

Search Overview

Search: search4
Date/Time done: Sat Oct 23 06:44:11 2010
Database(s): CSD version 5.31 (November 2009)
CSD version 5.31 updates (Nov 2009)
CSD version 5.31 updates (Feb 2010)
CSD version 5.31 updates (May 2010)
CSD version 5.31 updates (Aug 2010)
Restriction Info: No refcode restrictions applied
Filters: 3D coordinates determined R factor <= 0.1
No powder structures Only Organics
Percentage Completed: 100%
Number of Hits: 73

Summary of queries used. Search found structures that:

match

Query 1

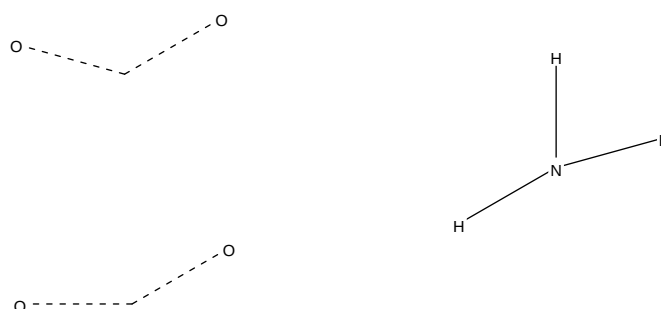
Query 2

do not match

Query 3

Query 4

Query 1



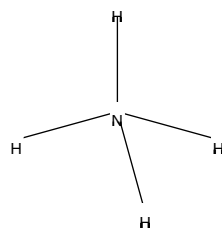
Query 2

Formula **O₄N₂C₁₋₄₀H₂₋₈₀**
Search on: **Sum of molecules**
Allow other elements: **Yes**

Query 3

Formula **N₂**
Search on: **each molecule in turn**
Allow other elements: **Yes**

Query 4



Search: search4 (Sat Oct 23 06:44:11 2010): Hits 1-4

BUCQAR

Reference: T.Odani, A.Matsumoto, K.Sada, M.Miyata (2001)
Chem.Commun. , 2004

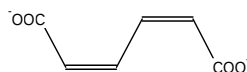
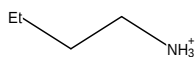
Formula: $2(\text{C}_4 \text{H}_{12} \text{N}_1^{1+}), \text{C}_6 \text{H}_4 \text{O}_4^{2-}$

Compound Name: bis(n-Butylammonium) (Z,Z)-hexa-2,4-diene-1,6-dioate

Synonym: bis(n-Butylammonium) (Z,Z)-muconate

Space Group: P21/n
Space Group No.: 14
Cell: $(\text{\AA}, ^\circ)$
 α 5.772(0) β 20.005(1) γ 14.749(1)
 α 90.00 β 96.51(0) γ 90.00

R-Factor (%): 6.33
Temperature(K): 200
Density(g/cm³): 1.132



BUCQEV

Reference: T.Odani, A.Matsumoto, K.Sada, M.Miyata (2001)
Chem.Commun. , 2004

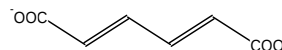
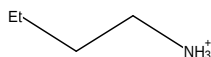
Formula: $2(\text{C}_4 \text{H}_{12} \text{N}_1^{1+}), \text{C}_6 \text{H}_4 \text{O}_4^{2-}$

Compound Name: bis(n-Butylammonium) (E,E)-hexa-2,4-diene-1,6-dioate

Synonym: bis(n-Butylammonium) (E,E)-muconate

Space Group: P-1
Space Group No.: 2
Cell: $(\text{\AA}, ^\circ)$
 α 5.525(0) β 7.433(1) γ 10.865(2)
 α 98.88(1) β 100.86(1) γ 104.38(1)

R-Factor (%): 4.60
Temperature(K): 296
Density(g/cm³): 1.154



IDOGUE

Reference: K.Ejsmont, J.Zaleski (2006)
Acta Crystallogr., Sect.E: Struct. Rep. Online , **62**, o2512

Formula: $2(\text{C}_4 \text{H}_{12} \text{N}_1^{1+}), \text{C}_2 \text{O}_4^{2-}$

Compound Name: bis(t-Butylammonium) oxalate

Space Group: C2/m
Space Group No.: 12
Cell: $(\text{\AA}, ^\circ)$
 α 11.264(2) β 7.512(1) γ 9.324(1)
 α 90.00 β 111.91(1) γ 90.00

R-Factor (%): 3.54
Temperature(K): 298
Density(g/cm³): 1.072



JEKJAL

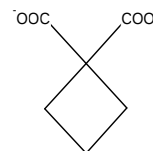
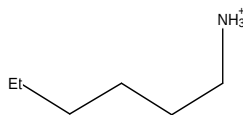
Reference: A.Ballabh, D.R.Trivedi, P.Dastidar (2006) *Org.Lett.* , **8**, 1271

Formula: $2(\text{C}_6 \text{H}_{16} \text{N}_1^{1+}), \text{C}_6 \text{H}_6 \text{O}_4^{2-}$

