

# Search Overview

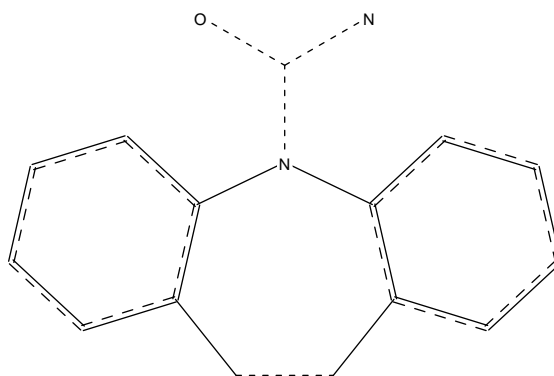
**Search:** search1  
**Date/Time done:** Fri Dec 07 16:17:43 2012  
**Database(s):** CSD version 5.33 (November 2011)  
CSD version 5.33 updates (Nov 2011)  
CSD version 5.33 updates (Feb 2012)  
CSD version 5.33 updates (May 2012)  
**Restriction Info:** No reffcode restrictions applied  
**Filters:** 3D coordinates determined No powder structures  
**Percentage Completed:** 100%  
**Number of Hits:** 82

**Single query used. Search found structures that:**

match

**Query 1**

**Query 1**



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 1

## AFEVEN

**Reference:** A.Johnston, A.J.Florence, P.Fernandes, N.Shankland, A.R.Kennedy (2007) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,**63**, o3888

**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>1</sub> H<sub>3</sub> N<sub>1</sub> O<sub>1</sub>

**Compound Name:** 10,11-dihydro-5H-dibenz(b,f)azepine-5-carboxamide formamide solvate

**Synonym:** Dihydrocarbamazepine formamide solvate

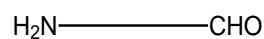
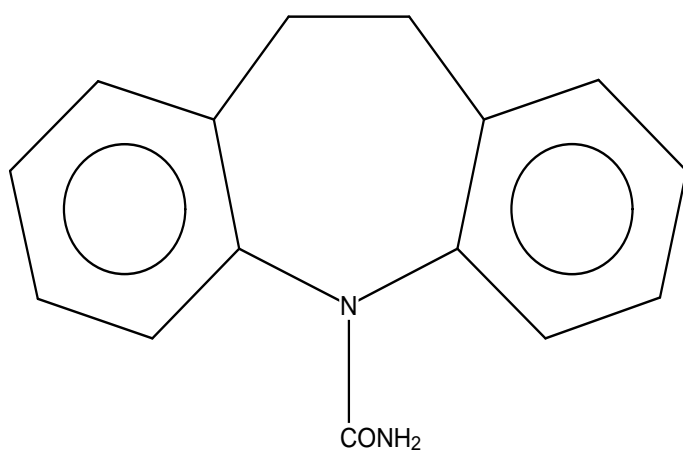
**Space Group:** P-1      **Cell:**    **a** 8.469(0)    **b** 9.021(0)    **c** 10.314(0)  
**Space Group No.:** 2      (**Å, °**)     $\alpha$  74.36(0)     $\beta$  83.63(0)     $\gamma$  70.85(0)

**R-Factor (%):** 7.38      **Temperature(K):** 120      **Density(g/cm<sup>3</sup>):** 1.313

### Parameters

Fragment 1

**DIST1 (D)**      1.245  
**DIST2 (D)**      1.366  
**DIST3 (D)**      1.345



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 2

## AFEZOB

**Reference:** A.Johnston, A.J.Florence, K.Shankland, C.K.Leech,  
N.Shankland, P.Fernandes (2007)  
*Acta Crystallogr., Sect.E: Struct.Rep. Online* ,**63**,o3918

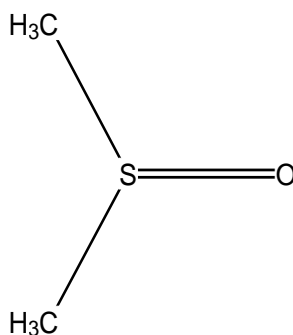
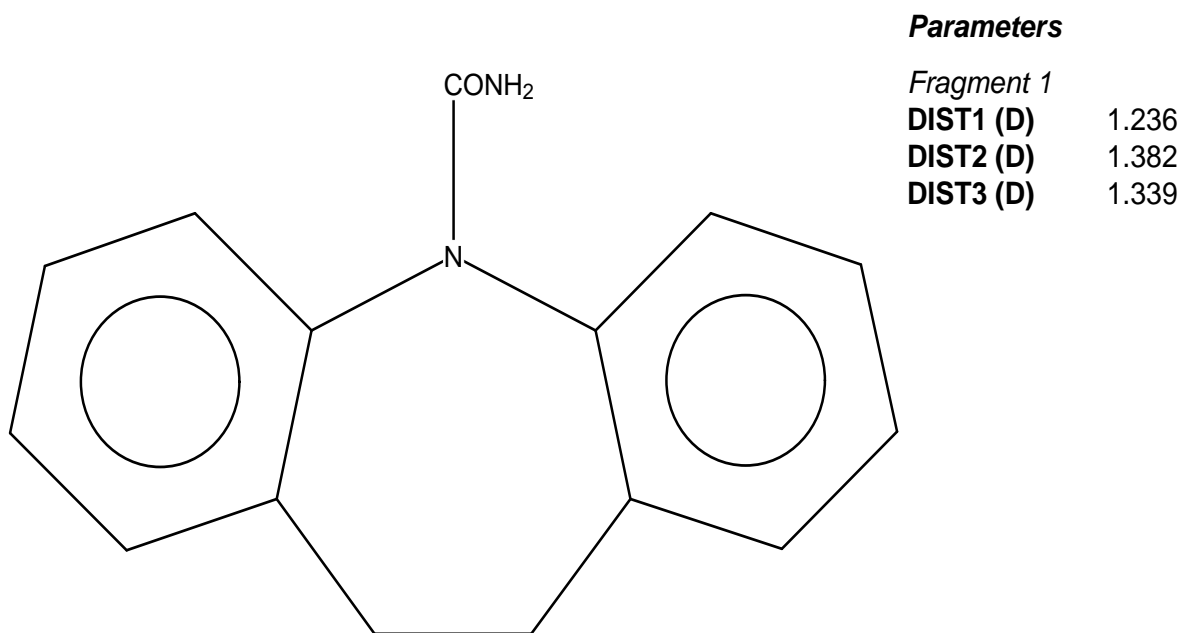
**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>2</sub> H<sub>6</sub> O<sub>1</sub> S<sub>1</sub>

**Compound Name:** 10,11-Dihydro-5H-dibenz(b,f)azepine-5-carboxamide dimethylsulfoxide solvate

**Synonym:** 10,11-Dihydrocarbamazepine dimethylsulfoxide solvate

**Space Group:** P21/c      **Cell:**      **a** 10.270(0)      **b** 6.854(0)      **c** 23.360(0)  
**Space Group No.:** 14      (**Å, °**)      **α** 90.00      **β** 98.93(0)      **γ** 90.00

**R-Factor (%):** 4.21      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.294



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 3

CBMZPN01

**Reference:** J.P.Reboul, B.Cristau, J.C.Soyfer, J.P.Astier (1981)  
*Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem.* ,**37**,1844

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 5H-Dibenz(b,f)azepine-5-carboxamide

**Synonym:** Carbamazepine

**Space Group:** P21/c      **Cell:**      **a** 7.529(1)      **b** 11.148(2)      **c** 15.470(2)

**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 116.17(1)      **γ** 90.00

**R-Factor (%):** 3.50      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.347

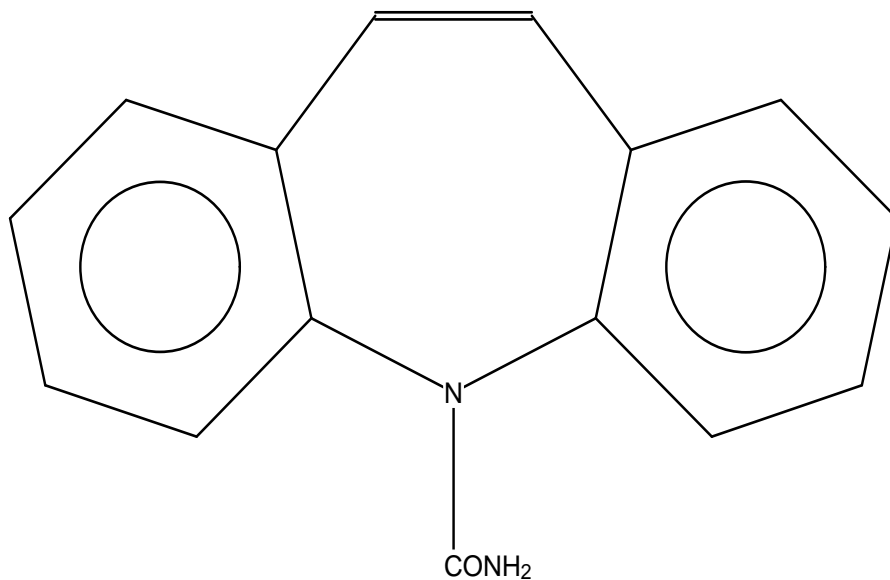
## Parameters

Fragment 1

**DIST1 (D)** 1.230

**DIST2 (D)** 1.380

**DIST3 (D)** 1.341



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 4

CBMZPN02

**Reference:** J.N.Lisgarten, R.A.Palmer, J.W.Saldanha (1989)  
*J.Crystallogr.Spectrosc.Res.* ,19,641

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 5-Carbamoyl-5H-dibenzo(b,f)azepine

**Synonym:** Carbamazepine

**Space Group:** P21/n      **Cell:**    **a** 7.534(1)    **b** 11.150(2)    **c** 13.917(3)

**Space Group No.:** 14      **(Å, °)**    **α** 90.00      **β** 92.94(4)    **γ** 90.00

**R-Factor (%):** 8.40      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.344

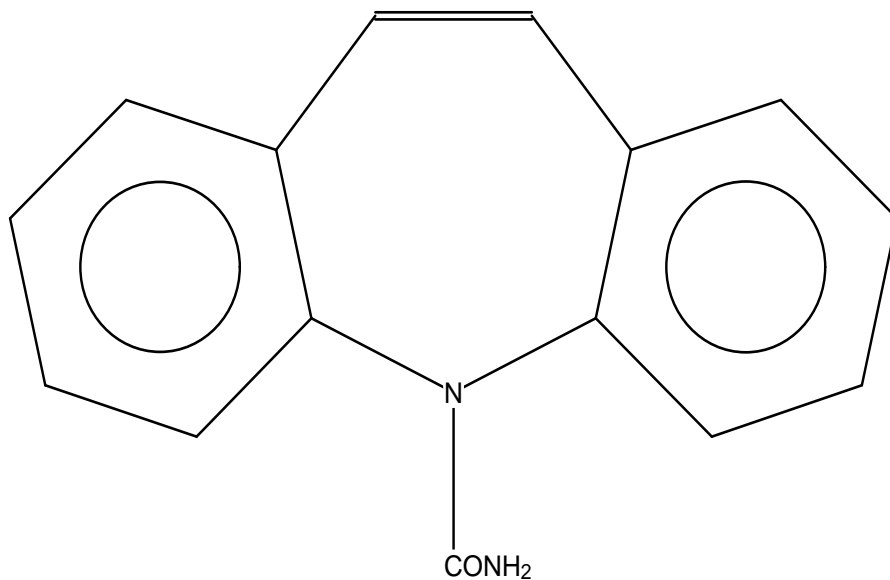
## Parameters

Fragment 1

**DIST1 (D)**      1.234

**DIST2 (D)**      1.386

**DIST3 (D)**      1.363



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 5

CBMZPN03

**Reference:** M.M.J.Lowes, M.R.Cairo, A.P.Lotter, J.G.van der Watt  
(1987) *J.Pharm.Sci.* ,76,744

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 5H-Dibenz(b,f)azepine-5-carboxamide

**Synonym:** Carbamazepine

**Space Group:** R-3      **Cell:**    **a** 35.454(3)    **b** 35.454(3)    **c** 5.253(1)

**Space Group No.:** 148      **(Å, °)**    **α** 90.00      **β** 90.00      **γ** 120.00

**R-Factor (%):** 6.90      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.235

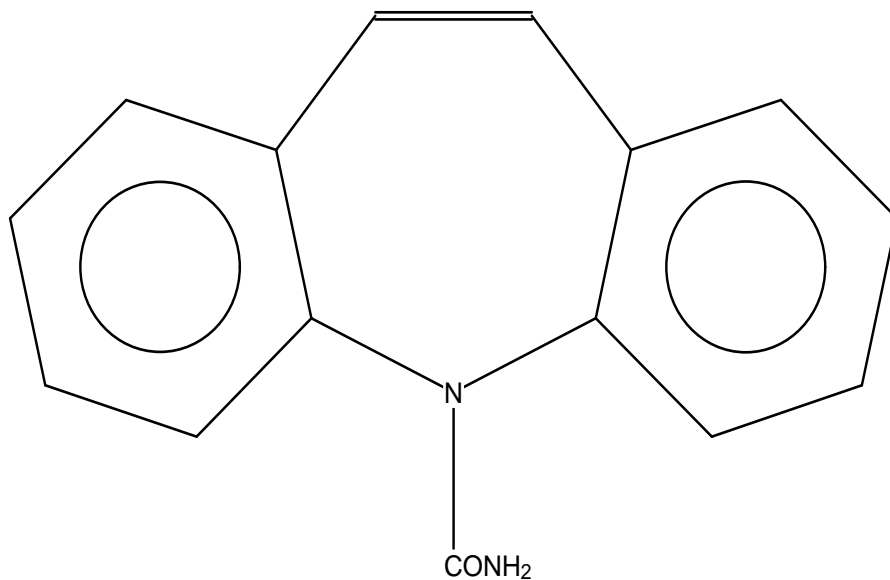
## Parameters

Fragment 1

**DIST1 (D)**      1.240

**DIST2 (D)**      1.377

**DIST3 (D)**      1.354



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 6

## CBMZPN10

**Reference:** V.L.Himes, A.D.Mighell, W.H.DeCamp (1981)  
*Acta Crystallogr., Sect.B: Struct. Crystallogr. Cryst. Chem.* ,**37**,2242

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 5H-Dibenz(b,f)azepine-5-carboxamide

**Synonym:** Carbamazepine

**Space Group:** P21/n      **Cell:**      **a** 7.537(1)      **b** 11.156(2)      **c** 13.912(3)

**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 92.86(2)      **γ** 90.00

**R-Factor (%):** 3.90      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.343

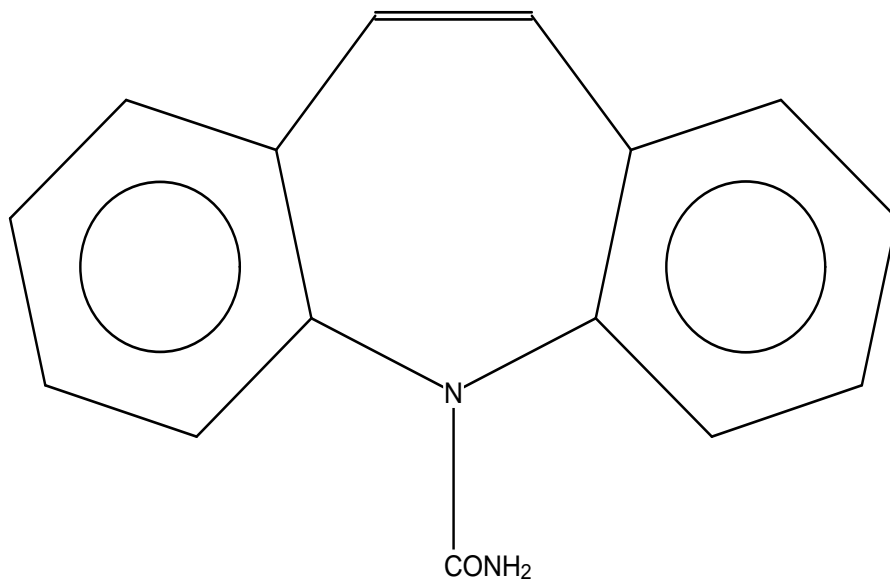
### Parameters

Fragment 1

**DIST1 (D)**      1.230

**DIST2 (D)**      1.379

**DIST3 (D)**      1.346



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 7

## CBMZPN11

**Reference:** A.L.Grzesiak, Meidong Lang, Kibum Kim, A.J.Matzger  
(2003) *J.Pharm.Sci.* ,**92**,2260

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

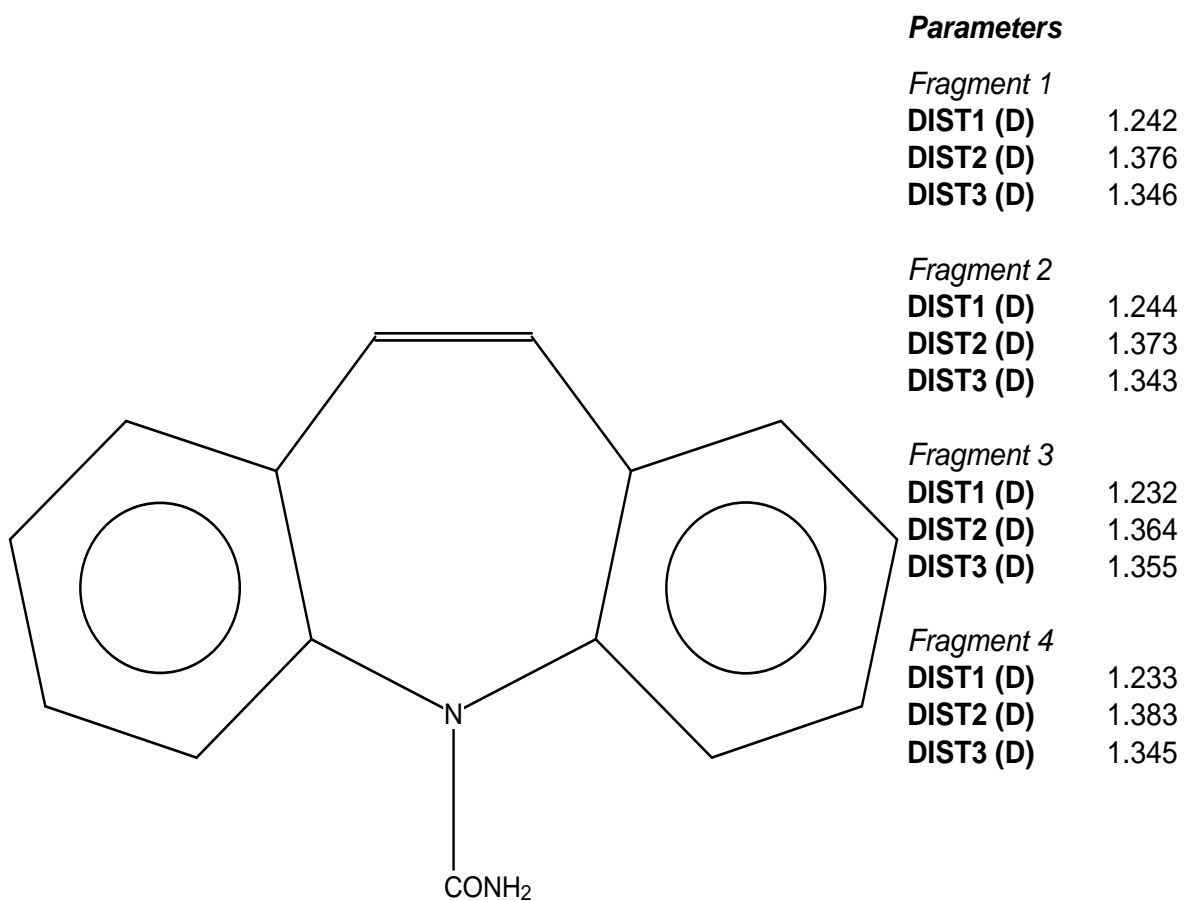
**Compound Name:** Carbamazepine

**Synonym:** 5H-Dibenz(b,f)azepine-5-carboxamide

**Space Group:** P-1      **Cell:**    **a** 5.171(0)    **b** 20.574(2)    **c** 22.245(2)

**Space Group No.:** 2      **(Å, °)**    **α** 84.12(0)    **β** 88.01(0)    **γ** 85.19(0)

**R-Factor (%):** 5.06      **Temperature(K):** 158      **Density(g/cm<sup>3</sup>):** 1.339





# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 8

CBMZPN12

**Reference:** M.Lang, J.W.Kampf, A.J.Matzger (2002) *J.Pharm.Sci.* ,**91**, 1186

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** Carbamazepine

**Space Group:** C2/c      **Cell:**    **a** 26.609(4)    **b** 6.927(1)    **c** 13.957(2)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 109.70(0)    **γ** 90.00

**R-Factor (%):** 3.57      **Temperature(K):** 158      **Density(g/cm<sup>3</sup>):** 1.296

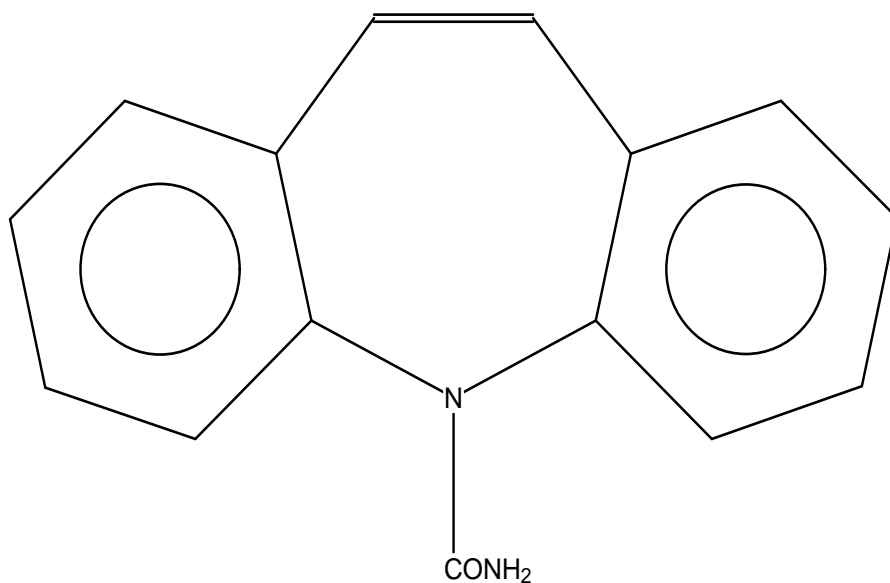
## Parameters

Fragment 1

**DIST1 (D)**      1.236

**DIST2 (D)**      1.377

**DIST3 (D)**      1.345



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 9

## CBMZPN14

**Reference:** K.S.Eccles, S.P.Stokes, C.A.Daly, N.M.Barry,  
S.P.McSweeney, D.J.O'Neill, D.M.Kelly, W.B.Jennings,  
O.M.N.Dhubhghaill, H.A.Moynihan, A.R.Maguire, S.E.Lawrence (2011)  
*J.Appl.Crystallogr.*, **44**,213

