

Polymorphism in cocrystals: a review and assessment of its significance

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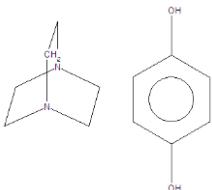
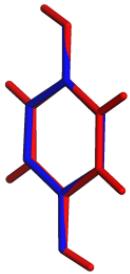
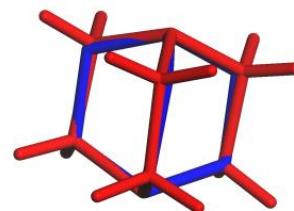
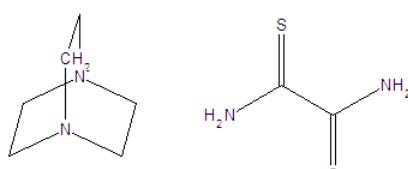
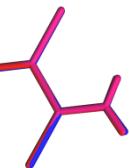
Email: reginald_tan@ices.a-star.edu.sg

Electronic Supplementary Information

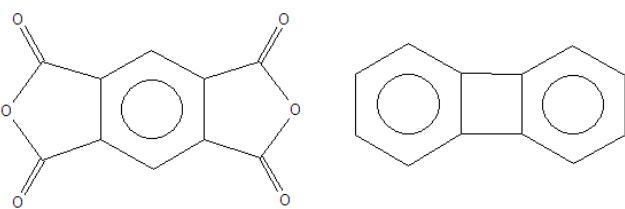
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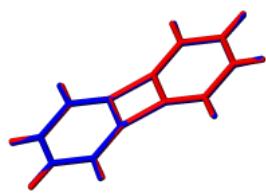
No.	Polymorphic cocrystal		
1	 <p>Benzene-1,4-diol 1,4-diazabicyclo[2.2.2]octane (COHWIF, COHWIF02)</p> <p>Reference: (a) T.C.W.Mak, W.-H.Yip, L.Book, <i>J.Crystallogr.Spectrosc.Res.</i> (1984), 14, 457; (b) Heng-Yun Ye, Jia-Zhen Ge, Fang Chen, Ren-Gen Xiong, <i>CrystEngComm</i> (2010), 12, 1705.</p>		
	 <p>Benzene-1,4-diol conformers</p>	 <p>1,4-diazabicyclo[2.2.2]octane conformers</p>	
2	 <p>1,4-Diazabicyclo(2.2.2)octane dithio-oxamide (DOKGUG, DOKGUG01)</p> <p>Reference: B.Piotrkowska, A.Wasilewska, M.Gdaniec, T.Polonski, <i>CrystEngComm</i> (2008), 10, 1421.</p>	 <p>1,4-Diazabicyclo(2.2.2)octane conformers</p>	 <p>Dithio-oxamide conformers</p>

3

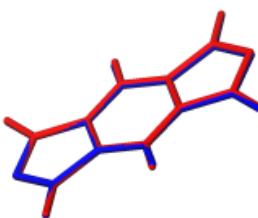


Biphenylene pyromellitic-dianhydride (DURZAR, DURZAR01)

Reference: J.J.Stezowski, R.-D.Stigler, N.Karl, *J.Chem.Phys.* (1986), 84, 5162.

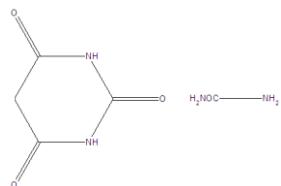


Biphenylene conformers



Pyromellitic-dianhydride conformers

4



2,4,6(1H,3H,5H)-Pyrimidinetrione urea (EFOZAB, EFOZAB01)

Reference: M.Gryl, A.Krawczuk, K.Stadnicka, *Acta Crystallogr., Sect.B:Struct.Sci.* (2008), 64, 623

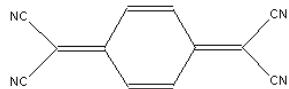
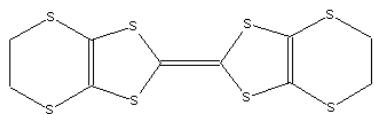


2,4,6(1H,3H,5H)-Pyrimidinetrione conformers



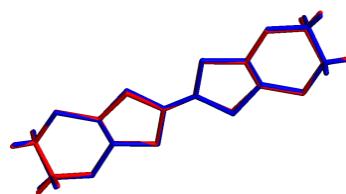
Urea conformers

5

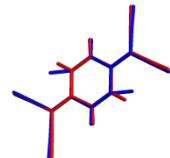


bis(Ethylenedithio)tetrathiafulvalene tetracyanoquinodimethane (FAHLEF01, FAHLEF02)

