# Benzene-1,3-Dihydrogensulfate as a Non-Cyclic Ionophore: Selective Extraction and Transport of Metal Ions

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## SUPPLEMENTARY INFORMATION

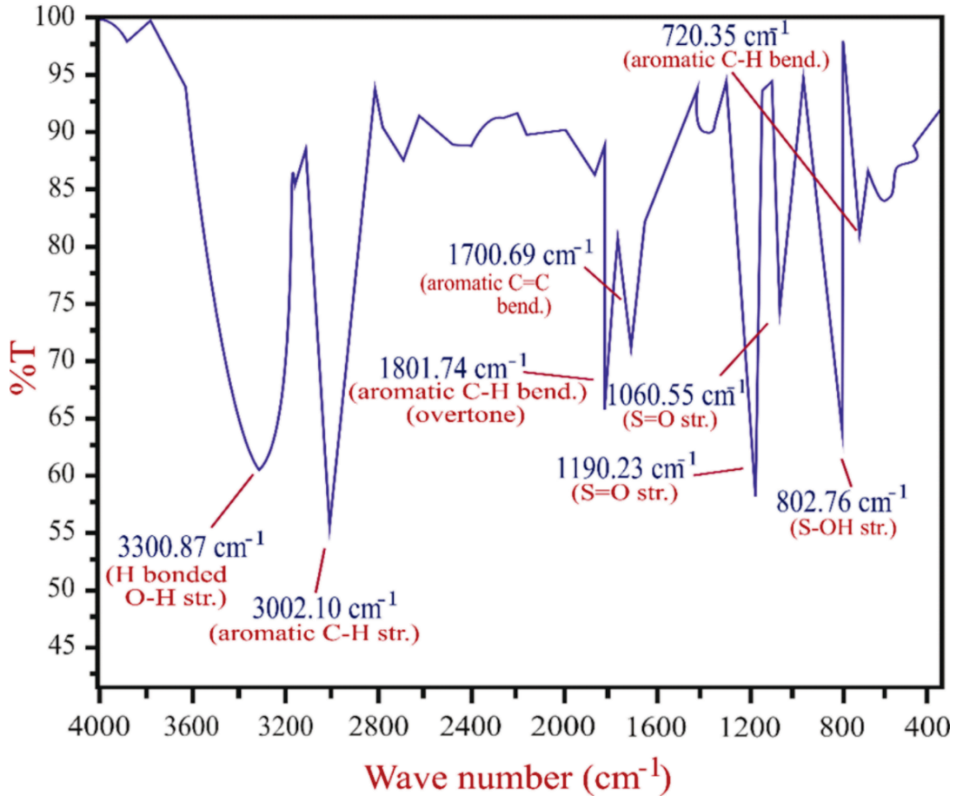



