Search Overview

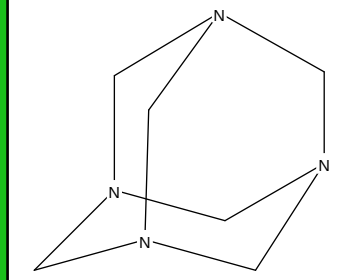
Search:	search1
Date/Time done:	Thu Dec 02 16:20:24 2010
Database(s):	CSD version 5.31 (November 2009) CSD version 5.31 updates (Nov 2009) CSD version 5.31 updates (Feb 2010) CSD version 5.31 updates (May 2010) CSD version 5.31 updates (Aug 2010)
Restriction Info:	No refcode restrictions applied
Filters:	3D coordinates determined No powder structures Only Organics
Percentage Completed:	100%
Number of Hits:	167

Single query used. Search found structures that:

match

Query 1

Query 1



Search: search1 (Thu Dec 02 16:20:24 2010): Hits 1-4

BOQBEO

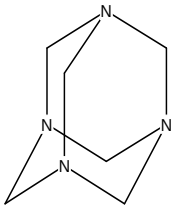
Reference: E.J.MacLean, C.Glidewell, G.Ferguson, R.M.Gregson, A.J.Lough (1999) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**55,** 1867

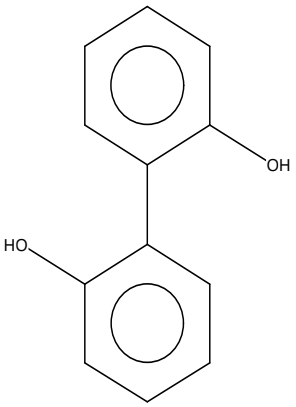
Formula: $C_6 H_{12} N_4,2(C_{12} H_{10} O_2)$

Compound Name: Hexamethylenetetramine bis(2,2'-biphenol)

Space Group:	P21	***Cell:***	***a***	9.761(0)	***b***	13.036(1)	***c***	9.788(0)
Space Group No.:	4	***(Å,°)***	α	90.00	β	90.20(0)	γ	90.00

R-Factor (%): 6.60 ***Temperature(K):*** 150 ***Density(g/cm^3):*** 1.367





BUQQAF04

Reference: S.W.Ng (2008) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* , **64,**o2195

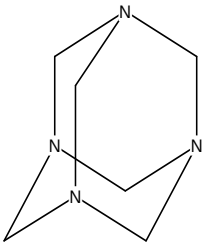
Formula: $C_6 H_{12} N_4,2(C_6 H_5 N_1 O_3),H_2 O_1$

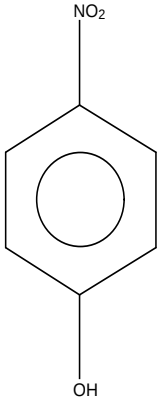
Compound Name: 1,3,5,7-tetraazatricyclo[3.3.1.1^{3,7}]decane bis(4-nitrophenol) monohydrate

Synonym: hexamethylenetetramine bis(4-nitrophenol) monohydrate

Space Group:	P1	***Cell:***	***a***	6.933(0)	***b***	11.687(0)	***c***	25.083(0)
Space Group No.:	1	***(Å,°)***	α	96.73(0)	β	92.45(0)	γ	89.97(0)

R-Factor (%): 7.86 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.438





H_2O

CERXIH

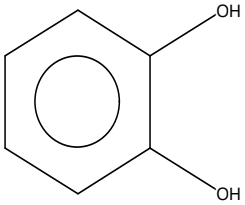
Reference: P.Daka, K.A.Wheeler (2006) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**62,**o5477

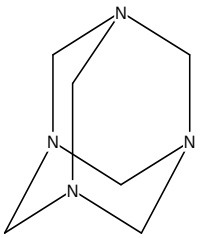
Formula: $2(C_6 H_6 O_2),C_6 H_{12} N_4$

Compound Name: bis(1,2-Dihydroxybenzene) hexamethylenetetramine

Space Group:	C2/c	***Cell:***	***a***	23.794(2)	***b***	6.842(0)	***c***	13.244(1)
Space Group No.:	15	***(Å,°)***	α	90.00	β	123.14(0)	γ	90.00

R-Factor (%): 5.10 ***Temperature(K):*** 298 ***Density(g/cm^3):*** 1.326





DIBZAQ

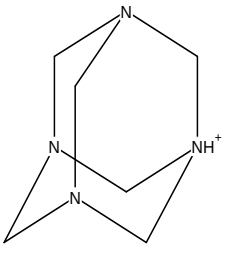
Reference: Hoong-Kun Fun, M.M.Rosli, Beck-Sim Lee, Lye-Hock Ong, S.Chantrapromma (2007) *J.Mol.Struct.* ,**837,**132

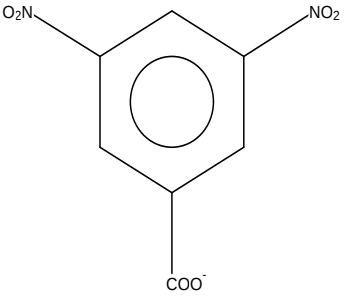
Formula: $C_6 H_{13} N_4^{1+},C_7 H_3 N_2 O_6^{1-},0.5(H_2 O_1)$

Compound Name: Hexamethylenetetraminium 3,5-dinitrobenzoate hemihydrate

Space Group:	P-1	***Cell:***	***a***	6.972(0)	***b***	10.721(0)	***c***	11.369(0)
Space Group No.:	2	***(Å,°)***	α	103.13(0)	β	98.43(0)	γ	105.83(0)

R-Factor (%): 4.60 ***Temperature(K):*** 297 ***Density(g/cm^3):*** 1.546





H_2O

Search: search1 (Thu Dec 02 16:20:24 2010): Hits 5-8

EKECOM01

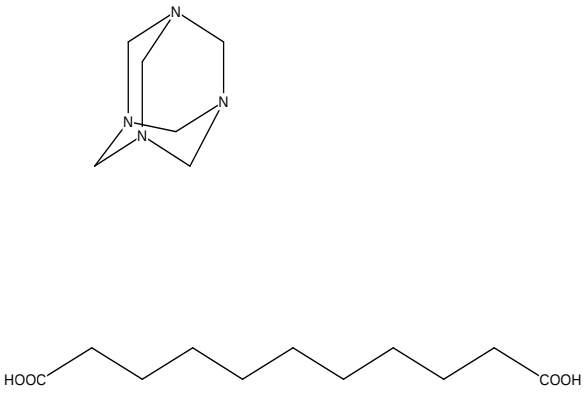
Reference: C.B.Pinheiro, M.Gardon, G.Chapuis (2003)
Acta Crystallogr.,Sect.B:Struct.Sci. ,**59,**416

Formula: $C_6 H_{12} N_4, C_{11} H_{20} O_4$

Compound Name: hexamethylenetetramine undecanedioic acid

Space Group:	P21/c	***Cell:***	***a***	5.897(0)	***b***	27.742(1)	***c***	23.497(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	102.98(0)	γ	90.00

R-Factor (%): 3.49 ***Temperature(K):*** 123 ***Density(g/cm³):*** 1.264



FEQXEF

Reference: K.Ghosh, M.Datta, R.Frohlich, N.C.Ganguly (2005)
J.Mol.Struct. ,**737,**201

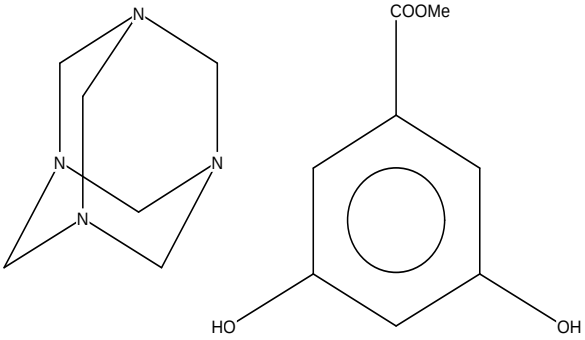
Formula: $C_6 H_{12} N_4, C_8 H_8 O_4$

Compound Name: Hexamethylenetetramine methyl 3,5-dihydroxybenzoate

Synonym: Urotropine methyl 3,5-dihydroxybenzoate

Space Group:	Cc	***Cell:***	***a***	22.621(1)	***b***	5.910(1)	***c***	12.325(1)
Space Group No.:	9	***(Å,°)***	α	90.00	β	116.32(1)	γ	90.00