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 5H-Dibenzo[b,f]azepine-5-carboxamide

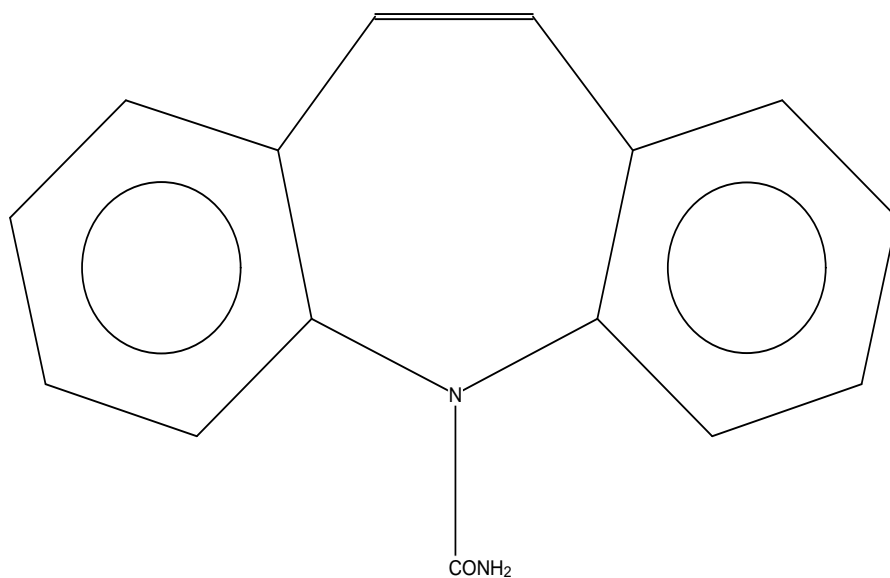
**Space Group:** P21/n      **Cell:**      **a** 7.550(1)      **b** 11.186(3)      **c** 13.954(3)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  92.94(0)       $\gamma$  90.00

**R-Factor (%):** 4.04      **Temperature(K):** 300      **Density(g/cm<sup>3</sup>):** 1.333

### Parameters

Fragment 1

**DIST1 (D)**      1.234  
**DIST2 (D)**      1.379  
**DIST3 (D)**      1.349



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 10

CRBMZA01

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>3</sub> H<sub>6</sub> O<sub>1</sub>

**Compound Name:** Carbamazepine acetone solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide acetone solvate

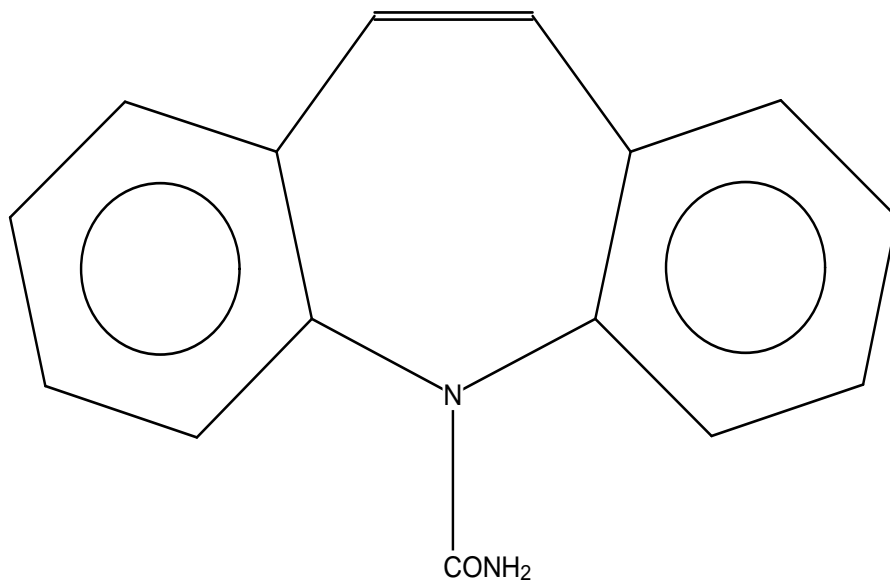
**Space Group:** P-1      **Cell:**    **a** 7.399(1)    **b** 8.905(1)    **c** 11.873(2)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  95.81(0)     $\beta$  93.40(0)     $\gamma$  101.36(0)

**R-Factor (%):** 7.68      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.285

## Parameters

Fragment 1

**DIST1 (D)**      1.226  
**DIST2 (D)**      1.399  
**DIST3 (D)**      1.352



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 11

## FEFNOT02

**Reference:** R.K.Harris, P.Y.Ghi, H.Puschmann, D.C.Apperley, U.J.Griesser, R.B.Hammond, Caiyun Ma, K.J.Roberts, G.J.Pearce, J.R.Yates, C.J.Pickard (2005) *Org.Process Res.Dev.* ,9,902

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,2</sub>(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** Carbamazepine dihydrate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide dihydrate

**Space Group:** P21/c      **Cell:**      **a** 10.066(2)      **b** 28.719(5)      **c** 4.831(1)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 103.45(1)      **γ** 90.00

**R-Factor (%):** 7.29      **Temperature(K):** 120      **Density(g/cm<sup>3</sup>):** 1.332

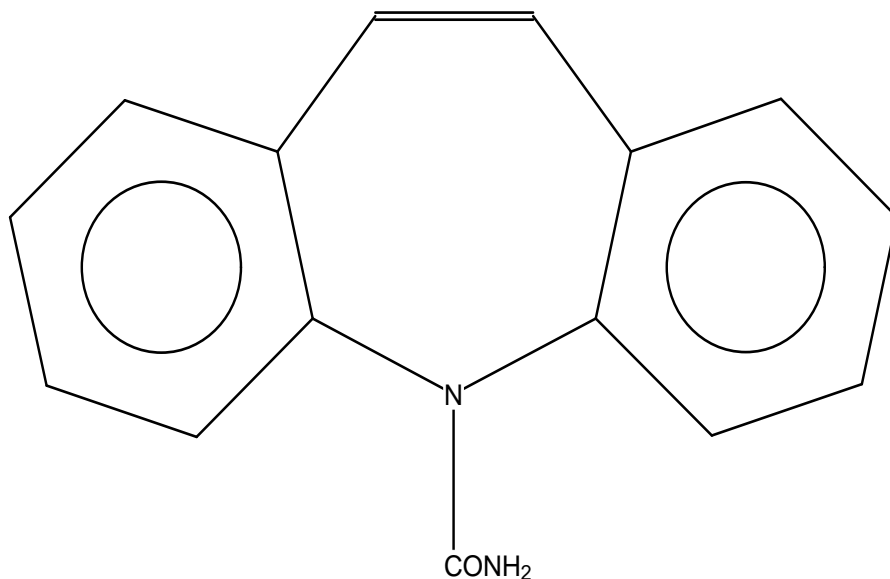
### Parameters

Fragment 1

**DIST1 (D)** 1.263

**DIST2 (D)** 1.376

**DIST3 (D)** 1.318



H<sub>2</sub>O

# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 12

FEFNOT03

**Reference:** T.Gelbrich, M.B.Hursthouse (2006) *CrystEngComm* ,8,448

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,2</sub>(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** Carbamazepine dihydrate

**Space Group:** P21/c      **Cell:**      **a** 10.105(0)      **b** 28.809(1)      **c** 4.838(0)

**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 103.87(1)      **γ** 90.00

**R-Factor (%):** 5.06      **Temperature(K):** 120      **Density(g/cm<sup>3</sup>):** 1.323

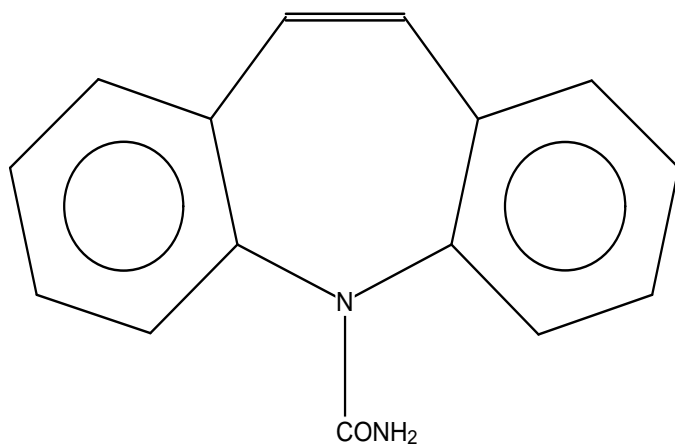
## Parameters

Fragment 1

**DIST1 (D)** 1.257

**DIST2 (D)** 1.378

**DIST3 (D)** 1.328



H<sub>2</sub>O

# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 13

FEFNOT04

**Reference:** A.Kogan, I.Popov, V.Uvarov, S.Cohen, A.Aserin, N.Garti  
(2007) *Journal of Dispersion Science and Technology* ,28,1008

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,2</sub>(H<sub>2</sub> O<sub>1</sub>)

**Compound Name:** 5H-Dibenzo[b,f]azepine-5-carboxamide dihydrate

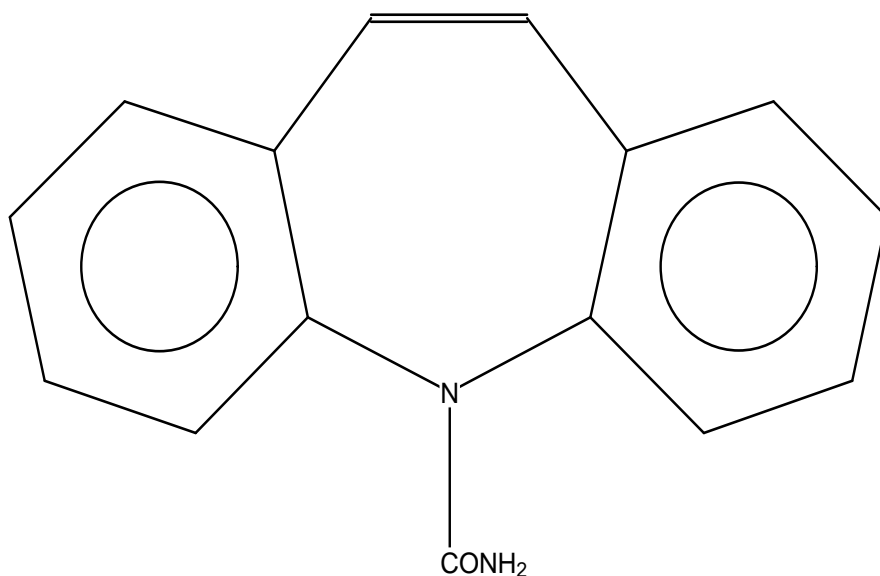
**Space Group:** P21/c      **Cell:**      **a** 10.162(0)      **b** 28.705(3)      **c** 4.935(0)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 103.33(0)      **γ** 90.00

**R-Factor (%):** 6.87      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.291

## Parameters

Fragment 1

**DIST1 (D)**      1.244  
**DIST2 (D)**      1.372  
**DIST3 (D)**      1.321



H<sub>2</sub>O

# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 14

FOMXAH

**Reference:** A.Johnston, A.J.Florence, A.R.Kennedy (2005)  
*Acta Crystallogr., Sect.E:Struct.Rep.Online* ,61,o1777

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,0.5</sub>(C<sub>5</sub> H<sub>4</sub> O<sub>2</sub>)

**Compound Name:** 5H-Dibenzo(b,f)azepine-5-carboxamide furan-2-carbaldehyde solvate

**Synonym:** Carbamazepine furfural solvate

**Space Group:** P21/n      **Cell:**      **a** 5.182(0)      **b** 26.045(1)      **c** 20.573(1)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 91.30(0)      **γ** 90.00

**R-Factor (%):** 5.65      **Temperature(K):** 120      **Density(g/cm<sup>3</sup>):** 1.361

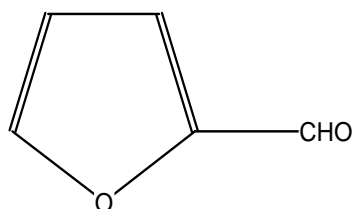
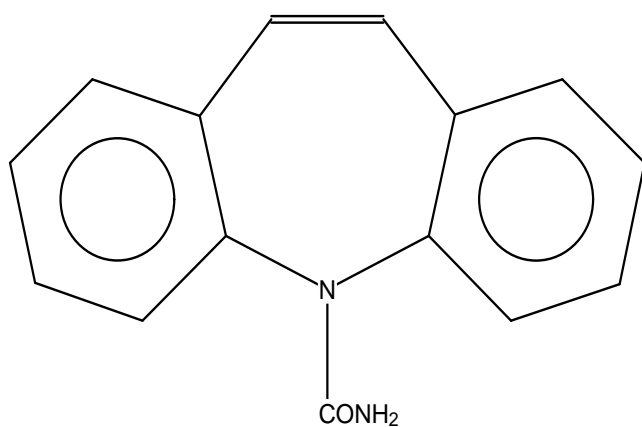
## Parameters

### Fragment 1

**DIST1 (D)** 1.235  
**DIST2 (D)** 1.385  
**DIST3 (D)** 1.344

### Fragment 2

**DIST1 (D)** 1.239  
**DIST2 (D)** 1.381  
**DIST3 (D)** 1.341



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 15

## GINFOZ

**Reference:** P.Fernandes, J.Bardin, A.Johnston, A.J.Florence,  
C.K.Leech, W.I.F.David, K.Shankland (2007)  
*Acta Crystallogr., Sect.E: Struct.Rep. Online* ,**63**,o4269

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>2</sub> H<sub>1</sub> F<sub>3</sub> O<sub>2</sub>

**Compound Name:** Carbamazepine trifluoroacetic acid solvate

**Synonym:** 5H-Dibenzo(b,f)azepine-5-carboxamide trifluoroacetic acid solvate

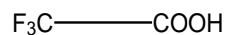
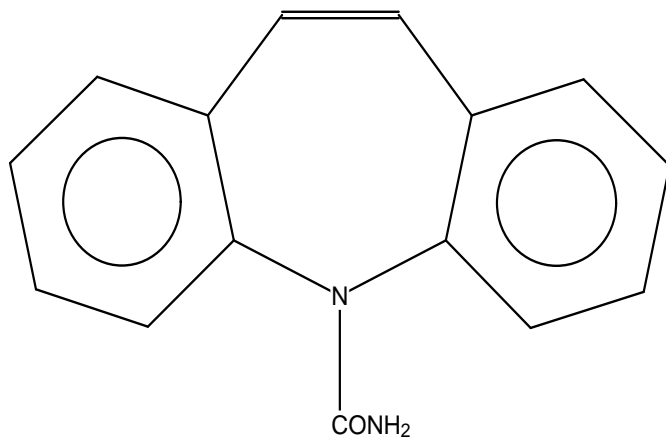
**Space Group:** P21/n      **Cell:**      **a** 15.014(0)      **b** 5.287(0)      **c** 20.249(0)  
**Space Group No.:** 14      (**Å, °**)      **α** 90.00      **β** 101.74(0)      **γ** 90.00

**R-Factor (%):** 3.86      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.478

### Parameters

Fragment 1

**DIST1 (D)**      1.270  
**DIST2 (D)**      1.353  
**DIST3 (D)**      1.320





# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 16

KIWBEY

**Reference:** A.Johnston, B.F.Johnston, A.R.Kennedy, A.J.Florence  
(2008) *CrystEngComm*, **10**,23

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>4</sub> H<sub>9</sub> N<sub>1</sub> O<sub>1</sub>

**Compound Name:** (5H-Dibenz(b,f)azepine-5-carboxamide) N,N-dimethyl acetamide solvate

**Synonym:** Carbamazepine N,N-dimethyl acetamide solvate

**Space Group:** P21/c      **Cell:**      **a** 7.505(0)      **b** 19.506(2)      **c** 11.781(1)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 96.60(0)      **γ** 90.00

**R-Factor (%):** 6.76      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.254

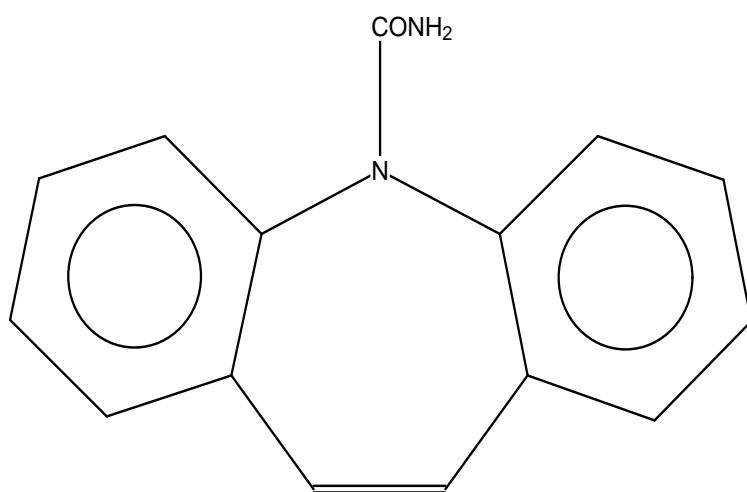
## Parameters

Fragment 1

**DIST1 (D)** 1.240

**DIST2 (D)** 1.387

**DIST3 (D)** 1.334



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 17

KIWBIC

**Reference:** A.Johnston, B.F.Johnston, A.R.Kennedy, A.J.Florence  
(2008) *CrystEngComm*, **10**,23

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>5</sub> H<sub>9</sub> N<sub>1</sub> O<sub>1</sub>

**Compound Name:** (5H-Dibenz(b,f)azepine-5-carboxamide) N-methylpyrrolidone solvate

**Synonym:** Carbamazepine N-methylpyrrolidone solvate

**Space Group:** P21/c      **Cell:**      **a** 7.545(0)      **b** 19.512(1)      **c** 11.878(0)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  98.01(0)       $\gamma$  90.00

**R-Factor (%):** 5.45      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.287

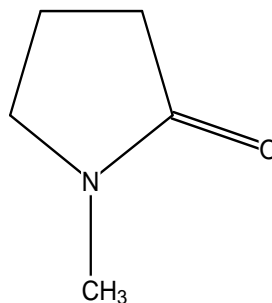
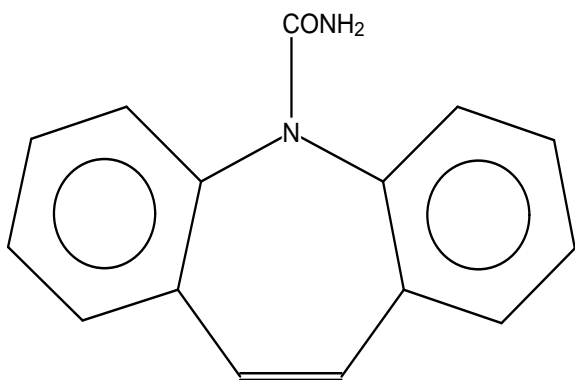
## Parameters

Fragment 1

**DIST1 (D)** 1.237

**DIST2 (D)** 1.382

**DIST3 (D)** 1.340



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 18

KIWBOI

**Reference:** A.Johnston, B.F.Johnston, A.R.Kennedy, A.J.Florence  
(2008) *CrystEngComm*, **10**,23

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>1</sub> H<sub>3</sub> N<sub>1</sub> O<sub>2</sub>

**Compound Name:** (5H-Dibenz(b,f)azepine-5-carboxamide) nitromethane solvate

**Synonym:** Carbamazepine nitromethane solvate

**Space Group:** P21/n      **Cell:**      **a** 10.924(1)      **b** 5.162(0)      **c** 26.309(3)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 100.10(0)      **γ** 90.00

**R-Factor (%):** 5.16      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.352

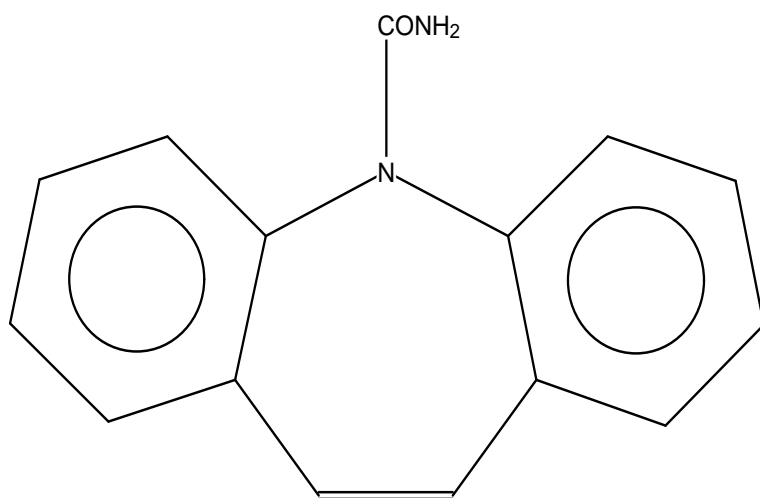
## Parameters

Fragment 1

**DIST1 (D)** 1.237

**DIST2 (D)** 1.380

**DIST3 (D)** 1.340



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 19

LOFKIB

**Reference:** J.H.ter Horst, P.W.Cains (2008) *Cryst.Growth Des.* ,8,2537

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>6</sub> H<sub>6</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** Carbamazepine isonicotinamide

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide isonicotinamide

**Space Group:** P-1      **Cell:**    **a** 7.048(2)    **b** 9.626(2)    **c** 14.399(5)

**Space Group No.:** 2      **(Å, °)**    **α** 105.75(1)    **β** 93.06(1)    **γ** 107.89(1)

**R-Factor (%):** 4.81      **Temperature(K):** 120      **Density(g/cm<sup>3</sup>):** 1.345

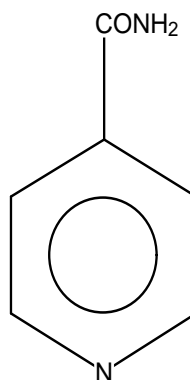
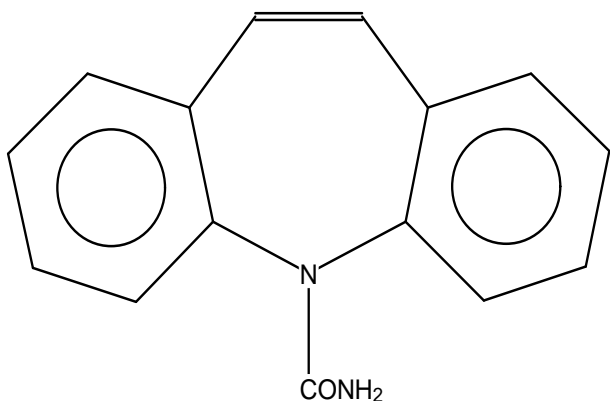
## Parameters

