

Search Overview

Search: search9
Date/Time done: Mon Aug 10 17:30:07 2009
Database(s): CSD version 5.30 (November 2008)
CSD version 5.30 updates (Nov 2008)
CSD version 5.30 updates (Feb 2009)
CSD version 5.30 updates (May 2009)
Restriction Info: No refcode restrictions applied
Filters: 3D coordinates determined Not disordered
No errors No powder structures
Only Organics
Percentage Completed: 100%
Number of Hits: 113

Summary of queries used. Search found structures that:

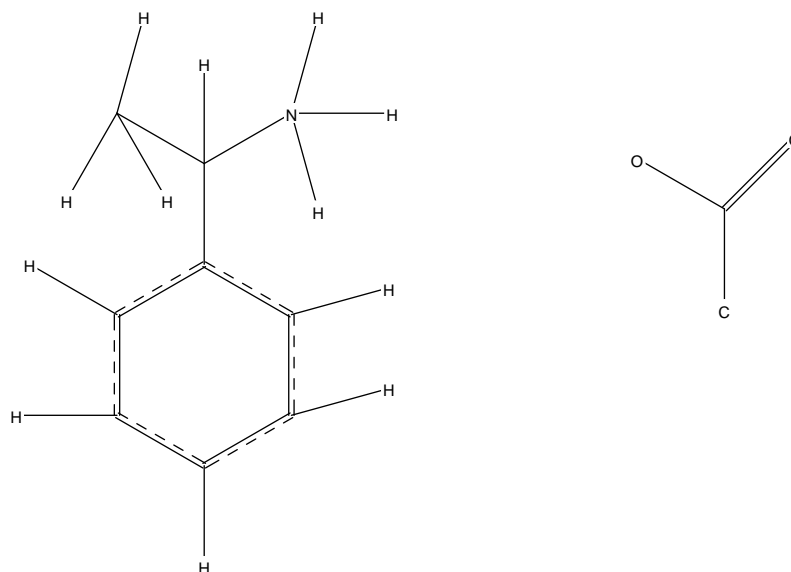
match

Query 7

Query 8

Query 9

Query 7



Query 8

Formula **C₁₋₄₀H₁₋₈₀N₁₋₂O₂₋₄**
Search on: **Sum of molecules**
Allow other elements: **Yes**

Query 9

Include only: **Sohncke (or chiral) space groups**

Search: search9 (Mon Aug 10 17:30:07 2009): Hits 1-4

AFINEJ

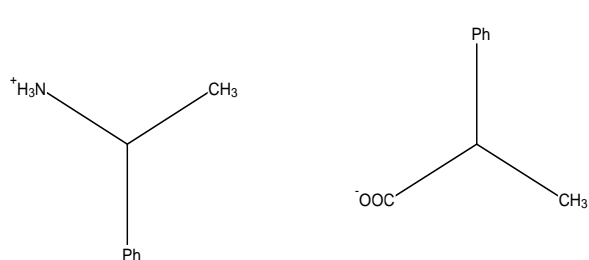
Reference: P.G.Karamertzanis, P.R.Anandamanoharan, P.Fernandes, P.W.Cains, M.Vickers, D.A.Tocher, A.J.Florence, S.L.Price (2007) *J.Phys.Chem.B* ,111,5326

Formula: C₈ H₁₂ N₁¹⁺.C₉ H₉ O₂¹⁻

Compound Name: (R)-1-Phenylethylammonium (S)-2-phenylpropanoate

Space Group: P21 **Cell:** a 11.008(1) b 6.539(0) c 12.161(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 116.01(0) γ 90.00

R-Factor (%): 4.07 **Temperature(K):** 150 **Density(g/cm³):** 1.146



CEFZUJ

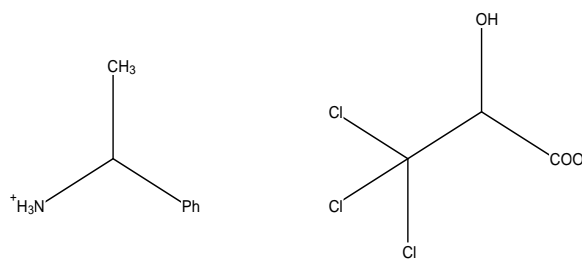
Reference: S.Takahashi, T.Jukurogi, T.Katagiri, K.Uneyama (2006) *CrystEngComm* ,8,320

Formula: C₈ H₁₂ N₁¹⁺.C₃ H₂ Cl₃ O₃¹⁻

Compound Name: (+)-(S)-1-Phenylethylammonium (S)-3,3,3-trichlorolactate

Space Group: P21 **Cell:** a 9.213(0) b 6.662(0) c 12.514(0)
Space Group No.: 4 **(Å, °)** α 90.00 β 103.89(0) γ 90.00

R-Factor (%): 6.07 **Temperature(K):** 296 **Density(g/cm³):** 1.401



DAZSON

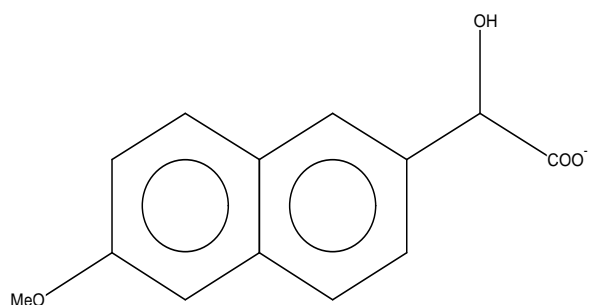
Reference: T.Shimada, Y.Kobayashi, K.Saigo (2005) *Tetrahedron:Asymm.* ,16,3807

Formula: C₈ H₁₂ N₁¹⁺.C₁₃ H₁₁ O₄¹⁻

Compound Name: (R)-1-Phenylethylammonium (R)-6-methoxy-2-naphthylglycolate

Space Group: P21 **Cell:** a 8.365(2) b 6.823(1) c 16.988(5)
Space Group No.: 4 **(Å, °)** α 90.00 β 103.25(0) γ 90.00

R-Factor (%): 7.90 **Temperature(K):** 296 **Density(g/cm³):** 1.244



DEWLIA

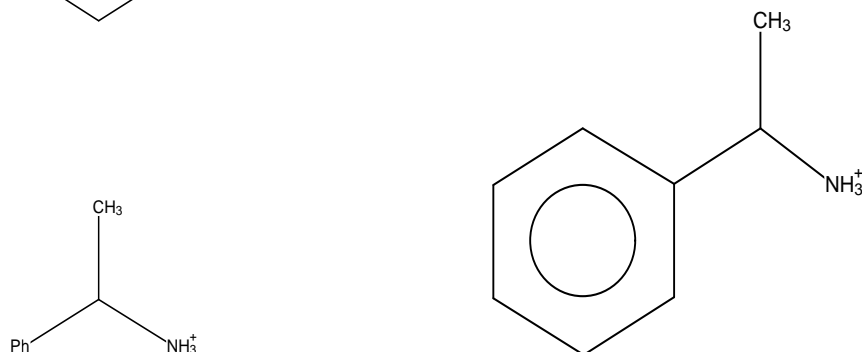
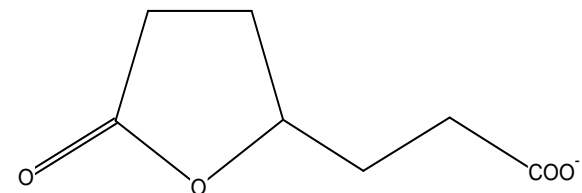
Reference: K.Fuji, M.Node, S.Terada, M.Murata, H.Nagasawa (1985) *J.Am.Chem.Soc.* ,107,6404

Formula: C₇ H₉ O₄¹⁻.C₈ H₁₂ N₁¹⁺

Compound Name: (S)-(-)-4-Hydroxypimelic acid lactone (S)-(-)-2-methylbenzylammonium

Space Group: P21 **Cell:** a 10.855(2) b 6.705(2) c 10.710(2)
Space Group No.: 4 **(Å, °)** α 90.00 β 90.34(1) γ 90.00

R-Factor (%): 5.20 **Temperature(K):** 295 **Density(g/cm³):** 1.190



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 5-8

FAPXUP

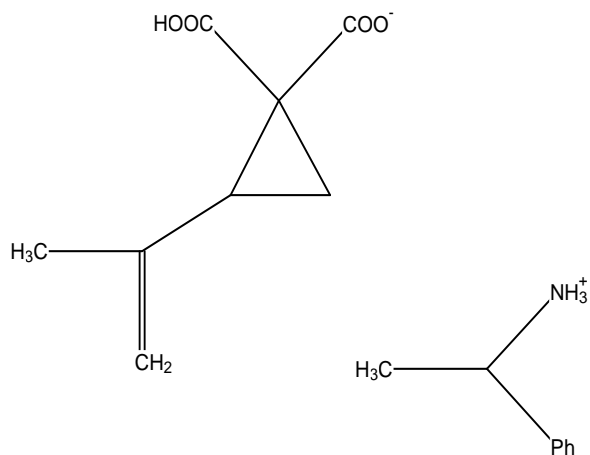
Reference: G.Quinkert, H.-G.Schmalz, E.Walzer, S.Gross, G.Durner, J.W.Bats (1986) *Angew.Chem.,Int.Ed.* ,25,732

Formula: C₈ H₉ O₄¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (S)-(-)-1-Phenylethylammonium (R)-2-(isopropen-2-yl)cyclopropane-1-carboxylate-1-carboxylic acid

Space Group: P21 **Cell:** a 9.271(0) b 6.178(2) c 14.114(0)
Space Group No.: 4 **(Å,°)** α 90.00 β 93.90(0) γ 90.00

R-Factor (%): 4.20 **Temperature(K):** 295 **Density(g/cm³):** 1.200



FEMGAF

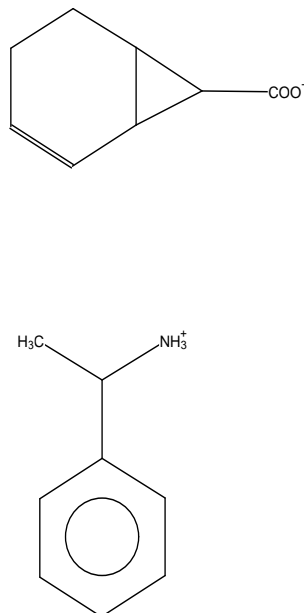
Reference: K.Yanagi, T.Aratani (1987) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,43,263

Formula: C₈ H₉ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (+)-(R)-α-Methylbenzylammonium (+)-(1S,6R,7S)-bicyclo(4.1.0)hept-2-ene-7-carboxylate

Space Group: P212121 **Cell:** a 12.582(1) b 19.537(2) c 6.159(1)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.50 **Temperature(K):** 295 **Density(g/cm³):** 1.138



FEMGEJ

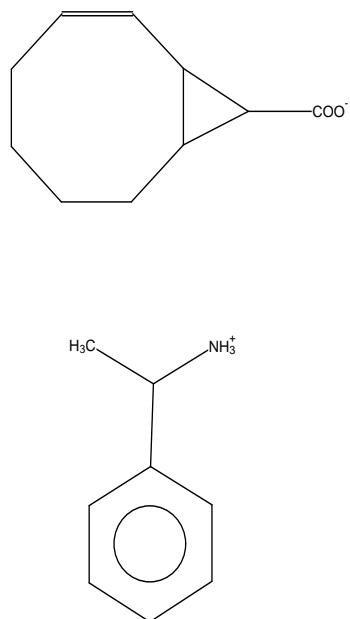
Reference: K.Yanagi, T.Aratani (1987) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,43,263

Formula: C₁₀ H₁₃ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (+)-(R)-α-Methylbenzylammonium (+)-(1R,8S,9R)-bicyclo(6.1.0)non-2-ene-9-carboxylate

Space Group: P21 **Cell:** a 15.625(1) b 5.639(2) c 9.717(1)
Space Group No.: 4 **(Å,°)** α 90.00 β 101.87(1) γ 90.00

R-Factor (%): 4.90 **Temperature(K):** 295 **Density(g/cm³):** 1.139



FUMNOQ10

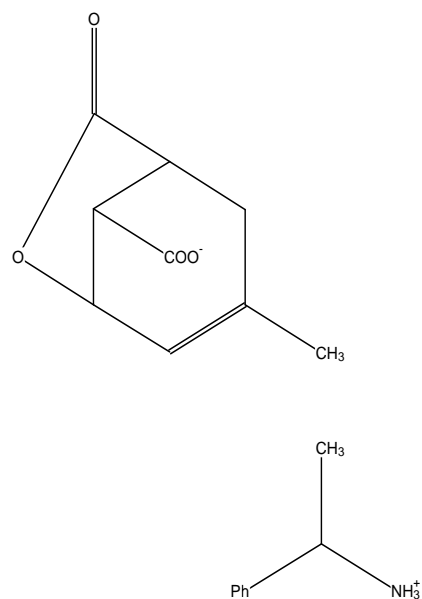
Reference: J.D.White, G.L.Bolton, A.P.Dantanarayana, C.M.J.Fox, R.N.Hiner, R.W.Jackson, K.Sakuma, U.S.Warrier (1995) *J.Am.Chem.Soc.* ,117,1908

Formula: C₉ H₉ O₄¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (S)-(-)-α-Methylbenzylammonium rac-anti-3-methyl-7-oxo-6-oxabicyclo(3.2.1)oct-3-ene-8-carboxylate

Space Group: P212121 **Cell:** a 6.715(5) b 12.602(1) c 19.451(2)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.90 **Temperature(K):** 295 **Density(g/cm³):** 1.224



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 9-12

FUSJAE

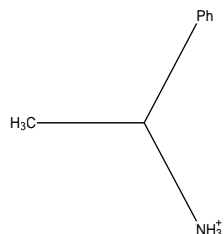
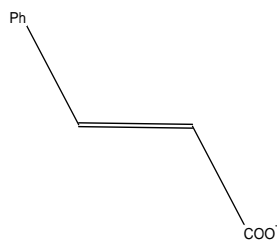
Reference: K.Saigo, H.Kimoto, H.Nohira, K.Yanagi, M.Hasegawa (1987) *Bull.Chem.Soc.Jpn.* **60**,3655

Formula: C₉ H₇ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: 1-Phenylethylammonium cinnamate

Space Group: P212121 **Cell:** a 9.368(1) b 26.703(2) c 6.043(1)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.60 **Temperature(K):** 295 **Density(g/cm³):** 1.183



GARLAN

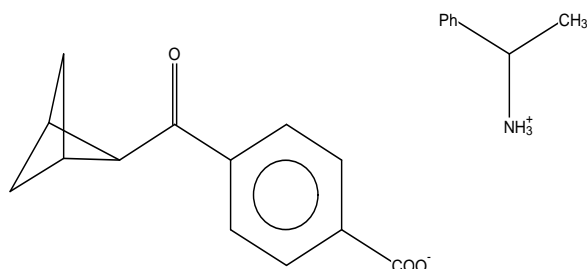
Reference: Chao Yang, Wujiong Xia, J.R.Scheffer, M.Botoshansky, M.Kafory (2005) *Angew.Chem.,Int.Ed.* **44**,5087

Formula: C₁₃ H₁₁ O₃¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: 1-phenylethylammonium 4-((2,4-methanocyclobutyl)carbonyl)benzoate

Space Group: P21 **Cell:** a 10.635(2) b 6.492(1) c 13.387(3)
Space Group No.: 4 **(Å, °)** α 90.00 β 93.03(3) γ 90.00