R-Factor (%): 2.82 ***Temperature(K):*** 198 ***Density(g/cm³):*** 1.387



FEQXIJ

Reference: K.Ghosh, M.Datta, R.Frohlich, N.C.Ganguly (2005)
J.Mol.Struct. ,**737,**201

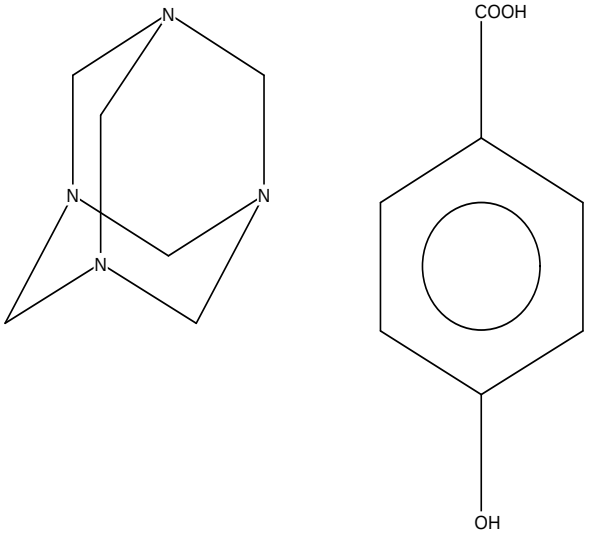
Formula: $C_6 H_{12} N_4, C_7 H_6 O_3$

Compound Name: Hexamethylenetetramine 4-hydroxybenzoic acid

Synonym: Urotropine 4-hydroxybenzoic acid

Space Group:	P21/n	***Cell:***	***a***	5.976(1)	***b***	11.796(1)	***c***	18.777(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	93.84(1)	γ	90.00

R-Factor (%): 4.40 ***Temperature(K):*** 198 ***Density(g/cm³):*** 1.400



FIFFIK

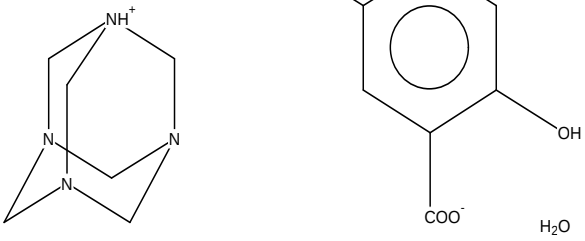
Reference: G.Smith, A.W.Hartono, U.D.Wermuth, P.C.Healy, J.M.White, A.D.Rae (2005) *Aust.J.Chem.* ,**58,**47

Formula: $C_6 H_{13} N_4^{1+}, C_7 H_4 N_1 O_5^{1-}, H_2 O_1$

Compound Name: 3,5,7-Triaza-1-azoniatricyclo(3.3.1.1^{3,7})decane 5-nitrosalicylate monohydrate

Space Group:	P21/c	***Cell:***	***a***	12.290(0)	***b***	6.549(0)	***c***	19.805(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	107.76(0)	γ	90.00

R-Factor (%): 5.30 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.493



Search: search1 (Thu Dec 02 16:20:24 2010): Hits 9-12

FITQII

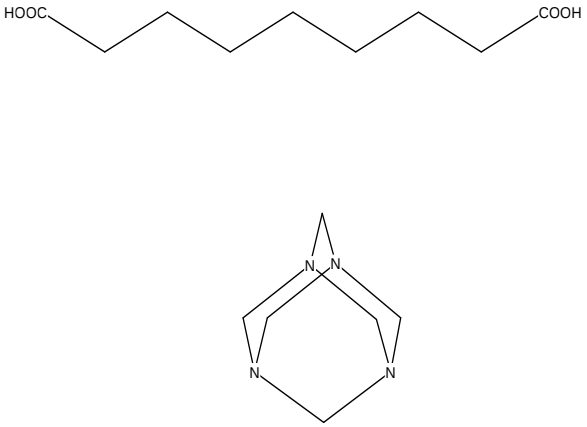
Reference: M.Hostettler, H.Birkedal, M.Gardon, G.Chapuis, D.Schwarzenbach, M.Bonin (1999) *Acta Crystallogr.,Sect.B:Struct.Sci.* ,**55,**448

Formula: $C_9 H_{16} O_4$,$C_6 H_{12} N_4$

Compound Name: Azelaic acid hexamethylenetetramine

Space Group:	P21/c	***Cell:***	***a***	5.891(0)	***b***	26.071(2)	***c***	11.887(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β	106.12(0)	γ	90.00

R-Factor (%): 4.69 ***Temperature(K):*** 258 ***Density(g/cm³):*** 1.244



GUTSIX

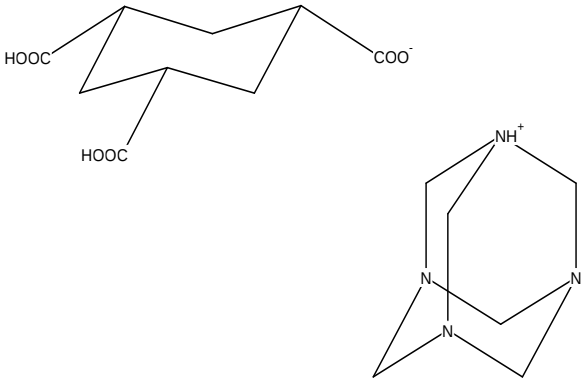
Reference: Ning Shan, A.D.Bond, W.Jones (2003) *New J.Chem.* ,**27,** 365

Formula: $C_6 H_{13} N_4^{1+}$,$C_9 H_{11} O_6^{1-}$

Compound Name: Hexamethylenetetramine cyclohexane-1,3cis,5cis-tricarboxylic acid

Space Group:	P21/c	***Cell:***	***a***	10.955(0)	***b***	14.487(0)	***c***	10.429(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	93.99(0)	γ	90.00

R-Factor (%): 4.49 ***Temperature(K):*** 180 ***Density(g/cm³):*** 1.434



HEXAIF10

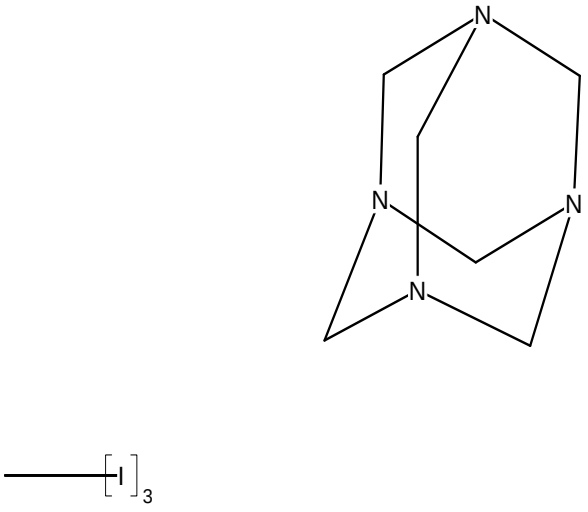
Reference: T.Dahl, O.Hassel (1970) *Acta Chem.Scand.* ,**24,**377

Formula: $C_6 H_{12} N_4$,$C_1 H_1 I_3$

Compound Name: Hexamethylenetetramine-iodoform complex

Space Group:	Cmc21	***Cell:***	***a***	10.681(1)	***b***	9.296(1)	***c***	13.988(2)
Space Group No.:	36	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.55 ***Temperature(K):*** 295 ***Density(g/cm³):*** 2.553