Compound Name: bis(hexylammonium) cyclobutane-1,1-dicarboxylate

Space Group: P21/c
Space Group No.: 14
Cell: $(\text{\AA}, ^\circ)$
 α 10.545(1) β 13.643(1) γ 29.180(3)
 α 90.00 β 99.87(0) γ 90.00

R-Factor (%): 6.42
Temperature(K): 100
Density(g/cm³): 1.113



Search: search4 (Sat Oct 23 06:44:11 2010): Hits 5-8

JEKJEP

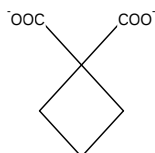
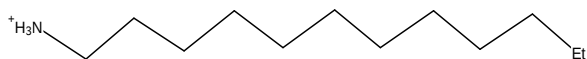
Reference: A.Ballabh, D.R.Trivedi, P.Dastidar (2006) *Org.Lett.* ,8,1271

Formula: $2(\text{C}_{12}\text{H}_{28}\text{N}_1^{1+}), \text{C}_6\text{H}_6\text{O}_4^{2-}$

Compound Name: bis(dodecylammonium) cyclobutane-1,1-dicarboxylate

Space Group: P21/c
Space Group No.: 14
Cell: (Å, °)
 α 7.099(1)
 β 43.266(7)
 γ 10.568(1)
 α 90.00
 β 91.74(0)
 γ 90.00

R-Factor (%): 6.15
Temperature(K): 293
Density(g/cm³): 1.054



JEKJIT

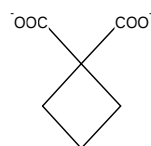
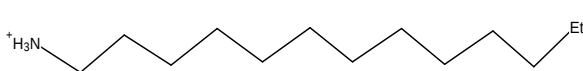
Reference: A.Ballabh, D.R.Trivedi, P.Dastidar (2006) *Org.Lett.* ,8,1271

Formula: $2(\text{C}_{13}\text{H}_{30}\text{N}_1^{1+}), \text{C}_6\text{H}_6\text{O}_4^{2-}$

Compound Name: bis(tridecylammonium) cyclobutane-1,1-dicarboxylate

Space Group: P21/c
Space Group No.: 14
Cell: (Å, °)
 α 7.071(0)
 β 45.852(3)
 γ 10.697(0)
 α 90.00
 β 91.54(0)
 γ 90.00

R-Factor (%): 7.10
Temperature(K): 293
Density(g/cm³): 1.040



JEKJOZ

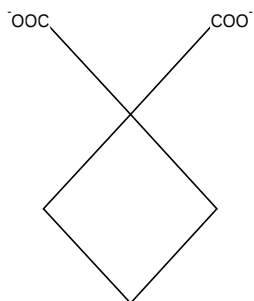
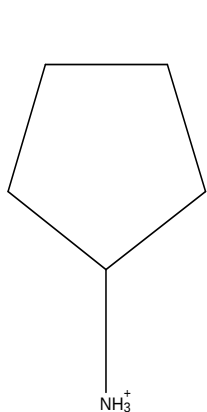
Reference: A.Ballabh, D.R.Trivedi, P.Dastidar (2006) *Org.Lett.* ,8,1271

Formula: $2(\text{C}_5\text{H}_{12}\text{N}_1^{1+}), \text{C}_6\text{H}_6\text{O}_4^{2-}$

Compound Name: bis(cyclopentylammonium) cyclobutane-1,1-dicarboxylate

Space Group: P-1
Space Group No.: 2
Cell: (Å, °)
 α 10.774(0)
 β 12.471(0)
 γ 14.930(1)
 α 68.44(0)
 β 71.44(0)
 γ 68.55(0)

R-Factor (%): 5.32
Temperature(K): 293
Density(g/cm³): 1.231



JEKJUF

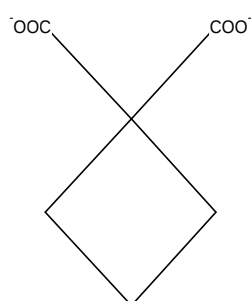
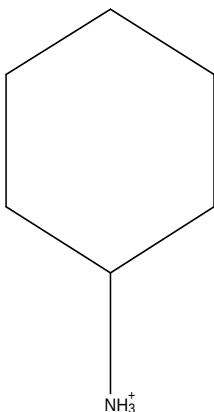
Reference: A.Ballabh, D.R.Trivedi, P.Dastidar (2006) *Org.Lett.* ,8,1271

Formula: $2(\text{C}_6\text{H}_{14}\text{N}_1^{1+}), \text{C}_6\text{H}_6\text{O}_4^{2-}$

Compound Name: bis(cyclohexylammonium) cyclobutane-1,1-dicarboxylate

Space Group: P21/c
Space Group No.: 14
Cell: (Å, °)
 α 30.215(2)
 β 15.406(1)
 γ 26.042(1)
 α 90.00
 β 110.10(0)
 γ 90.00