Reference: (a) T. Mori, H. Inokuchi, *Bull. Chem. Soc. Jpn.* (1987), 60, 402; (b) H. M. Yamamoto, M. Hagiwara, R. Kato, *Synth. Met.* (2003), 133, 449

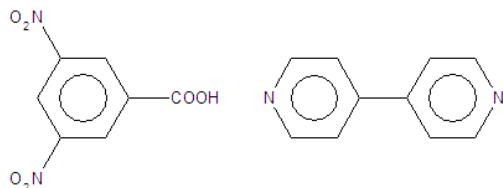


bis(Ethylenedithio)tetrathiafulvalene conformers



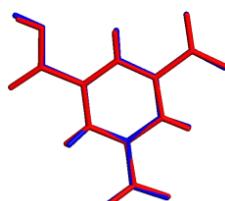
tetracyanoquinodimethane conformers

6

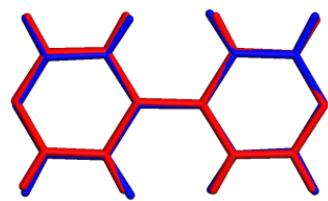


3,5-Dinitrobenzoic acid hemikis(4,4-bipyridine) (FIHYEA, FIHYEA02)

Reference: (a) V.R.Pedireddi, A.Ranganathan, S.Chatterjee, *Tetrahedron Lett.* (1998), 39, 9831; (b) Ting-Feng Tan, Jie Han, Mei-Li Pang, Hai-Bin Song, Yu-Xin Ma, Ji-Ben Meng, *Cryst.Growth Des.* (2006), 6, 1186.



3,5-Dinitrobenzoic acid hemikis conformers



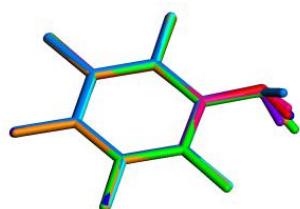
4,4'-bipyridine conformers

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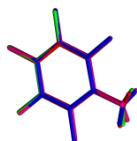


bis(2,3,4,5,6-Pentafluorophenol) 2,3,4,5,6-pentafluoroaniline (KIBQOC, KIBQOC01)

Reference: (a) M.T.Kirchner, D.Blaser, R.Boese, G.R.Desiraju, *CrystEngComm* (2009), 11, 229; (b) M.Gdaniec, *CrystEngComm* (2007), 9, 286

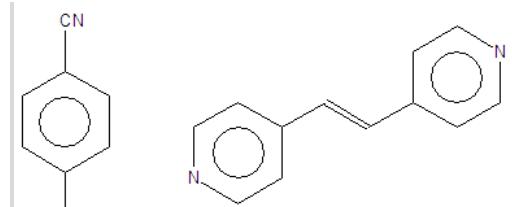


bis(2,3,4,5,6-Pentafluorophenol) conformers



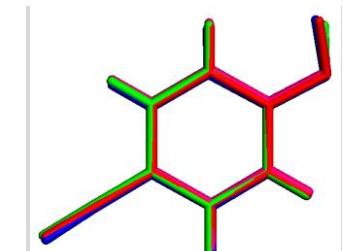
2,3,4,5,6-pentafluoroaniline conformers

8

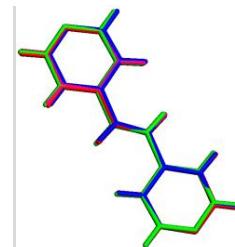


4-Cyanophenol trans-1,2-bis(4-pyridyl)ethylene (KIHYOQ, KIHYOQ01)

Reference: J.A.Bis, P.Vishweshwar, D.Weyna, M.J.Zaworotko, *Mol.Pharmaceutics* (2007), 4, 401.