HIFZIF

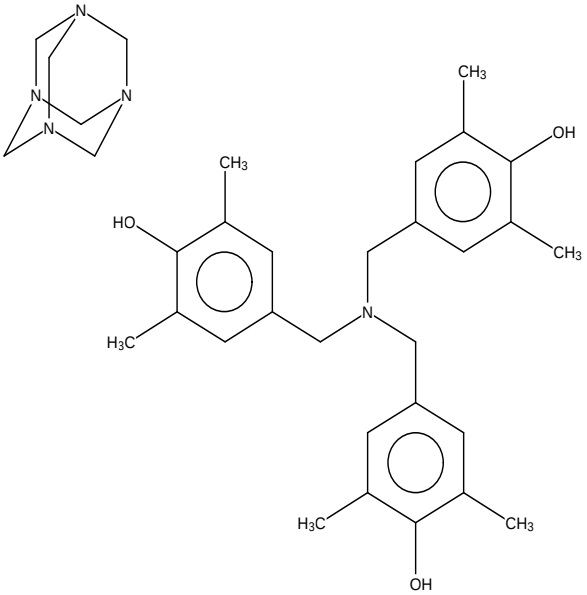
Reference: P.J.de Bruyn, R.W.Gable, A.C.Potter, D.H.Solomon (1996) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**52,**466

Formula: $C_6 H_{12} N_4$,$C_{27} H_{33} N_1 O_3$

Compound Name: 1,3,5,7-Tetra-azatricyclo(3.3.1.1^{3,7})decane 4,4',4"-(nitrilomethylene)-tris(2,6-dimethylphenol)

Space Group:	R-3	***Cell:***	***a***	14.109(1)	***b***	14.109(1)	***c***	26.697(5)
Space Group No.:	148	***(Å,°)***	α	90.00	β	90.00	γ	120.00

R-Factor (%): 3.53 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.212



Search: search1 (Thu Dec 02 16:20:24 2010): Hits 13-16

HMTHQU

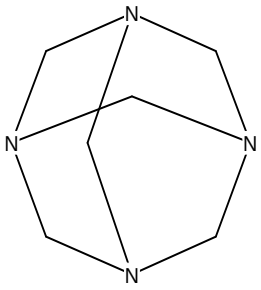
Reference: T.C.W.Mak, C.-S.Tse, Y.-H.Chong, F.-C.Mok (1977)
Acta Crystallogr.,Sect.B:Struct.Crystallogr.Cryst.Chem. ,**33,**2980

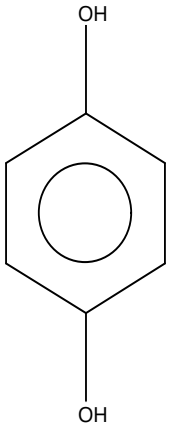
Formula: $C_6 H_{12} N_4, C_6 H_6 O_2$

Compound Name: Hexamethylenetetramine-hydroquinone

Space Group:	P21/m	***Cell:***	***a***	6.056(5)	***b***	16.700(10)	***c***	6.628(5)
Space Group No.:	11	***(Å,°)***	α	90.00	β	110.80(10)	γ	90.00

R-Factor (%): 9.90 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.327





HMTMCR

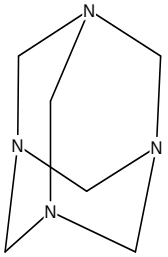
Reference: T.C.W.Mak, W.-H.Yu, Y.-S.Lam (1978)
Acta Crystallogr.,Sect.B:Struct.Crystallogr.Cryst.Chem. ,**34,**2061

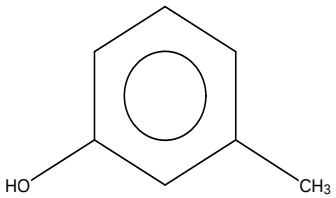
Formula: $C_6 H_{12} N_4, 2(C_7 H_8 O_1)$

Compound Name: Hexamethylenetetramine bis(m-cresol)

Space Group:	Ccc2	***Cell:***	***a***	10.630(10)	***b***	26.330(20)	***c***	7.199(5)
Space Group No.:	37	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 10.90 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.175





HMTNTI

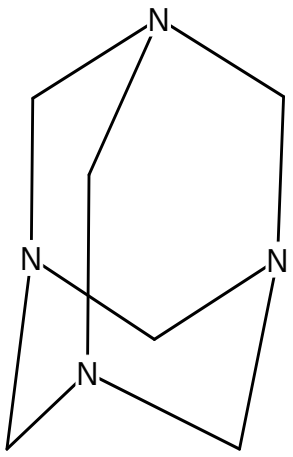
Reference: H.Pritzkow (1974) *Z.Anorg.Allg.Chem.* ,**409,**237

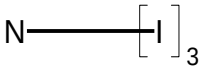
Formula: $C_6 H_{12} N_4, I_3 N_1, I_2$

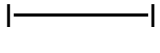
Compound Name: Hexamethylenetetramine tri-iodo-nitrogen iodine

Space Group:	Ama2	***Cell:***	***a***	10.017(1)	***b***	24.065(3)	***c***	7.152(1)
Space Group No.:	40	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.60 ***Temperature(K):*** 295 ***Density(g/cm³):*** 3.039







HMTTPO10

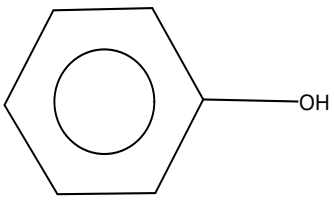
Reference: T.H.Jordan, T.C.W.Mak (1970) *J.Chem.Phys.* ,**52,**3790

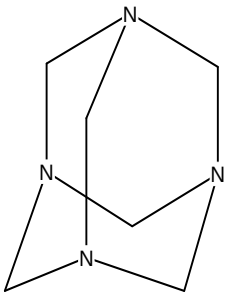
Formula: $C_6 H_{12} N_4, 3(C_6 H_6 O_1)$

Compound Name: Hexamethylenetetramine tri(phenol) complex

Space Group:	P-3	***Cell:***	***a***	14.880(10)	***b***	14.880(10)	***c***	6.007(5)
Space Group No.:	147	***(Å,°)***	α	90.00	β	90.00	γ	120.00

R-Factor (%): 10.10 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.218





Search: search1 (Thu Dec 02 16:20:24 2010): Hits 17-20

HUSWIB

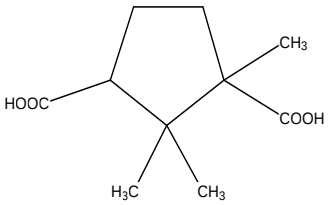
Reference: C.M.Zakaria, G.Ferguson, A.J.Lough, C.Glidewell (2003) *Acta Crystallogr.,Sect.B:Struct.Sci.* ,**59,**118

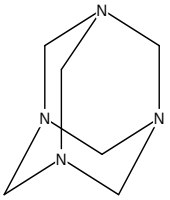
Formula: $2(C_{10}H_{16}O_4),C_6H_{12}N_4$

Compound Name: bis((1R,3S)-Camphoric acid) hexamethylenetetramine

Space Group:	P21212	***Cell:***	***a***	19.917(0)	***b***	6.752(0)	***c***	10.627(0)
Space Group No.:	18	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.27 ***Temperature(K):*** 150 ***Density(g/cm³):*** 1.256





HXMIOD

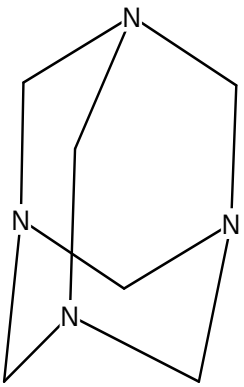
Reference: H.Pritzkow (1975) *Acta Crystallogr.,Sect.B:Struct.Crystallogr.Cryst.Chem.* ,**31,**1589