R-Factor (%): 5.26
Temperature(K): 293
Density(g/cm³): 1.199



Search: search4 (Sat Oct 23 06:44:11 2010): Hits 9-12

JIPKOJ

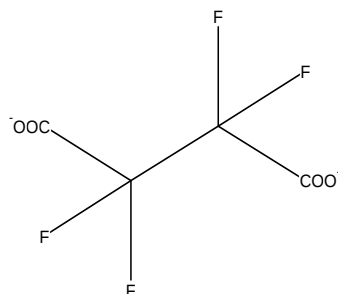
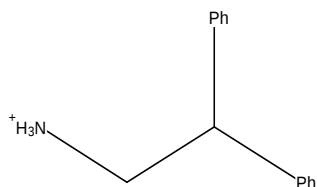
Reference: S.Parsons, N.Casati, D.Leigh (2007)
Private Communication ,

Formula: $2(\text{C}_{14}\text{H}_{16}\text{N}_1^{1+})\cdot\text{C}_4\text{F}_4\text{O}_4^{2-}$

Compound Name: bis(2,2-Diphenylethylammonium) tetrafluorosuccinate

Space Group: P21/c **Cell:** **a** 13.996(2) **b** 11.803(2) **c** 8.916(1)
Space Group No.: 14 **(Å,°)** α 90.00 β 101.37(0) γ 90.00

R-Factor (%): 5.32 **Temperature(K):** 150 **Density(g/cm³):** 1.345



KOLMAA

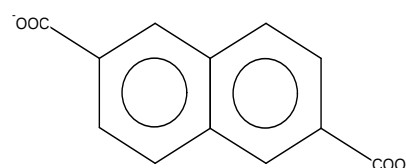
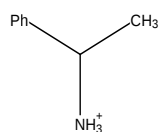
Reference: A.Lemmerer, S.Bourne, M.A.Fernandes (2008)
CrystEngComm ,10,1605

Formula: $2(\text{C}_8\text{H}_{12}\text{N}_1^{1+})\cdot\text{C}_{12}\text{H}_6\text{O}_4^{2-}$

Compound Name: bis((R)-1-Phenylethylammonium) naphthalene-2,6-dicarboxylate

Space Group: P21 **Cell:** **a** 9.663(0) **b** 6.373(0) **c** 19.721(0)
Space Group No.: 4 **(Å,°)** α 90.00 β 96.04(0) γ 90.00

R-Factor (%): 3.29 **Temperature(K):** 173 **Density(g/cm³):** 1.261



KONBAR

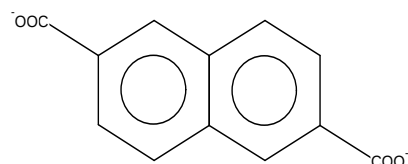
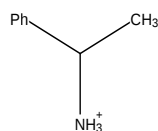
Reference: A.Lemmerer, S.Bourne, M.A.Fernandes (2008)
CrystEngComm ,10,1605

Formula: $2(\text{C}_8\text{H}_{12}\text{N}_1^{1+})\cdot\text{C}_{12}\text{H}_6\text{O}_4^{2-}$

Compound Name: bis((S)-1-Phenylethylammonium) naphthalene-2,6-dicarboxylate

Space Group: P21 **Cell:** **a** 9.666(1) **b** 6.371(0) **c** 19.708(2)
Space Group No.: 4 **(Å,°)** α 90.00 β 96.03(0) γ 90.00

R-Factor (%): 5.79 **Temperature(K):** 173 **Density(g/cm³):** 1.262



KONBEV

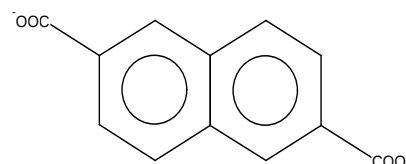
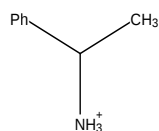
Reference: A.Lemmerer, S.Bourne, M.A.Fernandes (2008)
CrystEngComm ,10,1605

Formula: $2(\text{C}_8\text{H}_{12}\text{N}_1^{1+})\cdot\text{C}_{12}\text{H}_6\text{O}_4^{2-}$

Compound Name: bis((RS)-1-Phenylethylammonium) naphthalene-2,6-dicarboxylate

Space Group: P-1 **Cell:** **a** 6.121(0) **b** 9.648(0) **c** 10.581(1)
Space Group No.: 2 **(Å,°)** α 94.48(0) β 98.50(0) γ 103.13(0)

R-Factor (%): 5.04 **Temperature(K):** 173 **Density(g/cm³):** 1.274



Search: search4 (Sat Oct 23 06:44:11 2010): Hits 13-16

LAYGAT

Reference: A.Matsumoto, T.Odani, M.Chikada, K.Sada, M.Miyata (1999) *J.Am.Chem.Soc.* ,**121**,11122

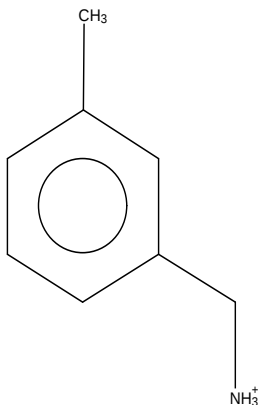
Formula: $2(\text{C}_8\text{H}_{12}\text{N}_1^{1+}), \text{C}_6\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(3-Methylbenzylammonium) 2,4-hexadienedioate

Synonym: bis(3-Methylbenzylammonium) (Z,Z)-muconate

Space Group: P21/a **Cell:** **a** 8.614(2) **b** 13.731(4) **c** 8.795(3)
Space Group No.: 14 **(Å,°)** α 90.00 β 103.06(2) γ 90.00