**Figure S1.** IR spectrum of benzene-1,3-dihydrogensulfate.

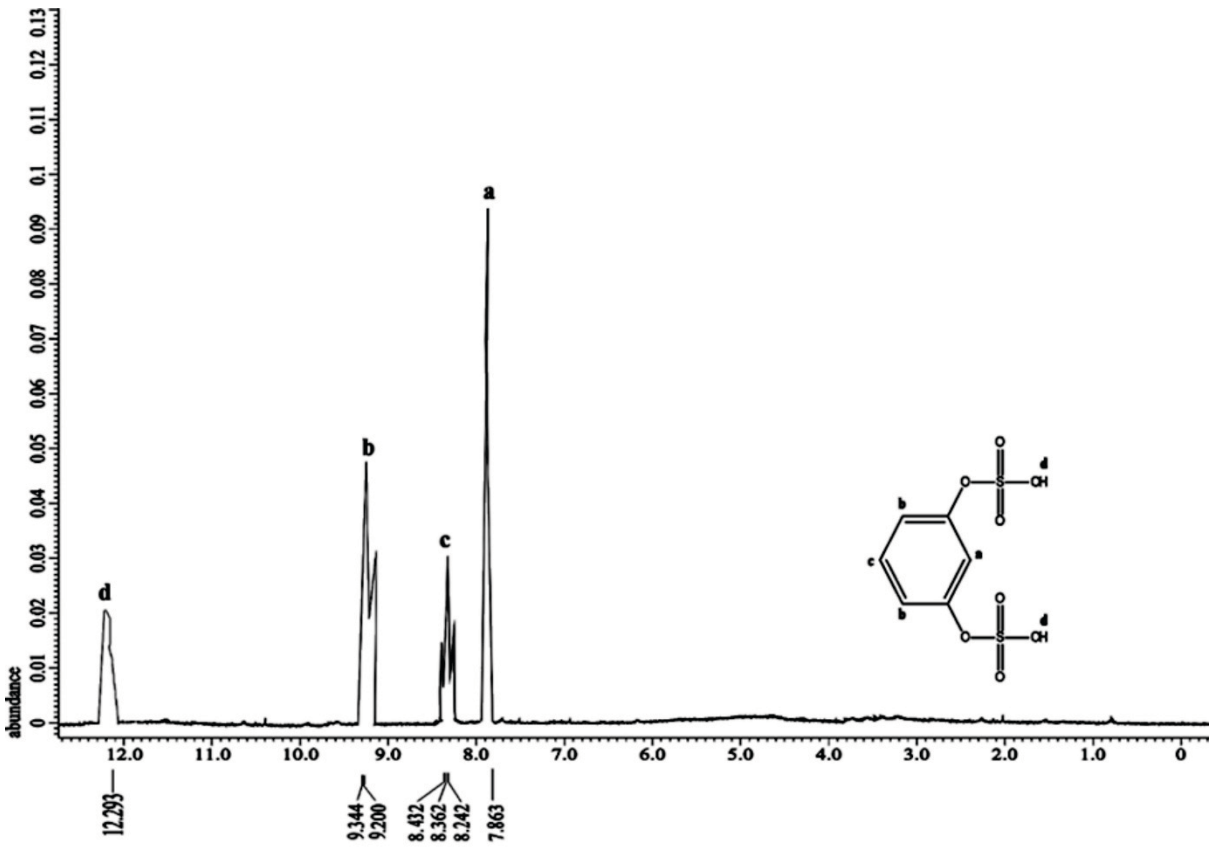



**Figure 2.** $^{1}$H NMR spectrum of benzene-1,3-dihydrogensulfate.

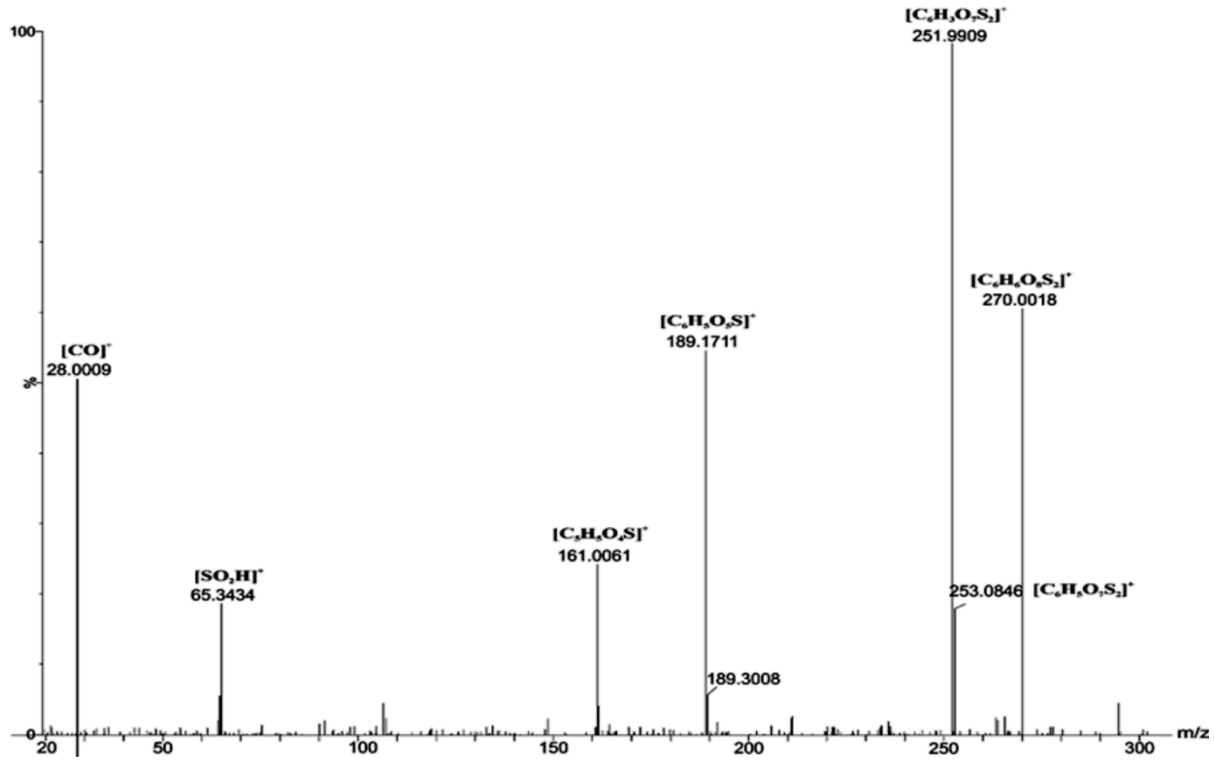
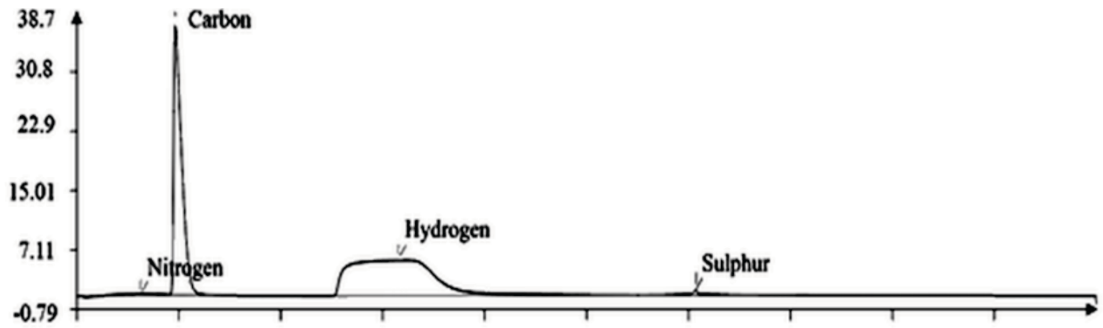