Formula: $C_6H_{12}N_4,2(I_2)$

Compound Name: Hexamethylenetetramine bis(iodine)

Space Group:	P21/c	***Cell:***	***a***	6.097(2)	***b***	16.754(3)	***c***	14.771(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	91.91	γ	90.00

R-Factor (%): 5.30 ***Temperature(K):*** 295 ***Density(g/cm³):*** 2.853



HXMTDI

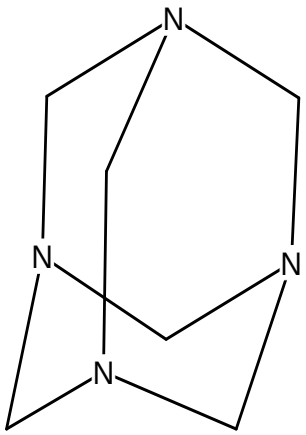
Reference: H.Pritzkow (1975) *Acta Crystallogr.,Sect.B:Struct.Crystallogr.Cryst.Chem.* ,**31,**1589

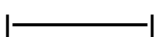
Formula: $C_6H_{12}N_4,I_2$

Compound Name: Hexamethylenetetramine iodine

Space Group:	Cmc21	***Cell:***	***a***	9.307(2)	***b***	7.603(2)	***c***	15.577(3)
Space Group No.:	36	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.40 ***Temperature(K):*** 295 ***Density(g/cm³):*** 2.374





HXMTHH

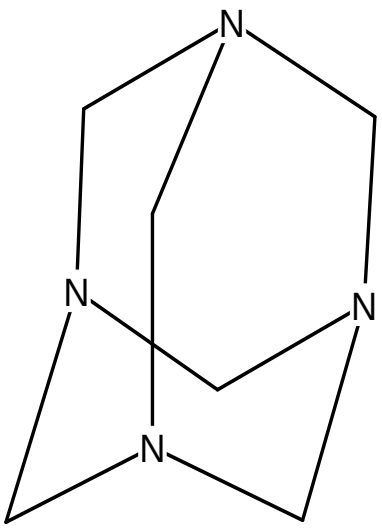
Reference: T.C.W.Mak (1965) *J.Chem.Phys.* ,**43,**2799

Formula: $C_6H_{12}N_4,6(H_2O_1)$

Compound Name: Hexamethylenetetramine hexahydrate clathrate

Space Group:	R3m	***Cell:***	***a***	11.620	***b***	11.620	***c***	8.670
Space Group No.:	160	***(Å,°)***	α	90.00	β	90.00	γ	120.00

R-Factor (%): 9.60 ***Temperature(K):*** 253 ***Density(g/cm³):*** 1.220



H_2O

Search: search1 (Thu Dec 02 16:20:24 2010): Hits 21-24

IDUTUX

Reference: Hai Feng, Ya-Ping Lu, Hui-Min Zhang, Bing Tu, Zhi-Min Jin (2006) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**62,** o3122

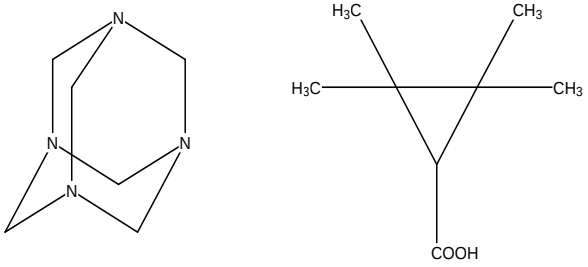
Formula: $C_6\,H_{12}\,N_4,C_8\,H_{14}\,O_2$

Compound Name: Hexamethylene triamine 2,2,3,3-tetramethylcyclopropanecarboxylic acid

Synonym: Urotropine 2,2,3,3-tetramethylcyclopropanecarboxylic acid

Space Group:	C2/c	***Cell:***	***a***	10.244(1)	***b***	7.072(0)	***c***	42.491(6)
Space Group No.:	15	***(Å,°)***	α	90.00	β	96.88(0)	γ	90.00

R-Factor (%): 8.10 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.228



IHERIW

Reference: S.Chantrapromma, A.Usman, Hoong-Kun Fun, Bo-Long Poh, C.Karalai (2002) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**58,**o675

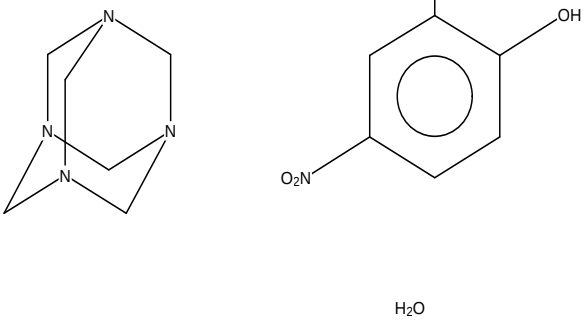
Formula: $C_6\,H_{12}\,N_4,2(C_6\,H_5\,N_1\,O_4),H_2\,O_1$

Compound Name: Hexamethylenetetraamine 4-nitrocatechol monohydrate

Synonym: 1,3,5,7-tetraazatricycl[3.3.1.1^{3,7}]decane 4-nitrobenzene-1,2-diol monohydrate

Space Group:	P-1	***Cell:***	***a***	9.352(0)	***b***	9.767(0)	***c***	11.826(0)
Space Group No.:	2	***(Å,°)***	α	99.49(0)	β	107.50(0)	γ	91.44(0)

R-Factor (%): 3.98 ***Temperature(K):*** 213 ***Density(g/cm³):*** 1.536



H_2O

IJETOG

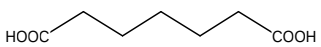
Reference: M.Gardon, C.B.Pinheiro, G.Chapuis (2003) *Acta Crystallogr.,Sect.B:Struct.Sci.* ,**59,**527

Formula: $C_6\,H_{12}\,N_4,C_7\,H_{12}\,O_4$

Compound Name: Hexamethylenetetramine pimelic acid

Space Group:	Pccn	***Cell:***	***a***	9.501(0)	***b***	22.660(1)	***c***	14.400(0)
Space Group No.:	56	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.87 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.287



IZAXIQ

Reference: R.Venkatraman, P.C.Ray, F.R.Fronczek (2004) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**60,**o633

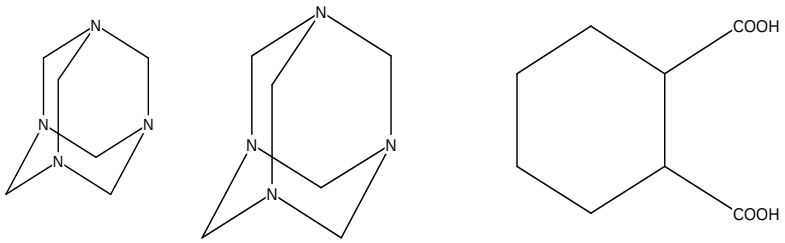
Formula: $C_6\,H_{12}\,N_4,C_8\,H_{12}\,O_4$

Compound Name: Hexamethylenetetramine rac-trans-1,2-cyclohexanedicarboxylic acid

Synonym: Urotropine rac-trans-1,2-cyclohexanedicarboxylic acid

Space Group:	Aba2	***Cell:***	***a***	11.990(3)	***b***	11.814(3)	***c***	22.606(6)
Space Group No.:	41	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.10 ***Temperature(K):*** 102 ***Density(g/cm³):*** 1.296



Search: search1 (Thu Dec 02 16:20:24 2010): Hits 25-28

MEVXIU01

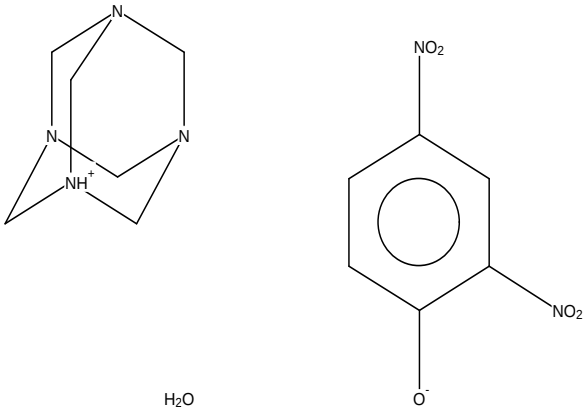
Reference: A.Usman, S.Chantrapromma, Hoong-Kun Fun (2001) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**57,**1443