Fragment 1

**DIST1 (D)** 1.247

**DIST2 (D)** 1.371

**DIST3 (D)** 1.350



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 20

MIMQIJ

**Reference:** F.P.A.Fabbiani, L.T.Byrne, J.J.McKinnon, M.A.Spackman  
(2007) *CrystEngComm*, **9**,728

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>,0.1(C<sub>4</sub> H<sub>8</sub> O<sub>1</sub>)

**Compound Name:** 5H-Dibenz(b,f)azepine-5-carboxamide tetrahydrofuran solvate

**Synonym:** Carbamazepine tetrahydrofuran solvate

**Space Group:** R-3      **Cell:**    **a** 35.243(5)    **b** 35.243(5)    **c** 5.185(1)

**Space Group No.:** 148      **(Å, °)**    **α** 90.00      **β** 90.00      **γ** 120.00

**R-Factor (%):** 5.12      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.305

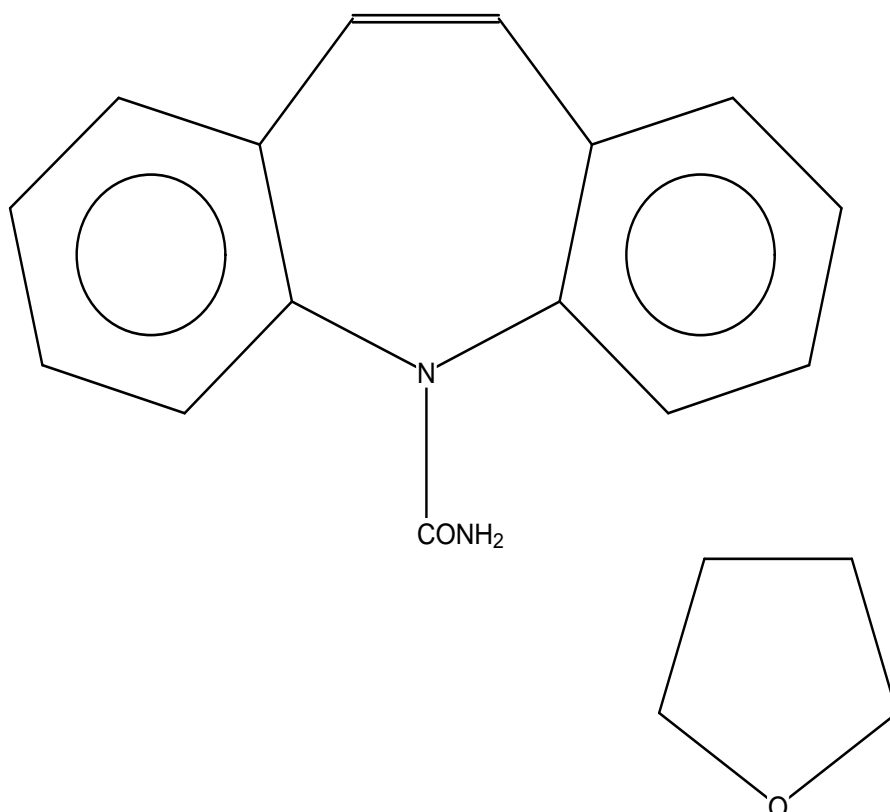
## Parameters

Fragment 1

**DIST1 (D)**      1.243

**DIST2 (D)**      1.384

**DIST3 (D)**      1.344



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 21

## MOXVAX

**Reference:** S.L.Childs, P.A.Wood, N.Rodriguez-Hornedo, L.S.Reddy, K.I.Hardcastle (2009) *Cryst.Growth Des.* ,**9**,1869

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>7</sub> H<sub>6</sub> O<sub>2</sub>

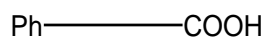
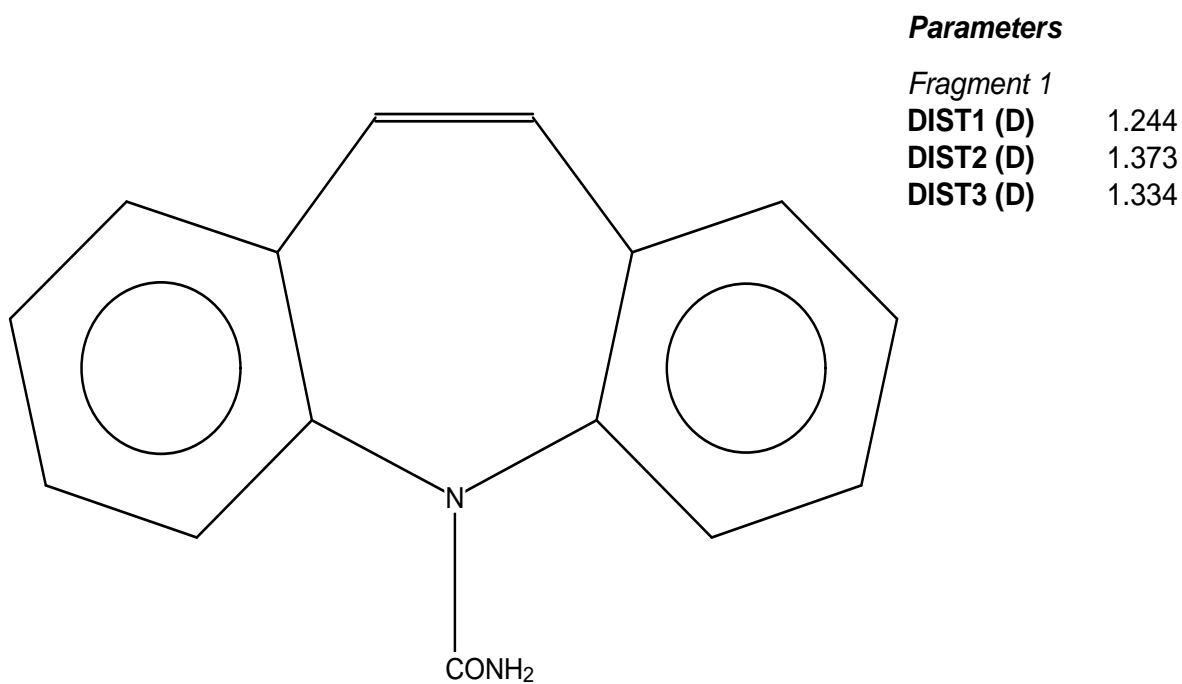
**Compound Name:** Carbamazepine benzoic acid

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide benzoic acid

**Space Group:** C2/c      **Cell:**    **a** 28.519(1)    **b** 5.161(0)    **c** 24.736(1)

**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 103.45(0)    **γ** 90.00

**R-Factor (%):** 4.39      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.345



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 22

## MOXVEB

**Reference:** S.L.Childs, P.A.Wood, N.Rodriguez-Hornedo, L.S.Reddy, K.I.Hardcastle (2009) *Cryst.Growth Des.* ,**9**,1869

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,0.5</sub>(C<sub>6</sub> H<sub>10</sub> O<sub>4</sub>)

**Compound Name:** Carbamazepine hemikis(adipic acid)

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide hemikis(hexanedioic acid)

**Space Group:** P-1      **Cell:**    **a** 7.338(0)    **b** 14.772(1)    **c** 15.889(1)  
**Space Group No.:** 2      **(Å, °)**    **α** 69.38(0)    **β** 84.18(0)    **γ** 88.27(0)

**R-Factor (%):** 5.15      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.281

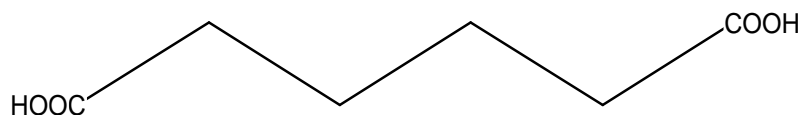
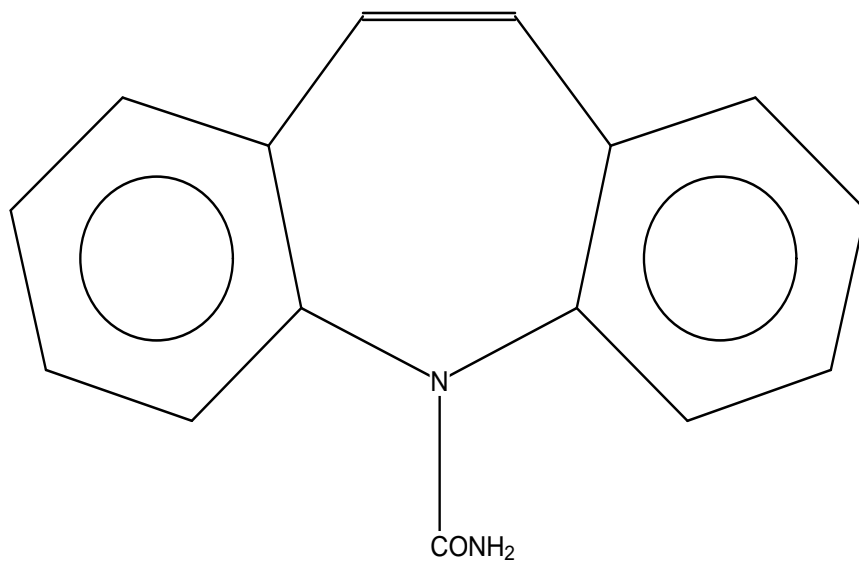
### Parameters

#### Fragment 1

**DIST1 (D)**      1.237  
**DIST2 (D)**      1.383  
**DIST3 (D)**      1.341

#### Fragment 2

**DIST1 (D)**      1.267  
**DIST2 (D)**      1.363  
**DIST3 (D)**      1.347



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 23

## MOXVIF

**Reference:** S.L.Childs, P.A.Wood, N.Rodriguez-Hornedo, L.S.Reddy, K.I.Hardcastle (2009) *Cryst.Growth Des.* ,**9**,1869

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>,C<sub>7</sub> H<sub>6</sub> O<sub>3</sub>

**Compound Name:** Carbamazepine 4-hydroxybenzoic acid

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide 4-hydroxybenzoic acid

**Space Group:** P21/c      **Cell:**      **a** 7.099(0)      **b** 12.709(0)      **c** 20.111(0)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  91.87(0)       $\gamma$  90.00

**R-Factor (%):** 2.88      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.371

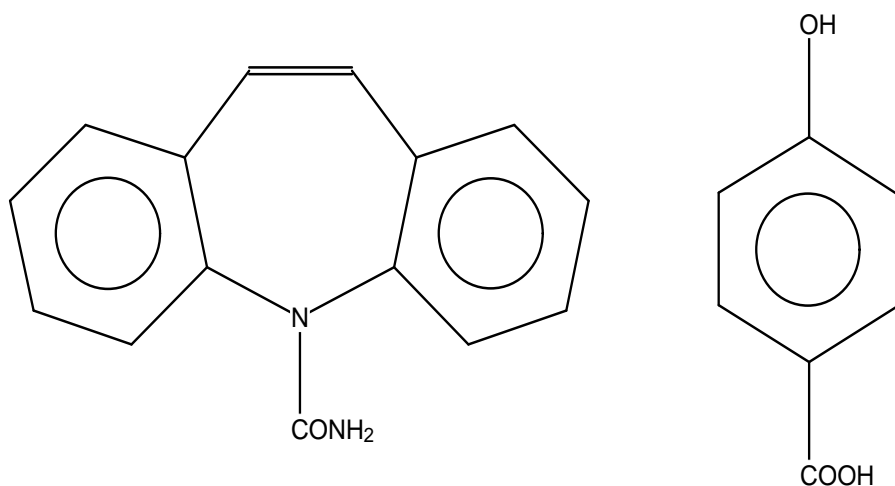
### Parameters

Fragment 1

**DIST1 (D)** 1.238

**DIST2 (D)** 1.378

**DIST3 (D)** 1.346





# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 24

MOXVIF01

**Reference:** S.L.Childs, P.A.Wood, N.Rodriguez-Hornedo, L.S.Reddy, K.I.Hardcastle (2009) *Cryst.Growth Des.* ,**9**,1869

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>,C<sub>7</sub> H<sub>6</sub> O<sub>3</sub>

**Compound Name:** Carbamazepine 4-hydroxybenzoic acid

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide 4-hydroxybenzoic acid

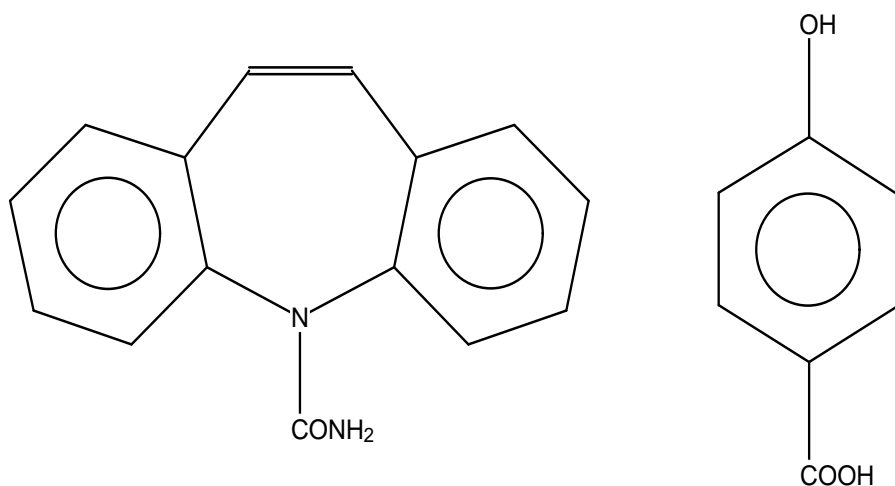
**Space Group:** P21/n      **Cell:**    **a** 13.306(0)    **b** 6.666(0)    **c** 20.709(1)  
**Space Group No.:** 14      **(Å, °)**     $\alpha$  90.00       $\beta$  91.01(0)     $\gamma$  90.00

**R-Factor (%):** 4.11      **Temperature(K):** 85      **Density(g/cm<sup>3</sup>):** 1.354

## Parameters

Fragment 1

**DIST1 (D)**      1.243  
**DIST2 (D)**      1.370  
**DIST3 (D)**      1.342



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 25

## MOXVOL

**Reference:** S.L.Childs, P.A.Wood, N.Rodriguez-Hornedo, L.S.Reddy, K.I.Hardcastle (2009) *Cryst.Growth Des.* ,**9**,1869

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>5</sub> H<sub>8</sub> O<sub>4</sub>

**Compound Name:** Carbamazepine glutaric acid

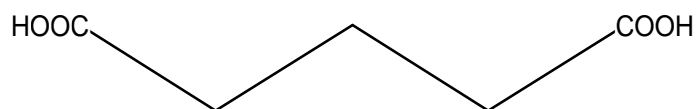
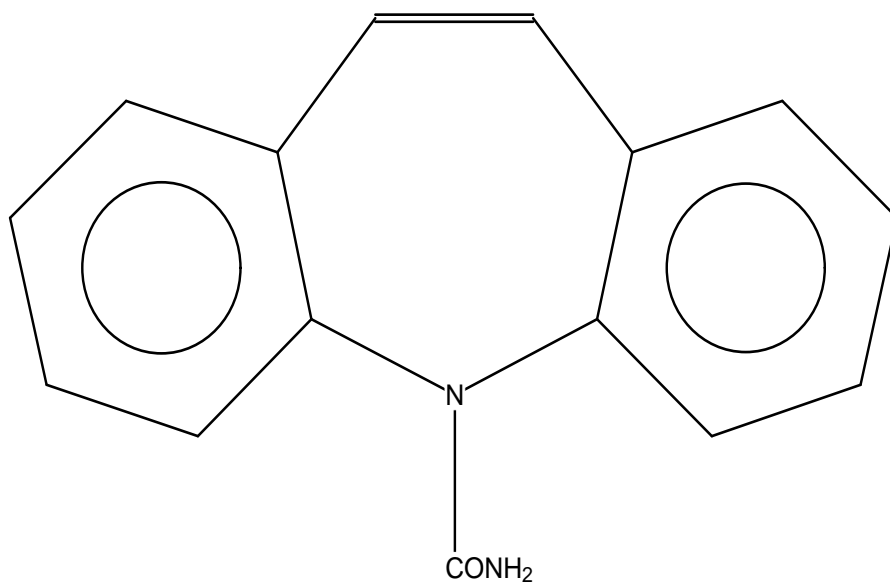
**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide 1,5-pentanedioic acid

**Space Group:** P21/n      **Cell:**      **a** 18.562(1)      **b** 5.120(0)      **c** 19.459(0)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  106.84(0)       $\gamma$  90.00

**R-Factor (%):** 3.71      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.382

### Parameters

Fragment 1  
**DIST1 (D)** 1.248  
**DIST2 (D)** 1.364  
**DIST3 (D)** 1.346



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 26

## MOXWAY

**Reference:** S.L.Childs, P.A.Wood, N.Rodriguez-Hornedo, L.S.Reddy, K.I.Hardcastle (2009) *Cryst.Growth Des.* ,**9**,1869

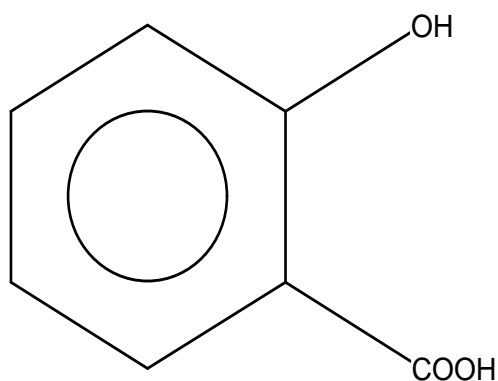
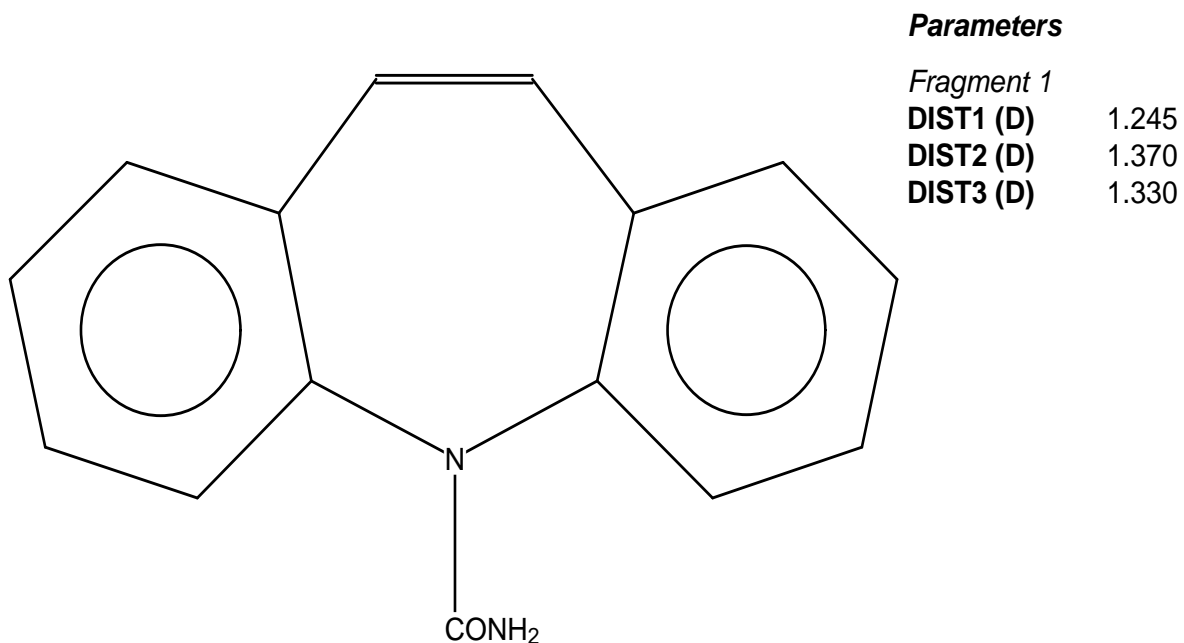
**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>,C<sub>7</sub> H<sub>6</sub> O<sub>3</sub>

**Compound Name:** Carbamazepine salicylic acid

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide 2-hydroxybenzoic acid

**Space Group:** P21/n      **Cell:**      **a** 5.106(0)      **b** 19.783(2)      **c** 18.328(2)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  97.90(0)       $\gamma$  90.00

**R-Factor (%):** 4.43      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.356



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 27

## MOXWEC

**Reference:** S.L.Childs, P.A.Wood, N.Rodriguez-Hornedo, L.S.Reddy, K.I.Hardcastle (2009) *Cryst.Growth Des.* ,**9**,1869

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>11</sub> H<sub>8</sub> O<sub>3</sub>

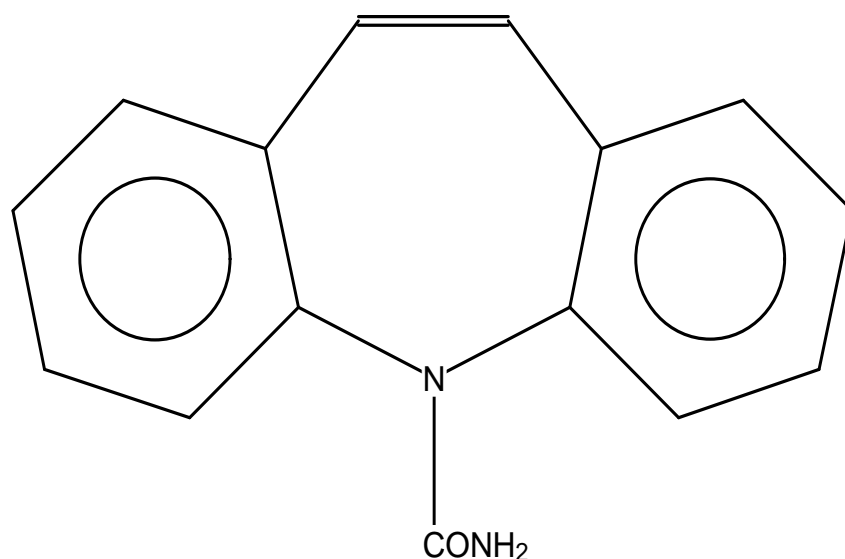
**Compound Name:** Carbamazepine L-1-hydroxy-2-naphthoic acid

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide L-1-hydroxy-2-naphthoic acid