R-Factor (%): 4.08 **Temperature(K):** 293 **Density(g/cm³):** 1.214



GARLER

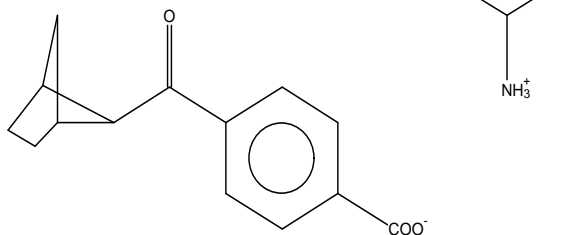
Reference: Chao Yang, Wujiong Xia, J.R.Scheffer, M.Botoshansky, M.W.Wieczorek, W.R.Majzner (1998) *Tetrahedron:Asymm.* **9**,2641

Formula: C₁₄ H₁₃ O₃¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: 1-phenylethylammonium 4-((2,5-methanocyclopentyl)carbonyl)benzoate

Space Group: P21 **Cell:** a 12.654(3) b 6.347(1) c 12.841(3)
Space Group No.: 4 **(Å, °)** α 90.00 β 108.86(3) γ 90.00

R-Factor (%): 4.73 **Temperature(K):** 293 **Density(g/cm³):** 1.196



GIVQOR

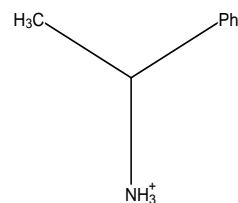
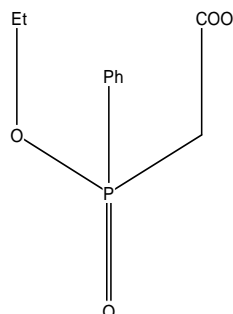
Reference: P.Kielbasinski, P.Goralczyk, M.Mikolajczyk, M.W.Wieczorek, W.R.Majzner (1998) *Tetrahedron:Asymm.* **9**,2641

Formula: C₁₀ H₁₂ O₄ P₁¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (-)-(S)-α-Phenylethylammonium (+)-(R)-(ethoxy(phenyl)oxyphosphinyl)acetate

Space Group: P212121 **Cell:** a 7.113(6) b 14.010(7) c 19.290(10)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.80 **Temperature(K):** 295 **Density(g/cm³):** 1.207



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 13-16

GOZDAA

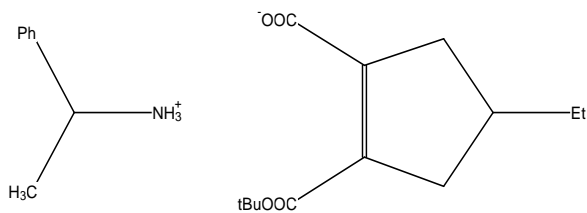
Reference: J.D.White, J.Kim, N.E.Drapela (2000) *J.Am.Chem.Soc.*, **122**,8665

Formula: C₁₃ H₁₉ O₄¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (S)-(-)-α-Methylbenzylammonium 2-t-butoxycarbonyl-4-ethylcyclopentene-1-carboxylate

Space Group: C2 **Cell:** a 35.202(1) b 6.072(0) c 10.471(0)
Space Group No.: 5 **(Å, °)** α 90.00 β 101.41(0) γ 90.00

R-Factor (%): 4.40 **Temperature(K):** 295 **Density(g/cm³):** 1.094



HIFRIX

Reference: L.Dupont, B.Pirotte, P.De Tullio, J.Delarge (1996) *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.*, **52**,393

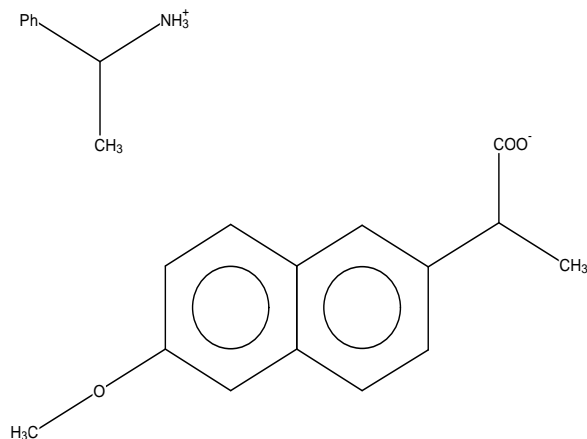
Formula: C₈ H₁₂ N₁¹⁺·C₁₄ H₁₃ O₃¹⁻

Compound Name: (R)-1-Phenylethylammonium (S)-2-(6-methoxy-2-naphthyl)propionate

Synonym: Naproxen

Space Group: P21 **Cell:** a 11.640(0) b 5.981(0) c 13.691(0)
Space Group No.: 4 **(Å, °)** α 90.00 β 94.46(1) γ 90.00

R-Factor (%): 3.76 **Temperature(K):** 295 **Density(g/cm³):** 1.228



HISREG

Reference: S.Houlemare-Druot, G.Coquerel (1998) *J.Chem.Soc., Perkin Trans.2*, 2211

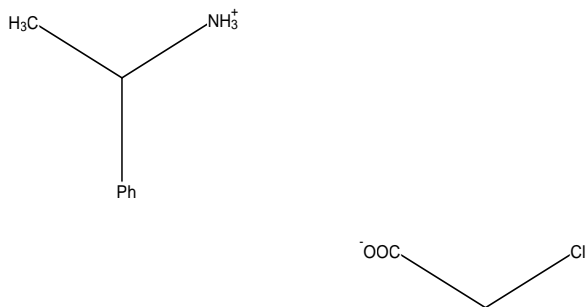
Formula: C₈ H₁₂ N₁¹⁺·C₂ H₂ Cl₁ O₂¹⁻

Compound Name: (R)-(+)-α-Methylbenzylammonium chloroacetate

Synonym: (R)-(+)-1 Phenylethylammonium chloroacetate

Space Group: P21 **Cell:** a 11.591(1) b 6.528(7) c 7.955(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 109.52(1) γ 90.00

R-Factor (%): 3.30 **Temperature(K):** 295 **Density(g/cm³):** 1.263



IBOPIY

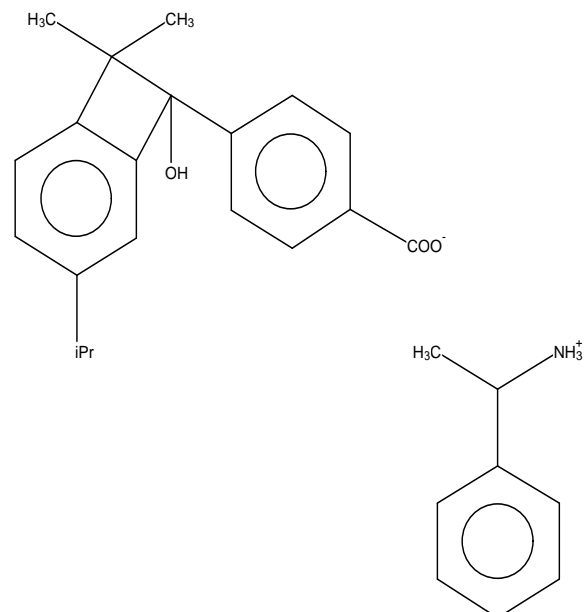
Reference: H.Koshima, D.Matsushige, M.Miyauchi (2001) *CrystEngComm*, **3**,141

Formula: C₈ H₁₂ N₁¹⁺·C₂₀ H₂₁ O₃¹⁻

Compound Name: (S)-Phenylethylammonium 4-(1-hydroxy-2,2-dimethyl-5-isopropyl-benzocyclobuten-1-yl)benzoate

Space Group: P212121 **Cell:** a 13.776(1) b 28.510(2) c 6.331(0)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.70 **Temperature(K):** 296 **Density(g/cm³):** 1.153



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 17-20

IBOPOE

Reference: H.Koshima, D.Matsushige, M.Miyauchi (2001) *CrystEngComm* ,3,141

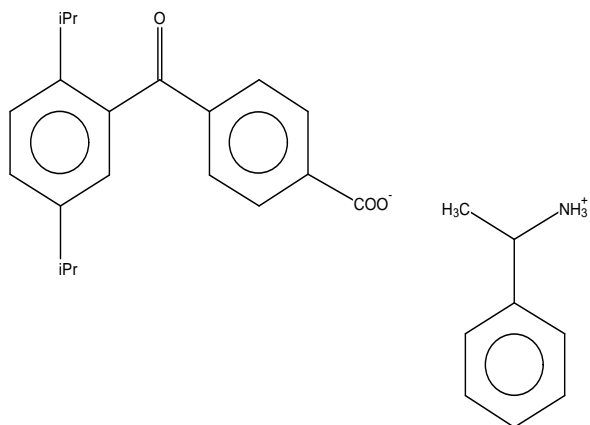
Formula: C₈ H₁₂ N₁¹⁺, C₂₀ H₂₁ O₃¹⁻

Compound Name: (S)-Phenylethylammonium 4-(2,5-di-isopropylbenzoyl)benzoate

Space Group: P212121 **Cell:** a 14.411(1) b 28.732(2) c 6.189(0)

Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.22 **Temperature(K):** 296 **Density(g/cm³):** 1.119



IRUYEZ

Reference: M.Hatano, K.Mikami (2003) *J.Mol.Catal.A:Chem.* ,196,165

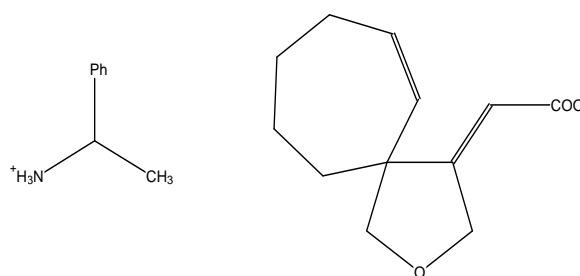
Formula: C₈ H₁₂ N₁¹⁺, C₁₂ H₁₅ O₃¹⁻

Compound Name: (S)-Phenylethylammonium (2-oxa-spiro(4.6)undec-6-en-4-ylidene)acetate

Space Group: P212121 **Cell:** a 14.205(2) b 19.760(3) c 6.735(3)

Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.47 **Temperature(K):** 253 **Density(g/cm³):** 1.157



IWUWUS

Reference: T.B.Mikhailova, E.V.Pakhmutova, A.E.Malkov, I.F.Golovaneva, A.A.Sidorov, I.G.Fomina, G.G.Aleksandrov, V.N.Ikorski, V.M.Novotortsev, I.L.Eremenko, I.I.Moiseev (2003) *Izv.Akad.Nauk SSSR,Ser.Khim.(Russ.)(Russ.Chem.Bull.)* ,1994

Formula: C₈ H₁₂ N₁¹⁺, C₅ H₉ O₂¹⁻

Compound Name: 1-Phenylethylammonium pivalate

Space Group: P212121 **Cell:** a 6.044(6) b 12.366(16) c 17.349(17)

Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.49 **Temperature(K):** 110 **Density(g/cm³):** 1.144



JAGHEE

Reference: R.B.Cain, A.A.Freer, G.W.Kirby, G.V.Rao (1989) *J.Chem.Soc.,Perkin Trans.1* ,202

Formula: C₇ H₇ O₄¹⁻, C₈ H₁₂ N₁¹⁺

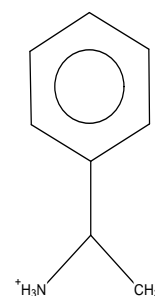
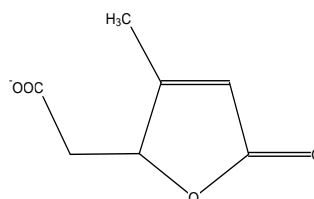
Compound Name: (S)-(-)-1-Phenylethylammonium (S)-(-)-2-(3-methyl-5-oxo-2,5-dihydro-2-furyl)acetate

Synonym: (S)-(-)-1-Phenylethylammonium (S)-(-)-3-methylmuconolactone

Space Group: P212121 **Cell:** a 5.988(3) b 12.472(3) c 20.857(3)

Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.70 **Temperature(K):** 295 **Density(g/cm³):** 1.183



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 21-24

JAGHII

Reference: R.B.Cain, A.A.Freer, G.W.Kirby, G.V.Rao (1989)
J.Chem.Soc.,Perkin Trans.1, 202

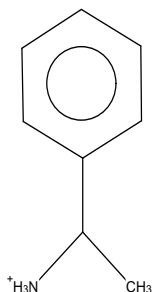
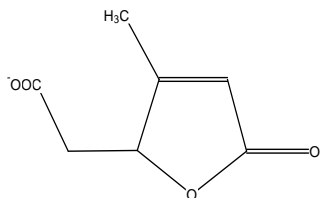
Formula: C₇ H₇ O₄¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (S)-(-)-1-Phenylethylammonium (R)-(+)-2-(3-methyl-5-oxo-2,5-dihydro-2-furyl)acetate

Synonym: (S)-(-)-1-Phenylethylammonium (R)-(+)-3-methylmuconolactone

Space Group: P212121 **Cell:** a 6.192(3) b 12.599(3) c 19.376(3)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.80 **Temperature(K):** 295 **Density(g/cm³):** 1.219



JASJIX

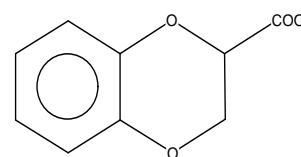
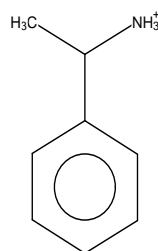
Reference: N.Marchini, G.Bombieri, R.Artali, C.Bolchi, M.Pallavicini, E.Valoti (2005) *Tetrahedron:Asymm.*, 16,2099

Formula: C₈ H₁₂ N₁¹⁺·C₉ H₇ O₄¹⁻

Compound Name: (S)-(-)-1-Phenylethylammonium (R)-1,4-benzodioxane-2-carboxylate

Space Group: P212121 **Cell:** a 6.738(7) b 12.246(8) c 38.507(9)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 7.17 **Temperature(K):** 293 **Density(g/cm³):** 1.260



JEQSII

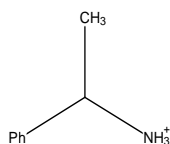
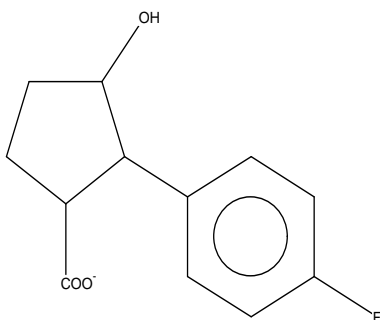
Reference: L.C.Meurer, P.E.Finke, K.A.Owens, N.N.Tsou, R.G.Ball, S.G.Mills, M.MacCoss, S.Sadowski, M.A.Cascieri, Kwei-Lan Tsao, G.G.Chicchi, L.A.Egger, S.Luell, J.M.Metzger, D.E.MacIntyre, N.M.J.Rupniak, A.R.Williams, R.J.Hargreaves (2006) *Bioorg.Med.Chem.Lett.*, 16,4504

Formula: C₈ H₁₂ N₁¹⁺·C₁₂ H₁₂ F₁ O₃¹⁻

Compound Name: (S)-α-Methylbenzylammonium 2-(4-fluorophenyl)-3-hydroxycyclopentanecarboxylate