Formula: $C_6 H_{13} N_4^{1+}$,$C_6 H_3 N_2 O_5^{1-}$,$H_2 O_1$

Compound Name: 3,5,7-triaza-1-azoniatricyclo(3.3.1.1^{3,7})decane 2,4-dinitrophenolate monohydrate

Space Group:	P21/m	***Cell:***	***a***	7.861(0)	***b***	6.598(0)	***c***	14.434(0)
Space Group No.:	11	***(Å,°)***	α	90.00	β	94.92(0)	γ	90.00

R-Factor (%): 5.89 ***Temperature(K):*** 300 ***Density(g/cm^3):*** 1.524



MIPVAI

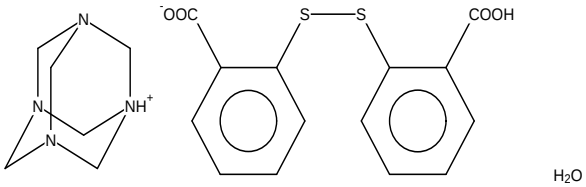
Reference: Wei Li, Jie-Peng Zhang, Ming-Liang Tong, Xiao-Ming Chen (2001) *Aust.J.Chem.* ,**54,**213

Formula: $C_6 H_{13} N_4^{1+}$,$C_{14} H_9 O_4 S_2^{1-}$,0.5($H_2 O_1$)

Compound Name: Hexamethylenetetraamine 2,2'-dithiosalicylic acid hemihydrate

Space Group:	C2/c	***Cell:***	***a***	14.181(7)	***b***	12.190(5)	***c***	24.942(13)
Space Group No.:	15	***(Å,°)***	α	90.00	β	101.29(2)	γ	90.00

R-Factor (%): 5.73 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.431



MIPVEM

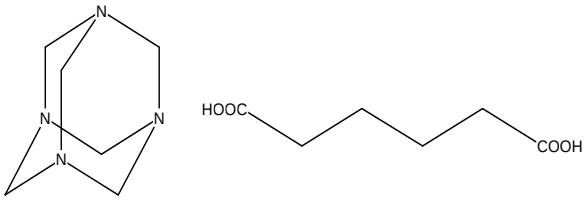
Reference: Wei Li, Jie-Peng Zhang, Ming-Liang Tong, Xiao-Ming Chen (2001) *Aust.J.Chem.* ,**54,**213

Formula: $C_6 H_{12} N_4$,$C_6 H_{10} O_4$

Compound Name: Hexamethylenetetraamine adipic acid

Space Group:	Cmcm	***Cell:***	***a***	9.267(3)	***b***	7.417(2)	***c***	22.222(7)
Space Group No.:	63	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 6.92 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.245



MIPVIQ

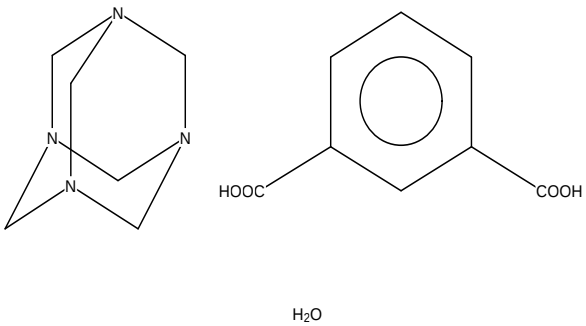
Reference: Wei Li, Jie-Peng Zhang, Ming-Liang Tong, Xiao-Ming Chen (2001) *Aust.J.Chem.* ,**54,**213

Formula: $C_6 H_{12} N_4$,2($C_8 H_6 O_4$),$H_2 O_1$

Compound Name: Hexamethylenetetraamine bis(m-benzenedicarboxylic acid) monohydrate

Space Group:	P21/m	***Cell:***	***a***	6.935(2)	***b***	23.859(12)	***c***	6.954(4)
Space Group No.:	11	***(Å,°)***	α	90.00	β	97.88	γ	90.00

R-Factor (%): 6.03 ***Temperature(K):*** 293 ***Density(g/cm^3):*** 1.429



Search: search1 (Thu Dec 02 16:20:24 2010): Hits 29-32

MIPVOW

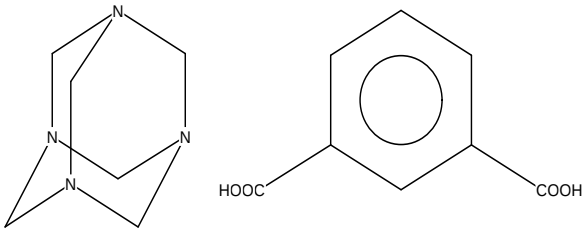
Reference: Wei Li, Jie-Peng Zhang, Ming-Liang Tong, Xiao-Ming Chen (2001) *Aust.J.Chem.* ,**54**,213

Formula: $2(C_6H_{12}N_4),C_8H_6O_4$

Compound Name: bis(Hexamethylenetetraamine) m-benzenedicarboxylic acid

Space Group:	P212121	***Cell:***	***a***	7.044(2)	***b***	14.024(6)	***c***	21.745(10)
Space Group No.:	19	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 5.53 ***Temperature(K):*** 293 ***Density(g/cm³):*** 1.381



PIZDUX

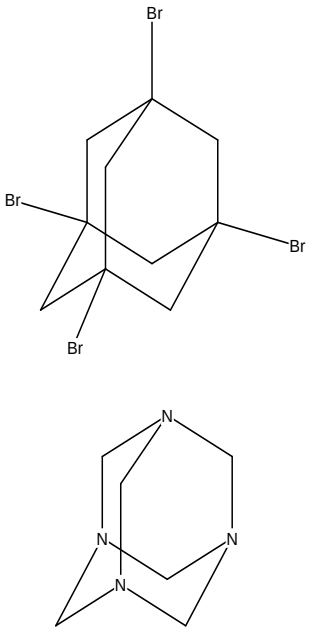
Reference: D.S.Reddy, D.C.Craig, G.R.Desiraju (1994) *Chem.Commun.* ,1457

Formula: $C_{10}H_{12}Br_4,2(C_6H_{12}N_4)$

Compound Name: 1,3,5,7-Tetrabromo-adamantane bis(hexamethylenetetramine)

Space Group:	F-43m	***Cell:***	***a***	13.801(1)	***b***	13.801(1)	***c***	13.801(1)
Space Group No.:	216	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.20 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.850



PIZFAF

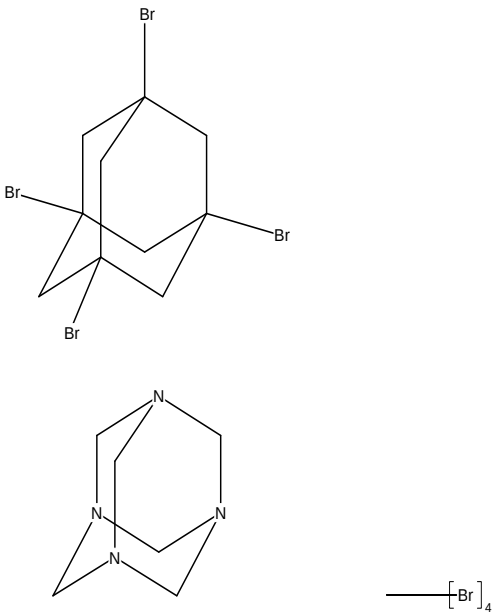
Reference: D.S.Reddy, D.C.Craig, G.R.Desiraju (1994) *Chem.Commun.* ,1457