**Space Group:** P21/c      **Cell:**      **a** 16.641(1)      **b** 5.053(0)      **c** 24.493(2)

**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 99.06(0)      **γ** 90.00

**R-Factor (%):** 5.29      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.386



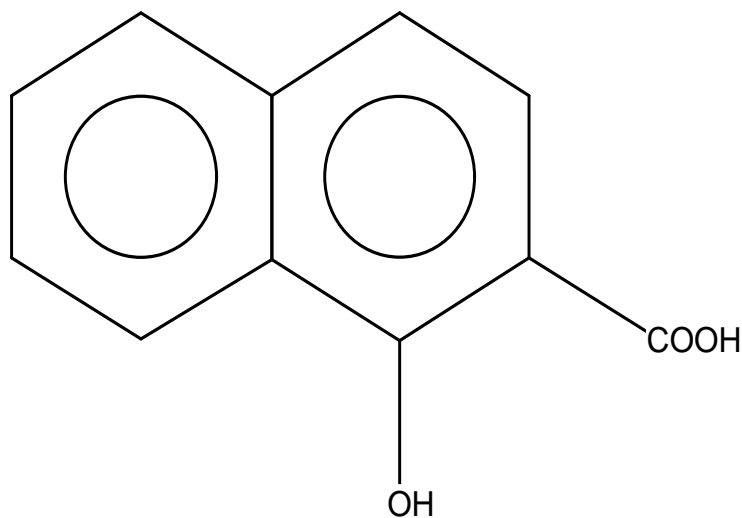
### Parameters

Fragment 1

**DIST1 (D)** 1.247

**DIST2 (D)** 1.378

**DIST3 (D)** 1.337



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 28

## MOXXAZ

**Reference:** S.L.Childs, P.A.Wood, N.Rodriguez-Hornedo, L.S.Reddy, K.I.Hardcastle (2009) *Cryst.Growth Des.* ,9,1869

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>10</sub> H<sub>16</sub> O<sub>4</sub>

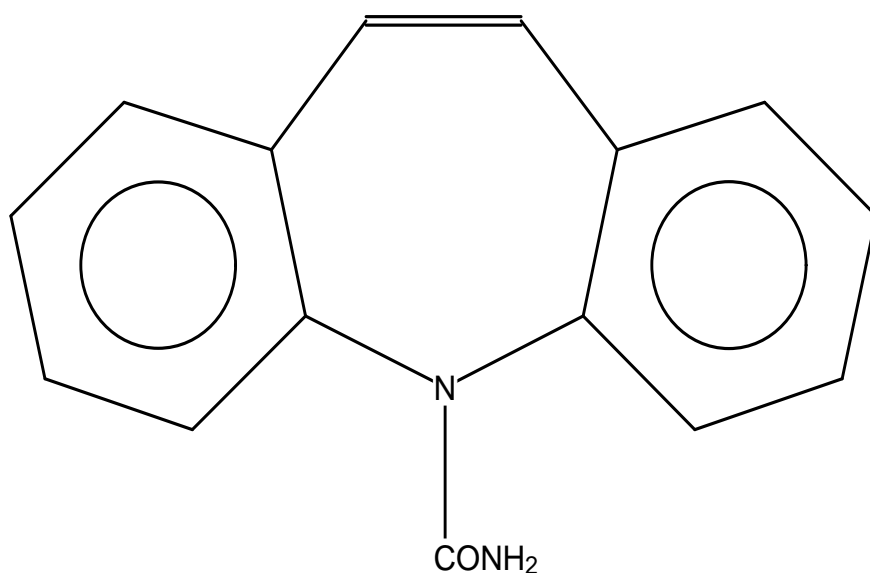
**Compound Name:** Carbamazepine (+)-camphoric acid

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide 1,2,2-trimethyl-1,3-cyclopentanedicarboxylic acid

**Space Group:** P21      **Cell:**    **a** 12.589(0)    **b** 13.145(0)    **c** 14.482(0)

**Space Group No.:** 4      **(Å, °)**    **α** 90.00      **β** 105.75(0)    **γ** 90.00

**R-Factor (%):** 2.68      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.257



### Parameters

#### Fragment 1

**DIST1 (D)** 1.245

**DIST2 (D)** 1.364

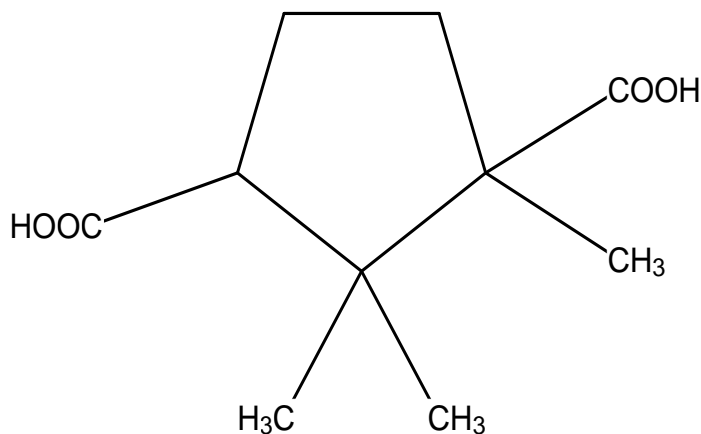
**DIST3 (D)** 1.342

#### Fragment 2

**DIST1 (D)** 1.245

**DIST2 (D)** 1.361

**DIST3 (D)** 1.341



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 29

## QANQUS

**Reference:** A.Johnston, A.J.Florence, A.R.Kennedy (2005)  
*Acta Crystallogr., Sect.E: Struct. Rep. Online* ,61,o1509

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>3</sub> H<sub>7</sub> N<sub>1</sub> O<sub>1</sub>

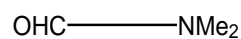
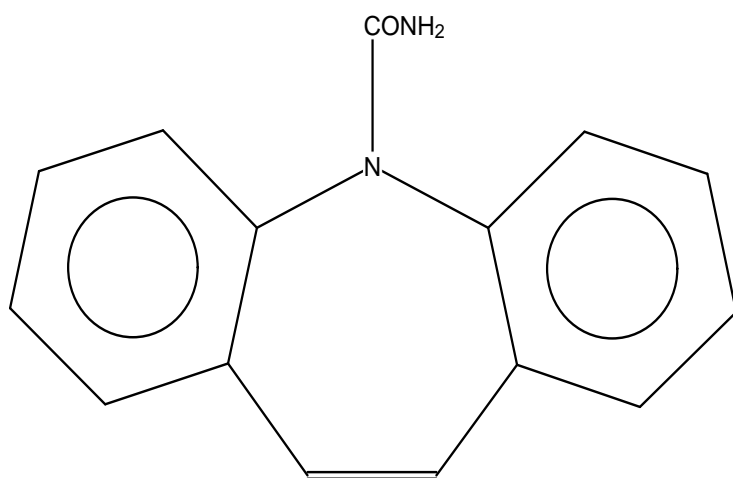
**Compound Name:** Carbamazepine N,N-dimethylformamide solvate

**Space Group:** P-1      **Cell:**    **a** 7.712(0)    **b** 9.150(0)    **c** 11.697(0)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  100.19(0)     $\beta$  95.38(0)     $\gamma$  101.91(0)

**R-Factor (%):** 4.77      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.305

### Parameters

Fragment 1  
**DIST1 (D)**      1.238  
**DIST2 (D)**      1.388  
**DIST3 (D)**      1.344



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 30

SAPDUJ

**Reference:** S.Lohani, Yuegang Zhang, L.J.Chyall, P.Mougin-Andres, F.X.Muller, D.J.W.Grant (2005)  
*Acta Crystallogr., Sect.E: Struct.Rep. Online* ,61,o1312

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>2</sub> H<sub>3</sub> F<sub>3</sub> O<sub>1</sub>

**Compound Name:** Carbamazepine 2,2,2-trifluoroethanol solvate

**Synonym:** 5H-Dibenzo(b,f)azepine-5-carboxamide 2,2,2-trifluoroethanol solvate

**Space Group:** P-1      **Cell:**    **a** 10.236(2)    **b** 12.937(2)    **c** 13.614(2)  
**Space Group No.:** 2      **(Å, °)**    **α** 62.42(0)    **β** 88.22(0)    **γ** 84.29(0)

**R-Factor (%):** 4.64      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.405

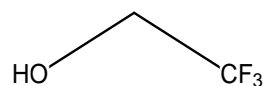
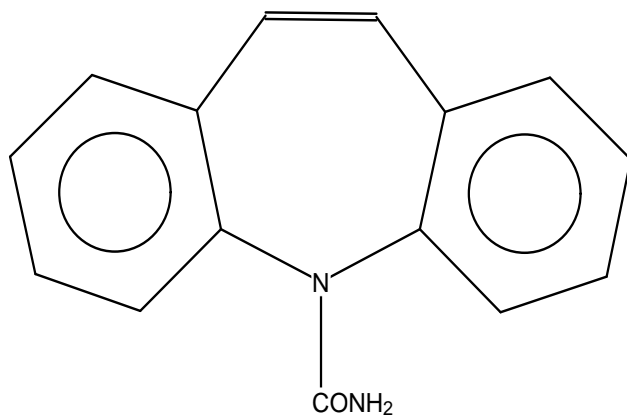
## Parameters

### Fragment 1

**DIST1 (D)**      1.233  
**DIST2 (D)**      1.374  
**DIST3 (D)**      1.346

### Fragment 2

**DIST1 (D)**      1.247  
**DIST2 (D)**      1.369  
**DIST3 (D)**      1.334



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 31

## SEZDIL

**Reference:** A.Johnston, A.J.Florence, P.Fernandes, N.Shankland, A.R.Kennedy (2007) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,**63**, o1469

**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>1</sub> H<sub>2</sub> O<sub>2</sub>

**Compound Name:** 10,11-Dihydro-5H-dibenz(b,f)azepine-5-carboxamide formic acid solvate

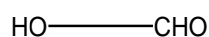
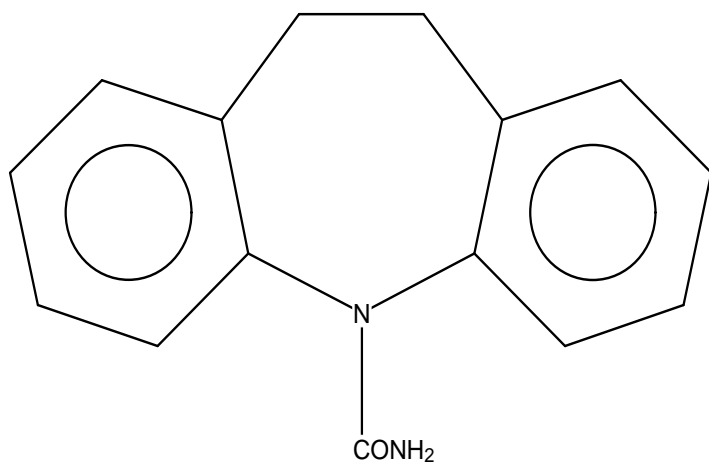
**Synonym:** 10,11-Dihydrocarbamazepine formic acid solvate

**Space Group:** P-1      **Cell:**      **a** 5.230(0)      **b** 9.385(1)      **c** 14.486(1)  
**Space Group No.:** 2      (**Å, °**)      **α** 83.85(0)      **β** 88.23(0)      **γ** 88.22(0)

**R-Factor (%):** 4.90      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.337

### Parameters

Fragment 1  
**DIST1 (D)**      1.248  
**DIST2 (D)**      1.370  
**DIST3 (D)**      1.341





# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 32

## TAZRAO

**Reference:** P.Vishweshwar, J.A.McMahon, M.Oliveira, M.L.Peterson, M.J.Zaworotko (2005) *J.Am.Chem.Soc.* ,**127**,16802

**Formula:** C<sub>9</sub> H<sub>8</sub> O<sub>4</sub>, C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

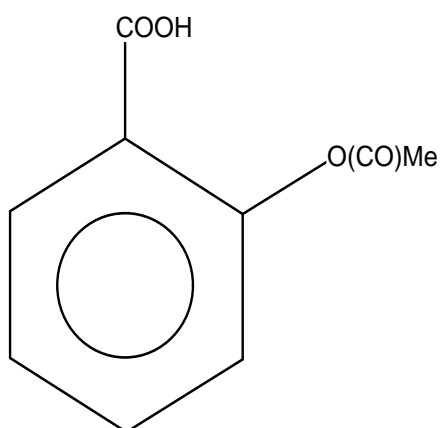
**Compound Name:** Aspirin carbamazepine

**Synonym:** Acetylsalicylic acid 5H-dibenzo(b,f)azepine-5-carboxamide

**Space Group:** P-1      **Cell:**      **a** 9.032(1)      **b** 11.364(2)      **c** 11.424(2)

**Space Group No.:** 2      **(Å, °)**      **α** 60.35(0)      **β** 85.60(0)      **γ** 84.72(0)

**R-Factor (%):** 5.71      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.364



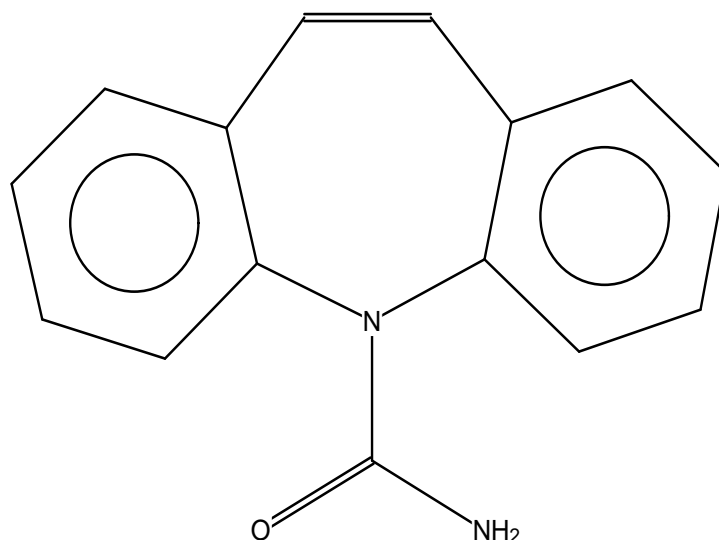
### Parameters

Fragment 1

**DIST1 (D)** 1.249

**DIST2 (D)** 1.366

**DIST3 (D)** 1.341



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 33

UNEYIV

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

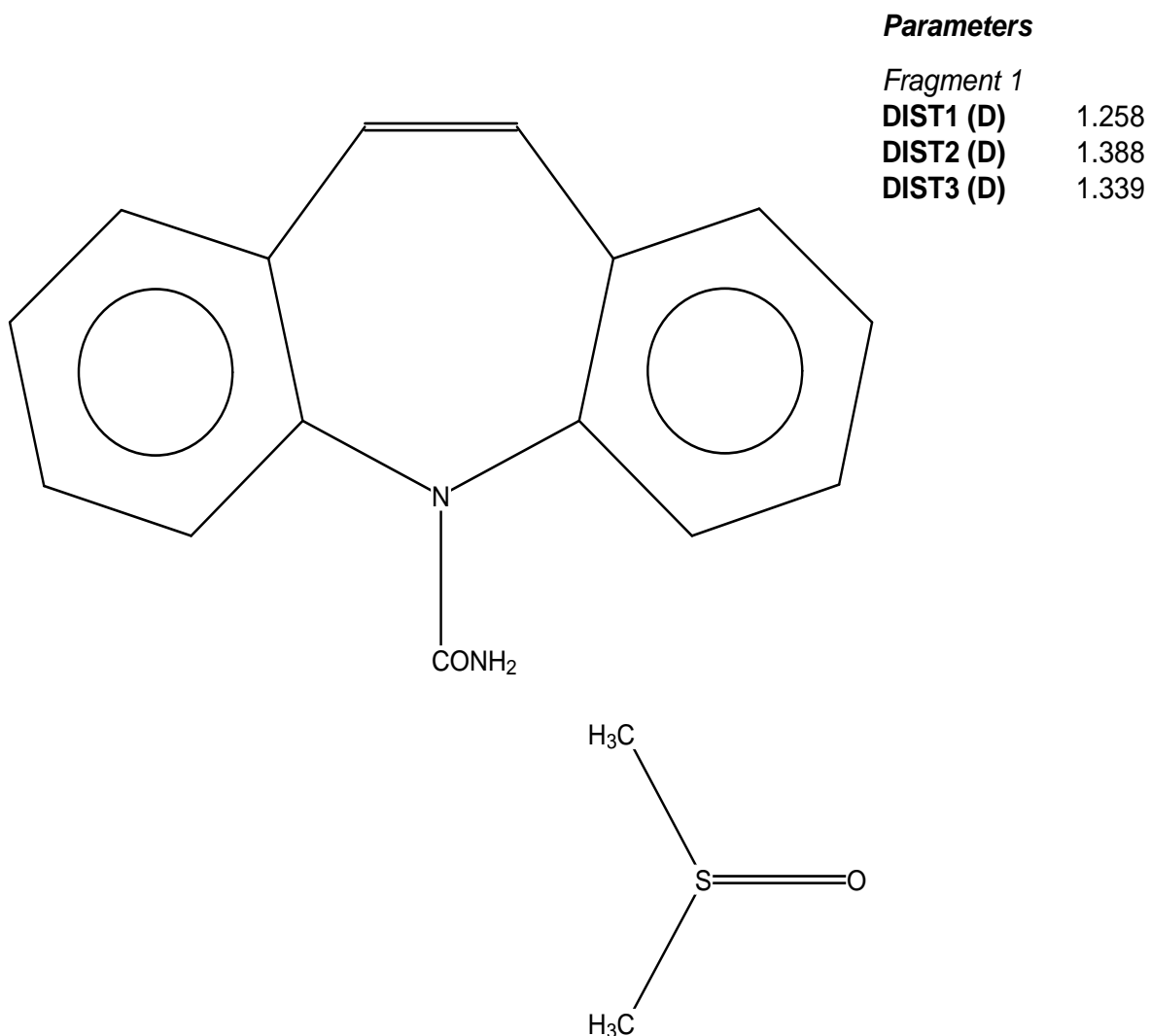
**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>,C<sub>2</sub> H<sub>6</sub> O<sub>1</sub> S<sub>1</sub>

**Compound Name:** Carbamazepine dimethylsulfoxide solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide dimethylsulfoxide solvate

**Space Group:** P-1      **Cell:**    **a** 7.325(1)    **b** 8.889(2)    **c** 12.208(3)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  94.84(0)     $\beta$  94.93(0)     $\gamma$  100.05(0)

**R-Factor (%):** 7.95      **Temperature(K):** 200      **Density(g/cm<sup>3</sup>):** 1.346



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 34

## UNEYOB

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

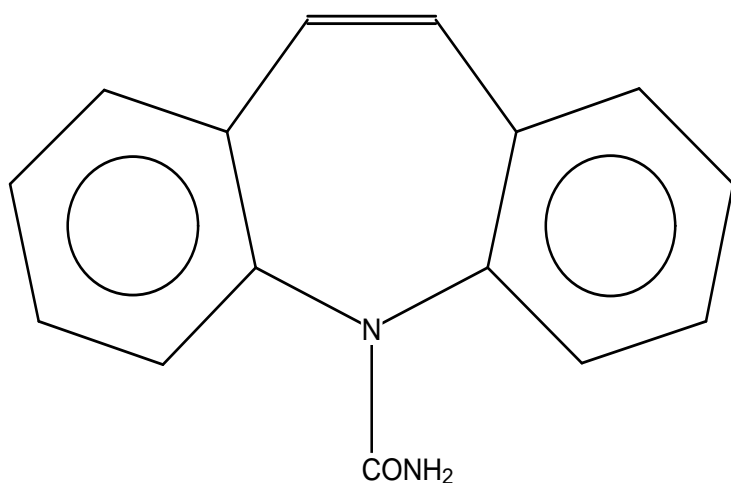
**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,0.5</sub>(C<sub>6</sub> H<sub>4</sub> O<sub>2</sub>)

**Compound Name:** Carbamazepine benzoquinone solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide benzoquinone solvate

**Space Group:** P21/c      **Cell:**      **a** 10.334(1)      **b** 27.611(5)      **c** 4.996(0)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 102.28(0)      **γ** 90.00

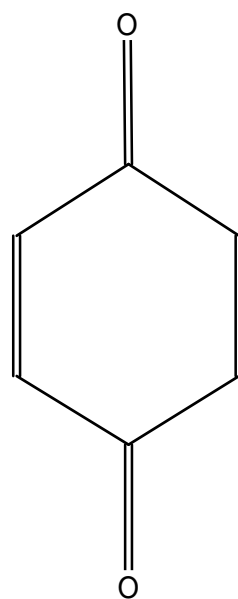
**R-Factor (%):** 5.45      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.384



### Parameters

Fragment 1

**DIST1 (D)** 1.237  
**DIST2 (D)** 1.378  
**DIST3 (D)** 1.353



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 35

UNEYUH

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

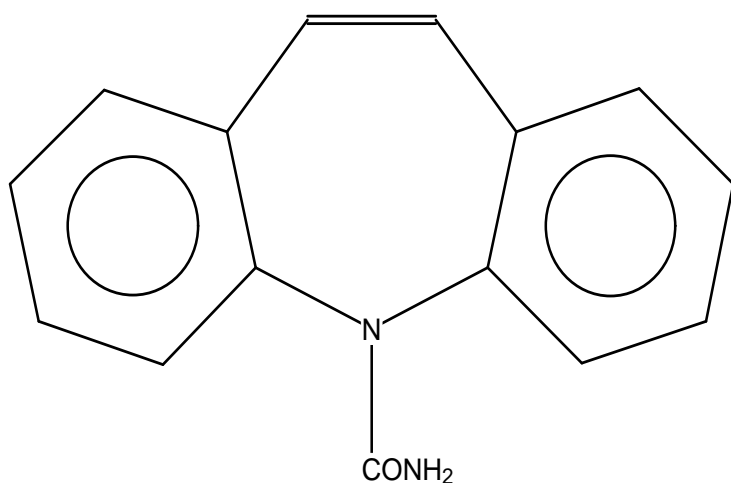
**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,0.5</sub>(C<sub>8</sub> H<sub>6</sub> O<sub>2</sub>)

**Compound Name:** Carbamazepine terephthalaldehyde solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide terephthalaldehyde solvate

**Space Group:** C2/c      **Cell:**    **a** 29.191(16)    **b** 4.962(3)    **c** 20.316(11)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 92.11(0)    **γ** 90.00

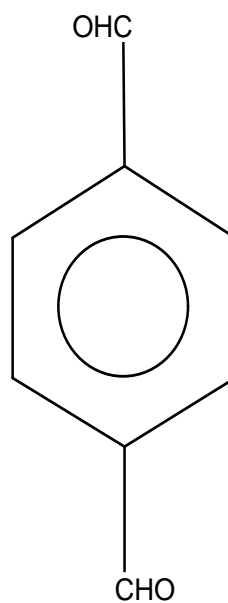
**R-Factor (%):** 3.51      **Temperature(K):** 200      **Density(g/cm<sup>3</sup>):** 1.370