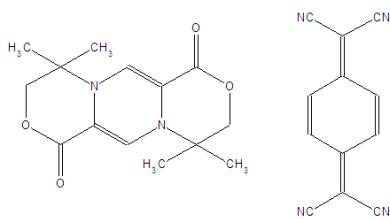


4-Cyanophenol conformers



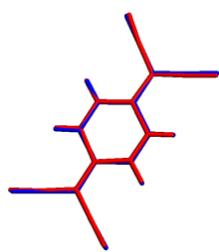
trans-1,2-bis(4-pyridyl)ethylene conformers

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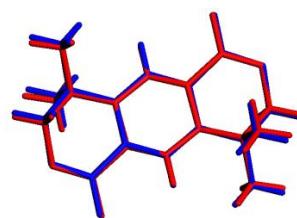


(4a,8a-Diaza-2,6-dioxa-3,4,7,8-tetrahydro-4,4,8,8-tetramethylanthracene-1,5-dione)
bis(tetracyanoquinodimethane) (TAMBUE, TAMBUE01)

Reference: (a) D.J.R.Brook, R.C.Haltiwanger, T.H.Koch, *J.Am.Chem.Soc.* (1991), 113, 5910; (b) D.J.R.Brook, T.H.Koch, *J.Mater.Chem.* (1997), 7, 2381.

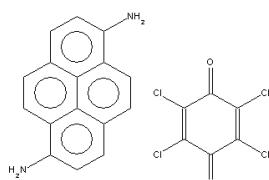


4a,8a-Diaza-2,6-dioxa-3,4,7,8-tetrahydro-4,4,8,8-tetramethylanthracene-1,5-dione conformers



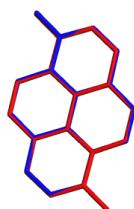
tetracyanoquinodimethane conformers

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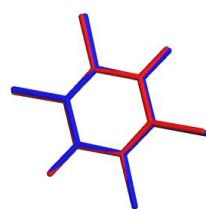


1,6-Diaminopyrene p-chloranil (TECCAF01, TECCAR02)

Reference: H.Goto, T.Fujinawa, H.Asahi, T.Inabe, H.Ogata, S.Miyajima, Y.Muruyama, *Bull.Chem.Soc.Jpn.* (1996), 69, 85.

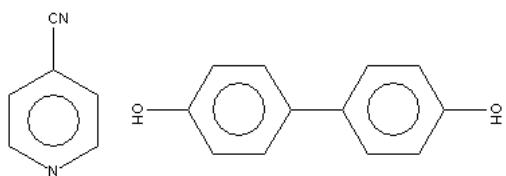


1,6-Diaminopyrene conformers



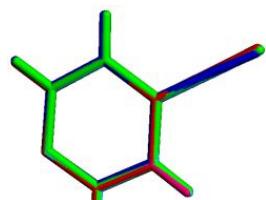
p-chloranil conformers

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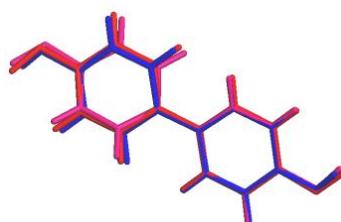


bis(4-Cyanopyridine) 4,4'-biphenol (TEHNAW, TEHNAW01)

Reference: J.A.Bis, P.Vishweshwar, R.A.Middleton, M.J.Zaworotko, *Cryst.Growth Des.* (2006), 6, 1048

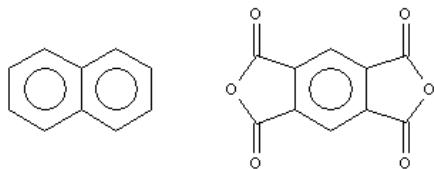


4-Cyanopyridine conformers



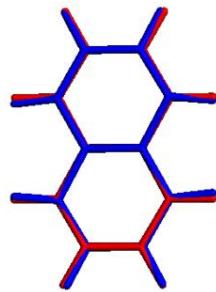
4,4'-biphenol conformers

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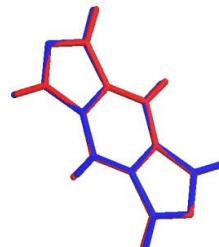


Naphthalene-pyromellitic dianhydride complex (NAPYMA, NAPYMA01)

Reference: M.Le Bars-Combe, B.Chion, J.Lajzerowicz-Bonneteau, *Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem.* (1979), 35, 913