Formula: $C_{10}H_{12}Br_4,C_6H_{12}N_4,C_1Br_4$

Compound Name: 1,3,5,7-Tetrabromoadamantane hexamethylenetetramine carbon tetrabromide solvate

Space Group:	F-43m	***Cell:***	***a***	13.571(1)	***b***	13.571(1)	***c***	13.571(1)
Space Group No.:	216	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 2.80 ***Temperature(K):*** 295 ***Density(g/cm³):*** 2.455



QIHCIT

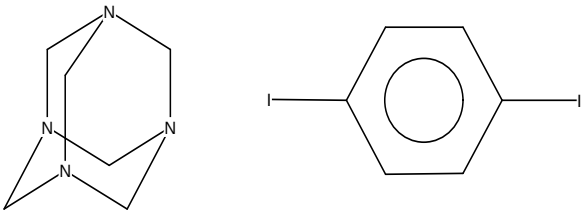
Reference: R.B.Walsh, C.W.Padgett, P.Metrangolo, G.Resnati, T.W.Hanks, W.T.Pennington (2001) *Cryst.Growth Des.* ,**1**,165

Formula: $C_6H_{12}N_4,C_6H_4I_2$

Compound Name: hexamethylethylenetetramine 1,4-diiodobenzene

Space Group:	Pmcm	***Cell:***	***a***	9.552(1)	***b***	7.577(1)	***c***	20.642(3)
Space Group No.:	51	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.18 ***Temperature(K):*** 295 ***Density(g/cm³):*** 2.090



Search: search1 (Thu Dec 02 16:20:24 2010): Hits 33-36

QIHCOZ01

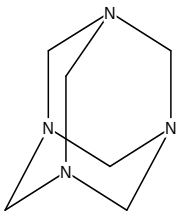
Reference: M.Bolte (2003) *Private Communication* ,

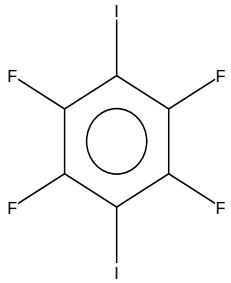
Formula: $C_6 H_{12} N_4, C_6 F_4 I_2$

Compound Name: Hexamethylenetetramine 1,4-di-iodotetrafluorobenzene

Space Group:	P21/m	***Cell:***	***a***	5.870(0)	***b***	21.186(2)	***c***	6.316(0)
Space Group No.:	11	***(Å,°)***	α	90.00	β	91.03(0)	γ	90.00

R-Factor (%): 2.09 ***Temperature(K):*** 100 ***Density(g/cm³):*** 2.292





QIHCUF

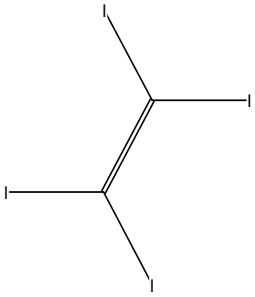
Reference: R.B.Walsh, C.W.Padgett, P.Metrangolo, G.Resnati, T.W.Hanks, W.T.Pennington (2001) *Cryst.Growth Des.* ,**1,**165

Formula: $C_6 H_{12} N_4, C_2 I_4$

Compound Name: hexamethylethylenetetramine tetraiodoethylene

Space Group:	P2/m	***Cell:***	***a***	8.826(0)	***b***	11.060(0)	***c***	15.914(0)
Space Group No.:	10	***(Å,°)***	α	90.00	β	92.61	γ	90.00

R-Factor (%): 2.81 ***Temperature(K):*** 295 ***Density(g/cm³):*** 2.875



RAWCOH

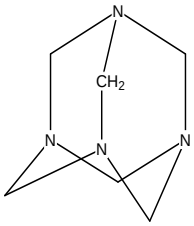
Reference: P.I.Coupar, C.Glidewell, G.Ferguson (1997) *Acta Crystallogr.,Sect.B:Struct.Sci.* ,**53,**521

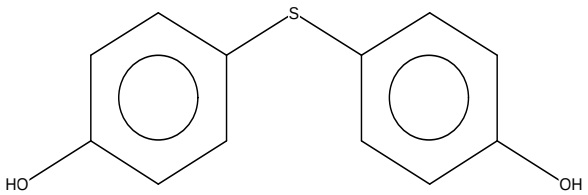
Formula: $C_6 H_{12} N_4, C_{12} H_{10} O_2 S_1$

Compound Name: Hexamethylenetetramine 4,4'-thiodiphenol

Space Group:	Pmn21	***Cell:***	***a***	15.029(2)	***b***	9.795(0)	***c***	5.982(1)
Space Group No.:	31	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 3.23 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.352





RAWCUN

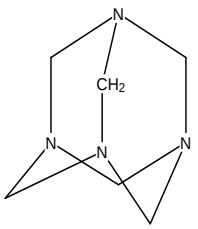
Reference: P.I.Coupar, C.Glidewell, G.Ferguson (1997) *Acta Crystallogr.,Sect.B:Struct.Sci.* ,**53,**521

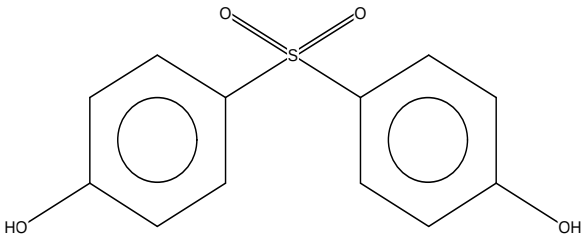
Formula: $C_6 H_{12} N_4, C_{12} H_{10} O_4 S_1$

Compound Name: Hexamethylenetetramine 4,4'-sulfonyldiphenol

Space Group:	Pmn21	***Cell:***	***a***	14.779(2)	***b***	10.256(1)	***c***	5.982(0)
Space Group No.:	31	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.21 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.430





Search: search1 (Thu Dec 02 16:20:24 2010): Hits 37-40

RAWDAU

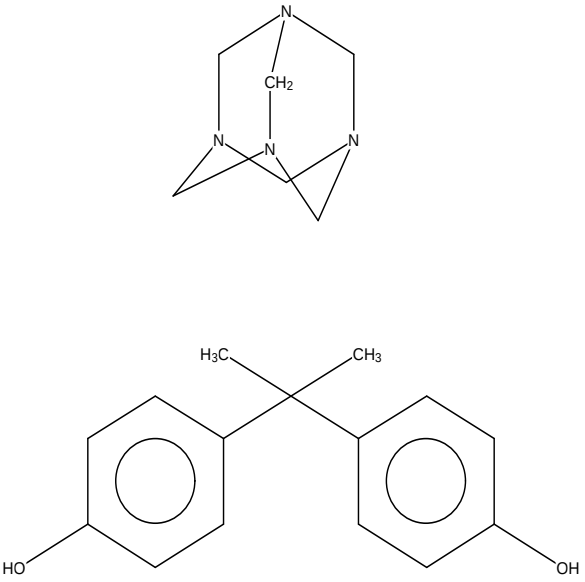
Reference: P.I.Coupar, C.Glidewell, G.Ferguson (1997)
Acta Crystallogr.,Sect.B:Struct.Sci. ,**53,**521

Formula: $C_6 H_{12} N_4,C_{15} H_{16} O_2$

Compound Name: Hexamethylenetetramine 4,4'-isopropylidenediphenol

Space Group:	C2/c	***Cell:***	***a***	25.093(6)	***b***	7.174(1)	***c***	23.612(7)
Space Group No.:	15	***(Å,°)***	α	90.00	β	110.42(2)	γ	90.00