## Parameters

Fragment 1

<b>DIST1 (D)</b>	1.237
<b>DIST2 (D)</b>	1.380
<b>DIST3 (D)</b>	1.352



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 36

UNEZAO

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

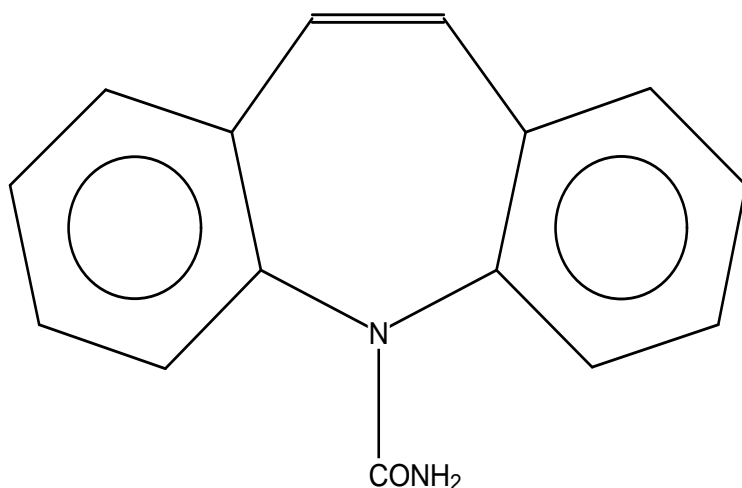
**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>7</sub> H<sub>5</sub> N<sub>1</sub> O<sub>3</sub> S<sub>1</sub>

**Compound Name:** 5H-Dibenz(b,f)azepine-5-carboxamide saccharin

**Synonym:** Carbamazepine saccharin

**Space Group:** P-1      **Cell:**    **a** 7.514(1)    **b** 10.454(1)    **c** 12.683(1)  
**Space Group No.:** 2      (**Å, °**)    **α** 83.64(0)    **β** 85.70(0)    **γ** 75.41(0)

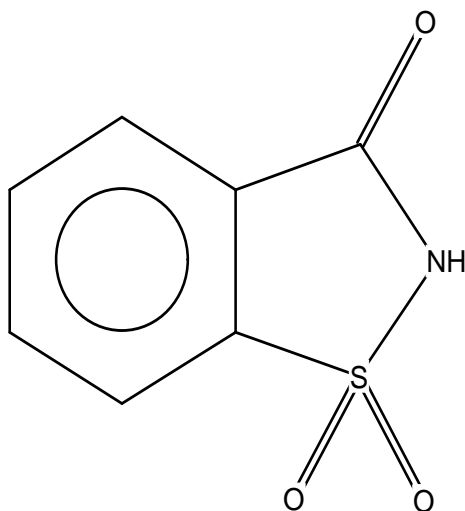
**R-Factor (%):** 4.58      **Temperature(K):** 200      **Density(g/cm<sup>3</sup>):** 1.456



## Parameters

Fragment 1

<b>DIST1 (D)</b>	1.246
<b>DIST2 (D)</b>	1.371
<b>DIST3 (D)</b>	1.336



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 37

UNEZAO01

**Reference:** W.W.Porter III, S.C.Elie, A.J.Matzger (2008)  
*Cryst.Growth Des.* ,8,14

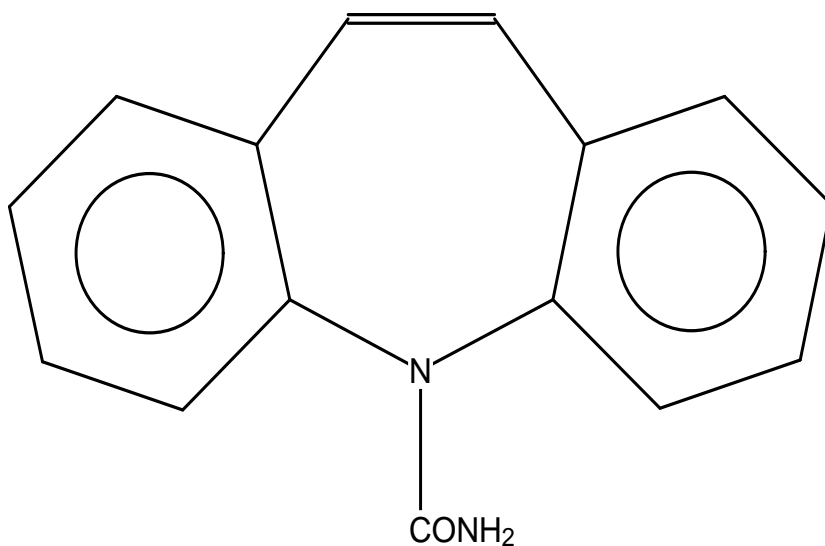
**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>7</sub> H<sub>5</sub> N<sub>1</sub> O<sub>3</sub> S<sub>1</sub>

**Compound Name:** 5H-Dibenz(b,f)azepine-5-carboxamide saccharin

**Synonym:** Carbamazepine saccharin

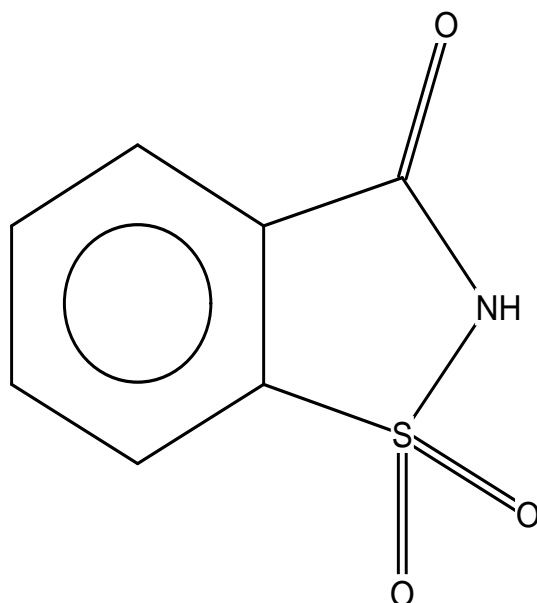
**Space Group:** C2/c      **Cell:**    **a** 35.719(1)    **b** 6.837(0)    **c** 16.111(0)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 98.03(0)    **γ** 90.00

**R-Factor (%):** 7.78      **Temperature(K):** 200      **Density(g/cm<sup>3</sup>):** 1.430



## Parameters

Fragment 1  
**DIST1 (D)** 1.246  
**DIST2 (D)** 1.376  
**DIST3 (D)** 1.332



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 38

## UNEZES

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>6</sub> H<sub>6</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** Carbamazepine nicotinamide solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide nicotinamide solvate

**Space Group:** P21/n      **Cell:**      **a** 5.096(0)      **b** 17.595(3)      **c** 19.647(3)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 90.92(0)      **γ** 90.00

**R-Factor (%):** 5.22      **Temperature(K):** 200      **Density(g/cm<sup>3</sup>):** 1.351

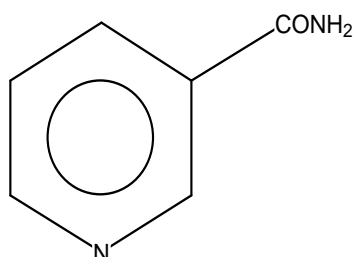
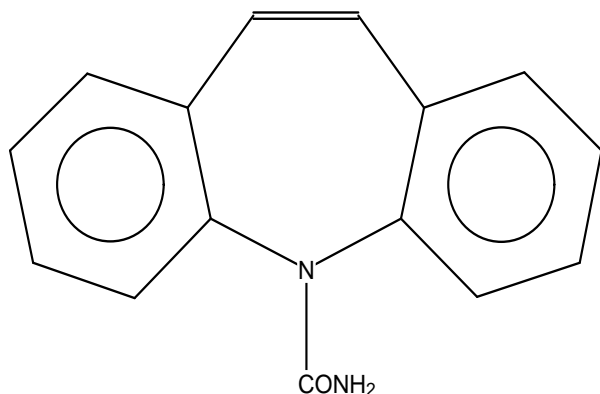
### Parameters

Fragment 1

**DIST1 (D)** 1.236

**DIST2 (D)** 1.371

**DIST3 (D)** 1.335



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 39

UNEZIW

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>2</sub> H<sub>4</sub> O<sub>2</sub>

**Compound Name:** Carbamazepine acetic acid solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide acetic acid solvate

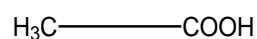
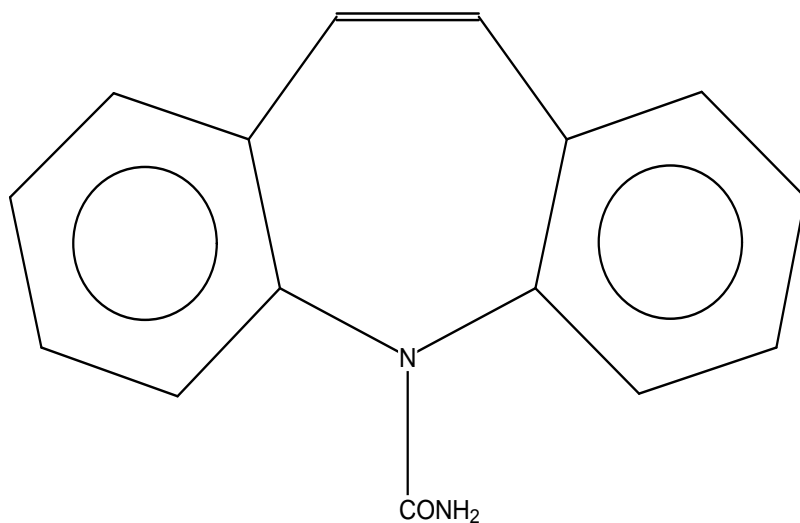
**Space Group:** P21/c      **Cell:**      **a** 5.121(0)      **b** 15.714(1)      **c** 18.499(1)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 96.55(0)      **γ** 90.00

**R-Factor (%):** 4.92      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.331

## Parameters

Fragment 1

**DIST1 (D)**      1.254  
**DIST2 (D)**      1.367  
**DIST3 (D)**      1.339





# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 40

## UNEZOC

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>1</sub> H<sub>2</sub> O<sub>2</sub>

**Compound Name:** Carbamazepine formic acid solvate

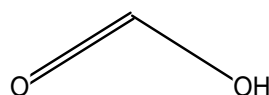
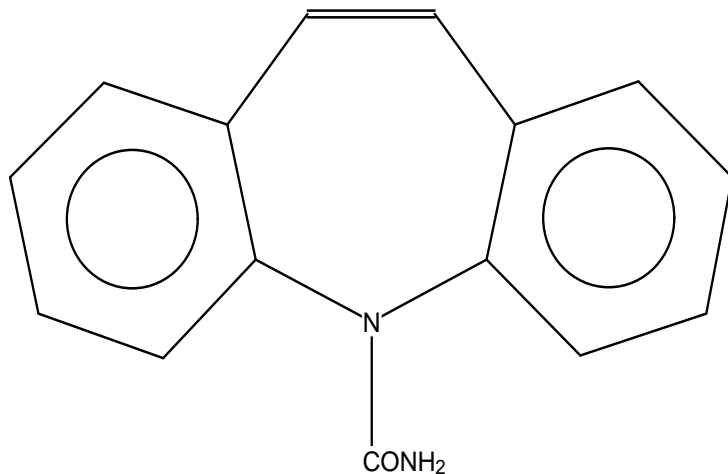
**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide formic acid solvate

**Space Group:** P21/c      **Cell:**    **a** 5.203(0)    **b** 14.741(2)    **c** 17.882(3)  
**Space Group No.:** 14      **(Å, °)**    **α** 90.00      **β** 98.13(0)    **γ** 90.00

**R-Factor (%):** 5.33      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.381

### Parameters

Fragment 1  
**DIST1 (D)**      1.254  
**DIST2 (D)**      1.361  
**DIST3 (D)**      1.336



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 41

UNEZUI

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>4</sub> H<sub>8</sub> O<sub>2</sub>

**Compound Name:** Carbamazepine butyric acid solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide butyric acid solvate

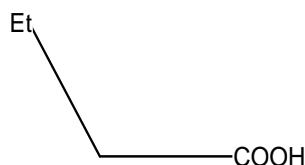
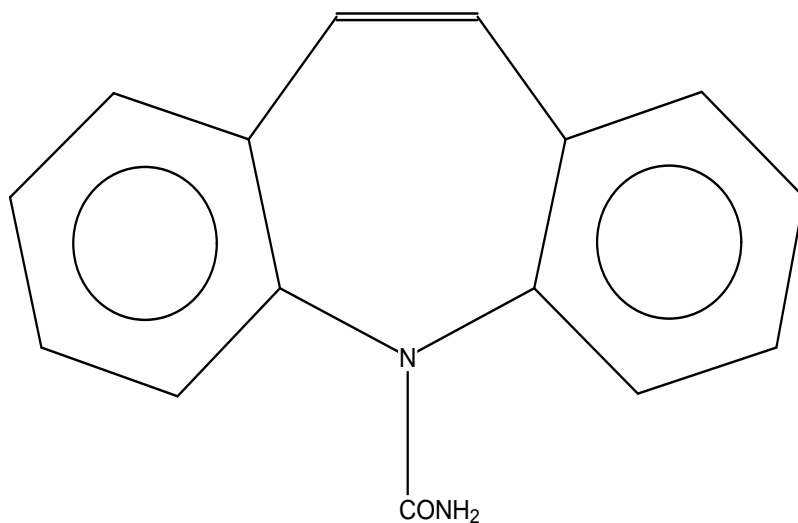
**Space Group:** P-1      **Cell:**    **a** 9.157(1)    **b** 10.175(1)    **c** 10.512(1)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  72.85(0)     $\beta$  70.29(0)     $\gamma$  67.27(0)

**R-Factor (%):** 4.99      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.290

## Parameters

Fragment 1

**DIST1 (D)**    1.241  
**DIST2 (D)**    1.374  
**DIST3 (D)**    1.346



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 42

## UNIBEY

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

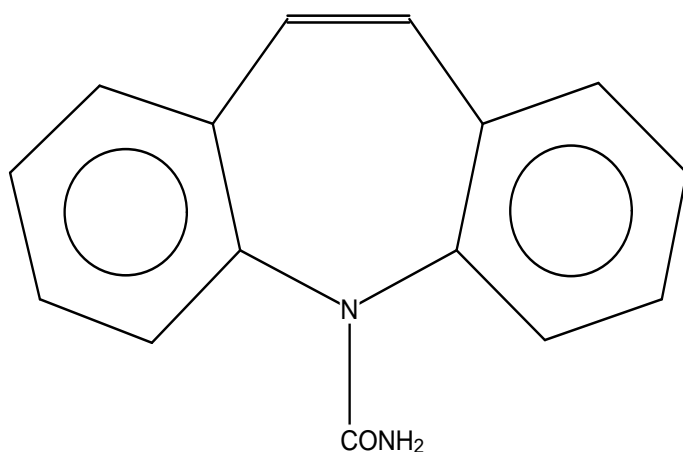
**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>8</sub> H<sub>5</sub> N<sub>1</sub> O<sub>6</sub>, 0.5(C<sub>1</sub> H<sub>4</sub> O<sub>1</sub>)

**Compound Name:** Carbamazepine 5-nitroisophthalic acid methanol solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide 5-nitroisophthalic acid methanol solvate

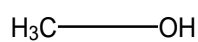
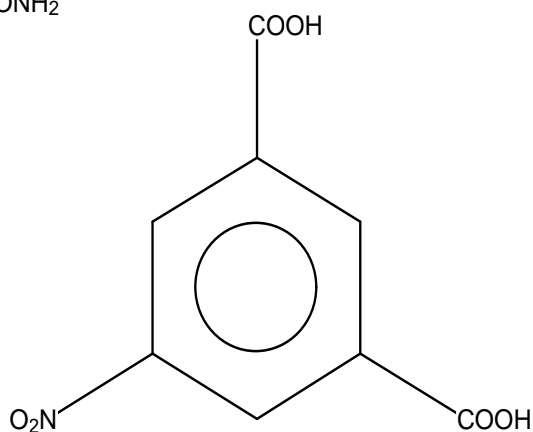
**Space Group:** C2/c      **Cell:**    **a** 34.355(8)    **b** 5.380(1)    **c** 23.654(6)  
**Space Group No.:** 15      **(Å, °)**    **α** 90.00      **β** 93.95(0)    **γ** 90.00

**R-Factor (%):** 6.19      **Temperature(K):** 200      **Density(g/cm<sup>3</sup>):** 1.412



### Parameters

Fragment 1  
**DIST1 (D)** 1.252  
**DIST2 (D)** 1.372  
**DIST3 (D)** 1.317



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 43

## UNIBIC

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

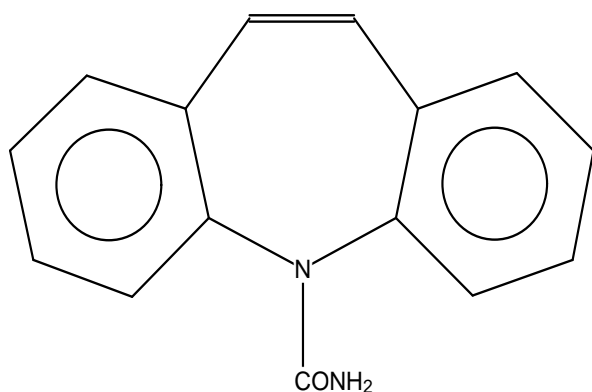
**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,0.5</sub>(C<sub>14</sub> H<sub>16</sub> O<sub>8</sub>)

**Compound Name:** Carbamazepine adamantane-1,3,5,7-tetracarboxylic acid solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide adamantane-1,3,5,7-tetracarboxylic acid solvate

**Space Group:** C2/c      **Cell:**    **a** 18.388(4)    **b** 12.682(3)    **c** 16.429(3)  
**Space Group No.:** 15      **(Å, °)**     $\alpha$  90.00       $\beta$  100.49(0)     $\gamma$  90.00

**R-Factor (%):** 4.33      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.384



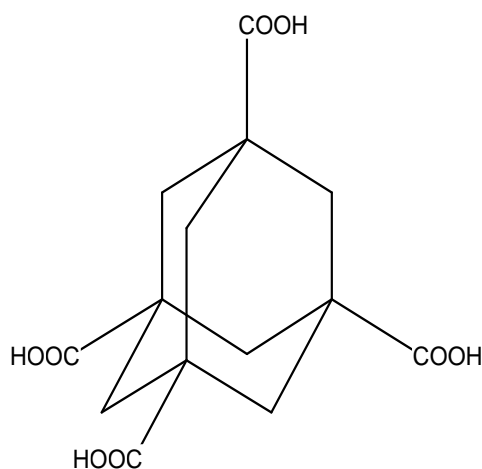
### Parameters

Fragment 1

**DIST1 (D)** 1.264

**DIST2 (D)** 1.366

**DIST3 (D)** 1.333



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 44

UNIBOI

**Reference:** S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko (2003) *Cryst.Growth Des.* ,3,909

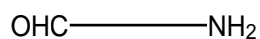
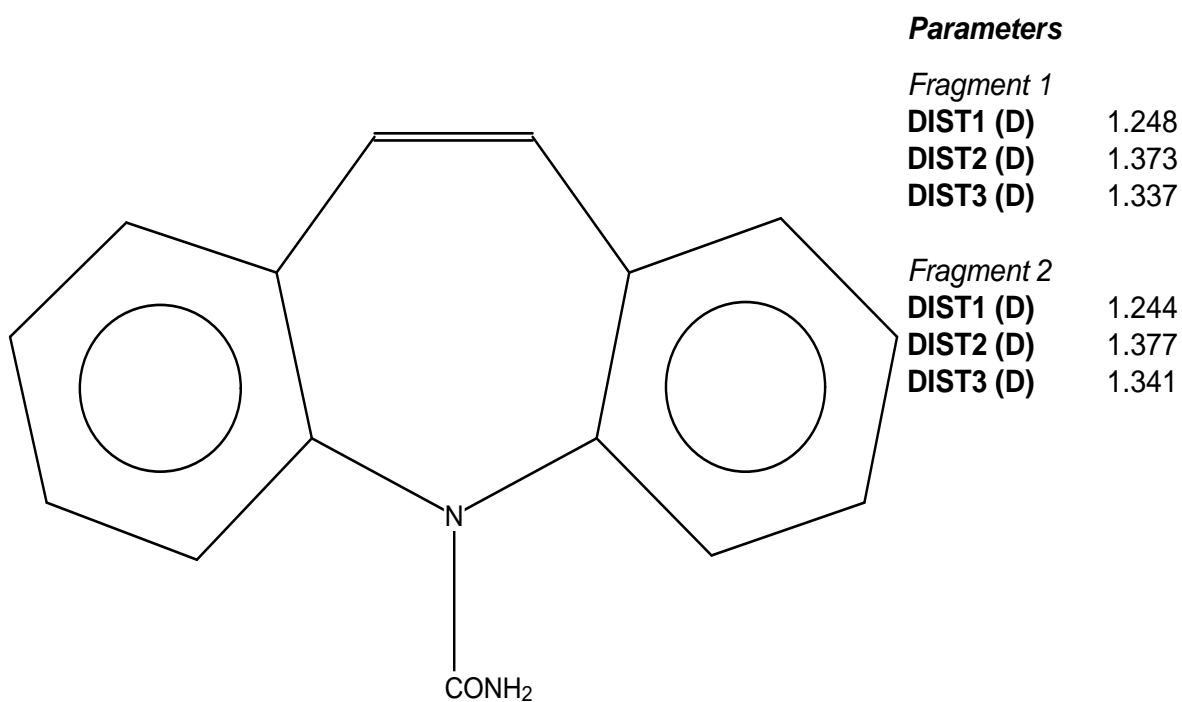
**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>1</sub> H<sub>3</sub> N<sub>1</sub> O<sub>1</sub>

**Compound Name:** Carbamazepine formamide solvate

**Synonym:** 5H-dibenz(b,f)azepine-5-carboxamide formamide solvate

**Space Group:** P-1      **Cell:**    **a** 5.108(1)    **b** 16.057(3)    **c** 17.752(4)  
**Space Group No.:** 2      (**Å, °**)    **α** 73.71(0)    **β** 89.35(0)    **γ** 88.64(0)