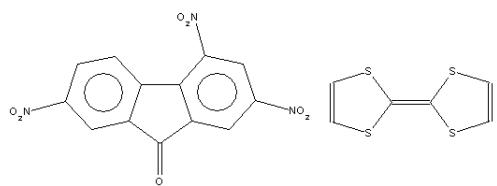


Naphthalene conformers



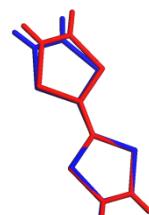
pyromellitic dianhydride conformers

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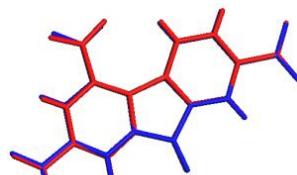


tris(Tetrathiafulvalene) bis(2,4,7-trinitro-9-fluorenone) (NARSOP, NARSOP01, NARSOP02)

Reference: A.Salmeron-Valverde, S.Bernes, *Comptes Rendus Chimie* (2005), 8, 1017

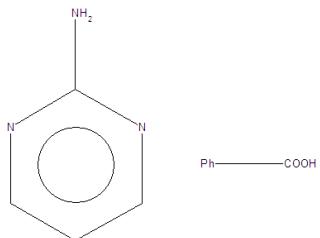


tris(Tetrathiafulvalene) conformers



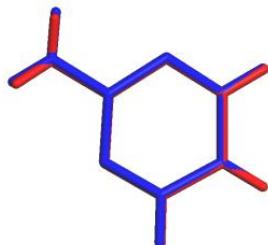
bis(2,4,7-trinitro-9-fluorenone) conformers

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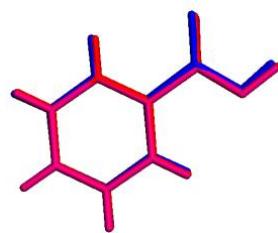


2-Aminopyrimidine bis(benzoic acid) (NUKWEW, NUKWEW01)

Reference: S.Skovsgaard, A.D.Bond, *CrystEngComm* (2009), 11, 444

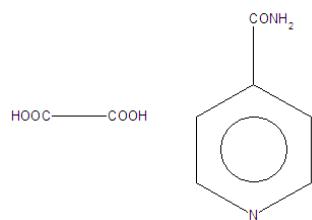


2-Aminopyrimidine conformers



benzoic acid conformers

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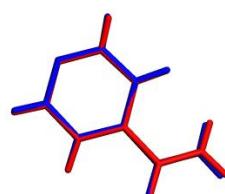


trans-oxalic acid bis(isonicotinamide) (ULAWAF, ULAWAF01, ULAWAF02)

Reference: M.Schmidtmann, M.J.Gutmann, D.S.Middlemiss, C.C.Wilson, *CrystEngComm* (2007), 9, 743.

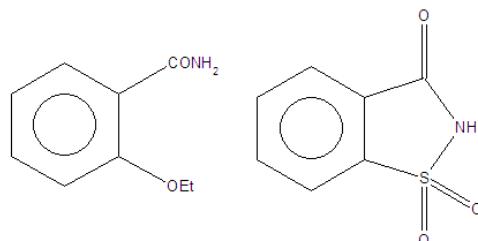


trans-oxalic acid conformers



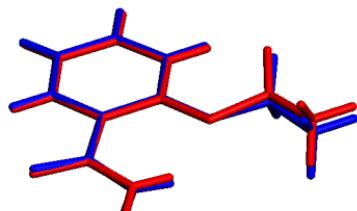
isonicotinamide conformers

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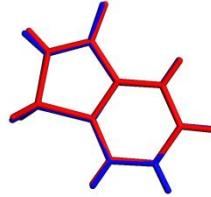


2-Ethoxybenzamide 1,2-benzothiazol-3(2H)-one 1,1-dioxide (VUHFIO, VUHFIO01)

Reference: S.Aitipamula, Pui Shan Chow, R.B.H.Tan, *CrystEngComm* (2009), 11, 889

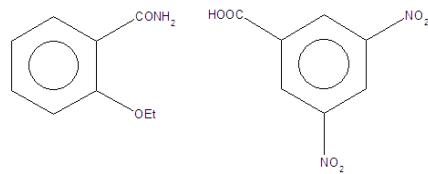


2-Ethoxybenzamide conformers

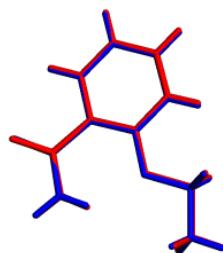


1,2-benzothiazol-3(2H)-one 1,1-dioxide conformers

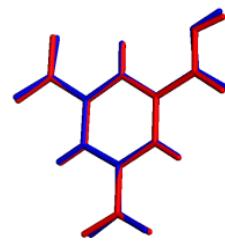
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ethenzamide 3,5-dinitrobenzoic acid (WUZHOP, WUZHOP01)

