemical shifts is denoted by  $(\delta_{\text{CO}})$ , the IR carbonyl stretching frequencies by  $(\nu_{\text{CO}})$ , the alkaline hydrolysis is denoted by (AH), and the susceptibility to the steric factor by  $\delta_{\text{S}}$ .

The results of correlations of the carbonyl and the single-bonded oxygen  $^{17}\text{O}$  NMR chemical shifts,  $\delta(^{17}\text{O})$ , for *para*-, *meta*-, and *ortho*-substituted phenyl esters of benzoic acid,  $\text{C}_6\text{H}_4\text{CO}_2\text{C}_6\text{H}_4\text{-X}$ , and alkyl benzoates,  $\text{C}_6\text{H}_5\text{CO}_2\text{R}$ , with Eqs (6)-(9) are shown in Table IV.