Space Group: P21 **Cell:** a 6.338(2) b 11.805(2) c 12.595(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 101.69(1) γ 90.00

R-Factor (%): 10.51 **Temperature(K):** 294 **Density(g/cm³):** 1.243



KEBYAS

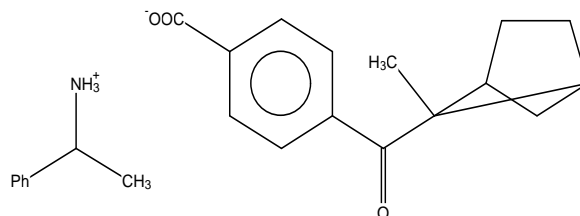
Reference: Wujiong Xia, J.R.Scheffer, B.O.Patrick (2005) *CrystEngComm*, 7,728

Formula: C₈ H₁₂ N₁¹⁺·C₁₅ H₁₅ O₃¹⁻

Compound Name: (S)-(-)-1-Phenylethylammonium 4-((5-methylbicyclo[2.1.1]hex-5-yl)carbonyl)benzoate

Space Group: P212121 **Cell:** a 6.127(0) b 7.262(1) c 45.252(6)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.44 **Temperature(K):** 173 **Density(g/cm³):** 1.206



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 25-28

KEBYEW

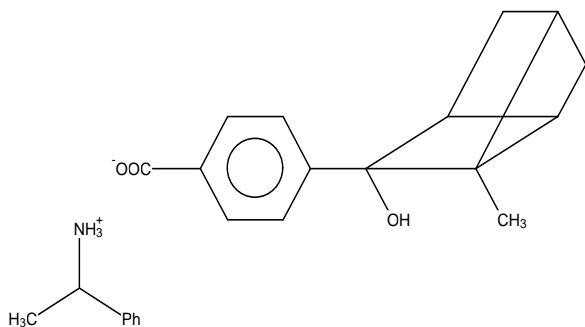
Reference: Wujiong Xia, J.R.Scheffer, B.O.Patrick (2005) *CrystEngComm*, 7,728

Formula: C₈ H₁₂ N₁⁺·C₁₅ H₁₅ O₃¹⁻

Compound Name: (S)-(-)-1-Phenylethylammonium 4-(4-hydroxy-5-methyltricyclo(3.2.0.0^{3,6})hept-4-yl)benzoate

Space Group: P212121 **Cell:** a 6.212(1) b 7.213(2) c 44.481(9)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 8.43 **Temperature(K):** 173 **Density(g/cm³):** 1.218



KEDYEX

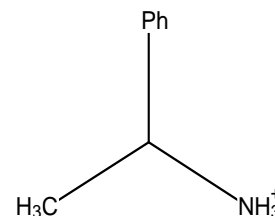
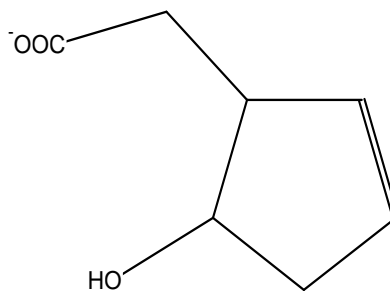
Reference: M.Czugler, I.Csoregh, A.Kalman, F.Faigl, M.Acs (1989) *J.Mol.Struct.*, 196,157

Formula: C₇ H₉ O₃¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: R-1-Phenylethylammonium 1R,2S(+)-cis-2-hydroxycyclopent-4-enylacetate

Space Group: P212121 **Cell:** a 5.806(1) b 9.261(1) c 27.624(2)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.56 **Temperature(K):** 295 **Density(g/cm³):** 1.178



KUYKOE

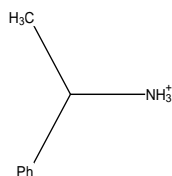
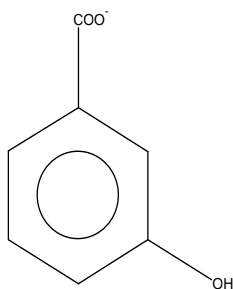
Reference: C.B.Aakeroy, G.S.Bahra, P.B.Hitchcock, Y.Patell, K.R.Seddon (1993) *Chem.Comm.*, 152

Formula: C₇ H₅ O₃¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (S)-1-Phenylethylammonium 3-hydroxybenzoate

Space Group: P212121 **Cell:** a 6.358(1) b 11.620(5) c 18.310(9)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.10 **Temperature(K):** 173 **Density(g/cm³):** 1.273



KUYKUK

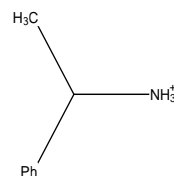
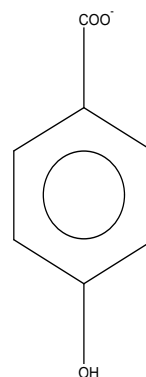
Reference: C.B.Aakeroy, G.S.Bahra, P.B.Hitchcock, Y.Patell, K.R.Seddon (1993) *Chem.Comm.*, 152

Formula: C₇ H₅ O₃¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (S)-1-Phenylethylammonium 4-hydroxybenzoate

Space Group: P212121 **Cell:** a 6.520(1) b 11.918(2) c 17.922(3)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.00 **Temperature(K):** 295 **Density(g/cm³):** 1.237



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 29-32

LAFDEC

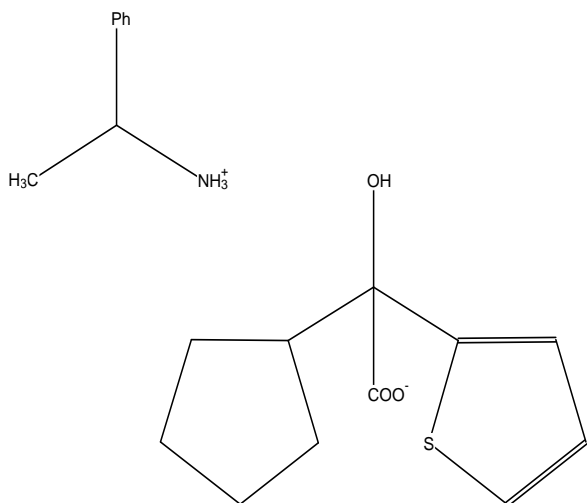
Reference: He Liu, Chun-he Liu, Xiang-Yu Han, Bo-Hua Zhong, Ke-Liang Liu (2004) *J.Chem.Res.*, 482

Formula: C₈ H₁₂ N₁¹⁺, C₁₁ H₁₃ O₃ S₁¹⁻

Compound Name: (R)- α -Methylbenzylamine (S)- α -cyclopentyl- α -hydroxy- α -thienylacetic acid

Space Group: P21 **Cell:** a 14.376(4) b 17.810(5) c 15.695(5)
Space Group No.: 4 **(\AA ,^o)** α 90.00 β 101.22(0) γ 90.00

R-Factor (%): 7.24 **Temperature(K):** 293 **Density(g/cm³):** 1.171



LIWHAA

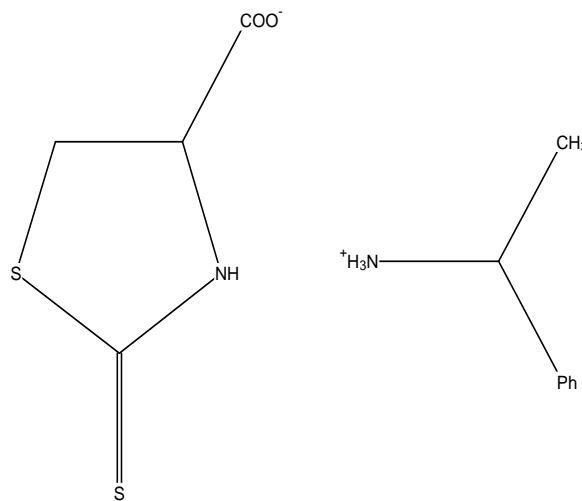
Reference: Yezhi Li, Chunxiao Guo, Weiming Bu, Huamin Huang (1998) *Sci.China,Ser.B:Chem.*, 41,361

Formula: C₄ H₄ N₁ O₂ S₂¹⁻, C₈ H₁₂ N₁¹⁺

Compound Name: (R)-(-)-Thiazolidine-2-thione-4-carboxylic acid (S)-(-)- α -phenylethylamine

Space Group: P21 **Cell:** a 13.878(2) b 6.641(1) c 15.800(2)
Space Group No.: 4 **(\AA ,^o)** α 90.00 β 90.84(1) γ 90.00

R-Factor (%): 5.26 **Temperature(K):** 295 **Density(g/cm³):** 1.297



LIWHEE

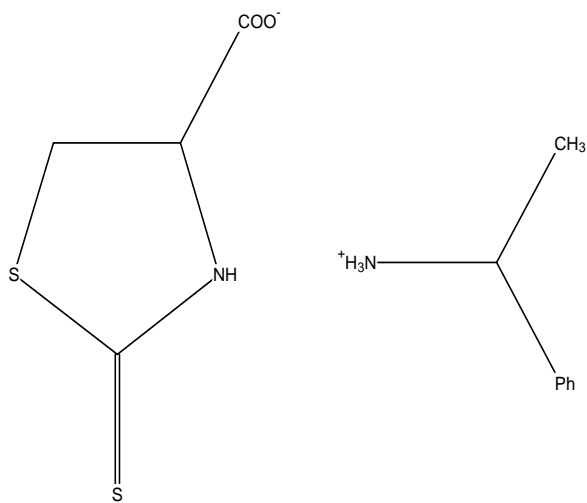
Reference: Yezhi Li, Chunxiao Guo, Weiming Bu, Huamin Huang (1998) *Sci.China,Ser.B:Chem.*, 41,361

Formula: C₄ H₄ N₁ O₂ S₂¹⁻, C₈ H₁₂ N₁¹⁺

Compound Name: (R)-(+)- α -Phenylethylammonium (R)-(-)-thiazolidine-2-thione-4-carboxylate

Space Group: P21 **Cell:** a 10.806(2) b 5.848(1) c 12.188(2)
Space Group No.: 4 **(\AA ,^o)** α 90.00 β 110.38(3) γ 90.00

R-Factor (%): 4.70 **Temperature(K):** 295 **Density(g/cm³):** 1.308



LUDWIQ

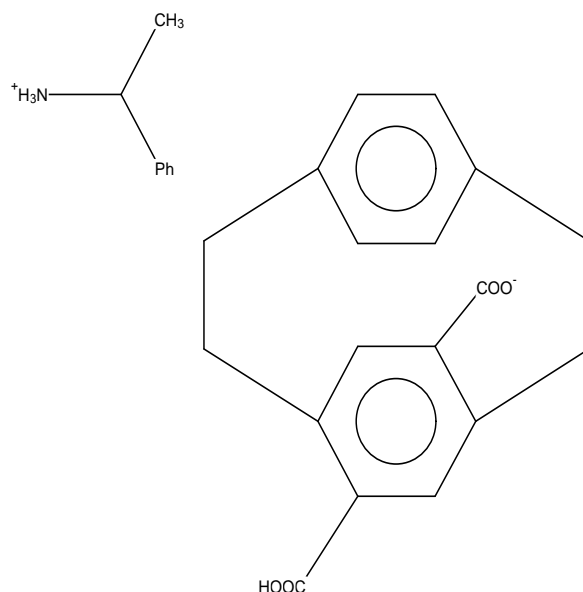
Reference: E.L.Popova, V.I.Rozenberg, Z.A.Starikova, S.Keuker-Baumann, H.-S.Kitzerow, H.Hopf (2002) *Angew.Chem.,Int.Ed.*, 41,3411

Formula: C₁₈ H₁₅ O₄¹⁻, C₈ H₁₂ N₁¹⁺

Compound Name: (S)-phenylethylammonium (R)-(2,2)paracyclophane-4-carboxylic acid-7-carboxylate

Space Group: C2 **Cell:** a 20.503(9) b 7.028(3) c 14.943(5)
Space Group No.: 5 **(\AA ,^o)** α 90.00 β 97.04(3) γ 90.00

R-Factor (%): 6.35 **Temperature(K):** 163 **Density(g/cm³):** 1.298



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 33-36

LUMQIT

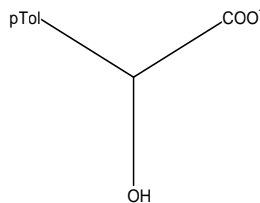
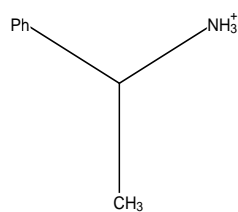
Reference: K.Kinbara, Y.Tagawa, K.Saigo (2001)
Tetrahedron:Asymm., **12**,2927

Formula: C₉ H₉ O₃¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: 1-Phenylethylammonium p-methylmandelate

Space Group: P212121 **Cell:** a 8.417(4) b 27.290(10) c 6.850(4)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 8.50 **Temperature(K):** 298 **Density(g/cm³):** 1.213



LUMQOZ

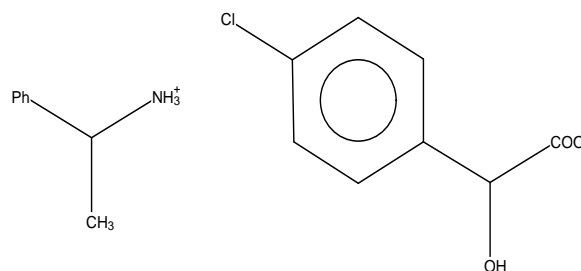
Reference: K.Kinbara, Y.Tagawa, K.Saigo (2001)
Tetrahedron:Asymm., **12**,2927

Formula: C₈ H₆ Cl₁ O₃¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: 1-Phenylethylammonium p-chloromandelate

Space Group: P212121 **Cell:** a 6.869(1) b 8.428(1) c 27.030(1)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.40 **Temperature(K):** 296 **Density(g/cm³):** 1.306



MEGVEZ

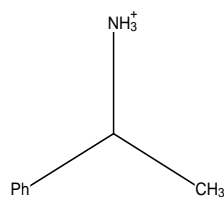
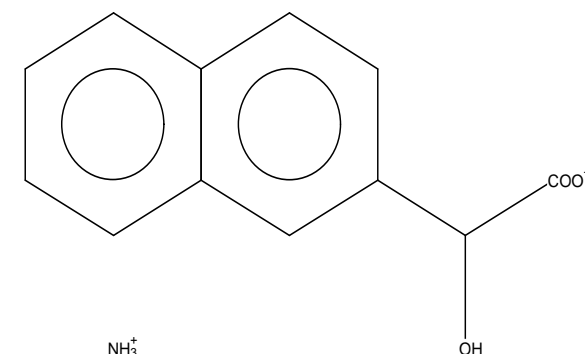
Reference: K.Kinbara, Y.Harada, K.Saigo (2000)
J.Chem.Soc.,Perkin Trans.2, 1339

Formula: C₈ H₁₂ N₁¹⁺·C₁₂ H₉ O₃¹⁻

Compound Name: (R)-1-Phenylethylammonium (R)-2-naphthylglycolate

Space Group: C2 **Cell:** a 30.573(7) b 6.835(2) c 8.446(2)
Space Group No.: 5 **(Å, °)** α 90.00 β 100.26(2) γ 90.00