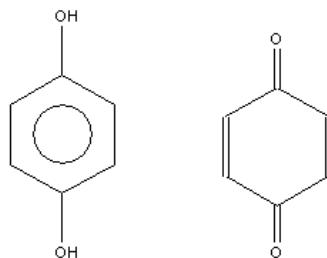
Reference: S.Aitipamula, Pui Shan Chow, R.B.H.Tan, *Cryst.Growth Des.* (2010), 10, 2229

ethenzamide conformers

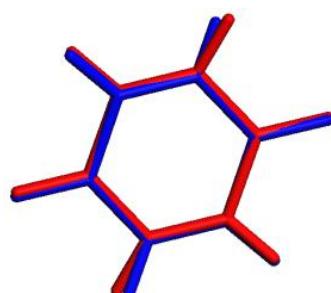


3,5-dinitrobenzoic acid conformers

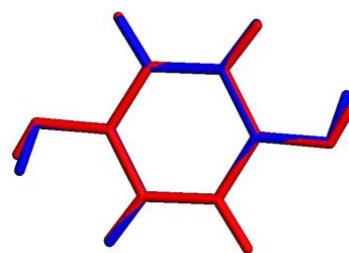
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Quinhydrone (QUIDON, QUIDON01, QUIDON02)

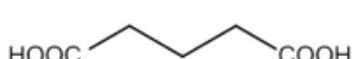
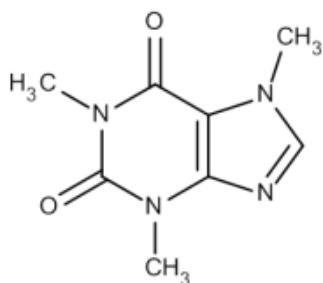
Reference: (a) T.Sakurai, *Acta Crystallogr.* (1965), 19, 320; (b) T.Sakurai, *Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem.* (1968), 24, 403

1,2-Benzoquinone conformers



Hydroquinone conformers

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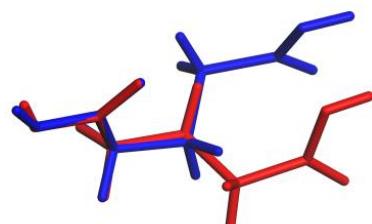


Caffeine-glutaric acid (1:1) (EXUQUJ, EXUQUJ01)

Reference: A.V.Trask, W.D.S.Motherwell, W.Jones, *Chem.Commun.* (2004), 890.

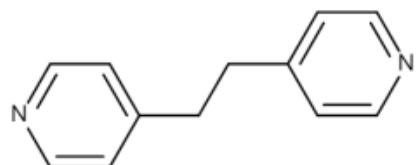
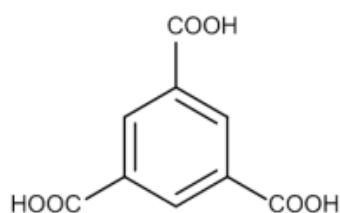


Caffeine conformers



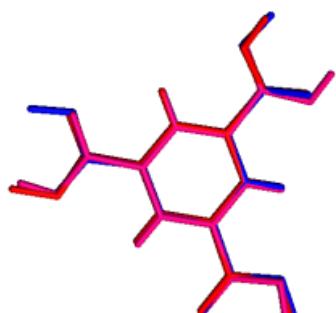
glutaric acid conformers

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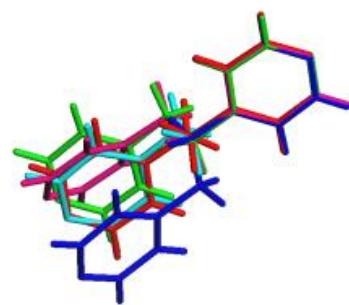


Trimesic acid (TA)-1,2-bis(4-pyridyl)ethane (BPE) (SAYMUB, SAYMUB01)

Reference: T.R.Shattock, P.Vishweshwar, Zhenqiang Wang, M.J.Zaworotko, *Cryst.Growth Des.* (2005), 5, 2046.