R-Factor (%): 4.44 **Temperature(K)**: 295 **Density(g/cm³)**: 1.260



LAYKAX

Reference: A.Matsumoto, T.Odani, M.Chikada, K.Sada, M.Miyata (1999) *J.Am.Chem.Soc.* ,**121**,11122

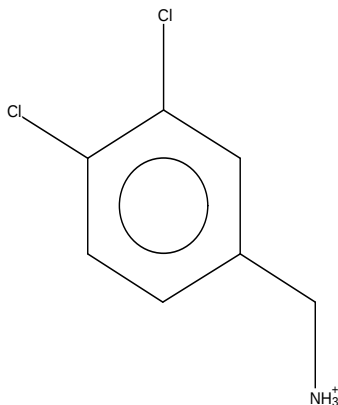
Formula: $2(\text{C}_7\text{H}_8\text{Cl}_2\text{N}_1^{1+}), \text{C}_6\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(3,4-Dichlorobenzylammonium) 2,4-hexadienedioate

Synonym: bis(3,4-Dichlorobenzylammonium) (Z,Z)-muconate

Space Group: P21/a **Cell:** **a** 8.842(1) **b** 13.678(2) **c** 9.902(0)
Space Group No.: 14 **(Å,°)** α 90.00 β 108.79(0) γ 90.00

R-Factor (%): 7.20 **Temperature(K)**: 295 **Density(g/cm³)**: 1.448



NARDIT

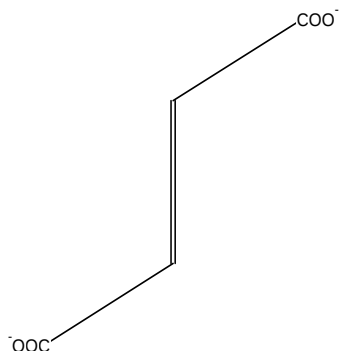
Reference: H.Hosomi, Y.Ito, S.Ohba (1998) *Acta Crystallogr., Sect.C:Cryst.Struct.Comm.* ,**54**,142

Formula: $\text{C}_4\text{H}_2\text{O}_4^{2-} \cdot 2(\text{C}_3\text{H}_{10}\text{N}_1^{1+})$

Compound Name: bis(Isopropylammonium) fumarate

Space Group: P21/n **Cell:** **a** 7.236(2) **b** 6.275(2) **c** 15.460(2)
Space Group No.: 14 **(Å,°)** α 90.00 β 99.55(1) γ 90.00

R-Factor (%): 4.50 **Temperature(K)**: 295 **Density(g/cm³)**: 1.124



PIHWOS

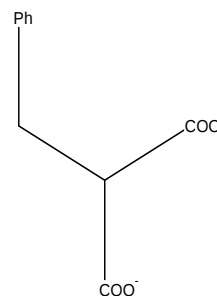
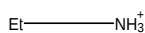
Reference: J.V.Beach, K.J.Shea (1994) *J.Am.Chem.Soc.* ,**116**,379

Formula: $2(\text{C}_2\text{H}_8\text{N}_1^{1+}), \text{C}_{10}\text{H}_8\text{O}_4^{2-}$

Compound Name: bis(Ethylammonium) benzylmalonate

Space Group: Pbca **Cell:** **a** 10.626(1) **b** 13.889(2) **c** 21.794(2)
Space Group No.: 61 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.80 **Temperature(K)**: 295 **Density(g/cm³)**: 1.174



Search: search4 (Sat Oct 23 06:44:11 2010): Hits 17-20

QEJWAE

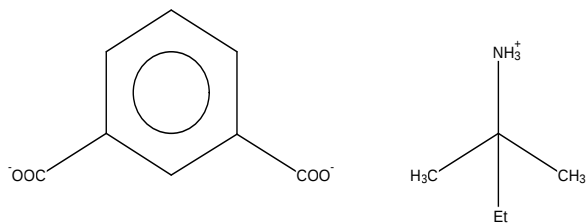
Reference: T.Yuge, M.Miyata, N.Tohnai (2006) *Cryst.Growth Des.* , **6**, 1271

Formula: $2(\text{C}_5\text{H}_{14}\text{N}_1^{1+})\cdot\text{C}_8\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(t-pentylammonium) isophthalate

Space Group: P21/c **Cell:** **a** 17.870(3) **b** 6.252(0) **c** 18.688(3)
Space Group No.: 14 **Cell:** **(Å,°)** α 90.00 β 111.01(1) γ 90.00

R-Factor (%): 5.27 **Temperature(K)**: 213 **Density(g/cm³)**: 1.160



QEJWEI

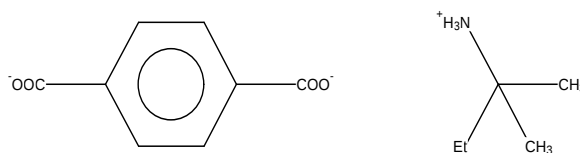
Reference: T.Yuge, M.Miyata, N.Tohnai (2006) *Cryst.Growth Des.* , **6**, 1271