R-Factor (%): 6.10 **Temperature(K):** 295 **Density(g/cm³):** 1.237



MUPNIU

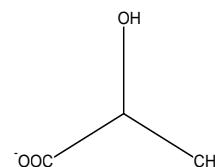
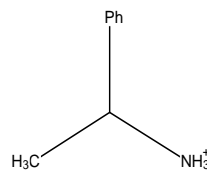
Reference: A.Langkilde, J.Oddershede, S.Larsen (2002)
Acta Crystallogr.,Sect.B:Struct.Sci., **58**,1044

Formula: C₈ H₁₂ N₁¹⁺·C₃ H₅ O₃¹⁻

Compound Name: (R)-1-Phenylethylammonium (S)-lactate

Space Group: P212121 **Cell:** a 6.847(1) b 6.970(0) c 24.248(4)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.81 **Temperature(K):** 122 **Density(g/cm³):** 1.213



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 37-40

NEBHIL

Reference: A.Jegorov, M.Husak, J.Ondracek, B.Kratochvil, M.Kuchar, P.Bulej, M.Gilar, E.Tesarova (1997) *J.Fluorine Chem.* ,**83**,111

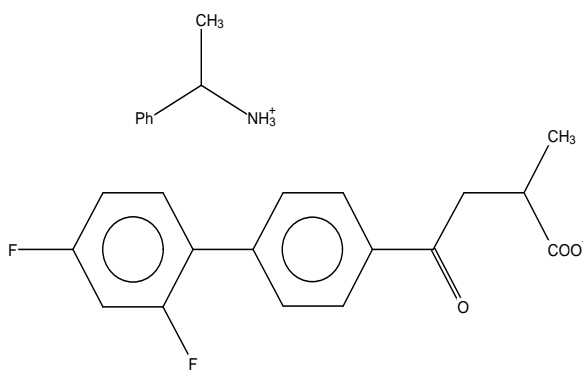
Formula: C₈ H₁₂ N₁⁺·C₁₇ H₁₃ F₂ O₃¹⁻

Compound Name: (R)-(+)-1-Phenylethylammonium (R)-(-)-4-(2',4'-difluorobiphenyl-4-yl)-2-methyl-4-oxobutanoic acid

Synonym: (R)-(+)-1-Phenylethylammonium (R)-(-)-flobufen

Space Group: P212121 **Cell:** a 5.959(2) b 11.179(3) c 32.992(3)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.61 **Temperature(K):** 295 **Density(g/cm³):** 1.286



NENYOU

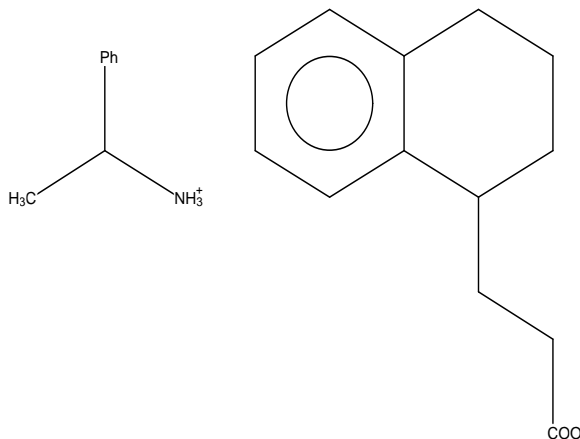
Reference: J.Wichmann, G.Adam, S.Rover, M.Hennig, M.Scalone, A.M.Cesura, F.M.Dautzenberg, F.Jenck (2000) *Eur.J.Med.Chem.* ,**35**, 839

Formula: C₈ H₁₂ N₁¹⁺·C₁₃ H₁₅ O₂¹⁻

Compound Name: (R)-(-)-1-Phenylethylammonium (S)-3-(1,2,3,4-tetrahydronaphthalen-1-yl)propionate

Space Group: P21 **Cell:** a 11.992 b 6.198 c 12.709
Space Group No.: 4 **(Å,°)** α 90.00 β 101.50 γ 90.00

R-Factor (%): 5.14 **Temperature(K):** 183 **Density(g/cm³):** 1.168



NIHDAJ01

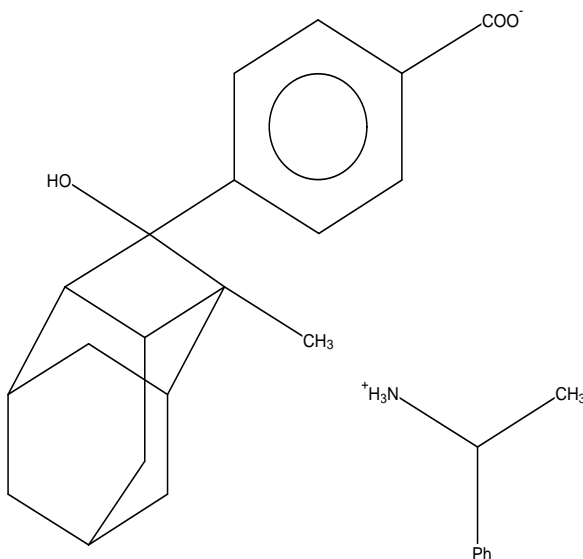
Reference: I.Turowska-Tyrk, E.Trzop, J.R.Scheffer, Shuang Chen (2006) *Acta Crystallogr., Sect.B:Struct.Cryst.Chem.* ,**62**,128

Formula: C₈ H₁₂ N₁¹⁺·C₁₉ H₂₁ O₃¹⁻

Compound Name: α-Methylbenzylamine 3-(4-carboxyphenyl)-3-hydroxy-2-methyltetracyclo(5.3.1.0^{2,5}.0^{4,9})undecane

Space Group: P212121 **Cell:** a 12.454(1) b 28.749(2) c 6.424(0)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 7.93 **Temperature(K):** 293 **Density(g/cm³):** 1.212



NMACEP

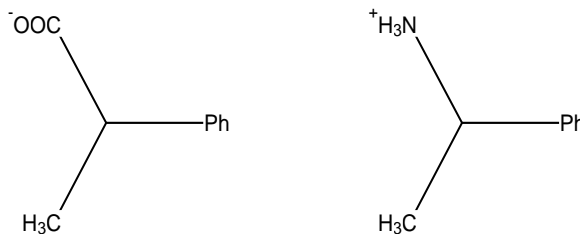
Reference: M.C.Briano (1976) *Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem.* ,**32**,3040

Formula: C₉ H₉ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (+)-α-Phenyl-ethylammonium (-)-α-phenyl-α-methylacetate

Space Group: P212121 **Cell:** a 17.080(10) b 15.470(10) c 5.800(10)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 7.80 **Temperature(K):** 295 **Density(g/cm³):** 1.176



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 41-44

PBUPEA

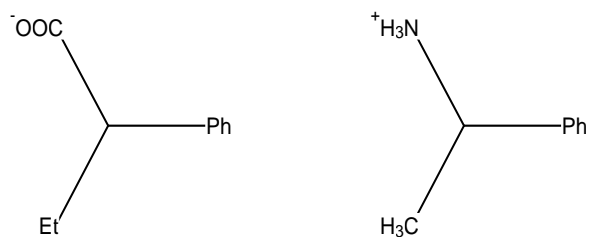
Reference: M.C.Brioso (1978)
Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem. ,**34**,679

Formula: C₁₀H₁₁O₂¹⁻·C₈H₁₂N₁¹⁺

Compound Name: α-Phenylethylammonium α-phenylbutyrate

Space Group: P212121 **Cell:** a 17.794(5) b 15.528(4) c 5.816(2)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 7.00 **Temperature(K):** 295 **Density(g/cm³):** 1.180



PBUPEA02

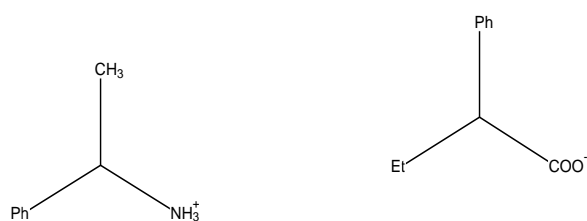
Reference: P.Fernandes, A.J.Florence, K.Shankland,
P.G.Karamertzanis, A.T.Hulme, R.P.Anandamanoharan (2007)
Acta Crystallogr., Sect.E:Struct.Rep.Online ,**63**,o202

Formula: C₈H₁₂N₁¹⁺·C₁₀H₁₁O₂¹⁻

Compound Name: (R)-1-Phenylethylammonium (R)-2-phenylbutyrate

Space Group: P21 **Cell:** a 11.882(0) b 5.976(0) c 13.075(0)
Space Group No.: 4 **(Å,°)** α 90.00 β 113.51(0) γ 90.00

R-Factor (%): 3.10 **Temperature(K):** 295 **Density(g/cm³):** 1.113



PBUPEA03

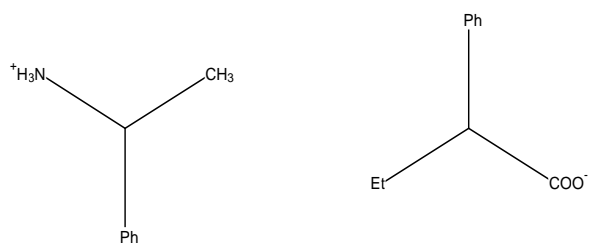
Reference: P.G.Karamertzanis, P.R.Anandamanoharan,
P.Fernandes, P.W.Cains, M.Vickers, D.A.Tocher, A.J.Florence,
S.L.Price (2007) *J.Phys.Chem.B* ,**111**,5326

Formula: C₈H₁₂N₁¹⁺·C₁₀H₁₁O₂¹⁻

Compound Name: (R)-1-Phenylethylammonium (R)-2-phenylbutyrate

Space Group: P212121 **Cell:** a 5.757(0) b 15.433(1) c 17.571(1)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.98 **Temperature(K):** 150 **Density(g/cm³):** 1.214



PEAMAN

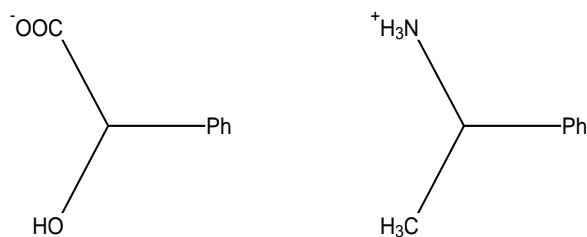
Reference: M.C.Brioso, M.Leclercq, J.Jacques (1979)
Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem. ,**35**,2751

Formula: C₈H₇O₃¹⁻·C₈H₁₂N₁¹⁺

Compound Name: (S)-1-Phenylethylammonium (S)-mandelate

Space Group: P212121 **Cell:** a 25.602(7) b 6.874(2) c 8.401(3)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.90 **Temperature(K):** 295 **Density(g/cm³):** 1.228



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 45-48

PEAPEA10

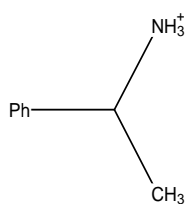
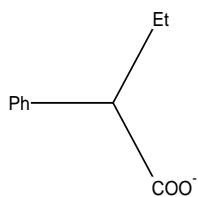
Reference: M.C.Brianso (1981) *Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem.* ,37,740

Formula: C₁₀ H₁₁ O₂¹⁻ · C₈ H₁₂ N₁¹⁺

Compound Name: 1-Phenylethylammonium 2-phenylbutyrate

Space Group: P41 **Cell:** a 16.642(4) b 16.642(4) c 6.408(2)
Space Group No.: 76 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.60 **Temperature(K):** 295 **Density(g/cm³):** 1.068



PEGVON

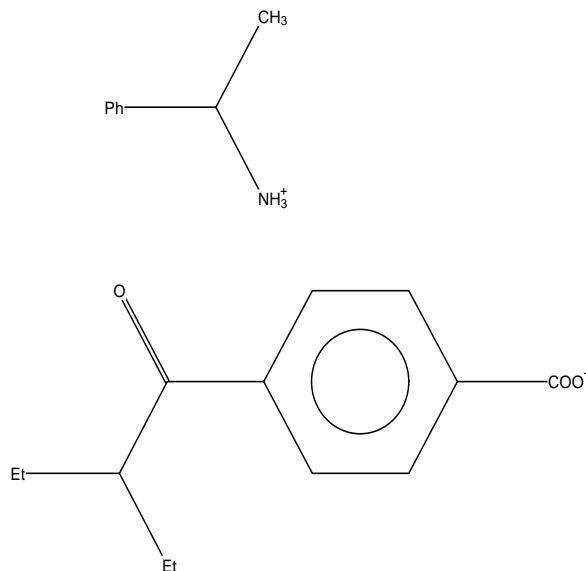
Reference: Wujiong Xia, Chao Yang, J.R.Scheffer, B.O.Patrick (2006) *CrystEngComm* ,8,388

Formula: C₈ H₁₂ N₁¹⁺ · C₁₃ H₁₅ O₃¹⁻

Compound Name: (S)-(-)-1-Phenylethylammonium 2,2-diethyl-1-(p-carboxylatophenyl) ethanone

Space Group: P212121 **Cell:** a 6.121(2) b 7.073(3) c 45.300(20)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 13.81 **Temperature(K):** 173 **Density(g/cm³):** 1.156



PIVGEG

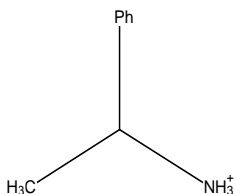
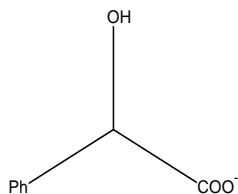
Reference: H.Lopez de Diego (1994) *Acta Chem.Scand.* ,48,306

Formula: C₈ H₁₂ N₁¹⁺ · C₈ H₇ O₃¹⁻

Compound Name: (S)-1-Phenylethylammonium (R)-mandelate

Space Group: P1 **Cell:** a 6.398(1) b 14.807(3) c 16.109(2)
Space Group No.: 1 **(Å,°)** α 75.33(1) β 82.97(0) γ 81.03(2)

R-Factor (%): 4.49 **Temperature(K):** 122 **Density(g/cm³):** 1.250



PIVGEH01

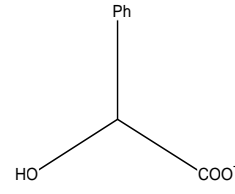
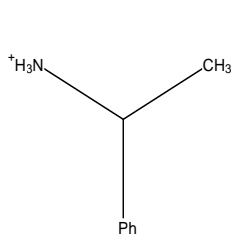
Reference: P.G.Karamertzanis, P.R.Anandamanoharan, P.Fernandes, P.W.Cains, M.Vickers, D.A.Tocher, A.J.Florence, S.L.Price (2007) *J.Phys.Chem.B* ,111,5326

Formula: C₈ H₁₂ N₁¹⁺ · C₈ H₇ O₃¹⁻

Compound Name: (R)-1-Phenylethylammonium (R)-mandelate

Space Group: P212121 **Cell:** a 6.849(0) b 8.325(0) c 25.441(2)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.88 **Temperature(K):** 150 **Density(g/cm³):** 1.252

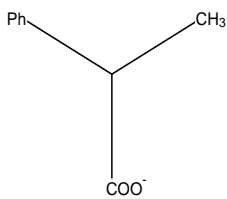
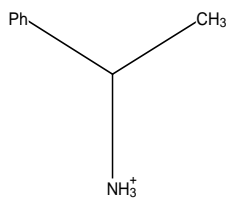