**R-Factor (%):** 7.66      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.337



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 45

VACTAU01

**Reference:** G.Bandoli, M.Nicolini, A.Ongaro, G.Volpe, A.Rubello  
(1992) *J.Crystallogr.Spectrosc.Res.* ,**22**,177

**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 10,11-Dihydro-5H-dibenz(b,f)azepine-5-carboxamide

**Space Group:** P21/c      **Cell:**      **a** 5.505(1)      **b** 9.158(2)      **c** 24.266(7)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  95.95(2)       $\gamma$  90.00

**R-Factor (%):** 4.10      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.301

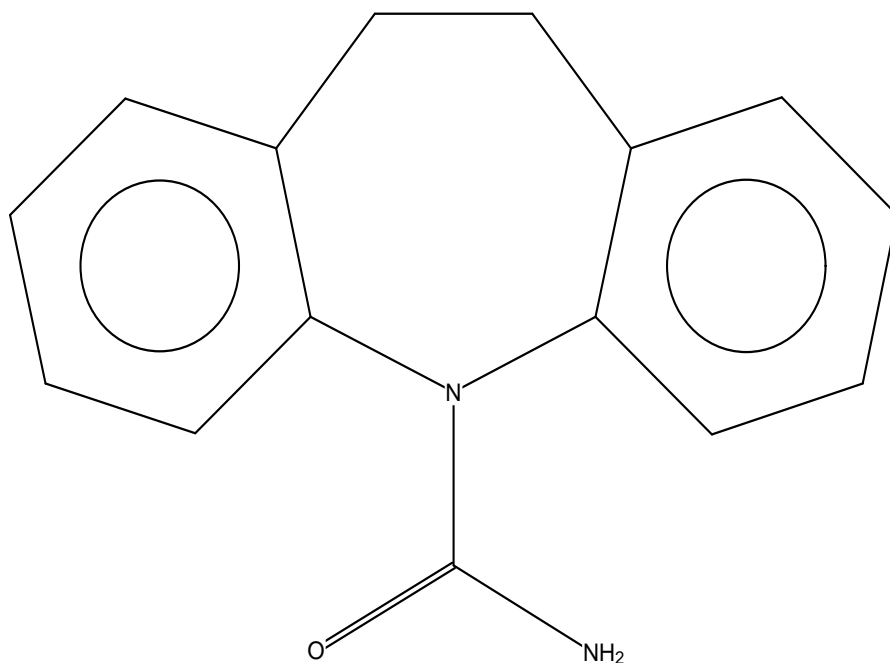
## Parameters

Fragment 1

**DIST1 (D)** 1.219

**DIST2 (D)** 1.377

**DIST3 (D)** 1.338



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 46

VACTAU02

**Reference:** W.T.A.Harrison, H.S.Yathirajan, H.G.Anilkumar (2006)  
*Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* ,62,o240

**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 10,11-Dihydro-5H-dibenzo(b,f)azepine-5-carboxamide

**Synonym:** 10,11-Dihydrocarbamazepine

**Space Group:** Pbc<sub>2</sub>      **Cell:**      **a** 9.059(0)      **b** 10.316(0)      **c** 25.053(1)  
**Space Group No.:** 61      **(Å, °)**       $\alpha$  90.00       $\beta$  90.00       $\gamma$  90.00

**R-Factor (%):** 4.16      **Temperature(K):** 120      **Density(g/cm<sup>3</sup>):** 1.352

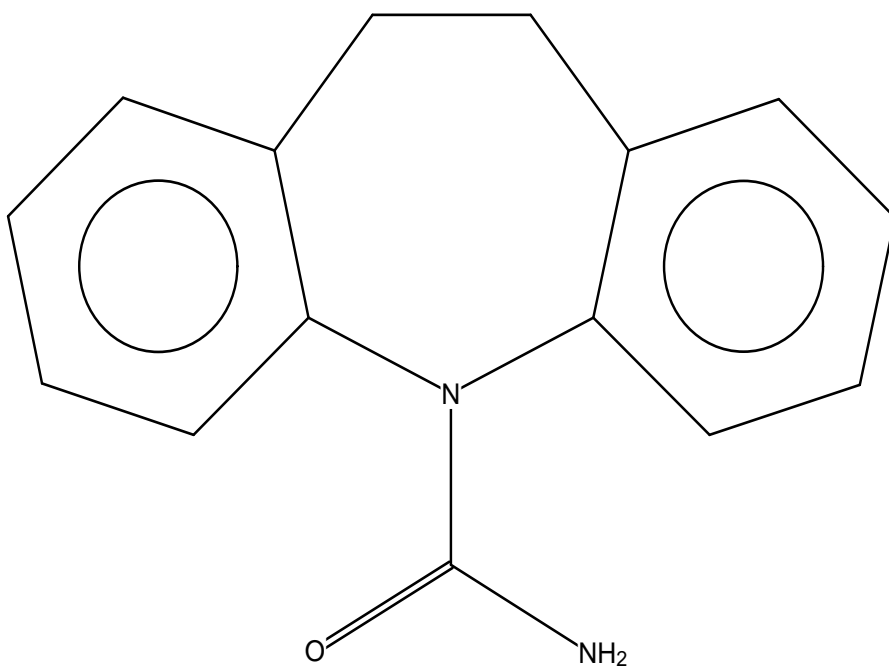
## Parameters

Fragment 1

**DIST1 (D)** 1.234

**DIST2 (D)** 1.384

**DIST3 (D)** 1.349



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 47

VACTAU03

**Reference:** C.K.Leech, A.J.Florence, K.Shankland, N.Shankland, A.Johnston (2007) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,63,o675

**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 10,11-Dihydrocarbamazepine

**Synonym:** 10,11-Dihydro-5H-dibenz(b,f)azepine-5-carboxamide

**Space Group:** P-1      **Cell:**    **a** 5.423(1)    **b** 9.200(5)    **c** 24.189(6)

**Space Group No.:** 2      **(Å, °)**    **α** 87.59(3)    **β** 84.23(2)    **γ** 88.93(3)

**R-Factor (%):** 4.08      **Temperature(K):** 150      **Density(g/cm<sup>3</sup>):** 1.319

## Parameters

### Fragment 1

**DIST1 (D)** 1.233

**DIST2 (D)** 1.392

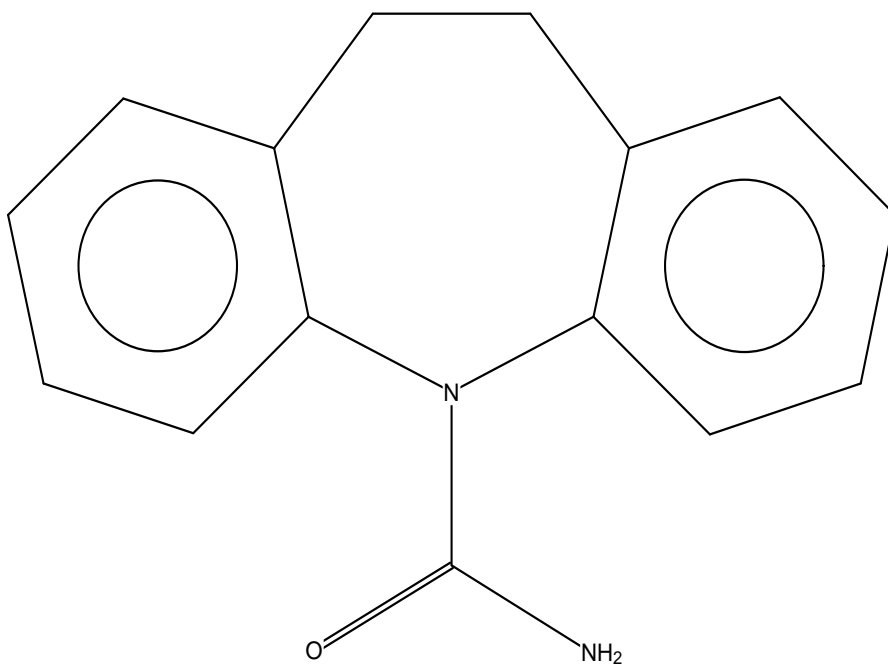
**DIST3 (D)** 1.337

### Fragment 2

**DIST1 (D)** 1.229

**DIST2 (D)** 1.389

**DIST3 (D)** 1.339





# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 48

VACTAU04

**Reference:** J.-B.Arlin, A.Johnston, G.J.Miller, A.R.Kennedy, S.L.Price, A.J.Florence (2010) *CrystEngComm* ,12,64

**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** 10,11-Dihydro-5H-dibenzo[b,f]azepine-5-carboxamide

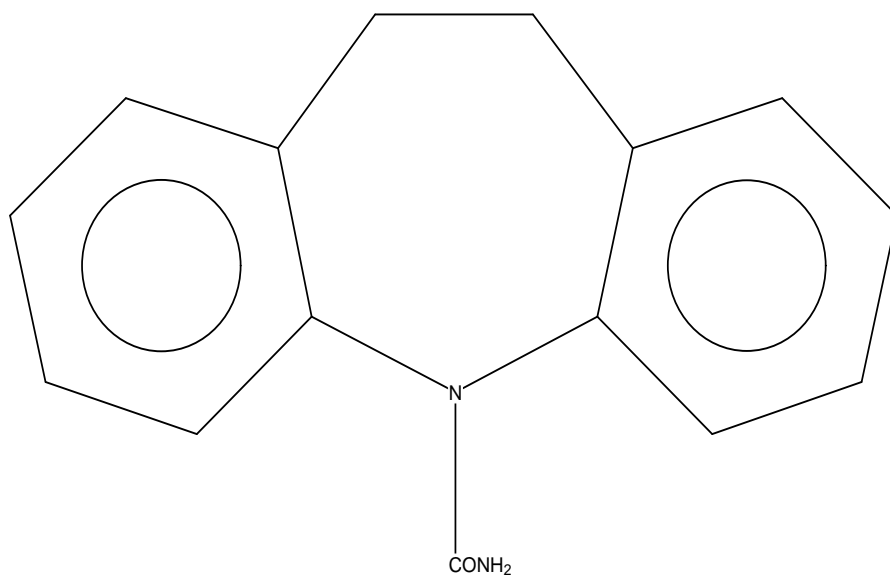
**Space Group:** P21/c      **Cell:**    **a** 13.207(6)    **b** 5.347(2)    **c** 18.891(7)  
**Space Group No.:** 14      **(Å, °)**     $\alpha$  90.00       $\beta$  116.37(2)     $\gamma$  90.00

**R-Factor (%):** 4.27      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.324

## Parameters

Fragment 1

**DIST1 (D)**      1.252  
**DIST2 (D)**      1.380  
**DIST3 (D)**      1.333



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 49

## VEXLOA

**Reference:** A.Johnston, A.J.Florence, P.Fernandes, N.Shankland, A.R.Kennedy (2006) *Acta Crystallogr., Sect.E:Struct.Rep.Online* ,**62**, o5361

**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>2</sub> H<sub>4</sub> O<sub>2</sub>

**Compound Name:** 10,11-Dihydro-5H-dibenz(b,f)azepine-5-carboxamide acetic acid solvate

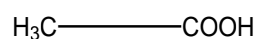
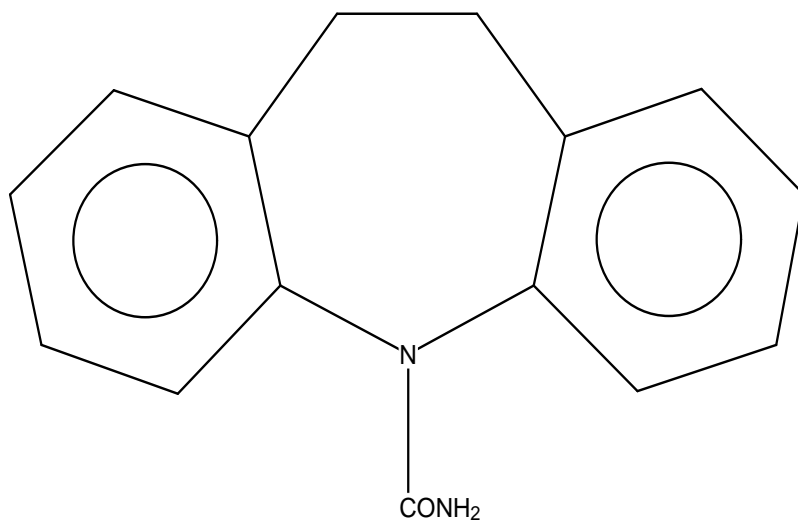
**Synonym:** 10,11-Dihydrocarbamazepine acetic acid solvate

**Space Group:** P21/c      **Cell:**      **a** 5.310(0)      **b** 15.425(1)      **c** 18.732(2)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  95.11(0)       $\gamma$  90.00

**R-Factor (%):** 7.60      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.297

### Parameters

Fragment 1  
**DIST1 (D)** 1.252  
**DIST2 (D)** 1.366  
**DIST3 (D)** 1.336



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 50

VEXLOA01

**Reference:** A.J.C.Cabeza, G.M.Day, W.D.S.Motherwell, W.Jones  
(2006) *J.Am.Chem.Soc.* ,**128**,14466

**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>,C<sub>2</sub> H<sub>4</sub> O<sub>2</sub>

**Compound Name:** 10,11-Dihydro-5H-dibenzo(b,f)azepine-5-carboxamide acetic acid solvate

**Synonym:** 10,11-Dihydrocarbamazepine acetic acid solvate

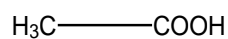
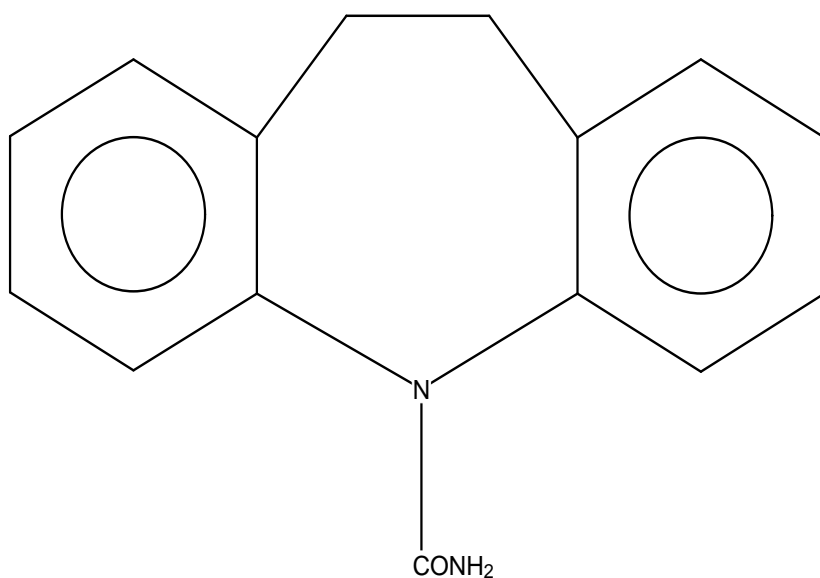
**Space Group:** P21/c      **Cell:**      **a** 5.300(0)      **b** 15.426(0)      **c** 18.720(0)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 95.17(0)      **γ** 90.00

**R-Factor (%):** 4.29      **Temperature(K):** 120      **Density(g/cm<sup>3</sup>):** 1.300

## Parameters

Fragment 1

**DIST1 (D)**      1.247  
**DIST2 (D)**      1.366  
**DIST3 (D)**      1.343



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 51

## VIGGOI

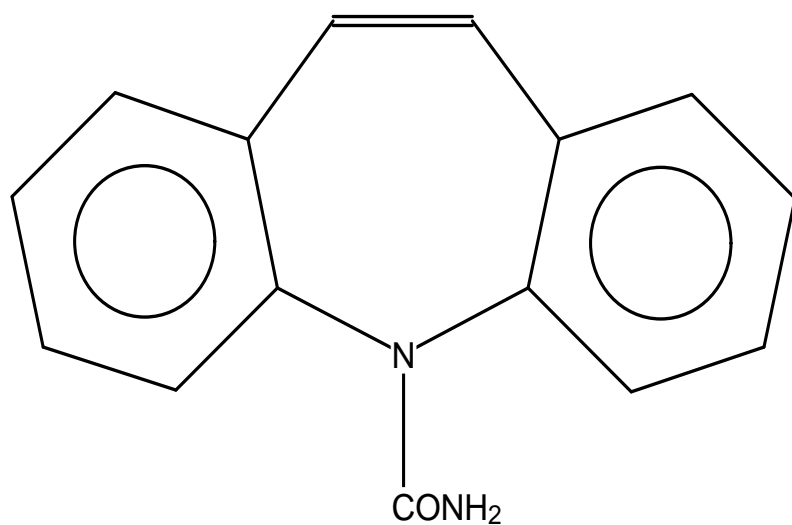
**Reference:** N.J.Babu, L.S.Reddy, A.Nangia (2007)  
*Mol.Pharmaceutics* ,4,417

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>8</sub> H<sub>6</sub> N<sub>2</sub> O<sub>2</sub>

**Compound Name:** Carbamazepine quinoxaline-N,N'-dioxide

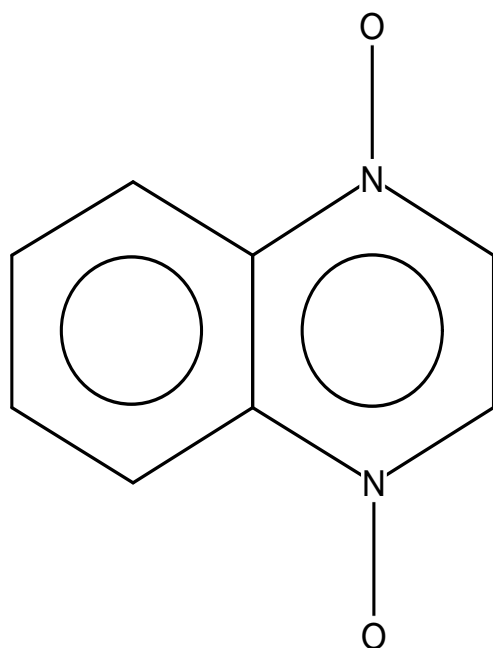
**Space Group:** P-1      **Cell:**    **a** 7.284(2)    **b** 10.688(4)    **c** 14.132(5)  
**Space Group No.:** 2      (**Å, °**)     $\alpha$  100.25(0)     $\beta$  102.46(0)     $\gamma$  109.08(0)

**R-Factor (%):** 5.48      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.353



### Parameters

Fragment 1  
**DIST1 (D)** 1.237  
**DIST2 (D)** 1.372  
**DIST3 (D)** 1.333



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 52

## VIGGUO

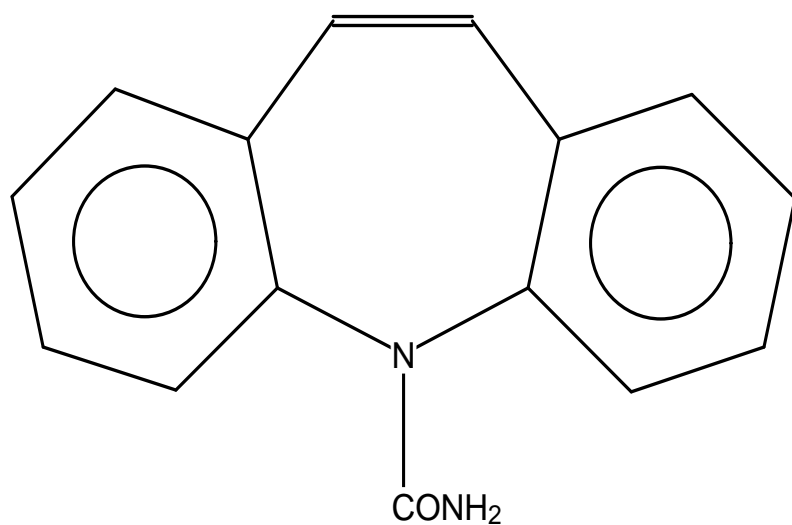
**Reference:** N.J.Babu, L.S.Reddy, A.Nangia (2007)  
*Mol.Pharmaceutics* ,4,417

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,0.5</sub>(C<sub>4</sub> H<sub>4</sub> N<sub>2</sub> O<sub>2</sub>)

**Compound Name:** Carbamazepine hemikis(pyrazine-N,N'-dioxide)

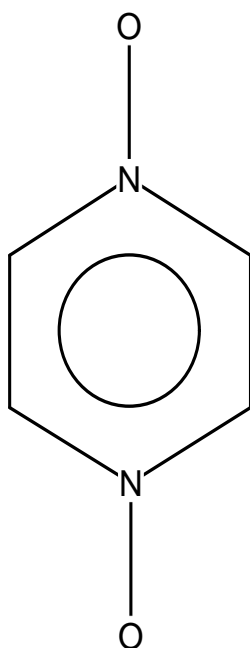
**Space Group:** P21/c      **Cell:**      **a** 10.237(4)      **b** 27.247(12)      **c** 5.135(2)  
**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 102.71(0)      **γ** 90.00

**R-Factor (%):** 13.80      **Temperature(K):** 293      **Density(g/cm<sup>3</sup>):** 1.390



### Parameters

Fragment 1  
**DIST1 (D)** 1.236  
**DIST2 (D)** 1.380  
**DIST3 (D)** 1.333



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 53

VUBCAW

**Reference:** G.Reck, W.Thiel (1991) *Pharmazie* ,46,509

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>,H<sub>4</sub> N<sub>1</sub><sup>1+</sup>,Cl<sub>1</sub><sup>1-</sup>

**Compound Name:** 5H-Dibenz(b,f)azepin-5-carboxamide ammonium chloride

**Synonym:** Carbamazepine ammonium chloride

**Space Group:** P21/n      **Cell:**      **a** 10.869(4)      **b** 5.341(3)      **c** 25.153(11)

**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 100.90(3)      **γ** 90.00

**R-Factor (%):** 11.00      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.342

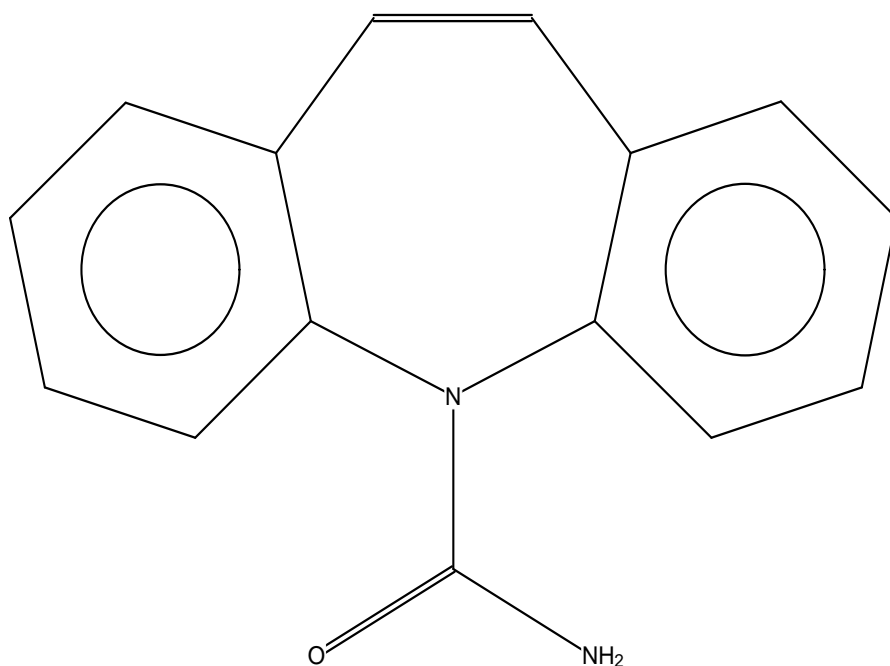
## Parameters

Fragment 1

**DIST1 (D)** 1.246

**DIST2 (D)** 1.352

**DIST3 (D)** 1.289



NH<sub>4</sub><sup>+</sup>

Cl<sup>-</sup>

# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 54

VUBCEA

**Reference:** G.Reck, W.Thiel (1991) *Pharmazie* ,**46**,509

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>,H<sub>4</sub> N<sub>1</sub><sup>1+</sup>,Br<sub>1</sub><sup>1-</sup>