Formula: $2(\text{C}_5\text{H}_{14}\text{N}_1^{1+})\cdot\text{C}_8\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(t-pentylammonium) terephthalate

Space Group: P21/n **Cell:** **a** 8.345(1) **b** 6.440(0) **c** 18.615(3)
Space Group No.: 14 **Cell:** **(Å,°)** α 90.00 β 96.02(1) γ 90.00

R-Factor (%): 5.21 **Temperature(K)**: 213 **Density(g/cm³)**: 1.137



QIYJOY

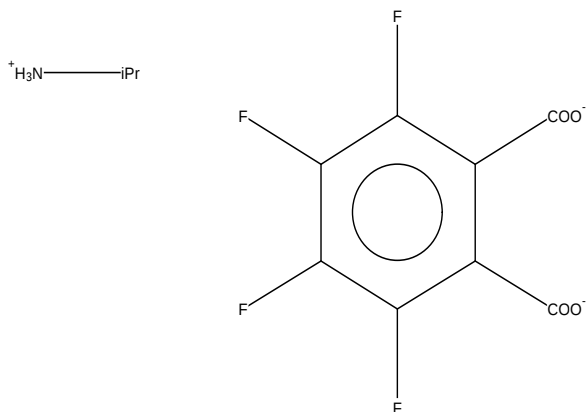
Reference: M.Pietsch, H.-G.Hacker, G.Schnakenburg, W.Hoffbauer, M.Nieger, M.Gutschow (2008) *J.Mol.Struct.* , **878**,131

Formula: $2(\text{C}_3\text{H}_{10}\text{N}_1^{1+})\cdot\text{C}_8\text{F}_4\text{O}_4^{2-}$

Compound Name: bis(isopropylammonium) tetrafluorophthalate

Space Group: C2/c **Cell:** **a** 12.196(1) **b** 19.608(2) **c** 7.339(0)
Space Group No.: 15 **Cell:** **(Å,°)** α 90.00 β 103.18(0) γ 90.00

R-Factor (%): 3.45 **Temperature(K)**: 123 **Density(g/cm³)**: 1.385



SOJMOT

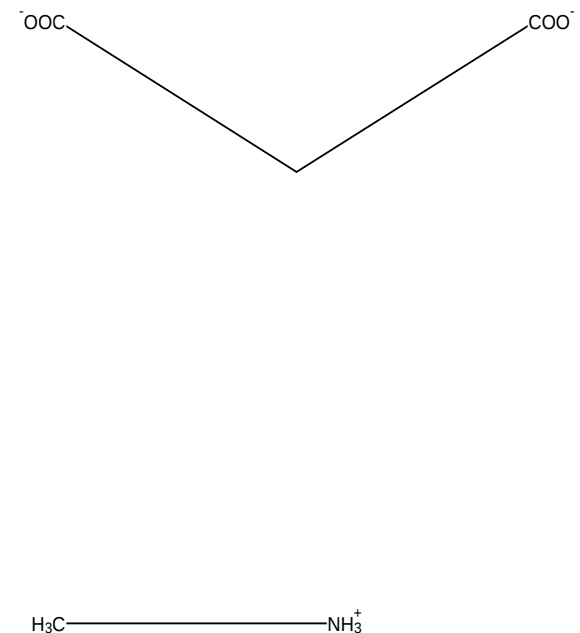
Reference: K.Djinovic, L.Golic (1991) *Acta Crystallogr., Sect.C:Cryst.Struct.Comm.* , **47**,2367

Formula: $\text{C}_3\text{H}_2\text{O}_4^{2-}\cdot 2(\text{C}_1\text{H}_6\text{N}_1^{1+})$

Compound Name: Methylammonium malonate(ii)

Space Group: P21/c **Cell:** **a** 9.185(1) **b** 11.225(1) **c** 8.810(1)
Space Group No.: 14 **Cell:** **(Å,°)** α 90.00 β 97.05(1) γ 90.00

R-Factor (%): 3.40 **Temperature(K)**: 295 **Density(g/cm³)**: 1.224



Search: search4 (Sat Oct 23 06:44:11 2010): Hits 21-24

SOVVEF

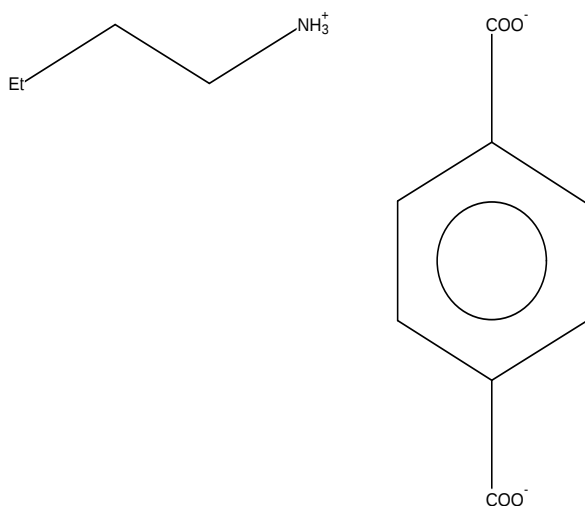
Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_4\text{H}_{12}\text{N}_1^{1+})\cdot\text{C}_8\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(n-Butylammonium) terephthalate