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PMACEP01

Reference: F.Dufour, G.Perez, G.Coquerel (2004) *Bull.Chem.Soc.Jpn.*, **77**,79
Formula: C₈ H₁₂ N₁⁺, C₉ H₉ O₂¹⁻
Compound Name: (S)-Phenylethylammonium (R)-2-phenylpropionate
Synonym: (S)- α -methylbenzylammonium (R)-hydratropate

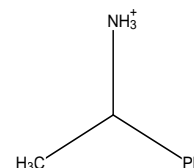
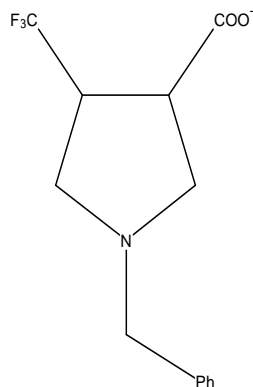
Space Group: P21 **Cell:** a 11.225(1) b 6.570(0) c 12.257(1)
Space Group No.: 4 **(\AA , $^\circ$)** α 90.00 β 115.83(0) γ 90.00
R-Factor (%): 4.49 **Temperature(K):** 296 **Density(g/cm³):** 1.108



PUGQUD

Reference: H.Fukui, K.Kobayashi, T.Nakata, T.Shibata, T.Naito, J.Nakano (1997) *Anal.Sci.*, **13**,689
Formula: C₁₃ H₁₃ F₃ N₁ O₂¹⁻, C₈ H₁₂ N₁⁺
Compound Name: (R)- α -Methylbenzylammonium (-)-(3S,4S)-1-benzyl-4-trifluoromethylpyrrolidine-3-carboxylate

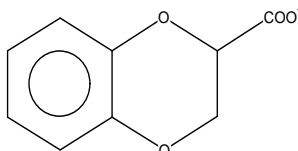
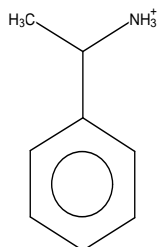
Space Group: P212121 **Cell:** a 14.459(1) b 22.755(1) c 6.420(1)
Space Group No.: 19 **(\AA , $^\circ$)** α 90.00 β 90.00 γ 90.00
R-Factor (%): 5.70 **Temperature(K):** 295 **Density(g/cm³):** 1.240



QANPIF

Reference: N.Marchini, G.Bombieri, R.Artali, C.Bolchi, M.Pallavicini, E.Valoti (2005) *Tetrahedron:Asymm.*, **16**,2099
Formula: C₈ H₁₂ N₁⁺, C₉ H₇ O₄¹⁻
Compound Name: (S)-(1-Phenylethyl)ammonium (S)-1,4-benzodioxane-2-carboxylate

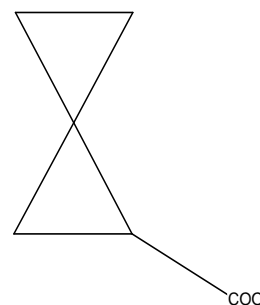
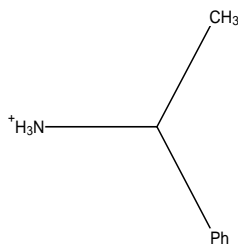
Space Group: P21 **Cell:** a 11.028(3) b 6.752(6) c 11.706(6)
Space Group No.: 4 **(\AA , $^\circ$)** α 90.00 β 111.50(5) γ 90.00
R-Factor (%): 5.40 **Temperature(K):** 293 **Density(g/cm³):** 1.234



QEBVOI

Reference: K.B.Wiberg, C.Osterle (1999) *J.Org.Chem.*, **64**,7763
Formula: C₈ H₁₂ N₁⁺, C₆ H₇ O₂¹⁻
Compound Name: (S)- α -methylbenzylammonium (R)-spiro[5.5]undecane-2-carboxylate

Space Group: P21 **Cell:** a 9.888(0) b 6.903(0) c 19.217(0)
Space Group No.: 4 **(\AA , $^\circ$)** α 90.00 β 91.34(0) γ 90.00
R-Factor (%): 4.50 **Temperature(K):** 295 **Density(g/cm³):** 1.182



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QEFQUN

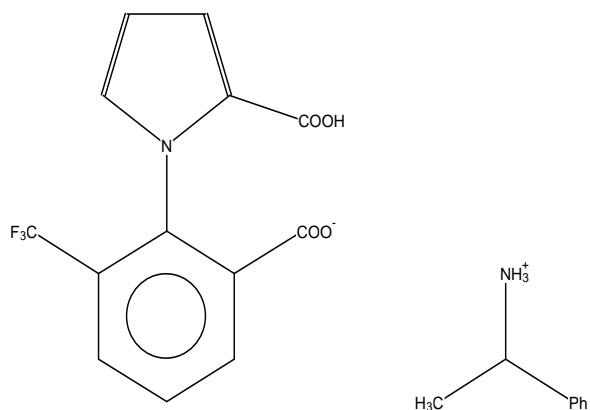
Reference: K.Fogassy, V.Harmat, Z.Bocskai, G.Tarkanyi, L.Toke, F.Faigl (2000) *Tetrahedron:Asymm.* ,11,4771

Formula: C₁₃ H₇ F₃ N₁ O₄¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (R)- α -methylbenzylamine (+)-1-(2-carboxy-6-(trifluoromethyl)phenyl)pyrrole-2-carboxylic acid

Space Group: P21 **Cell:** a 12.398(1) b 7.490(1) c 12.520(1)
Space Group No.: 4 **(\AA , $^\circ$)** α 90.00 β 118.95(0) γ 90.00

R-Factor (%): 5.29 **Temperature(K):** 295 **Density(g/cm³):** 1.372



QEFRAU

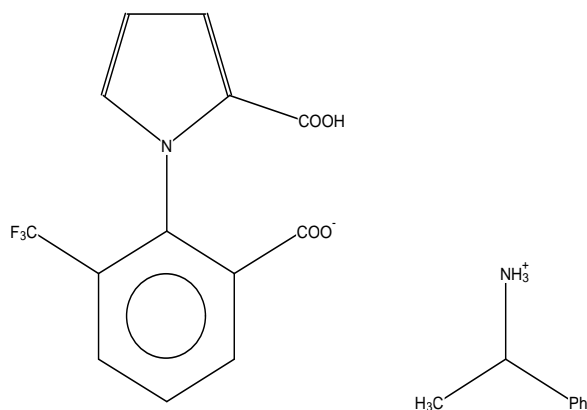
Reference: K.Fogassy, V.Harmat, Z.Bocskai, G.Tarkanyi, L.Toke, F.Faigl (2000) *Tetrahedron:Asymm.* ,11,4771

Formula: C₁₃ H₇ F₃ N₁ O₄¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (S)- α -methylbenzylamine (+)-1-(2-carboxy-6-(trifluoromethyl)phenyl)pyrrole-2-carboxylic acid

Space Group: P21 **Cell:** a 12.169(8) b 7.221(8) c 12.809(8)
Space Group No.: 4 **(\AA , $^\circ$)** α 90.00 β 115.10(2) γ 90.00

R-Factor (%): 7.81 **Temperature(K):** 295 **Density(g/cm³):** 1.370



QEJFUG

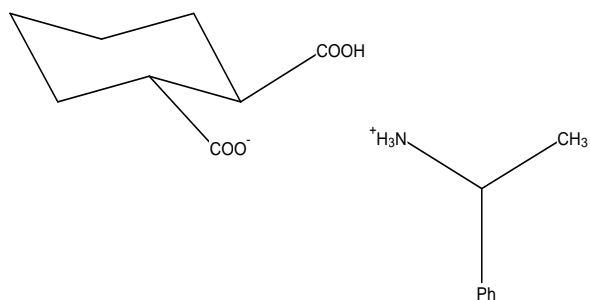
Reference: K.Kimura, Y.Watanabe, T.Suda, H.Senda, S.Hosoi, T.Ohta, K.Kunimoto (1999) *Anal.Sci.* ,15,609

Formula: C₈ H₁₂ N₁¹⁺·C₈ H₁₁ O₄¹⁻

Compound Name: (R)-1-Phenylethylammonium (1R,2R)-trans-cyclohexane-1-carboxylate-2-carboxylic acid

Space Group: P212121 **Cell:** a 9.988(0) b 26.034(2) c 6.083(0)
Space Group No.: 19 **(\AA , $^\circ$)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.10 **Temperature(K):** 295 **Density(g/cm³):** 1.232



RAHLIV

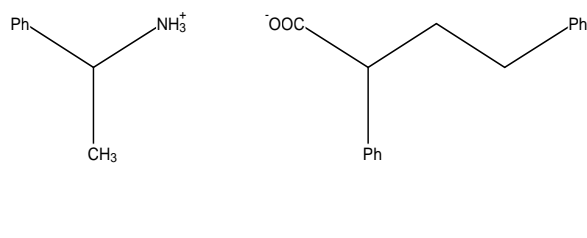
Reference: A.P.Kozikowski, W.Tuckmantel, C.George (2000) *J.Org.Chem.* ,65,5371

Formula: C₈ H₁₂ N₁¹⁺·C₁₆ H₁₅ O₂¹⁻

Compound Name: (R)-(+)- α -Methylbenzylammonium (R)-(-)-2,4-diphenylbutyrate

Space Group: C2 **Cell:** a 30.228(2) b 6.156(1) c 11.686(1)
Space Group No.: 5 **(\AA , $^\circ$)** α 90.00 β 108.21(1) γ 90.00

R-Factor (%): 3.16 **Temperature(K):** 293 **Density(g/cm³):** 1.162



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 57-60

RAYRAK

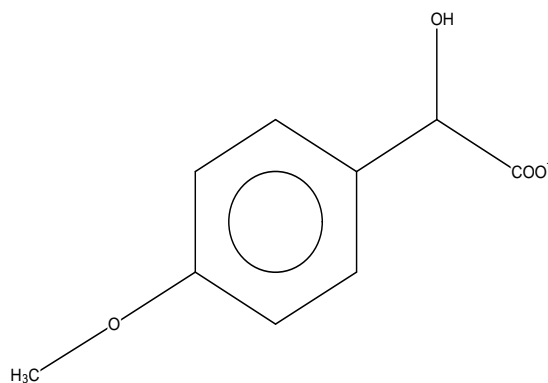
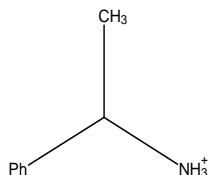
Reference: K.Kinbara, K.Sakai, Y.Hashimoto, H.Nohira, K.Saigo (1996) *J.Chem.Soc.,Perkin Trans.2* ,2615

Formula: C₈ H₁₂ N₁¹⁺, C₉ H₉ O₄¹⁻

Compound Name: (R)-1-Phenylethylammonium (R)-p-methoxymandelate

Space Group: P21 **Cell:** a 13.963(3) b 6.945(2) c 8.355(2)
Space Group No.: 4 **(Å, °)** α 90.00 β 96.19(2) γ 90.00

R-Factor (%): 3.29 **Temperature(K):** 295 **Density(g/cm³):** 1.251



RICGIU

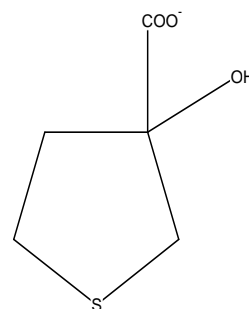
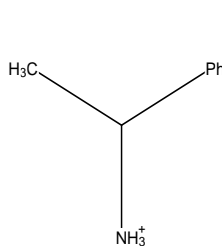
Reference: H.M.Fechter, K.Gruber, M.Avi, W.Skranc, C.Schuster, P.Pochlauer, K.O.Klepp, H.Griegl (2007) *Chem.-Eur.J.* ,13,3369

Formula: C₈ H₁₂ N₁¹⁺, C₅ H₇ O₃ S₁¹⁻

Compound Name: (S)-1-Phenylethylammonium (S)-3-hydroxytetrahydrothiophene-3-carboxylate

Space Group: P212121 **Cell:** a 6.449(2) b 13.267(6) c 16.220(11)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.10 **Temperature(K):** 294 **Density(g/cm³):** 1.289



ROLFAZ

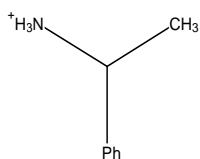
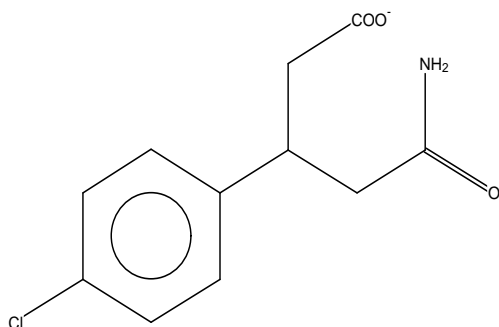
Reference: M.R.Caira, R.Clauss, L.R.Nassimbeni, J.L.Scott, A.F.Wildervanck (1997) *J.Chem.Soc.,Perkin Trans.2* ,763

Formula: C₁₁ H₁₁ Cl₁ N₁ O₃¹⁻, C₈ H₁₂ N₁¹⁺

Compound Name: (S)-(-)-α-Phenylethylammonium (R)-(+)-3-(p-chlorophenyl)glutaramate

Space Group: P21 **Cell:** a 5.728(2) b 20.671(3) c 8.354(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 107.39(2) γ 90.00

R-Factor (%): 2.96 **Temperature(K):** 295 **Density(g/cm³):** 1.277



RUTYUA

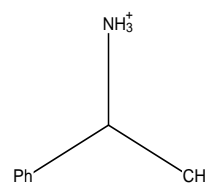
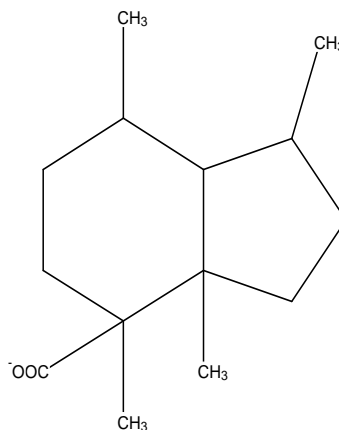
Reference: E.J.Corey, B.E.Roberts (1997) *Tetrahedron Lett.* ,38,8921

Formula: C₁₄ H₂₃ O₂¹⁻, C₈ H₁₂ N₁¹⁺

Compound Name: 1S-1-Methyl-1-phenylethylammonium 1R,2R,5R,6R,9S-2,5,6,9-tetramethylbicyclo[4.3.0]nonane-5-carboxylate

Space Group: P21212 **Cell:** a 14.181(2) b 21.243(2) c 13.934(2)
Space Group No.: 18 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 7.91 **Temperature(K):** 193 **Density(g/cm³):** 1.094



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SABJOU

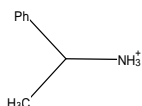
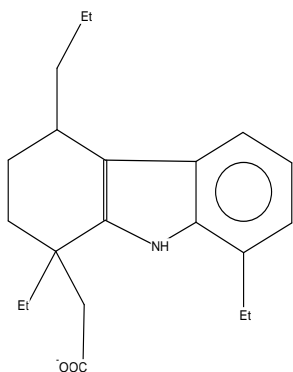
Reference: D.Mobilio, L.G.Humber, A.H.Katz, C.A.Demerson, P.Hughes, R.Brigance, K.Conway, U.Shah, G.Williams, F.Labbadia, B.de Lange, A.Asselin, J.Schmid, J.Newburger, N.P.Jensen, B.M.Weichman, T.Chau, G.Neuman, D.D.Wood, D.van Engen, N.Taylor (1988) *J.Med.Chem.* ,31,2211