R-Factor (%): 4.01 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.229



RAWDEY

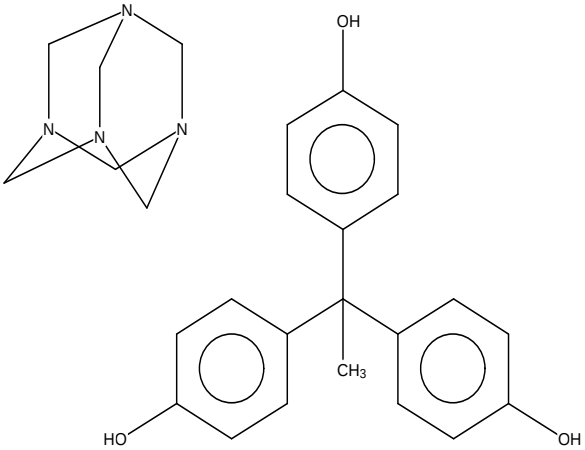
Reference: P.I.Coupar, C.Glidewell, G.Ferguson (1997)
Acta Crystallogr.,Sect.B:Struct.Sci. ,**53,**521

Formula: $2(C_6 H_{12} N_4),C_{20} H_{18} O_3$

Compound Name: bis(Hexamethylenetetramine) 1,1,1-tris(4-hydroxyphenyl)ethane

Space Group:	P212121	***Cell:***	***a***	6.993(1)	***b***	14.095(1)	***c***	30.999(4)
Space Group No.:	19	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 6.36 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.276



RAWDIC

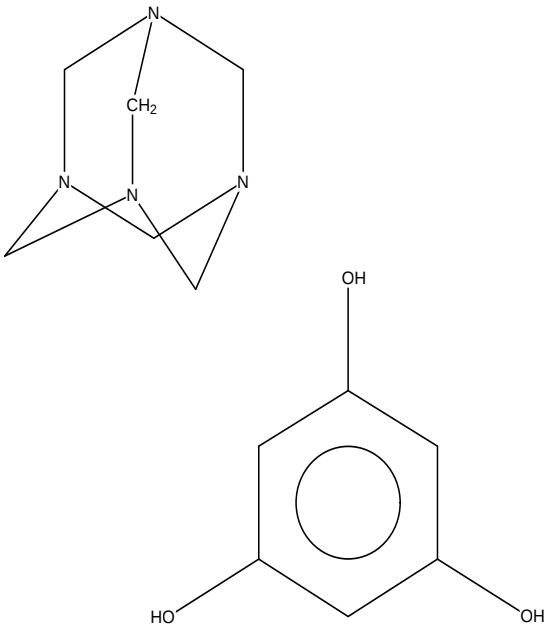
Reference: P.I.Coupar, C.Glidewell, G.Ferguson (1997)
Acta Crystallogr.,Sect.B:Struct.Sci. ,**53,**521

Formula: $3(C_6 H_{12} N_4),2(C_6 H_6 O_3)$

Compound Name: tris(Hexamethylenetetramine) bis(1,3,5-trihydroxybenzene)

Space Group:	C2/c	***Cell:***	***a***	23.598(2)	***b***	7.136(2)	***c***	19.445(3)
Space Group No.:	15	***(Å,°)***	α	90.00	β	96.82(1)	γ	90.00

R-Factor (%): 6.28 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.374



ROKQIR

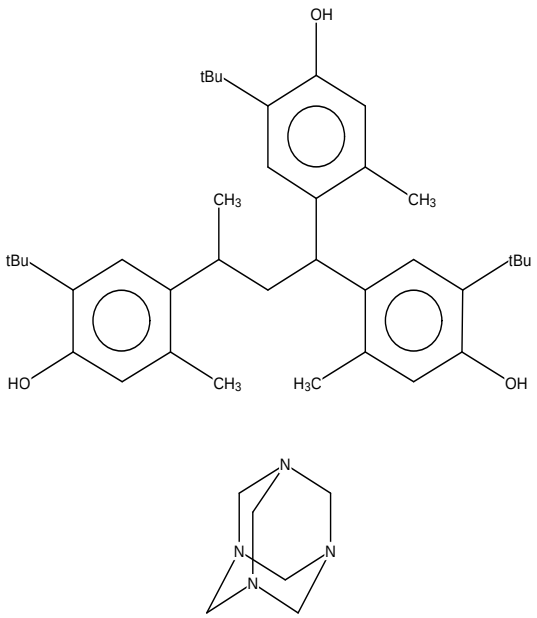
Reference: P.R.Meehan, R.M.Gregson, C.Glidewell, G.Ferguson
(1997) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**53,**1637

Formula: $C_{37} H_{52} O_3,C_6 H_{12} N_4$

Compound Name: 1,1,3-tris(2-Methyl-4-hydroxy-5-t-butylphenyl)butane
hexamethylenetetramine

Space Group:	P21/n	***Cell:***	***a***	10.114(0)	***b***	13.421(1)	***c***	30.576(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	98.92(0)	γ	90.00

R-Factor (%): 6.22 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.110



Search: search1 (Thu Dec 02 16:20:24 2010): Hits 41-44

RSHMTA02

Reference: S.W.Ng, P.Naumov, A.R.Ibrahim, H.-K.Fun, S.Chantrapromma, G.Wojciechowski, B.Brzezinski, J.V.Hanna (2002) *J.Mol.Struct.* ,**609,**89

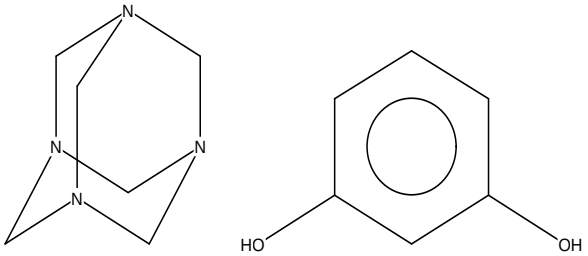
Formula: $C_6 H_{12} N_4$,$C_6 H_6 O_2$

Compound Name: Hexamethylenetetramine resorcinol

Synonym: Urotropine resorcinol

Space Group:	Cmcm	***Cell:***	***a***	10.353(0)	***b***	7.087(0)	***c***	16.856(1)
Space Group No.:	63	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 6.48 ***Temperature(K):*** 298 ***Density(g/cm³):*** 1.344



RUWJOI

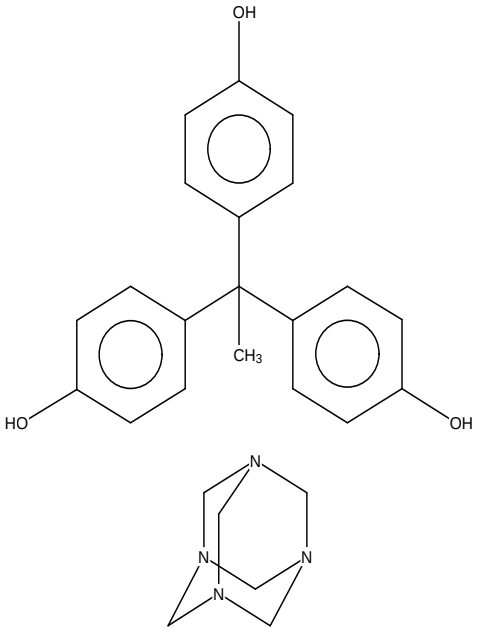
Reference: P.I.Coupar, G.Ferguson, C.Glidewell, P.R.Meehan (1997) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**53,**1978

Formula: $C_{20} H_{18} O_3$,$C_6 H_{12} N_4$

Compound Name: Hexamethylenetetramine 1,1,1-tris(4-hydroxyphenyl)ethane

Space Group:	Pbca	***Cell:***	***a***	13.307(2)	***b***	24.150(3)	***c***	14.740(2)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 6.01 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.252



TIPWAQ01

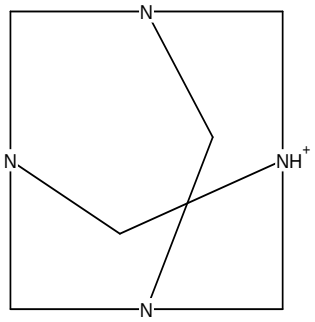
Reference: V.B.Gaillard, W.Paciorek, K.Schenk, G.Chapuis (1996) *Acta Crystallogr.,Sect.B:Struct.Sci.* ,**52,**1036