**Figure 3.** Mass spectrum benzene-1,3-dihydrogensulfate.




| Peak Number (#) | Retention Time (min) | Area (.1* uV * sec) | Element % | Component Name |
|---|---|---|---|---|
| 1 | 0.767 | 97082 | 0.0005 | Nitrogen |
| 2 | 1.158 | 2316367 | 26.5789 | Carbon |
| 3 | 3.892 | 3373631 | 2.1908 | Hydrogen |
| 4 | 7.292 | 50927 | 23.7989 | Sulphur |
| | | 0.531 | 52.5691 | |

**Figure 4.** Elemental analysis of benzene-1,3-dihydrogensulfate.

**Table 1.** Extraction of metal ions from picrate, dinitrophenolate, and *o*-nitrophenolate salts into chloroform.

| Metal Ion | Parameter | picrate | dinitrophenolate | *o*-nitrophenolate |
|---|---|---|---|---|
| **$Zn^{2+}$** | R1 | 0.35 | 0.32 | 0.05 |
| | R2 | 0.32 | 0.29 | 0.05 |
| | R3 | 0.31 | 0.30 | 0.04 |
| | **Mean(ppm)** | **0.33** | **0.30** | **0.05** |
| **$Na^{+}$** | R1 | 0.70 | 0.28 | 0.07 |
| | R2 | 0.69 | 0.29 | 0.06 |
| | R3 | 0.65 | 0.28 | 0.05 |
| | **Mean(ppm)** | **0.68** | **0.28** | **0.06** |
| **$K^{+}$** | R1 | 0.48 | 0.19 | 0.03 |
| | R2 | 0.47 | 0.17 | 0.02 |
| | R3 | 0.44 | 0.19 | 0.03 |
| | **Mean(ppm)** | **0.46** | **0.18** | **0.03** |
| **$Ni^{2+}$** | R1 | 0.30 | 0.21 | 0.04 |
| | R2 | 0.31 | 0.20 | 0.04 |
| | R3 | 0.32 | 0.21 | 0.04 |
| | **Mean(ppm)** | **0.31** | **0.21** | **0.04** |

**Table 2.** Extraction of metal ions from picrate, dinitrophenolate, and *o*-nitrophenolate salts into 1,2-dichloroethane membranes.