Formula: $C_{21}H_{28}N_1O_2^{1-} \cdot C_8H_{12}N_1^{1+}$

Compound Name: (R)- α -Methylbenzylammonium (1R-cis)-1,8-diethyl-2,3,4,9-tetrahydro-4-propyl-1H-carbazole-1-acetate

Space Group: P212121 **Cell:** **a** 6.081(2) **b** 15.850(5) **c** 27.919(8)
Space Group No.: 19 **(\AA , $^\circ$)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 0.00 **Temperature(K):** 295 **Density(g/cm 3):** 1.107



SAFCIM

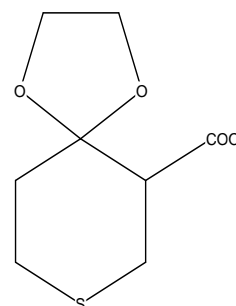
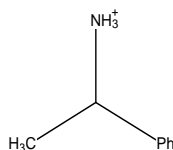
Reference: D.E.Ward, O.T.Akinnusi, I.Q.Alarcon, V.Jheengut, Jianheng Shen, J.W.Quail (2004) *Tetrahedron:Asymm.* ,15,2425

Formula: $C_8H_{12}N_1^{1+} \cdot C_8H_{11}O_4S_1^{1-}$

Compound Name: (S)-1-Phenylethylammonium (S)-1,4-diaza-8-thia-spiro(4.5)decane-6-carboxylate

Space Group: C2 **Cell:** **a** 21.880(0) **b** 5.830(0) **c** 15.277(0)
Space Group No.: 5 **(\AA , $^\circ$)** α 90.00 β 121.59(0) γ 90.00

R-Factor (%): 4.19 **Temperature(K):** 173 **Density(g/cm 3):** 1.302



SIRKUA

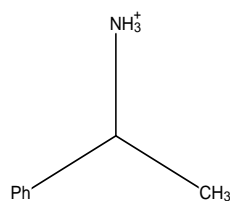
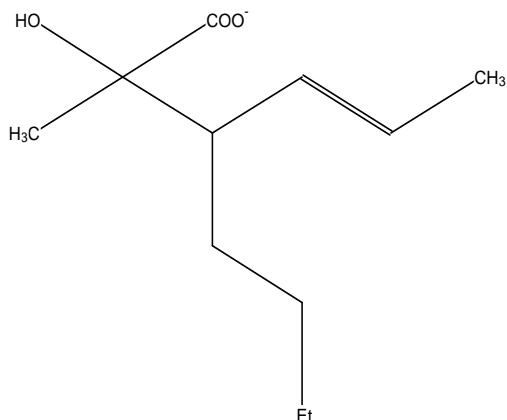
Reference: B.E.Howard, K.A.Woerpel (2007) *Org.Lett.* ,9,4651

Formula: $C_8H_{12}N_1^{1+} \cdot C_{11}H_{19}O_3^{1-}$

Compound Name: 1-Phenylethylammonium 2-hydroxy-2-methyl-3-(propenyl)heptanoate

Space Group: P21 **Cell:** **a** 17.558(3) **b** 5.405(0) **c** 20.711(3)
Space Group No.: 4 **(\AA , $^\circ$)** α 90.00 β 92.48(0) γ 90.00

R-Factor (%): 5.97 **Temperature(K):** 153 **Density(g/cm 3):** 1.087



TEPQIO

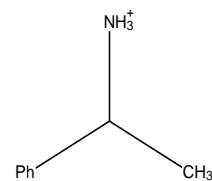
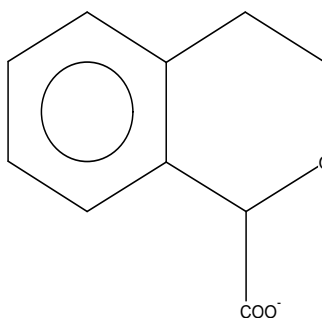
Reference: B.Unterhalt, B.Krebs, M.Lage, B.Nocon (1994) *Arch.Pharm.* ,327,799

Formula: $C_{10}H_9O_3^{1-} \cdot C_8H_{12}N_1^{1+}$

Compound Name: 1-Phenylethylammonium (S,S)-isochroman-1-carboxylate

Space Group: P212121 **Cell:** **a** 6.649(4) **b** 13.117(7) **c** 19.007(11)
Space Group No.: 19 **(\AA , $^\circ$)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.69 **Temperature(K):** 295 **Density(g/cm 3):** 1.200



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TERFOL

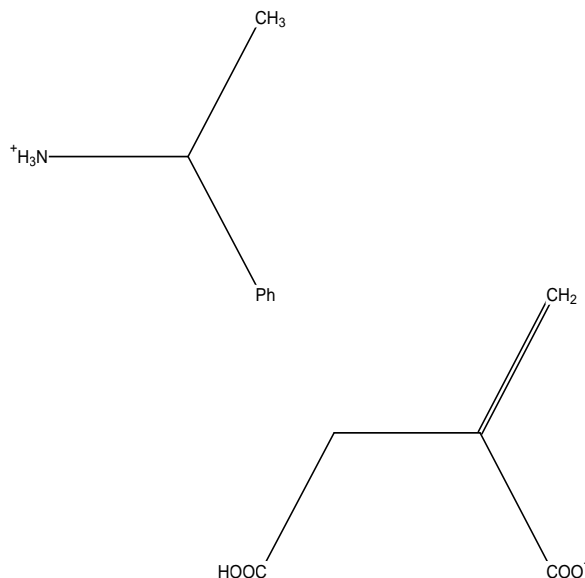
Reference: Z.Bocskai, C.Kassai, K.Simon, E.Fogassy, D.Kozma (1996) *J.Chem.Soc.,Perkin Trans.2* ,1511

Formula: C₈ H₁₂ N₁¹⁺, C₅ H₅ O₄¹⁻

Compound Name: (R)- α -Phenylethylammonium hydrogen itaconate

Space Group: P212121 **Cell:** a 11.049(5) b 18.758(4) c 6.317(3)
Space Group No.: 19 **(\AA , $^\circ$)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.97 **Temperature(K):** 295 **Density(g/cm³):** 1.275



TEWFOR

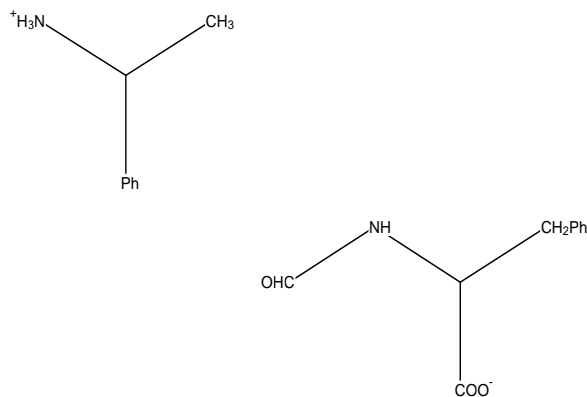
Reference: L.Bereczki, E.Palovics, P.Bombicz, G.Pokol, E.Fogassy, K.Marthi (2007) *Tetrahedron:Asymm.* ,18,260

Formula: C₈ H₁₂ N₁¹⁺, C₁₀ H₁₀ N₁ O₃¹⁻

Compound Name: (S)-(-)-1-Phenylethylammonium (S)-(+)-N-formylphenylalaninate

Space Group: P212121 **Cell:** a 6.104(0) b 16.255(1) c 16.790(1)
Space Group No.: 19 **(\AA , $^\circ$)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.03 **Temperature(K):** 93 **Density(g/cm³):** 1.254



TEYXOL

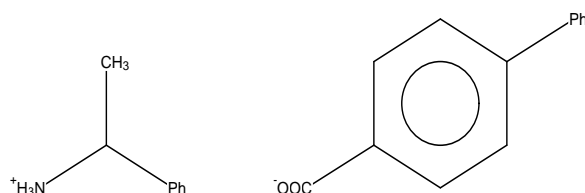
Reference: K.Kodama, Y.Kobayashi, K.Saigo (2007) *Chem.-Eur.J.* ,13, 2144

Formula: C₈ H₁₂ N₁¹⁺, C₁₃ H₉ O₂¹⁻

Compound Name: (R)-1-Phenylethylammonium 4-phenylbenzoate

Space Group: P21 **Cell:** a 7.210(1) b 6.353(0) c 20.224(4)
Space Group No.: 4 **(\AA , $^\circ$)** α 90.00 β 103.83(0) γ 90.00

R-Factor (%): 8.50 **Temperature(K):** 296 **Density(g/cm³):** 1.179



TEYXUR

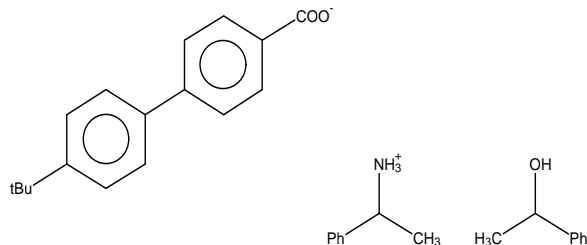
Reference: K.Kodama, Y.Kobayashi, K.Saigo (2007) *Chem.-Eur.J.* ,13, 2144

Formula: C₈ H₁₂ N₁¹⁺, C₁₇ H₁₇ O₂¹⁻, C₈ H₁₀ O₁

Compound Name: (R)-1-Phenylethylammonium 4-(4-t-butylphenyl)benzoate (R)-1-phenylethanol

Space Group: P212121 **Cell:** a 6.640(3) b 12.096(5) c 35.610(10)
Space Group No.: 19 **(\AA , $^\circ$)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.30 **Temperature(K):** 293 **Density(g/cm³):** 1.156



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 69-72

UKUMUI

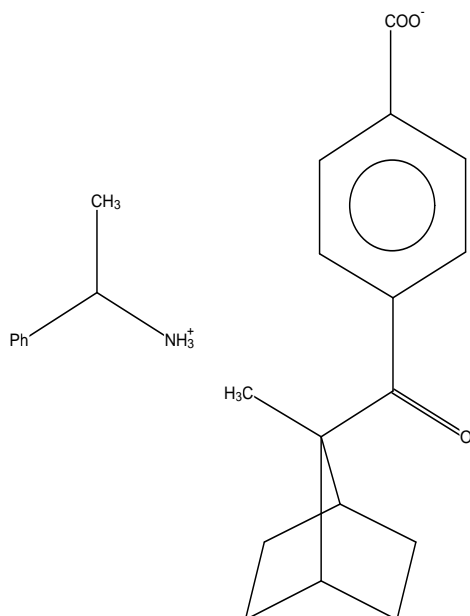
Reference: B.O.Patrick, J.R.Scheffer, C.Scott (2003)
Angew.Chem.,Int.Ed., **42**,3775

Formula: C₈ H₁₂ N₁¹⁺.C₁₆ H₁₇ O₃¹⁻

Compound Name: (S)-(-)-1-phenylethylammonium 4-((7-methylbicyclo(2.2.1)hept-7-yl) carbonyl)benzoate

Space Group: P212121 **Cell:** a 6.165(2) b 7.090(2) c 45.810(20)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.80 **Temperature(K):** 173 **Density(g/cm³):** 1.259



UKUNET02

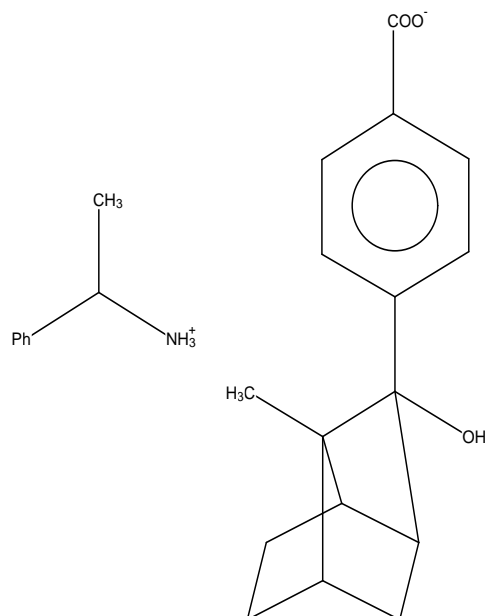
Reference: B.O.Patrick, J.R.Scheffer, C.Scott (2003)
Angew.Chem.,Int.Ed., **42**,3775

Formula: C₈ H₁₂ N₁¹⁺.C₁₆ H₁₇ O₃¹⁻

Compound Name: (S)-(-)-1-phenylethylammonium 4-((1S,2S,5R,7R,8S)-8-hydroxy-1-methyltricyclo(3.3.0.0(2,7))oct-8-yl)benzoate

Space Group: P21 **Cell:** a 12.258(1) b 6.990(0) c 12.665(1)
Space Group No.: 4 **(Å,°)** α 90.00 β 105.87(0) γ 90.00

R-Factor (%): 4.06 **Temperature(K):** 173 **Density(g/cm³):** 1.207



VIQPUH

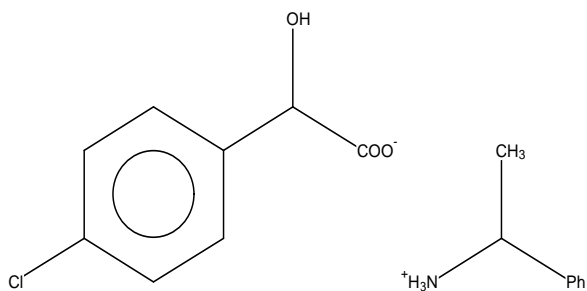
Reference: Quan He, M.C.Jennings, S.Rohani, J.Zhu, H.Gomaa (2008) *Acta Crystallogr., Sect.E: Struct.Rep.Online*, **64**,o559

Formula: C₈ H₁₂ N₁¹⁺.C₈ H₈ Cl₁ O₃¹⁻

Compound Name: (R)-1-Phenylethanaminium (S)-4-chloromandelate

Space Group: P21 **Cell:** a 10.409(0) b 5.764(0) c 13.254(1)
Space Group No.: 4 **(Å,°)** α 90.00 β 96.83(0) γ 90.00

R-Factor (%): 4.44 **Temperature(K):** 150 **Density(g/cm³):** 1.295



VISTAT

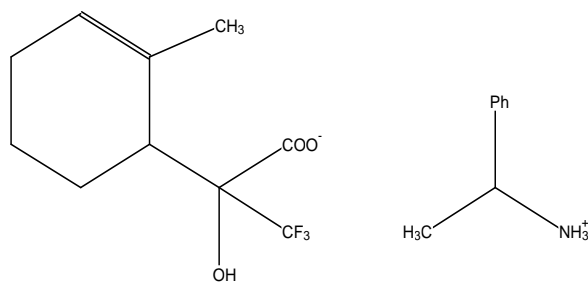
Reference: S.Doherty, J.G.Knight, C.H.Smyth, R.W.Harrington, W.Clegg (2007) *Organometallics*, **26**,6453

Formula: C₁₀ H₁₂ F₃ O₃¹⁻.C₈ H₁₂ N₁¹⁺

Compound Name: (S)-α-methylbenzylammonium (2R)-3,3,3-trifluoro-2-hydroxy-2-((1R)-2-methylcyclohex-2-en-1-yl)propanoate