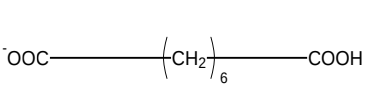
Formula: $C_6 H_{13} N_4^{1+}$,$C_8 H_{13} O_4^{1-}$

Compound Name: Hexamethylenetetramine suberate

Space Group:	P21	***Cell:***	***a***	5.908(0)	***b***	24.542(2)	***c***	5.915(0)
Space Group No.:	4	***(Å,°)***	α	90.00	β	102.04(0)	γ	90.00

R-Factor (%): 2.20 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.245





VIJTIR

Reference: T.C.W.Mak, Chen Xiaoming, Shi Kailiang, Yao Jiaxing, Zheng Chaode (1986) *J.Crystallogr.Spectrosc.Res.* ,**16,**639

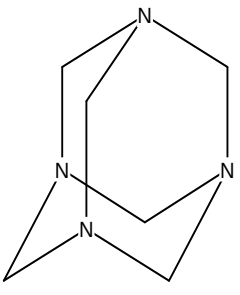
Formula: $C_6 H_{12} N_4$,$C_8 H_8 O_2$

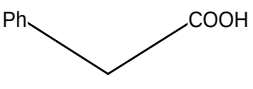
Compound Name: Hexamethylenetetramine phenylacetic acid

Synonym: 1,3,5,7-Tetra-aza-adamantane phenylacetic acid

Space Group:	I-4	***Cell:***	***a***	20.576(3)	***b***	20.576(3)	***c***	6.907(1)
Space Group No.:	82	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 7.10 ***Temperature(K):*** 295 ***Density(g/cm³):*** 1.255





Search: search1 (Thu Dec 02 16:20:24 2010): Hits 45-48

WISNER

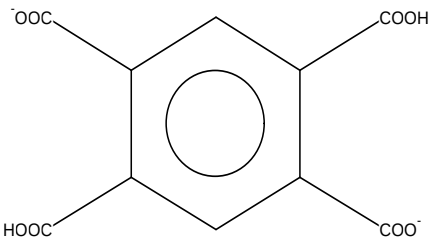
Reference: A.J.Lough, P.S.Wheatley, G.Ferguson, C.Glidewell (2000) *Acta Crystallogr.,Sect.B:Struct.Sci.* ,**56,**261

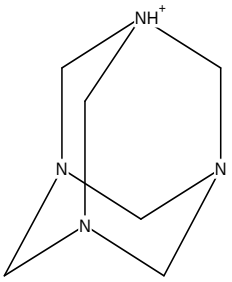
Formula: $2(C_6H_{13}N_4^{1+}),C_{10}H_4O_8^{2-}$

Compound Name: Benzene-1,2,4,5-tetracarboxylic acid bis(hexamethylenetetramine)

Space Group:	P-1	***Cell:***	***a***	9.703(0)	***b***	10.937(0)	***c***	16.765(1)
Space Group No.:	2	***(Å,°)***	α	84.27(0)	β	79.40(0)	γ	75.26(0)

R-Factor (%): 4.82 ***Temperature(K):*** 100 ***Density(g/cm³):*** 1.577





YEJKON

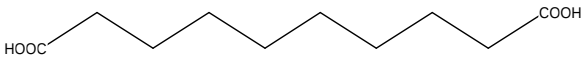
Reference: M.Gardon, A.Schonleber, G.Chapuis, M.Hostettler, M.Bonin (2001) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**57,**936

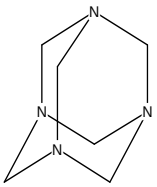
Formula: $C_6H_{12}N_4,C_{10}H_{18}O_4$

Compound Name: Decanedioic acid 1,3,5,7-tetra-azatricyclo(3.3.1.1^{3,7})decane

Space Group:	P21/c	***Cell:***	***a***	5.903(1)	***b***	27.549(6)	***c***	23.371(5)
Space Group No.:	14	***(Å,°)***	α	90.00	β	101.22(3)	γ	90.00

R-Factor (%): 5.70 ***Temperature(K):*** 215 ***Density(g/cm³):*** 1.220





YOLQIZ

Reference: A.Usman, S.Chantrapromma, Hoong-Kun Fun, Bo-Long Poh, C.Karalai (2002) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**58,**o46

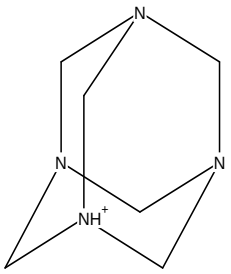
Formula: $C_6H_{13}N_4^{1+},C_6H_2N_3O_7^{1-}$

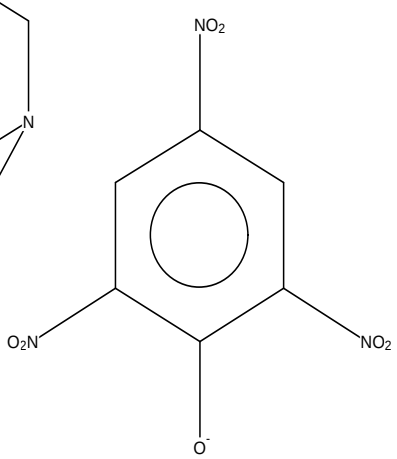
Compound Name: 3,5,7-Triaza-1-azoniatricyclo(3.3.1.1^{3,7})decane 2,4,6-trinitrophenolate

Synonym: Hexamethylenetetraminium picrate

Space Group:	P21/c	***Cell:***	***a***	12.500(0)	***b***	6.634(0)	***c***	18.620(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β	107.02(0)	γ	90.00

R-Factor (%): 5.80 ***Temperature(K):*** 183 ***Density(g/cm³):*** 1.661





YOLQOF

Reference: A.Usman, S.Chantrapromma, Hoong-Kun Fun, Bo-Long Poh, C.Karalai (2002) *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.* ,**58,**o48

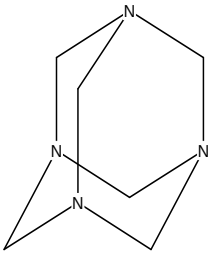
Formula: $C_6H_{12}N_4,C_8H_8O_3$

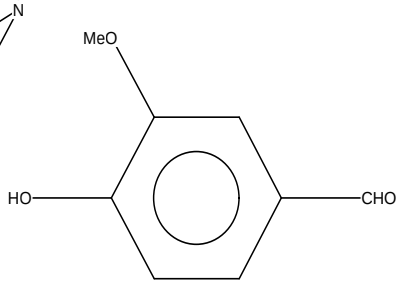
Compound Name: 1,3,5,7-Tetraazatricyclo(3.3.1.1^{3,7})decane 4-hydroxy-3-methoxybenzaldehyde

Synonym: Hexamethylenetetramine 4-hydroxy-3-methoxybenzaldehyde

Space Group:	Pca21	***Cell:***	***a***	27.121(0)	***b***	7.133(0)	***c***	7.478(0)
Space Group No.:	29	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.86 ***Temperature(K):*** 183 ***Density(g/cm³):*** 1.342





Search: search1 (Thu Dec 02 16:20:24 2010): Hit 49

YUYNUB

Reference: K.-F.Tebbe, K.Nagel (1995)
Acta Crystallogr.,Sect.C:Cryst.Struct.Commun. ,**51,**1388

Formula: $C_6 H_{12} N_4,3(I_2)$

Compound Name: 1,3,5,7-Tetra-azatricyclo(3.3.1.1^{3,7})decane tris(di-iodide)

Synonym: Urotropin-3-di-iode

Space Group:	R3cr	***Cell:***	***a*** 9.841(2)	***b*** 9.841(2)	***c*** 9.841(2)
Space Group No.:	161	***(Å,°)***	α 81.33(2)	β 81.33(2)	γ 81.33(2)

R-Factor (%): 2.62 ***Temperature(K):*** 295 ***Density(g/cm^3):*** 3.243