| **Metal Ion** | **Parameter** | **picrate** | **dinitrophenolate** | ***o*-nitrophenolate** |
|---|---|---|---|---|
| **$Zn^{2+}$** | R1 | 0.42 | 0.21 | 0.15 |
| | R2 | 0.41 | 0.19 | 0.16 |
| | R3 | 0.42 | 0.21 | 0.15 |
| | **Mean(ppm)** | **0.42** | **0.20** | **0.15** |
| **$Na^{+}$** | R1 | 0.68 | 0.25 | 0.11 |
| | R2 | 0.65 | 0.24 | 0.09 |
| | R3 | 0.67 | 0.25 | 0.10 |
| | **Mean(ppm)** | **0.67** | **0.25** | **0.10** |
| **$K^{+}$** | R1 | 0.55 | 0.18 | 0.08 |
| | R2 | 0.52 | 0.19 | 0.09 |
| | R3 | 0.54 | 0.18 | 0.08 |
| | **Mean(ppm)** | **0.54** | **0.18** | **0.08** |
| **$Ni^{2+}$** | R1 | 0.35 | 0.2 | 0.12 |
| | R2 | 0.34 | 0.21 | 0.11 |
| | R3 | 0.33 | 0.22 | 0.11 |
| | **Mean(ppm)** | **0.34** | **0.21** | **0.11** |

**Table 3.** Transport of metal ions from picrate, dinitrophenolate, and *o*-nitrophenolate salts into chloroform membrane.

| Metal Ion | Parameter | picrate | dinitrophenolate | *o*-nitrophenolate |
|---|---|---|---|---|
| **$Zn^{2+}$** | R1 | 0.91 | 0.52 | 0.02 |
| | R2 | 0.89 | 0.53 | 0.01 |
| | R3 | 0.88 | 0.52 | 0.02 |
| | **Mean(ppm)** | **0.89** | **0.52** | **0.02** |
| **$Na^{+}$** | R1 | 1.39 | 0.88 | 0.03 |
| | R2 | 1.35 | 0.87 | 0.01 |
| | R3 | 1.37 | 0.89 | 0.02 |
| | **Mean(ppm)** | **1.37** | **0.88** | **0.02** |
| **$K^{+}$** | R1 | 1.22 | 0.79 | 0.05 |
| | R2 | 1.20 | 0.79 | 0.04 |
| | R3 | 1.22 | 0.78 | 0.05 |
| | **Mean(ppm)** | **1.21** | **0.79** | **0.05** |
| **$Ni^{2+}$** | R1 | 0.51 | 0.32 | 0.01 |
| | R2 | 0.48 | 0.30 | 0.00 |
| | R3 | 0.49 | 0.29 | 0.01 |
| | **Mean(ppm)** | **0.49** | **0.30** | **0.01** |

**Table 4.** Transport of metal ions from picrate, dinitrophenolate and *o*-nitrophenolate salts into 1,2-dichloroethane membrane.

| Metal Ion | Parameter | Picrate | dinitrophenolate | *o*-nitrophenolate |
|---|---|---|---|---|
| **$Zn^{2+}$** | R1 | 0.98 | 0.87 | 0.11 |
| | R2 | 0.96 | 0.85 | 0.09 |
| | R3 | 0.96 | 0.85 | 0.10 |
| | **Mean(ppm)** | **0.97** | **0.86** | **0.10** |
| **$Na^{+}$** | R1 | 1.46 | 1.08 | 0.04 |
| | R2 | 1.44 | 1.06 | 0.03 |
| | R3 | 1.45 | 1.06 | 0.03 |
| | **Mean(ppm)** | **1.45** | **1.07** | **0.03** |
| **$K^{+}$** | R1 | 1.26 | 1.11 | 0.10 |
| | R2 | 1.20 | 1.10 | 0.09 |
| | R3 | 1.23 | 1.09 | 0.09 |
| | **Mean(ppm)** | **1.23** | **1.10** | **0.09** |
| **$Ni^{2+}$** | R1 | 0.62 | 0.55 | 0.01 |
| | R2 | 0.60 | 0.52 | 0.00 |
| | R3 | 0.62 | 0.53 | 0.01 |
| | **Mean(ppm)** | **0.61** | **0.53** | **0.01** |