**Compound Name:** 5H-Dibenz(b,f)azepin-5-carboxamide ammonium bromide

**Synonym:** Carbamazepine ammonium bromide

**Space Group:** P21/n      **Cell:**      **a** 11.051(3)      **b** 5.464(2)      **c** 24.928(9)

**Space Group No.:** 14      **(Å, °)**      **α** 90.00      **β** 100.81(4)      **γ** 90.00

**R-Factor (%):** 5.30      **Temperature(K):** 295      **Density(g/cm<sup>3</sup>):** 1.501

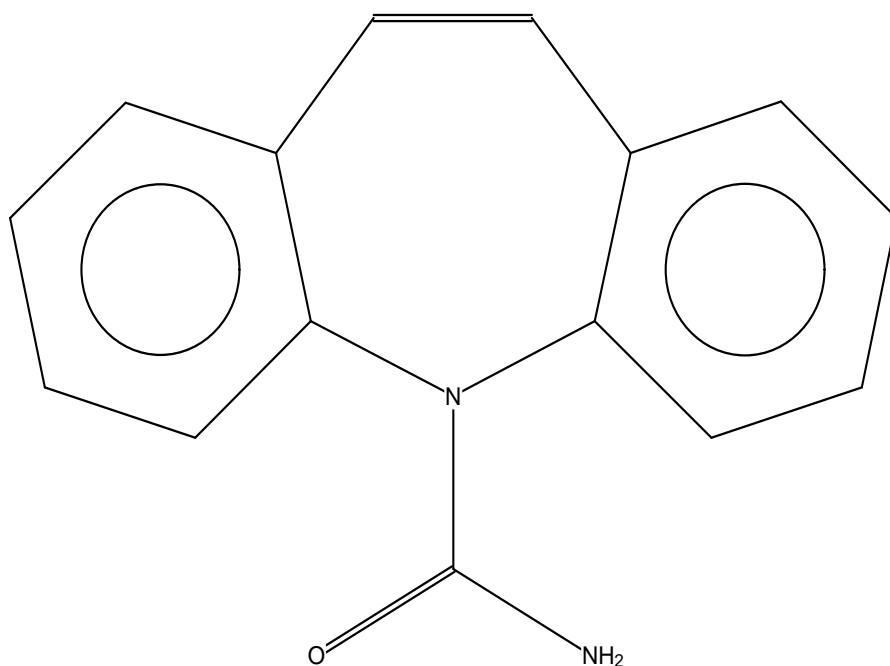
## Parameters

Fragment 1

**DIST1 (D)** 1.229

**DIST2 (D)** 1.387

**DIST3 (D)** 1.331



NH<sub>4</sub><sup>+</sup>

Br<sup>-</sup>

# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 55

XAQQUC

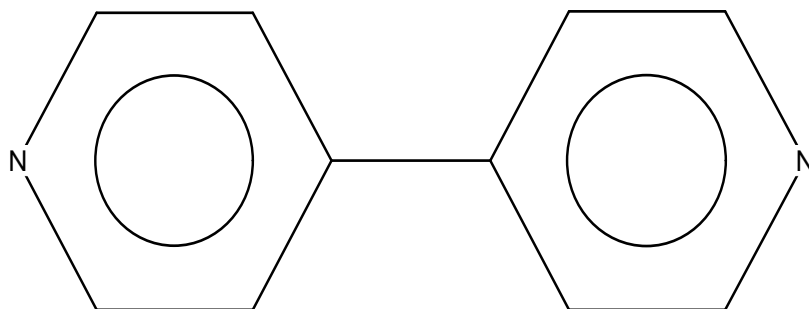
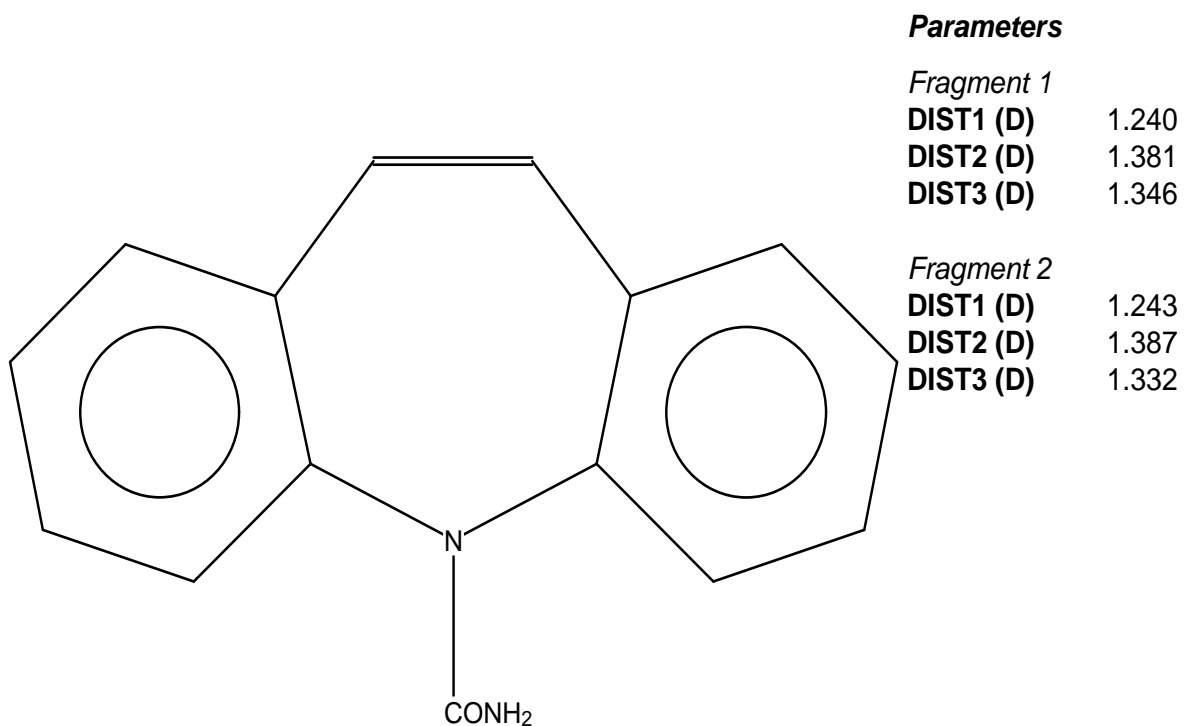
**Reference:** J.A.McMahon, J.A.Bis, P.Vishweshwar, T.R.Shattock,  
O.L.McLaughlin, M.J.Zaworotko (2005) *Z.Kristallogr.* ,**220**,340

**Formula:**  $2(C_{15}H_{12}N_2O_1), C_{10}H_8N_2$

**Compound Name:** bis(Carbamazepine) 4,4'-bipyridine

**Space Group:** P-1      **Cell:**    **a** 7.105(0)    **b** 11.801(1)    **c** 19.648(2)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  93.66(0)     $\beta$  92.80(0)     $\gamma$  91.06(0)

**R-Factor (%):** 4.87      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.272





# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 56

XAQRAJ

**Reference:** J.A.McMahon, J.A.Bis, P.Vishweshwar, T.R.Shattock,  
O.L.McLaughlin, M.J.Zaworotko (2005) *Z.Kristallogr.* ,**220**,340

**Formula:** 2(C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>),C<sub>7</sub> H<sub>7</sub> N<sub>1</sub> O<sub>2</sub>

**Compound Name:** bis(Carbamazepine) 4-aminobenzoic acid

**Space Group:** C2/c      **Cell:**    **a** 37.013(3)    **b** 12.132(0)    **c** 13.599(1)  
**Space Group No.:** 15      **(Å, °)**     $\alpha$  90.00       $\beta$  99.17(0)     $\gamma$  90.00

**R-Factor (%):** 4.16      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.344

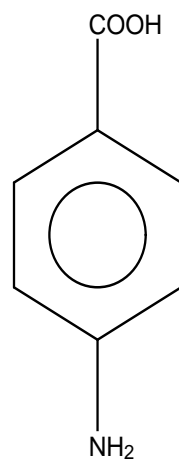
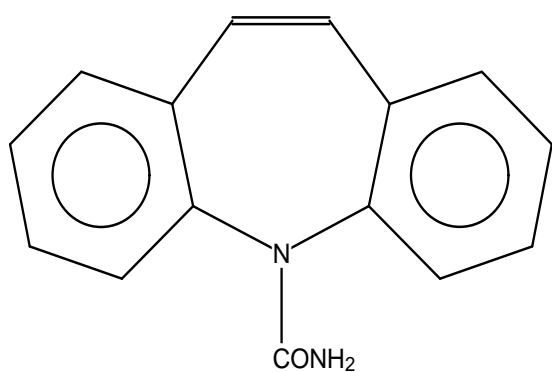
## Parameters

### Fragment 1

**DIST1 (D)** 1.240  
**DIST2 (D)** 1.374  
**DIST3 (D)** 1.343

### Fragment 2

**DIST1 (D)** 1.248  
**DIST2 (D)** 1.365  
**DIST3 (D)** 1.346



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 57

## XAQREN

**Reference:** J.A.McMahon, J.A.Bis, P.Vishweshwar, T.R.Shattock, O.L.McLaughlin, M.J.Zaworotko (2005) *Z.Kristallogr.* ,**220**,340

**Formula:** 2(C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>),C<sub>7</sub> H<sub>7</sub> N<sub>1</sub> O<sub>2</sub>,H<sub>2</sub> O<sub>1</sub>

**Compound Name:** bis(Carbamazepine) 4-aminobenzoic acid monohydrate

**Space Group:** P21/n      **Cell:**      **a** 13.761(1)      **b** 17.457(1)      **c** 14.624(1)  
**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  115.88(0)       $\gamma$  90.00

**R-Factor (%):** 4.31      **Temperature(K):** 100      **Density(g/cm<sup>3</sup>):** 1.319

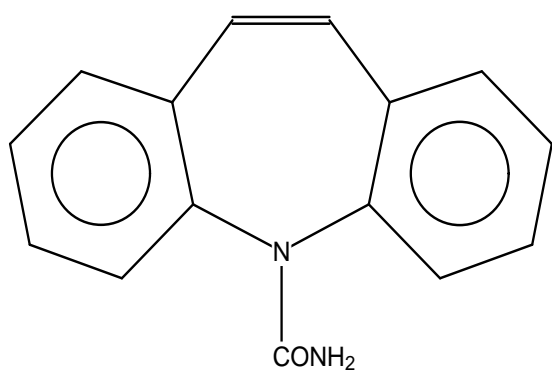
### Parameters

#### Fragment 1

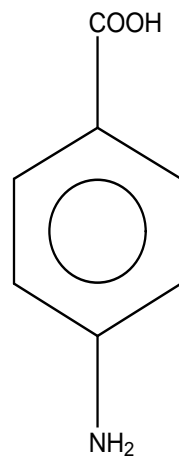
**DIST1 (D)** 1.243  
**DIST2 (D)** 1.375  
**DIST3 (D)** 1.338

#### Fragment 2

**DIST1 (D)** 1.240  
**DIST2 (D)** 1.368  
**DIST3 (D)** 1.342



H<sub>2</sub>O



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 58

XAQRIR

**Reference:** J.A.McMahon, J.A.Bis, P.Vishweshwar, T.R.Shattock,  
O.L.McLaughlin, M.J.Zaworotko (2005) *Z.Kristallogr.* ,**220**,340

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>7</sub> H<sub>5</sub> N<sub>1</sub> O<sub>4</sub>

**Compound Name:** Carbamazepine 2,6-pyridinedicarboxylic acid

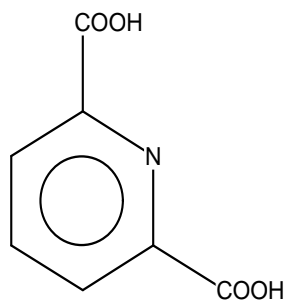
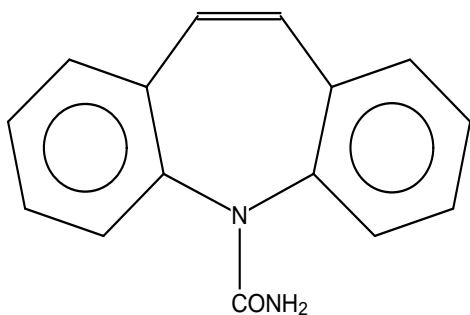
**Space Group:** P212121    **Cell:**    **a** 7.208(1)    **b** 14.644(3)    **c** 17.577(4)  
**Space Group No.:** 19    **(Å, °)**     $\alpha$  90.00     $\beta$  90.00     $\gamma$  90.00

**R-Factor (%):** 3.40    **Temperature(K):** 153    **Density(g/cm<sup>3</sup>):** 1.444

## Parameters

Fragment 1

**DIST1 (D)**    1.247  
**DIST2 (D)**    1.371  
**DIST3 (D)**    1.342



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 59

## XOBCEX

**Reference:** Enxian Lu, N.Rodriguez-Hornedo, R.Suryanarayanan  
(2008) *CrystEngComm*, **10**,665

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,0.5</sub>(C<sub>3</sub> H<sub>4</sub> O<sub>4</sub>)

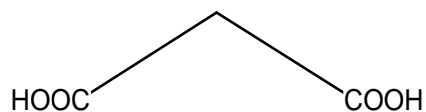
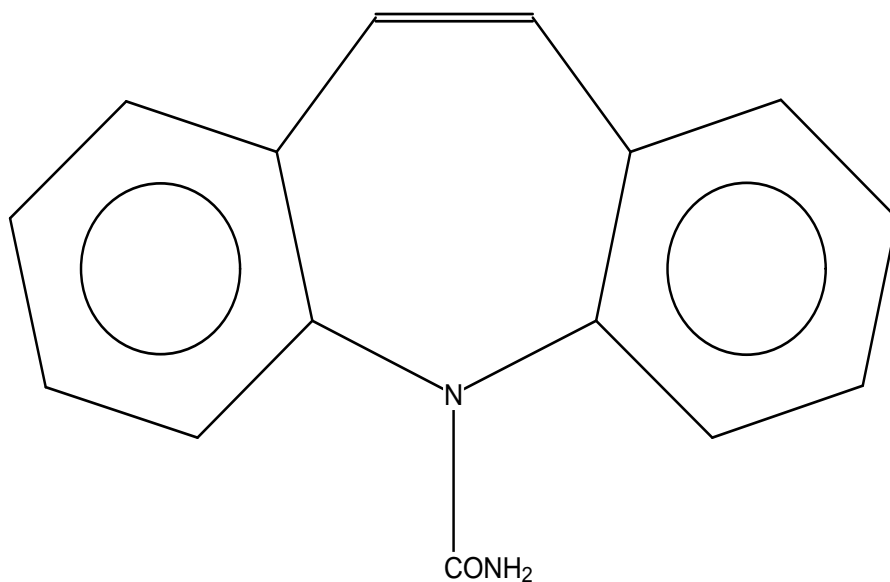
**Compound Name:** Carbamazepine hemikis(malonic acid)

**Space Group:** P2/n      **Cell:**    **a** 17.206(4)    **b** 4.993(1)    **c** 18.270(4)  
**Space Group No.:** 13      **(Å, °)**     $\alpha$  90.00       $\beta$  117.44(0)     $\gamma$  90.00

**R-Factor (%):** 4.57      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.375

### Parameters

Fragment 1  
**DIST1 (D)**    1.243  
**DIST2 (D)**    1.361  
**DIST3 (D)**    1.344



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 60

XOBCIB

**Reference:** Enxian Lu, N.Rodriguez-Hornedo, R.Suryanarayanan  
(2008) *CrystEngComm*, **10**,665

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1,0.5</sub>(C<sub>4</sub> H<sub>6</sub> O<sub>4</sub>)

**Compound Name:** Carbamazepine hemikis(succinic acid)

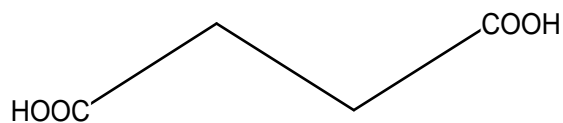
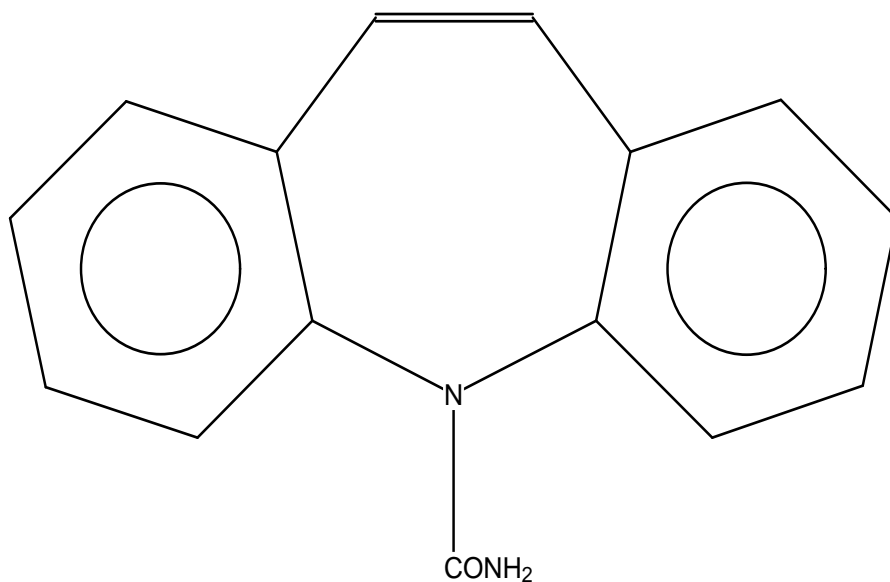
**Space Group:** P2/n      **Cell:**    **a** 17.536(2)    **b** 5.123(0)    **c** 18.308(2)  
**Space Group No.:** 13      **(Å, °)**     $\alpha$  90.00       $\beta$  118.51(0)     $\gamma$  90.00

**R-Factor (%):** 3.42      **Temperature(K):** 173      **Density(g/cm<sup>3</sup>):** 1.357

## Parameters

Fragment 1

**DIST1 (D)**    1.249  
**DIST2 (D)**    1.366  
**DIST3 (D)**    1.336



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 61

## XOXHEY

**Reference:** A.Jayasankar, L.S.Reddy, S.J.Bethune,  
N.Rodriguez-Hornedo (2009) *Cryst.Growth Des.* ,9,889

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>7</sub> H<sub>7</sub> N<sub>1</sub> O<sub>2</sub>

**Compound Name:** 4-Aminobenzoic acid 5H-dibenzo[b,f]azepine-5-carboxamide

**Synonym:** 4-Aminobenzoic acid carbamazepine

**Space Group:** P21/n      **Cell:**      **a** 5.191(0)      **b** 18.413(1)      **c** 19.048(1)

**Space Group No.:** 14      **(Å, °)**       $\alpha$  90.00       $\beta$  97.77(0)       $\gamma$  90.00

**R-Factor (%):** 4.06      **Temperature(K):** 85      **Density(g/cm<sup>3</sup>):** 1.375

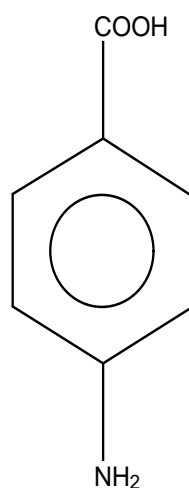
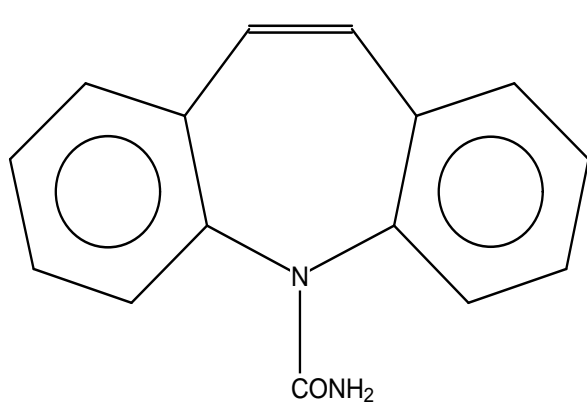
### Parameters

Fragment 1

**DIST1 (D)**      1.240

**DIST2 (D)**      1.372

**DIST3 (D)**      1.347



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 62

YABHIU

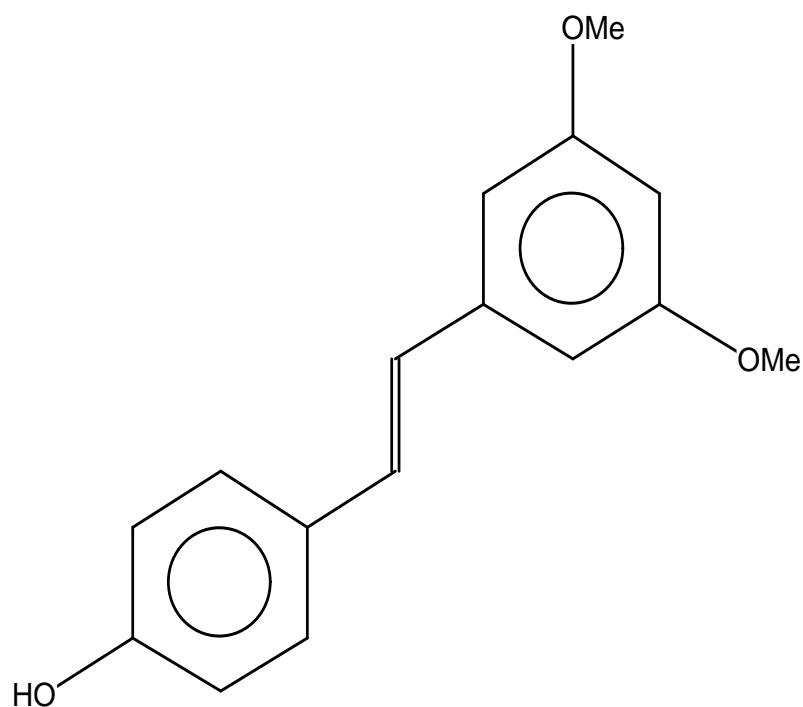
**Reference:** N.Schultheiss, S.Bethune, J.-O.Henck (2010)  
*CrystEngComm*, **12**,2436