Space Group: P21 **Cell:** a 11.271(1) b 6.647(1) c 13.145(2)
Space Group No.: 4 **(Å,°)** α 90.00 β 114.25(0) γ 90.00

R-Factor (%): 6.66 **Temperature(K):** 120 **Density(g/cm³):** 1.329



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 73-76

WALKIE

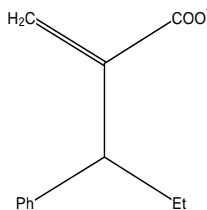
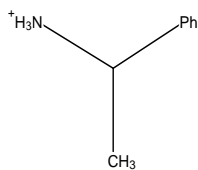
Reference: P.J.Goldsmith, S.J.Teate, S.Woodward (2005)
Angew.Chem.,Int.Ed., **44**,2235

Formula: C₈ H₁₂ N₁⁺, C₁₂ H₁₃ O₂¹⁻

Compound Name: (R)-1-Phenylethylammonium (R)-3-phenylpentene-2-carboxylate

Space Group: P21 **Cell:** a 11.927(2) b 19.015(3) c 12.876(2)
Space Group No.: 4 **(Å, °)** α 90.00 β 111.66(0) γ 90.00

R-Factor (%): 5.86 **Temperature(K):** 150 **Density(g/cm³):** 1.143



WANKUR

Reference: P.G.Jones, T.Laue, H.Hopf (1993)
Acta Crystallogr.,Sect.C:Cryst.Struct.Commun., **49**,1195

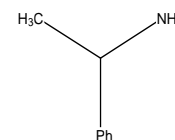
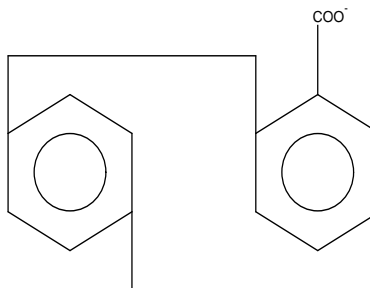
Formula: C₁₇ H₁₅ O₂¹⁻, C₈ H₁₂ N₁⁺

Compound Name: (-)-(S)-α-Phenylethylammonium tricyclo(8.2.2.2^{4,7})hexadeca-4,6,10,12,13,15-hexaene-5-carboxylate

Synonym: (-)-(S)-(α-Methylbenzyl)ammonium (-)-(R)-(2,2)paracyclophane-4-carboxylate

Space Group: C2 **Cell:** a 23.343(9) b 6.453(3) c 17.683(6)
Space Group No.: 5 **(Å, °)** α 90.00 β 128.48(3) γ 90.00

R-Factor (%): 3.80 **Temperature(K):** 178 **Density(g/cm³):** 1.190



WIKJEF

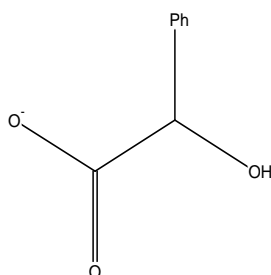
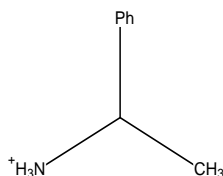
Reference: H.L.de Diego (1994)
Acta Crystallogr.,Sect.C:Cryst.Struct.Commun., **50**,1995

Formula: C₈ H₁₂ N₁⁺, C₈ H₇ O₃¹⁻

Compound Name: (R,S)-1-Phenylethylammonium (S)-mandelate

Space Group: P21 **Cell:** a 25.543(4) b 6.566(0) c 8.691(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 93.66(1) γ 90.00

R-Factor (%): 14.87 **Temperature(K):** 122 **Density(g/cm³):** 1.248



WIPBIH

Reference: Quan He, M.C.Jennings, S.Rohani, J.Zhu, H.Gomaa (2007) *Acta Crystallogr.,Sect.E:Struct.Rep.Online*, **63**,o4199

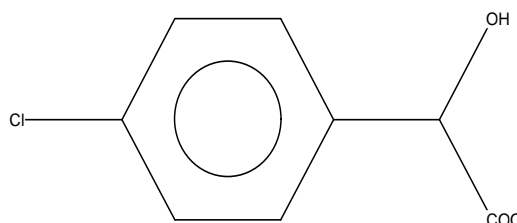
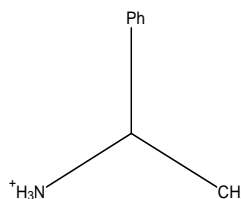
Formula: C₈ H₁₂ N₁⁺, C₈ H₆ Cl₁ O₃¹⁻

Compound Name: (R)-1-Phenylethylammonium (R)-2-(4-chlorophenyl)-2-hydroxyacetate

Synonym: (R)-1-Phenylethylammonium (R)-4-chloromandelate

Space Group: P212121 **Cell:** a 6.885(0) b 8.398(0) c 26.943(1)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.83 **Temperature(K):** 296 **Density(g/cm³):** 1.312



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 77-80

WOSTIH

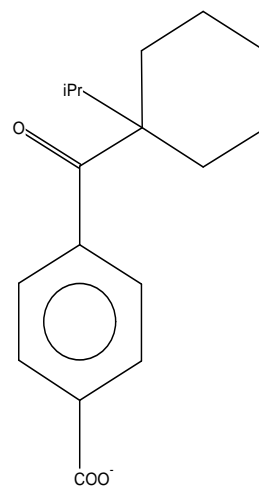
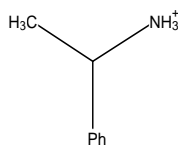
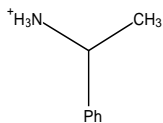
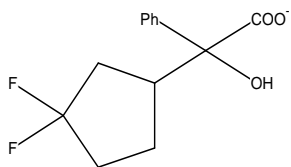
Reference: M.Mitsuya, Y.Ogino, N.Ohtake, T.Mase (2000) *Tetrahedron*, **56**,9901

Formula: C₈ H₁₂ N₁¹⁺·C₁₃ H₁₃ F₂ O₃¹⁻

Compound Name: (S)-1-Phenylethylammonium (2R)-2-((1R)-3,3-difluorocyclopentyl)-2-hydroxy-2-phenylacetate

Space Group: P21 **Cell:** **a** 12.430(2) **b** 5.743(2) **c** 14.608(2)
Space Group No.: 4 **(Å, °)** **α** 90.00 **β** 105.16(1) **γ** 90.00

R-Factor (%): 6.71 **Temperature(K):** 295 **Density(g/cm³):** 1.245



XAMWOY

Reference: Wujiang Xia, J.R.Scheffer, M.Botoshansky, M.Kaftory (2005) *Org.Lett.*, **7**,1315

Formula: C₈ H₁₂ N₁¹⁺·C₁₇ H₂₁ O₃¹⁻

Compound Name: α-Methylbenzylammonium 4-(1-isopropylcyclohexylcarbonyl)benzoate

Space Group: C2 **Cell:** **a** 48.050(10) **b** 6.381(1) **c** 14.630(3)
Space Group No.: 5 **(Å, °)** **α** 90.00 **β** 92.22(1) **γ** 90.00

R-Factor (%): 5.14 **Temperature(K):** 293 **Density(g/cm³):** 1.172

XOHFOP

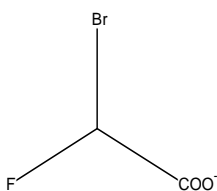
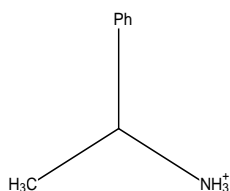
Reference: H.Boussac, J.Crassous, J.-P.Dutasta, L.Grosvalet, A.Thozet (2002) *Tetrahedron:Asymm.*, **13**,975

Formula: C₈ H₁₂ N₁¹⁺·C₂ H₁ Br₁ F₁ O₂¹⁻

Compound Name: (R)-(+)-α-methylbenzylammonium (S)-(+)-bromofluoroacetate

Space Group: P212121 **Cell:** **a** 6.954(1) **b** 8.691(1) **c** 18.312(4)
Space Group No.: 19 **(Å, °)** **α** 90.00 **β** 90.00 **γ** 90.00

R-Factor (%): 4.06 **Temperature(K):** 123 **Density(g/cm³):** 1.669



YELQAH

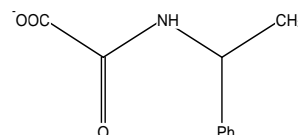
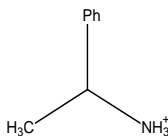
Reference: J.Balint, G.Egri, M.Czugler, J.Schindler, V.Kiss, Z.Juvancz, E.Fogassy (2001) *Tetrahedron:Asymm.*, **12**,1511

Formula: C₈ H₁₂ N₁¹⁺·C₁₀ H₁₀ N₁ O₃¹⁻

Compound Name: (R)-1-Phenylethylammonium (S)-N-(1-phenylethylamine)oxalamate

Space Group: P21 **Cell:** **a** 11.478(1) **b** 6.660(2) **c** 11.593(1)
Space Group No.: 4 **(Å, °)** **α** 90.00 **β** 103.06(1) **γ** 90.00

R-Factor (%): 4.73 **Temperature(K):** 295 **Density(g/cm³):** 1.209



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 81-84

YELQEL

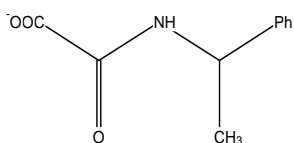
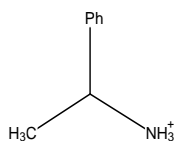
Reference: J.Balint, G.Egri, M.Czugler, J.Schindler, V.Kiss, Z.Juvancz, E.Fogassy (2001) *Tetrahedron:Asymm.* ,12,1511

Formula: C₈ H₁₂ N₁⁺·C₁₀ H₁₀ N₁ O₃¹⁻

Compound Name: (R)-1-Phenylethylammonium (R)-N-(1-phenylethylamine)oxalamate

Space Group: P21 **Cell:** a 9.869(1) b 6.750(1) c 13.548(1)
Space Group No.: 4 **(Å, °)** α 90.00 β 101.38(1) γ 90.00

R-Factor (%): 4.11 **Temperature(K):** 293 **Density(g/cm³):** 1.180



YUPYEN

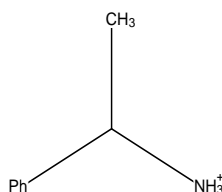
Reference: Z.Bocskei, D.Kozma, K.Simon, E.Fogassy (1995) *J.Opt.Soc.Am.* ,160

Formula: 2(C₈ H₁₂ N₁⁺)·C₂ O₄²⁻

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

Space Group: C2 **Cell:** a 10.786(1) b 7.430(0) c 11.493(0)
Space Group No.: 5 **(Å, °)** α 90.00 β 98.66(0) γ 90.00

R-Factor (%): 6.00 **Temperature(K):** 295 **Density(g/cm³):** 1.212



ZUNNIF

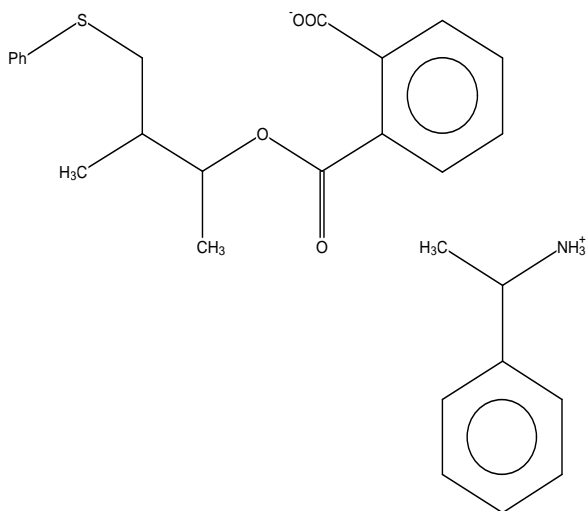
Reference: S.Koul, D.H.G.Crout, W.Errington, J.Tax (1995) *J.Chem.Soc.,Perkin Trans.1* ,2969

Formula: C₁₉ H₁₉ O₄ S₁¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (R)-1-Methylbenzylammonium (2S,3R)-3-methyl-4-phenylsulfanylbutan-2-yl phthalate

Space Group: P212121 **Cell:** a 6.111(7) b 15.850(20) c 25.960(40)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.96 **Temperature(K):** 295 **Density(g/cm³):** 1.230



ZUSLEE

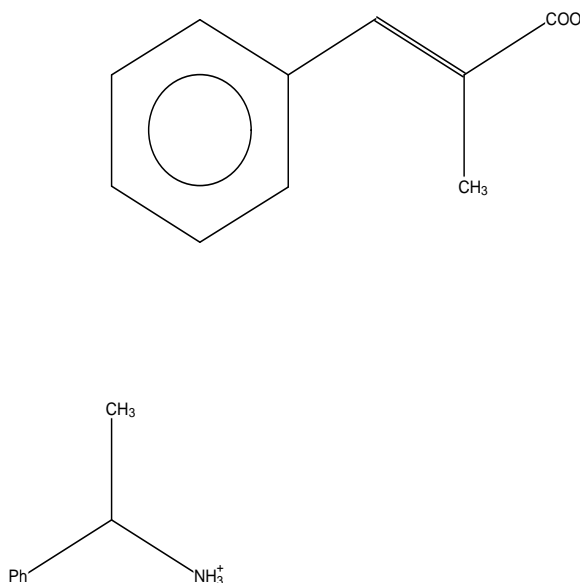
Reference: K.Kinbara, Y.Hashimoto, M.Sukegawa, H.Nohira, K.Saigo (1996) *J.Am.Chem.Soc.* ,118,3441

Formula: C₁₀ H₉ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (R)-1-Phenylethylammonium o-methylcinnamate

Space Group: P212121 **Cell:** a 7.572(1) b 34.424(6) c 6.321(1)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.31 **Temperature(K):** 295 **Density(g/cm³):** 1.142



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ZUSLOO

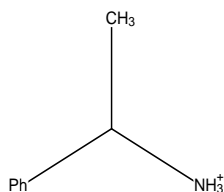
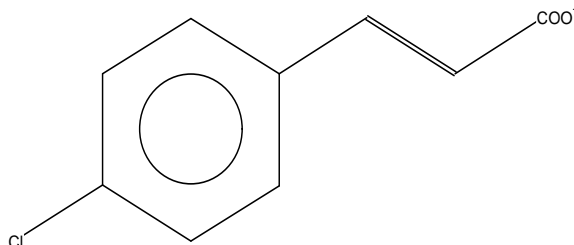
Reference: K.Kinbara, Y.Hashimoto, M.Sukegawa, H.Nohira, K.Saigo (1996) *J.Am.Chem.Soc.*, **118**,3441

Formula: C₉ H₆ Cl₁ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (R)-1-Phenylethylammonium p-chlorocinnamate

Space Group: P212121 **Cell:** a 9.376(1) b 28.353(4) c 6.076(1)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.46 **Temperature(K):** 295 **Density(g/cm³):** 1.249



ZUSLUU

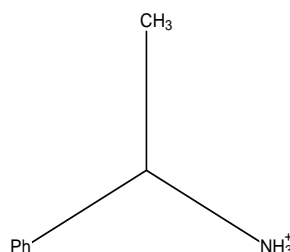
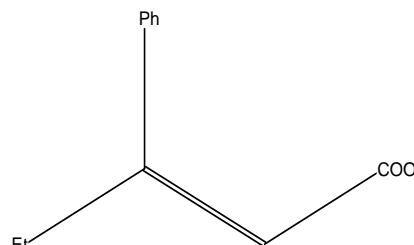
Reference: K.Kinbara, Y.Hashimoto, M.Sukegawa, H.Nohira, K.Saigo (1996) *J.Am.Chem.Soc.*, **118**,3441