**Table 5.** Spectral and elemental analysis data of ionophore

| Analysis Type | Key Findings |
|---|---|
| **IR Spectrum ($cm^{-1}$)** | 720.35 (aromatic C-H), 802.76 (S-OH stretching), 1190.23 and 1060.55 (S=O stretching), 1700.69 (aromatic C=C bending), 1801.74 (aromatic C-H bending, overtone), 3002.10 (aromatic C-H stretching), 3300.87 (H bonded O-H stretching) |
| **$^1$H-NMR (δ, ppm)** | 7.9 (s, 1H, CH), 9.2-9.3 (d, 1H, CH), 8.2-8.4 (t, 1H, CH), 12.0-12.3 (br, 1H, OH) |
| **Mass Spectrum (m/z)** | Calculated: 270.2384, Found: 270.0018 |
| **Elemental Analysis (%)** | Found: C 26.58; H 2.19; S 23.8. Calculated: C 26.67; H 2.22; S 23.7 |

**Coordinates from wxMacMolPlt**

| | | | | |
|---|---|---|---|---|
| C | 6.0 | -4.22105789 | 2.56104136 | 0.87929606 |
| C | 6.0 | -3.78582478 | 3.06105185 | 2.10459566 |
| C | 6.0 | -3.82661891 | 1.32444715 | 0.38240701 |
| C | 6.0 | -2.94572186 | 0.55710131 | 1.14697719 |
| H | 1.0 | -4.20384407 | 0.97606522 | -0.57165587 |
| C | 6.0 | -2.46966314 | 1.02734649 | 2.37027550 |
| H | 1.0 | -2.62313795 | -0.41402283 | 0.78671163 |
| C | 6.0 | -2.89707589 | 2.27168226 | 2.82995582 |
| H | 1.0 | -4.14578962 | 4.01444197 | 2.46638036 |
| O | 8.0 | -5.17554140 | 3.31973147 | 0.16655333 |
| H | 1.0 | -1.78084779 | 0.44589975 | 2.97276664 |
| O | 8.0 | -2.38414860 | 2.62434483 | 4.09527683 |
| S | 16.0 | -4.66585493 | 4.29821396 | -1.04557037 |
| S | 16.0 | -2.25384045 | 4.16454315 | 4.62257147 |
| O | 8.0 | -5.89506721 | 4.78596926 | -1.64086330 |
| O | 8.0 | -3.63000298 | 3.64115834 | -1.81722879 |
| O | 8.0 | -1.42265844 | 4.05043650 | 5.80344057 |
| O | 8.0 | -3.56048155 | 4.79236174 | 4.65689278 |
| O | 8.0 | -3.91954684 | 5.48352718 | -0.24967983 |
| H | 1.0 | -4.57415247 | 6.13096380 | 0.07627337 |
| O | 8.0 | -1.46493208 | 4.88559580 | 3.42304635 |
| H | 1.0 | -0.50483137 | 4.71732950 | 3.48836708 |

**Energies in solvent**

FREE ENERGY IN SOLVENT = <PSI| H(0)+V/2 |PSI> = -1629.7674850920 A.U.

INTERNAL ENERGY IN SOLVENT = <PSI| H(0) |PSI> = -1629.7412170299 A.U.

DELTA INTERNAL ENERGY = <D-PSI| H(0) |D-PSI> = 0.0000000000 A.U.

ELECTROSTATIC INTERACTION = -0.0262680621 A.U.

PIEROTTI CAVITATION ENERGY = 0.0000000000 A.U.

DISPERSION FREE ENERGY = 0.0000000000 A.U.

REPULSION FREE ENERGY = 0.0000000000 A.U.

TOTAL INTERACTION (DELTA + ES + CAV + DISP + REP) = -0.0262680621 A.U.

TOTAL FREE ENERGY IN SOLVENT = -1629.7674850920 A.U.

FREE ENERGY IN SOLVENT = -1022694.65 KCAL/MOL

INTERNAL ENERGY IN SOLVENT = -1022678.16 KCAL/MOL

DELTA INTERNAL ENERGY = 0.00 KCAL/MOL

ELECTROSTATIC INTERACTION = -16.48 KCAL/MOL

PIEROTTI CAVITATION ENERGY = 0.00 KCAL/MOL

DISPERSION FREE ENERGY = 0.00 KCAL/MOL

REPULSION FREE ENERGY = 0.00 KCAL/MOL

TOTAL INTERACTION = -16.48 KCAL/MOL

TOTAL FREE ENERGY IN SOLVENT = -1022694.65 KCAL/MOL