

Supporting Information for:

Mechanistic Studies of La^{3+} and Zn^{2+} -Catalyzed Methanolysis of *O*-Ethyl *O*-aryl methylphosphonate esters. Development of Effective Methods for the
Catalytic Destruction of Phosphonate CW Simulants.

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Physical data for characterization of *O*-ethyl *O*-aryl methylphosphonates **6a-f**

***O*-Ethyl *O*-*p*-Chloro-*o*-nitrophenyl Methylphosphonate 6a**

^1H -NMR (ppm, 400 MHz, d_3 -acetonitrile): δ 8.02 (s, 1H), 7.70 (d, $J = 8.0$ Hz, 1H), 7.54 (d, $J = 8.0$ Hz, 1H), 4.18 (m, $J = 8.0$ Hz, 2 Hz), 1.70 (d, $J = 16$ Hz, 3H), 1.30 (t, $J = 8.0$ Hz, 3H)

$^{31}\text{P}\{^1\text{H}\}$ -NMR (ppm, 400 MHz, d_3 -acetonitrile): δ 29.95

MS (TOF MS): m/z 301.99577 (M+Na)

Anal. Calc. for $\text{C}_9\text{H}_{11}\text{NO}_5\text{NaP}$: m/z 301.99610

***O*-Ethyl *O*-*p*-Nitrophenyl Methylphosphonate 6b**

^1H -NMR (ppm, 400 MHz, d_3 -acetonitrile): δ 8.26 (d, $J = 8.0$ Hz, 2H), 7.43 (d, $J = 8.0$ Hz, 2H), 4.20 (m, $J = 6$ Hz, 2H), 1.685 (d, $J = 20$, 3H), 1.32 (t, $J = 6$ Hz, 3H)

$^{31}\text{P}\{^1\text{H}\}$ -NMR (ppm, 400 MHz, d_3 -acetonitrile): δ 28.54

MS (TOF MS): m/z 268.03555 (M+Na)

Anal. Calc. for $\text{C}_9\text{H}_{12}\text{NO}_5\text{NaP}$: m/z 268.03508

O-Ethyl O-m-Nitrophenyl Methylphosphonate 6c

¹H-NMR (ppm, 400 MHz, d₃-acetonitrile): δ 8.08 (m, 2H), 7.635 (m, 2H), 4.20 (m, J = 8.0 Hz, 2H), 1.675 (d, J = 20 Hz, 3H), 1.32 (t, J = 8.0 Hz, 3H)

³¹P{¹H}-NMR (ppm, 400 MHz, d₃-acetonitrile): δ 28.82

MS (TOF MS): m/z 268.03294 (M+Na)

Anal. Calc. for C₉H₁₂NO₅NaP: m/z 268.03508

O-Ethyl O-p-Chlorophenyl Methylphosphonate 6d

¹H-NMR (ppm, 400 MHz, d₃-acetonitrile): δ 7.40 (d, J = 10 Hz, 2H), 7.215 (d, J = 10 Hz, 2H), 4.15 (m, J = 6.0 Hz, 2H), 1.61 (d, J = 16 Hz, 3H), 1.30 (t, J = 6.0 Hz, 3H)

³¹P{¹H}-NMR (ppm, 400 MHz, d₃-acetonitrile): δ 28.02

MS (TOF MS): m/z 257.01005 (M+Na)

Anal. Calc. for C₉H₁₂O₃NaPCl: m/z 257.01103

O-Ethyl O-Phenyl Methylphosphonate 6e

¹H-NMR (ppm, 400 MHz, d₃-acetonitrile): δ 7.41 (t, J = 8.0 Hz, 2H), 7.23 (m, J = 8.0 Hz, 3H), 4.16 (m, J = 8.0 Hz, 2H), 1.60 (d, J = 16 Hz, 3H), 1.30 (t, J = 8.0 Hz, 3H)

³¹P{¹H}-NMR (ppm, 400 MHz, d₃-acetonitrile): δ 27.50

MS (TOF MS): m/z 201.06726 (M+H)

Anal. Calc for C₉H₁₄O₃P: m/z 201.04211

O-Ethyl O-p-Methoxyphenyl Methylphosphonate 6f

¹H-NMR (ppm, 400 MHz, d₃-acetonitrile): δ 7.13 (d, J = 10 Hz, 2H), 6.925 (d, J = 10 Hz, 2H), 4.145 (m, J = 6.0 Hz, 2H), 1.57 (d, J = 8.0 Hz, 3H), 1.30 (t, J = 6.0 Hz, 3H)

³¹P{¹H}-NMR (ppm, 400 MHz, d₃-acetonitrile): δ 27.76

MS (TOF MS): m/z 231.07210 (M+H)

Anal. Calc. for C₁₀H₁₆O₄P: m/z 231.07862