Formula: C₁₁ H₁₁ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (R)-1-Phenylethylammonium (Z)-3-phenyl-2-pentenoate

Space Group: P21 **Cell:** a 13.326(4) b 6.172(2) c 11.885(3)
Space Group No.: 4 **(Å,°)** α 90.00 β 114.90(2) γ 90.00

R-Factor (%): 5.75 **Temperature(K):** 295 **Density(g/cm³):** 1.114



ZUSMIJ

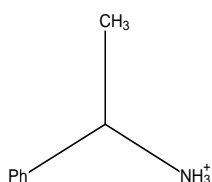
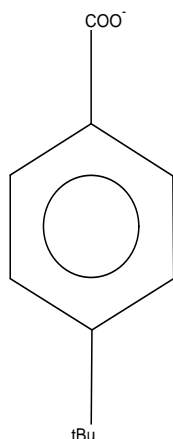
Reference: K.Kinbara, Y.Hashimoto, M.Sukegawa, H.Nohira, K.Saigo (1996) *J.Am.Chem.Soc.*, **118**,3441

Formula: C₁₁ H₁₃ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (R)-1-Phenylethylammonium p-t-butylbenzoate

Space Group: P21 **Cell:** a 19.838(6) b 6.356(2) c 7.032(2)
Space Group No.: 4 **(Å,°)** α 90.00 β 90.14(2) γ 90.00

R-Factor (%): 10.95 **Temperature(K):** 295 **Density(g/cm³):** 1.121



ZUSMUV

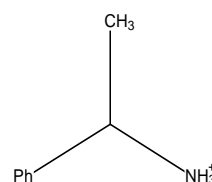
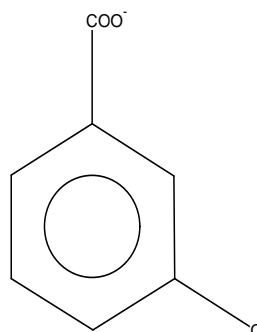
Reference: K.Kinbara, Y.Hashimoto, M.Sukegawa, H.Nohira, K.Saigo (1996) *J.Am.Chem.Soc.*, **118**,3441

Formula: C₇ H₄ Cl₁ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (R)-1-Phenylethylammonium m-chlorobenzoate

Space Group: P212121 **Cell:** a 7.182(1) b 32.302(6) c 6.256(2)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 5.74 **Temperature(K):** 295 **Density(g/cm³):** 1.271



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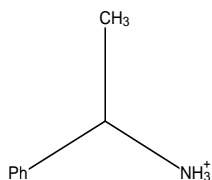
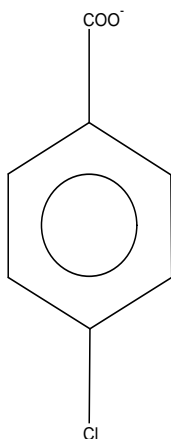
Reference: K.Kinbara, Y.Hashimoto, M.Sukegawa, H.Nohira, K.Saigo (1996) *J.Am.Chem.Soc.* ,118,3441

Formula: C₇ H₄ Cl₁ O₂¹⁻·C₈ H₁₂ N₁¹⁺

Compound Name: (R)-1-Phenylethylammonium p-chlorobenzoate

Space Group: P212121 **Cell:** a 10.089(0) b 23.117(2) c 5.973(0)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 4.92 **Temperature(K):** 295 **Density(g/cm³):** 1.324



KEBYAS01

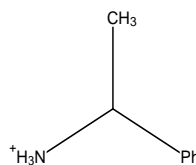
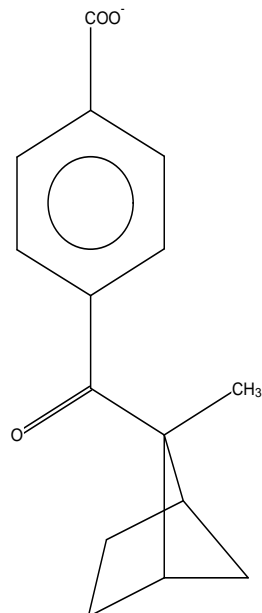
Reference: I.Turowska-Tyrk, I.Labecka, J.R.Scheffer, W.Xia (2007) *Pol.J.Chem.* ,81,813

Formula: C₈ H₁₂ N₁¹⁺·C₁₅ H₁₅ O₃¹⁻

Compound Name: (S)-(-)-1-Phenylethylammonium 5-(4-carboxybenzoyl)-5-methyl-endobicyclo(2.1.1)hexane

Space Group: P212121 **Cell:** a 6.181(1) b 7.303(1) c 45.496(7)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 6.21 **Temperature(K):** 293 **Density(g/cm³):** 1.182



KOBGIS

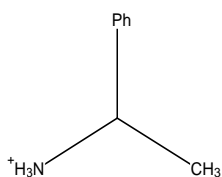
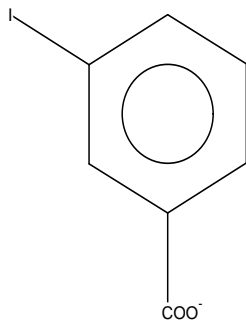
Reference: A.Lemmerer, S.A.Bourne, M.A.Fernandes (2008) *Cryst.Growth Des.* ,8,1106

Formula: C₈ H₁₂ N₁¹⁺·C₇ H₄ I₁ O₂¹⁻

Compound Name: (R)-1-phenylethylammonium m-iodobenzoate

Space Group: P212121 **Cell:** a 6.200(0) b 7.111(0) c 33.151(4)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.54 **Temperature(K):** 173 **Density(g/cm³):** 1.678



KOFMUO

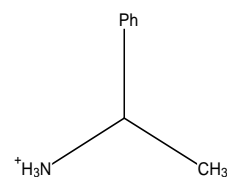
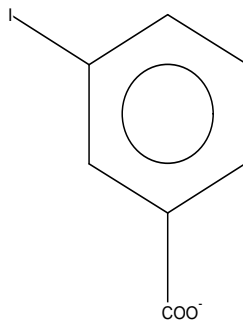
Reference: A.Lemmerer, S.A.Bourne, M.A.Fernandes (2008) *Cryst.Growth Des.* ,8,1106

Formula: C₈ H₁₂ N₁¹⁺·C₇ H₄ I₁ O₂¹⁻

Compound Name: (S)-1-phenylethylammonium m-iodobenzoate

Space Group: P212121 **Cell:** a 6.187(0) b 7.095(2) c 33.158(0)
Space Group No.: 19 **(Å,°)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 2.47 **Temperature(K):** 173 **Density(g/cm³):** 1.685

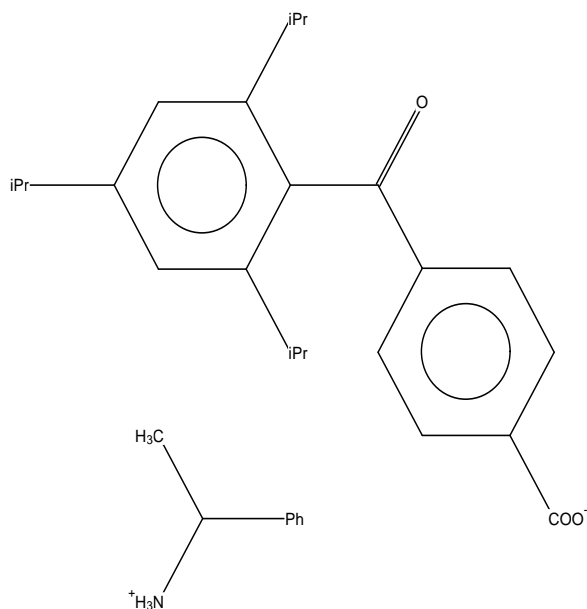


Search: search9 (Mon Aug 10 17:30:07 2009): Hits 93-96

SOFPEJ

Reference: H.Koshima, Y.Ide, M.Fukano, K.Fujii, H.Uekusa (2008) *Tetrahedron Lett.*, **49**,4346
Formula: C₂₃H₂₇O₃¹⁻·C₈H₁₂N₁¹⁺
Compound Name: (S)-1-Phenylethanaminium 4-(2,4,6-tri(isopropyl)benzoyl)benzoate

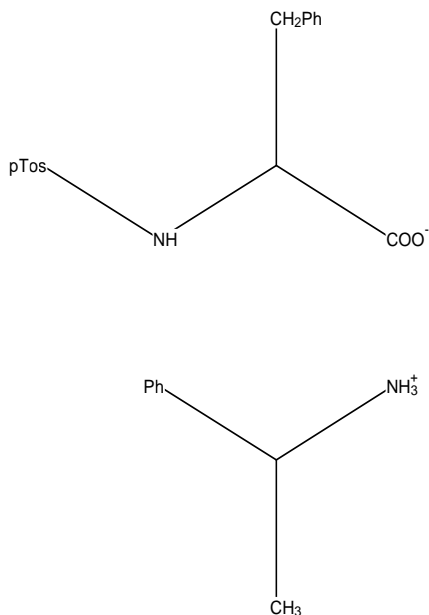
Space Group: P212121 **Cell:** a 6.243(1) b 13.787(3) c 32.470(8)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00
R-Factor (%): 6.53 **Temperature(K):** 296 **Density(g/cm³):** 1.126



UFUWUO

Reference: T.Hirose, M.Begum, Md.S.Islam, K.Taniguchi, M.Yasutake (2008) *Tetrahedron:Asymm.*, **19**,1641
Formula: C₈H₁₂N₁¹⁺·C₁₆H₁₆N₁O₄S₁¹⁻
Compound Name: (S)-1-Phenylethanaminium (S)-2-(((4-methylphenyl)sulfonyl)amino)-3-phenylpropanoate

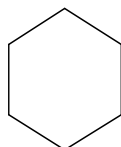
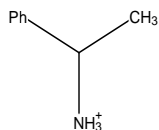
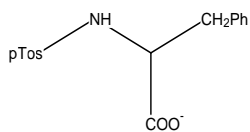
Space Group: P21 **Cell:** a 11.371(2) b 5.865(1) c 33.222(7)
Space Group No.: 4 **(Å, °)** α 90.00 β 92.99(3) γ 90.00
R-Factor (%): 4.49 **Temperature(K):** 123 **Density(g/cm³):** 1.322



UFUXAV

Reference: T.Hirose, M.Begum, Md.S.Islam, K.Taniguchi, M.Yasutake (2008) *Tetrahedron:Asymm.*, **19**,1641
Formula: C₈H₁₂N₁¹⁺·C₁₆H₁₆N₁O₄S₁¹⁻·C₆H₁₂
Compound Name: (R)-1-Phenylethanaminium (S)-2-(((4-methylphenyl)sulfonyl)amino)-3-phenylpropanoate cyclohexane solvate

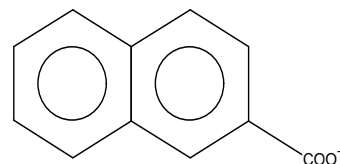
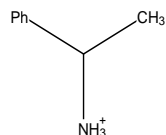
Space Group: P212121 **Cell:** a 6.182(1) b 20.039(4) c 22.350(5)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00
R-Factor (%): 10.33 **Temperature(K):** 123 **Density(g/cm³):** 1.259



KOLLUT

Reference: A.Lemmerer, S.Bourne, M.A.Fernandes (2008) *CrystEngComm*, **10**,1605
Formula: C₈H₁₂N₁¹⁺·C₁₁H₇O₂¹⁻
Compound Name: ((R)-1-Phenylethylammonium) naphthalene-2-carboxylate

Space Group: P212121 **Cell:** a 6.368(1) b 14.511(3) c 17.457(4)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00
R-Factor (%): 5.21 **Temperature(K):** 173 **Density(g/cm³):** 1.208



Search: search9 (Mon Aug 10 17:30:07 2009): Hits 97-100

KOLMAA

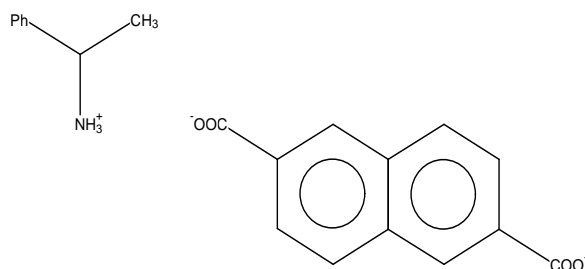
Reference: A.Lemmerer, S.Bourne, M.A.Fernandes (2008)
CrystEngComm, **10**,1605

Formula: $2(C_8H_{12}N_1^{1+}), C_{12}H_6O_4^{2-}$

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



KOMZOC

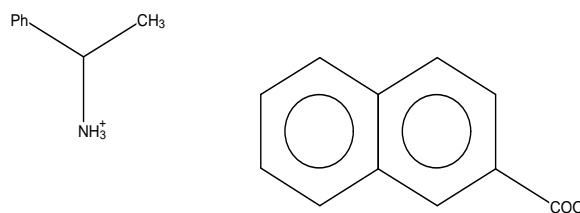
Reference: A.Lemmerer, S.Bourne, M.A.Fernandes (2008)
CrystEngComm, **10**,1605

Formula: $C_8H_{12}N_1^{1+}, C_{11}H_7O_2^{1-}$

Compound Name: ((S)-1-Phenylethylammonium) naphthalene-2-carboxylate

Space Group: P212121 **Cell:** a 6.371(1) b 14.513(3) c 17.445(4)
Space Group No.: 19 **(Å, °)** α 90.00 β 90.00 γ 90.00

R-Factor (%): 3.70 **Temperature(K):** 173 **Density(g/cm³):** 1.208



KONBAR

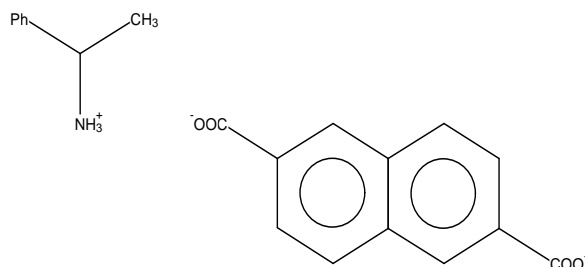
Reference: A.Lemmerer, S.Bourne, M.A.Fernandes (2008)
CrystEngComm, **10**,1605

Formula: $2(C_8H_{12}N_1^{1+}), C_{12}H_6O_4^{2-}$

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



QOQNAC

Reference: Y.Imai, K.Kamon, K.Murata, T.Harada, Y.Nakano, T.Sato, M.Fujiki, R.Kuroda, Y.Matsubara (2008) *Org.Biomol.Chem.*, **6**,3471

Formula: $C_8H_{12}N_1^{1+}, C_{15}H_9O_2^{1-}$

Compound Name: (R)-1-Phenylethylammonium anthracene-2-carboxylate

Space Group: P21 **Cell:** a 9.319(3) b 6.150(1) c 15.347(4)
Space Group No.: 4 **(Å, °)** α 90.00 β 90.09(0) γ 90.00

R-Factor (%): 5.18 **Temperature(K):** 120 **Density(g/cm³):** 1.297