Space Group: P21/n **Cell:** a 10.027(0) b 6.133(1) c 14.146(1)
Space Group No.: 14 **Cell:** ($^\circ$) α 90.00 β 106.95(1) γ 90.00

R-Factor (%): 5.47 **Temperature(K)**: 173 **Density(g/cm³)**: 1.247



SOVVIJ

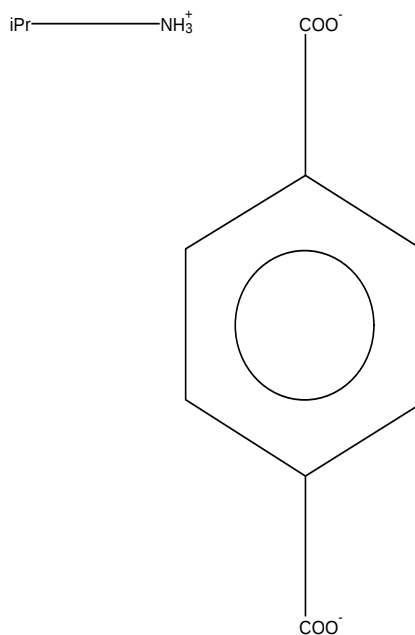
Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_3\text{H}_{10}\text{N}_1^{1+})\cdot\text{C}_8\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(Isopropylammonium) terephthalate

Space Group: C2/c **Cell:** a 20.784(3) b 6.372(0) c 13.321(2)
Space Group No.: 15 **Cell:** ($^\circ$) α 90.00 β 107.17(1) γ 90.00

R-Factor (%): 8.52 **Temperature(K)**: 273 **Density(g/cm³)**: 1.121



SOVUVJ

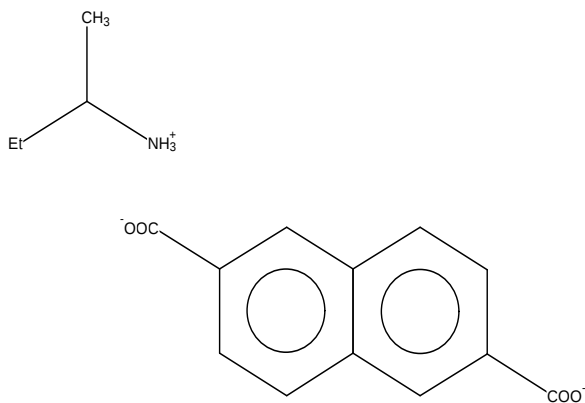
Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_4\text{H}_{12}\text{N}_1^{1+})\cdot\text{C}_{12}\text{H}_6\text{O}_4^{2-}$

Compound Name: bis(s-Butylammonium) 2,6-naphthalenedicarboxylate

Space Group: C2/c **Cell:** a 15.390(70) b 6.180(50) c 22.040(100)
Space Group No.: 15 **Cell:** ($^\circ$) α 90.00 β 96.10(40) γ 90.00

R-Factor (%): 9.69 **Temperature(K)**: 296 **Density(g/cm³)**: 1.155



SOVWEG

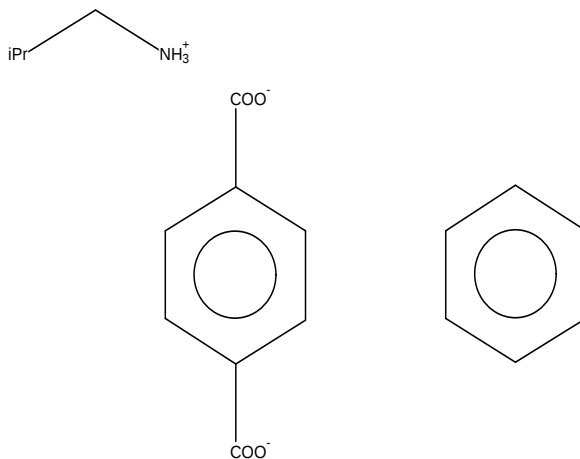
Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_4\text{H}_{12}\text{N}_1^{1+})\cdot\text{C}_8\text{H}_4\text{O}_4^{2-}\cdot\text{C}_6\text{H}_6$

Compound Name: bis(Isobutylammonium) terephthalate benzene solvate

Space Group: P21 **Cell:** a 17.308(5) b 6.272(0) c 20.611(6)
Space Group No.: 4 **Cell:** ($^\circ$) α 90.00 β 91.11(0) γ 90.00

R-Factor (%): 6.89 **Temperature(K)**: 213 **Density(g/cm³)**: 1.160



Search: search4 (Sat Oct 23 06:44:11 2010): Hits 25-28

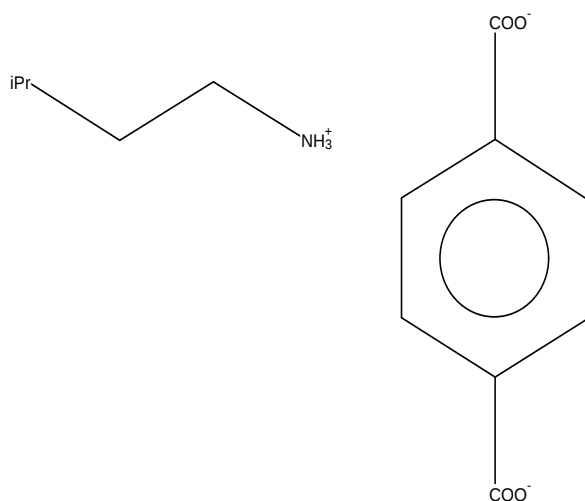
SOVWIK

Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohtnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_5\text{H}_{14}\text{N}_1^{1+})\cdot\text{C}_8\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(isopentylammonium) terephthalate