**Formula:** C<sub>16</sub> H<sub>16</sub> O<sub>3</sub>, C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** Carbamazepine pterostilbene

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide 4-(2-(3,5-dimethoxyphenyl)vinyl)phenol

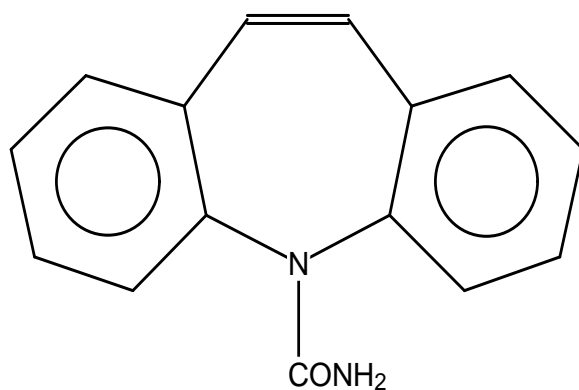
<b>Space Group:</b>	C2/c	<b>Cell:</b>	<b>a</b> 38.809(3)	<b>b</b> 5.392(0)	<b>c</b> 26.728(1)
<b>Space Group No.:</b>	15	(Å, °)	α 90.00	β 117.31(0)	γ 90.00
<b>R-Factor (%):</b>	5.15	<b>Temperature(K):</b>	120	<b>Density(g/cm<sup>3</sup>):</b>	1.317



## Parameters

Fragment 1

<b>DIST1 (D)</b>	1.246
<b>DIST2 (D)</b>	1.369
<b>DIST3 (D)</b>	1.339



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 63

## CBMZPN16

**Reference:** J.-B.Arlin, L.S.Price, S.L.Price, A.J.Florence (2011)  
*Chem.Comm.* ,47,7074

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>

**Compound Name:** Carbamazepine

**Synonym:** 5H-Dibenzo[b,f]azepine-5-carboxamide

**Space Group:** Pbcu      **Cell:**      **a** 9.125(0)      **b** 10.452(0)      **c** 24.822(1)  
**Space Group No.:** 61      **(Å, °)**      **α** 90.00      **β** 90.00      **γ** 90.00

**R-Factor (%):** 4.50      **Temperature(K):** 123      **Density(g/cm<sup>3</sup>):** 1.326

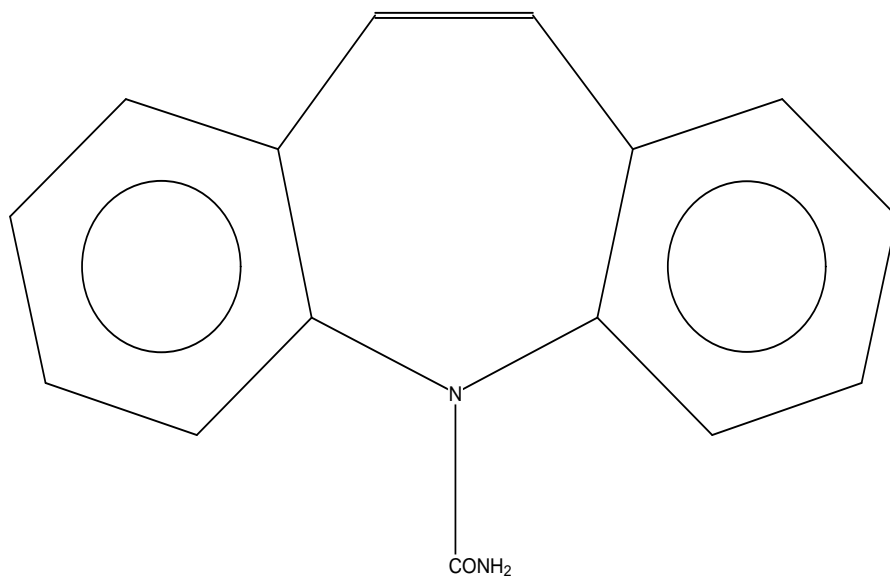
### Parameters

Fragment 1

**DIST1 (D)** 1.233

**DIST2 (D)** 1.374

**DIST3 (D)** 1.349





# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 64

## OTESSEM

**Reference:** M.A.Oliveira, M.L.Peterson, R.J.Davey (2011)  
*Cryst.Growth Des.* ,11,449

**Formula:** C<sub>15</sub> H<sub>14</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>7</sub> H<sub>5</sub> N<sub>1</sub> O<sub>3</sub> S<sub>1</sub>

**Compound Name:** 10,11-Dihydro-5H-dibenzo[b,f]azepine-5-carboxamide 1,2-benzothiazol-3(2H)-one 1,1-dioxide

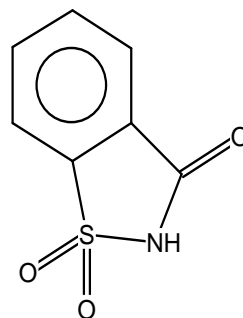
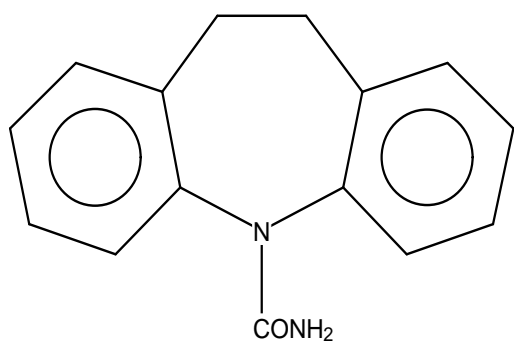
**Synonym:** dihydrocarbamazepine saccharin

<b>Space Group:</b>	P21/n	<b>Cell:</b>	<b>a</b> 7.582(1)	<b>b</b> 25.215(6)	<b>c</b> 10.554(3)
<b>Space Group No.:</b>	14	<b>(Å, °)</b>	<b>α</b> 90.00	<b>β</b> 105.88(0)	<b>γ</b> 90.00
<b>R-Factor (%):</b>	4.26	<b>Temperature(K):</b>	100	<b>Density(g/cm<sup>3</sup>):</b>	1.442

### Parameters

Fragment 1

<b>DIST1 (D)</b>	1.253
<b>DIST2 (D)</b>	1.369
<b>DIST3 (D)</b>	1.340



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 65

UNEYIV01

**Reference:** A.J.Cruz-Cabeza, G.M.Day, W.Jones (2011)  
*Phys.Chem.Chem.Phys.(PCCP)*, **13**,12808

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>2</sub> H<sub>6</sub> O<sub>1</sub> S<sub>1</sub>

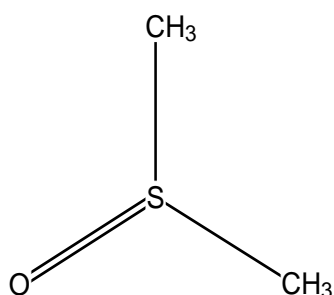
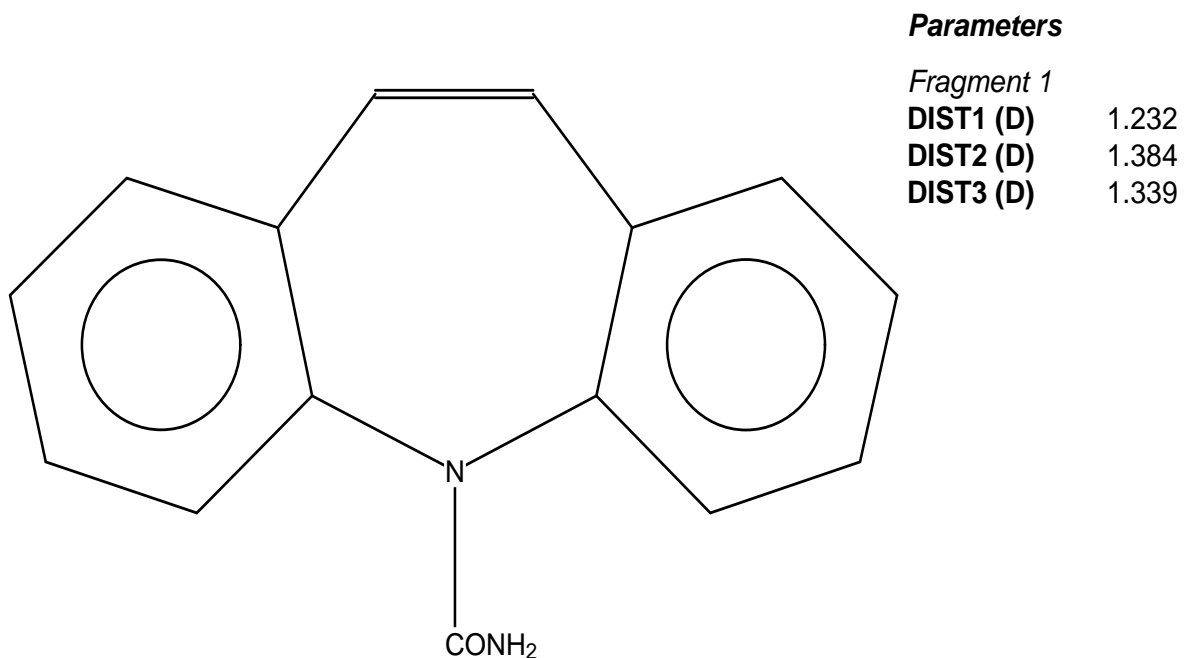
**Compound Name:** 5H-Dibenzo[b,f]azepine-5-carboxamide dimethylsulfoxide solvate

**Synonym:** Carbamazepine dimethylsulfoxide solvate

**Space Group:** P-1      **Cell:**    **a** 7.411(0)    **b** 8.975(0)    **c** 12.241(0)

**Space Group No.:** 2      **(Å, °)**    **α** 94.26(0)    **β** 94.53(0)    **γ** 100.20(0)

**R-Factor (%):** 4.86      **Temperature(K):** 280      **Density(g/cm<sup>3</sup>):** 1.313



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 66

UNEYIV02

**Reference:** A.J.Cruz-Cabeza, G.M.Day, W.Jones (2011)  
*Phys.Chem.Chem.Phys.(PCCP)*, **13**,12808

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>2</sub> H<sub>6</sub> O<sub>1</sub> S<sub>1</sub>

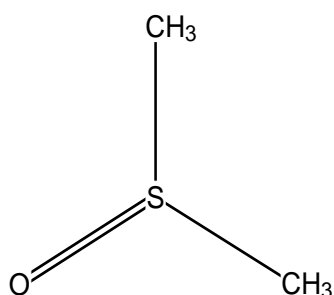
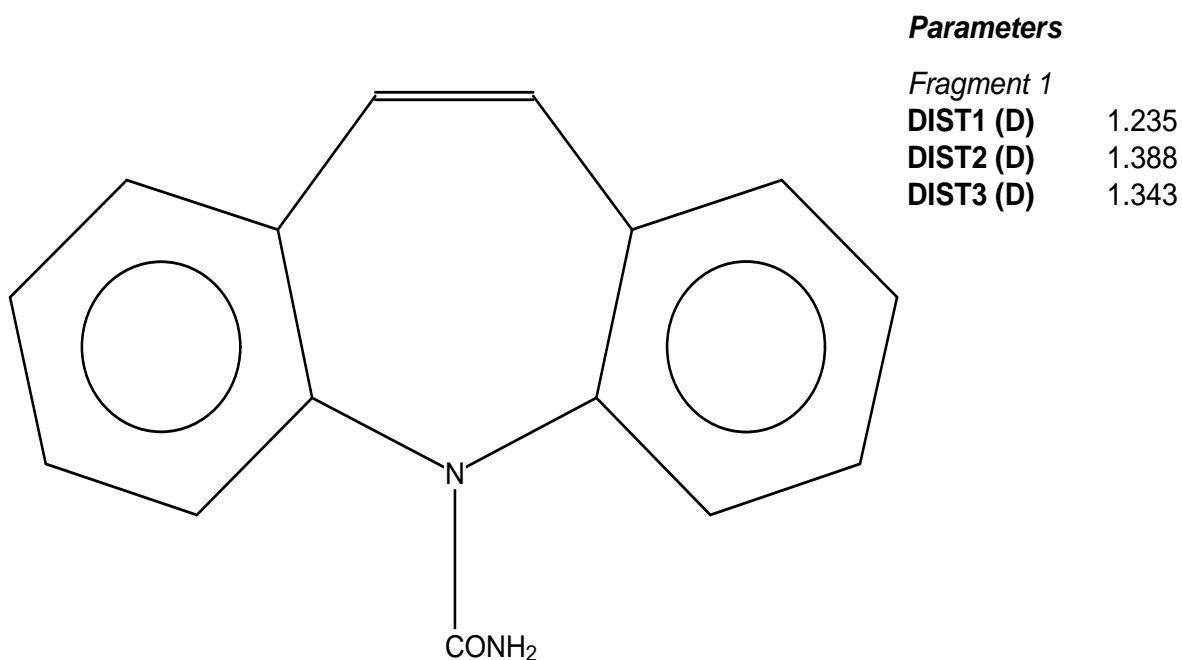
**Compound Name:** 5H-Dibenzo[b,f]azepine-5-carboxamide dimethylsulfoxide solvate

**Synonym:** Carbamazepine dimethylsulfoxide solvate

**Space Group:** P-1      **Cell:**    **a** 7.361(0)    **b** 8.929(0)    **c** 12.214(0)

**Space Group No.:** 2      **(Å, °)**    **α** 94.49(0)    **β** 94.72(0)    **γ** 100.07(0)

**R-Factor (%):** 5.40      **Temperature(K):** 200      **Density(g/cm<sup>3</sup>):** 1.332



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 67

UNEYIV03

**Reference:** A.J.Cruz-Cabeza, G.M.Day, W.Jones (2011)  
*Phys.Chem.Chem.Phys.(PCCP)* ,13,12808

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>2</sub> H<sub>6</sub> O<sub>1</sub> S<sub>1</sub>

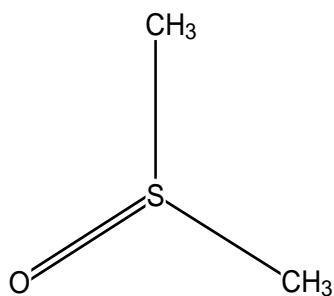
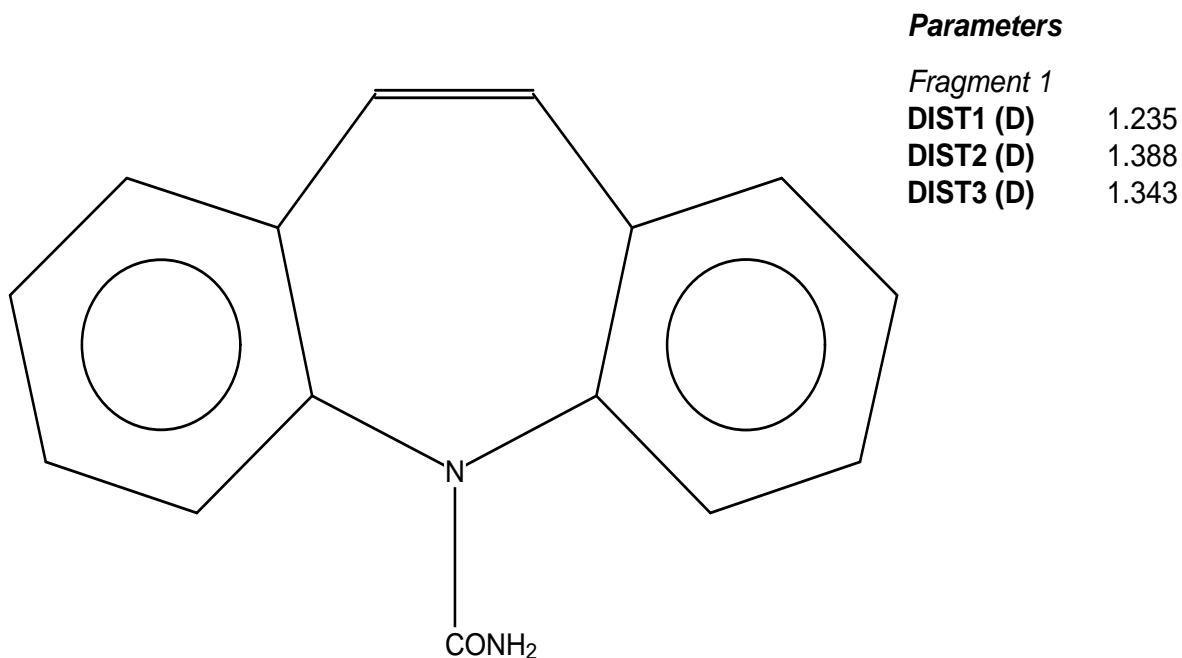
**Compound Name:** 5H-Dibenzo[b,f]azepine-5-carboxamide dimethylsulfoxide solvate

**Synonym:** Carbamazepine dimethylsulfoxide solvate

**Space Group:** P-1      **Cell:**    **a** 7.361(0)    **b** 8.929(0)    **c** 12.214(0)

**Space Group No.:** 2      **(Å, °)**    **α** 94.49(0)    **β** 94.72(0)    **γ** 100.07(0)

**R-Factor (%):** 5.40      **Temperature(K):** 200      **Density(g/cm<sup>3</sup>):** 1.332



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 68

UNEYIV04

**Reference:** A.J.Cruz-Cabeza, G.M.Day, W.Jones (2011)  
*Phys.Chem.Chem.Phys.(PCCP)*, **13**,12808

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>2</sub> H<sub>6</sub> O<sub>1</sub> S<sub>1</sub>

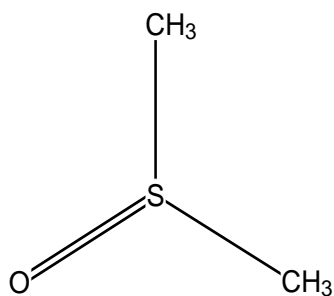
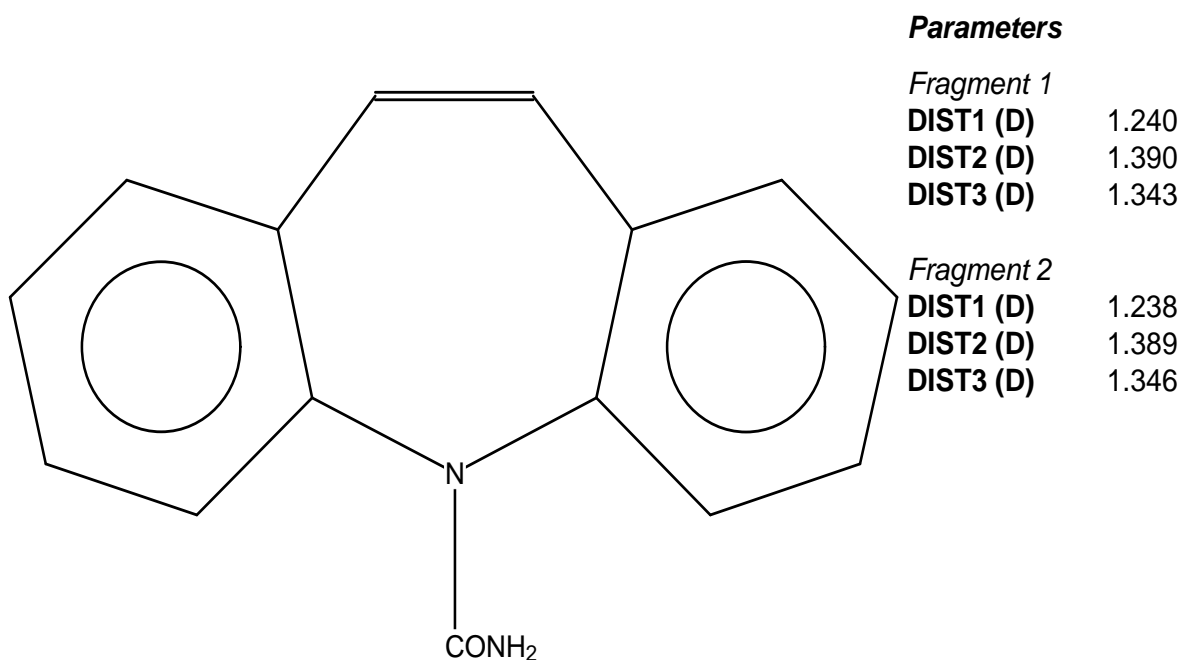
**Compound Name:** 5H-Dibenzo[b,f]azepine-5-carboxamide dimethylsulfoxide solvate

**Synonym:** Carbamazepine dimethylsulfoxide solvate

**Space Group:** P-1      **Cell:**    **a** 8.871(0)    **b** 12.190(0)    **c** 14.613(0)

**Space Group No.:** 2      **(Å, °)**    **α** 94.97(0)    **β** 100.22(0)    **γ** 95.04(0)

**R-Factor (%):** 4.75      **Temperature(K):** 110      **Density(g/cm<sup>3</sup>):** 1.355



# Search: search1 (Fri Dec 07 16:17:43 2012): Hit 69

## ABOQUF

**Reference:** S.Aitipamula, Pui Shan Chow, R.B.H.Tan (2011)  
*J.Chem.Cryst.* ,**41**,1604

**Formula:** C<sub>15</sub> H<sub>12</sub> N<sub>2</sub> O<sub>1</sub>, C<sub>6</sub> H<sub>6</sub> O<sub>2</sub>

**Compound Name:** 5H-Dibenzo[b,f]azepine-5-carboxamide benzene-1,4-diol

**Space Group:** P-1      **Cell:**    **a** 6.973(1)    **b** 8.818(1)    **c** 15.083(3)  
**Space Group No.:** 2      **(Å, °)**     $\alpha$  106.96(3)     $\beta$  92.16(3)     $\gamma$  103.23(3)

**R-Factor (%):** 8.01      **Temperature(K):** 110      **Density(g/cm<sup>3</sup>):** 1.341

### Parameters

*Fragment 1*  
**DIST1 (D)**      1.242  
**DIST2 (D)**      1.374  
**DIST3 (D)**      1.344