Space Group: P21/n
Space Group No.: 14
Cell: ($\text{\AA}$, $^\circ$)
 a 9.474(1) b 6.205(0) c 17.148(2)
 α 90.00 β 101.22(1) γ 90.00
R-Factor (%): 5.83
Temperature(K): 213
Density(g/cm³): 1.144



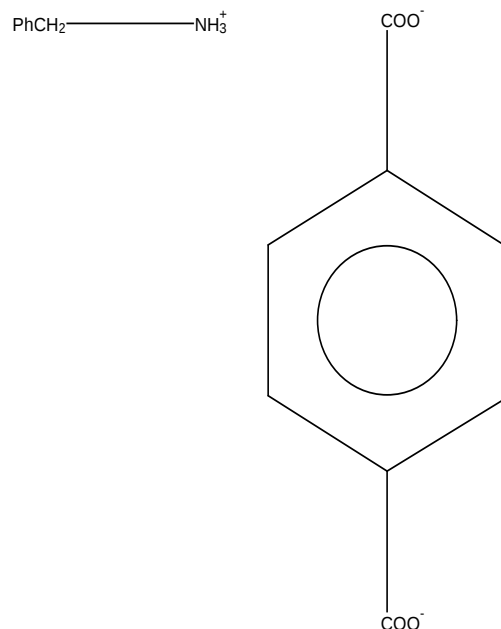
SOVWOQ

Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohtnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_7\text{H}_{10}\text{N}_1^{1+})\cdot\text{C}_8\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(Benzylammonium) terephthalate

Space Group: P21/n
Space Group No.: 14
Cell: ($\text{\AA}$, $^\circ$)
 a 12.660(2) b 6.317(1) c 13.262(2)
 α 90.00 β 107.10(1) γ 90.00
R-Factor (%): 5.89
Temperature(K): 213
Density(g/cm³): 1.246



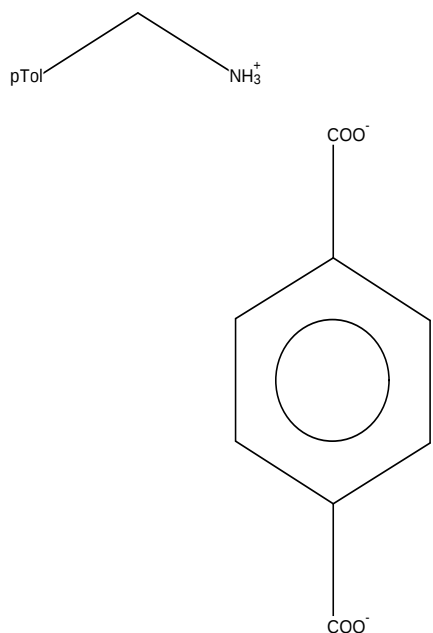
SOVXAD

Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohtnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_8\text{H}_{12}\text{N}_1^{1+})\cdot\text{C}_8\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(4-Methylbenzylammonium) terephthalate

Space Group: P21/n
Space Group No.: 14
Cell: ($\text{\AA}$, $^\circ$)
 a 8.421(3) b 6.385(3) c 20.696(7)
 α 90.00 β 98.97(3) γ 90.00
R-Factor (%): 6.32
Temperature(K): 213
Density(g/cm³): 1.234



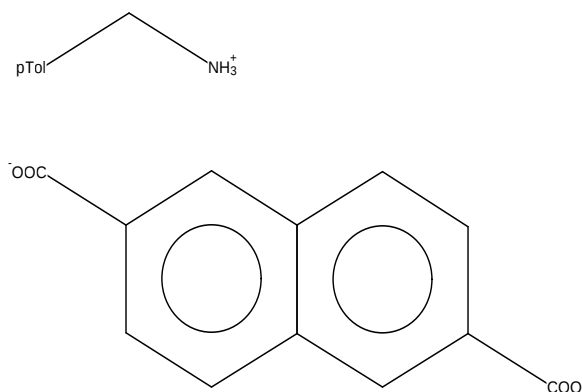
SOVXEh

Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohtnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_8\text{H}_{12}\text{N}_1^{1+})\cdot\text{C}_{12}\text{H}_6\text{O}_4^{2-}$

Compound Name: bis(4-Methylbenzylammonium) 2,6-naphthalenedicarboxylate

Space Group: P21/n
Space Group No.: 14
Cell: ($\text{\AA}$, $^\circ$)
 a 13.192(0) b 6.467(0) c 16.212(0)
 α 90.00 β 114.98(0) γ 90.00
R-Factor (%): 4.92
Temperature(K): 213
Density(g/cm³): 1.215



Search: search4 (Sat Oct 23 06:44:11 2010): Hits 29-32

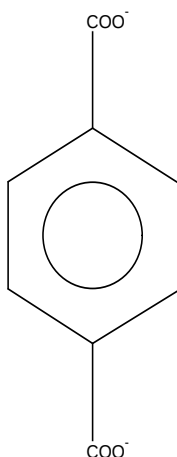
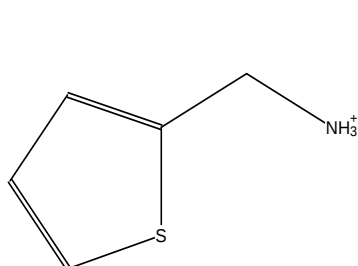
SOVZAF

Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohtnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_5\text{H}_8\text{N}_1\text{S}_1^{1+}), \text{C}_8\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(2-Thienylmethylammonium) terephthalate

Space Group: P21/n
Space Group No.: 14
Cell: (Å, °)
 a 12.326(1) b 6.145(0) c 13.186(2)
 α 90.00 β 108.86(0) γ 90.00
R-Factor (%): 7.07
Temperature(K): 93
Density(g/cm³): 1.379



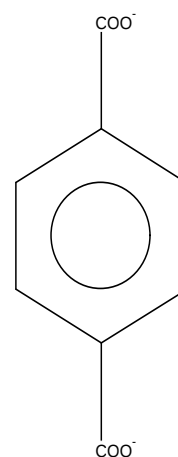
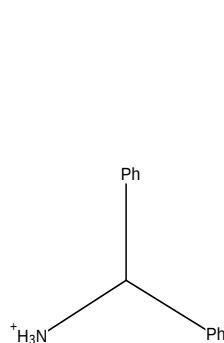
SOVZEJ

Reference: T.Yuge, T.Sakai, N.Kai, I.Hisaki, M.Miyata, N.Tohtnai (2008) *Chem.-Eur.J.*, **14**,2984

Formula: $2(\text{C}_{13}\text{H}_{14}\text{N}_1^{1+}), \text{C}_8\text{H}_4\text{O}_4^{2-}$

Compound Name: bis(1,1-(Diphenyl)methylammonium) terephthalate

Space Group: P21/c
Space Group No.: 14
Cell: (Å, °)
 a 10.517(0) b 6.320(0) c 20.879(1)
 α 90.00 β 90.98(0) γ 90.00
R-Factor (%): 5.73
Temperature(K): 213
Density(g/cm³): 1.275



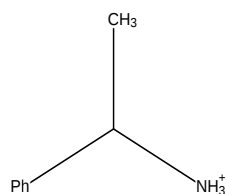
YUPYEN

Reference: Z.Bocskai, D.Kozma, K.Simon, E.Fogassy (1995) *J.Opt.Soc.Am.*, 160

Formula: $2(\text{C}_8\text{H}_{12}\text{N}_1^{1+}), \text{C}_2\text{O}_4^{2-}$

Compound Name: bis((R)-α-Phenylethylammonium) oxalate

Space Group: C2
Space Group No.: 5
Cell: (Å, °)
 a 10.786(1) b 7.430(0) c 11.493(0)
 α 90.00 β 98.66(0) γ 90.00
R-Factor (%): 6.00
Temperature(K): 295
Density(g/cm³): 1.212



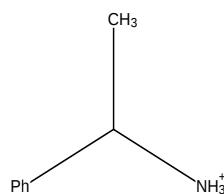
YUPYIR

Reference: Z.Bocskai, D.Kozma, K.Simon, E.Fogassy (1995) *J.Opt.Soc.Am.*, 160

Formula: $2(\text{C}_8\text{H}_{12}\text{N}_1^{1+}), \text{C}_2\text{O}_4^{2-}$

Compound Name: bis((R,S)-α-Phenylethylammonium) oxalate

Space Group: Pca21
Space Group No.: 29
Cell: (Å, °)
 a 12.237(4) b 6.786(5) c 21.859(4)
 α 90.00 β 90.00 γ 90.00
R-Factor (%): 4.10
Temperature(K): 295
Density(g/cm³): 1.216



Search: search4 (Sat Oct 23 06:44:11 2010): Hit 33

MOXDUZ

Reference: K.Inoue, N.Tohnai, M.Miyata, A.Matsumoto, T.Tani,
Y.Goto, S.Shinkai, K.Sada (2009) *Cryst.Growth Des.* ,9,1072

Formula: $2(\text{C}_{11}\text{H}_{12}\text{N}_1^{1+}), \text{C}_7\text{H}_{13}\text{O}_2^{1-}, \text{C}_9\text{H}_{17}\text{O}_2^{1-}$

Compound Name: bis(1-Naphthylmethylammonium) n-heptanoate n-nonanoate

Space Group: P-1 **Cell:** **a** 4.922(1) **b** 10.735(3) **c** 33.888(9)
Space Group No.: 2 ($\text{\AA}$, $^\circ$) α 87.80(3) β 85.85(2) γ 89.97(3)

R-Factor (%): 14.11 **Temperature(K)**: 300 **Density(g/cm³)**: 1.122