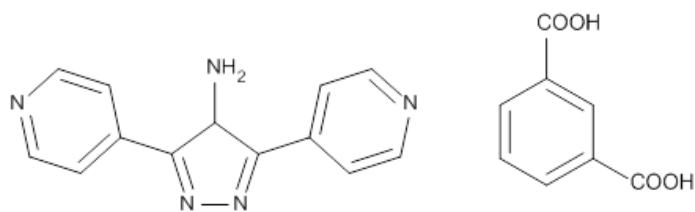


TA conformers



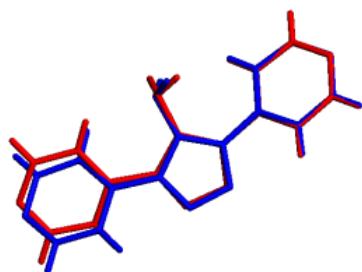
1,2-bis(4-pyridyl)ethane conformers

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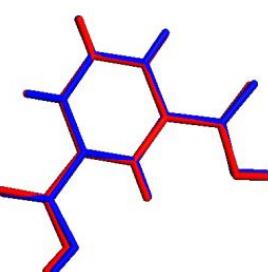


4-amino-3,5-bis(pyridin-4-yl)-1,2,4-triazole (APT)-Isophthalic acid (IA) (NUGZEV, NUGZEV01)

Reference: Miao Du, Xiu-Juan Jiang, Xue Tan, Zhi-Hui Zhang, Hua Cai, *CrystEngComm* (2009), 11, 454.

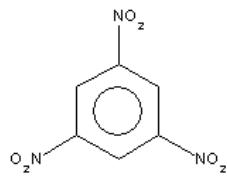
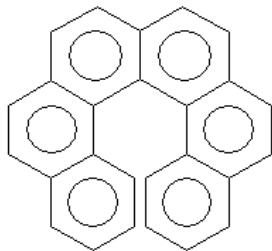


APT conformers



Isophthalic acid conformers

22

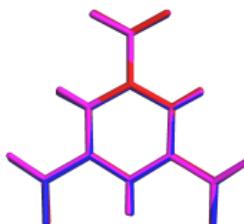


(+)-Phenanthro(3,4-c)phenanthrene 1,3,5-trinitrobenzene (ABUNIU, ABUNIU01)

Reference: O.Ermer, J.Neudorfl, *Helv.Chim.Acta* (2001), 84, 1268.

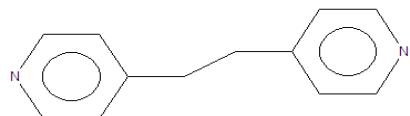
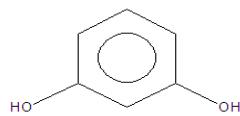


(+)-Phenanthro(3,4-c)phenanthrene



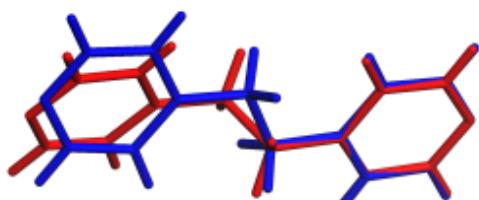
1,3,5-trinitrobenzene conformers

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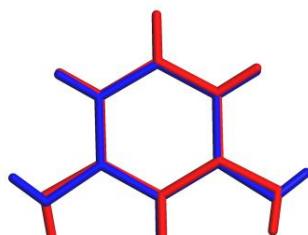


trans-1,2-bis(4-pyridyl)ethylene resorcinol (ABEKUN, ABEKUN01)

Reference: (a) L.R.MacGillivray, J.L.Reid, J.A.Ripmeester, *J.Am.Chem.Soc.* (2000), 122, 7817; (b) T.Frisic, L.R.MacGillivray, *Chem.Commun.* (2009), 773

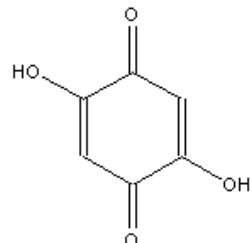
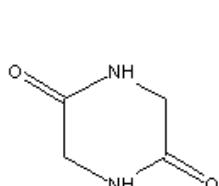


trans-1,2-bis(4-pyridyl)ethylene conformers



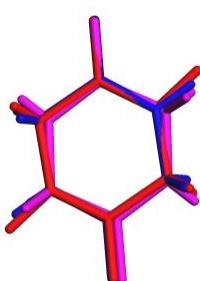
resorcinol conformers

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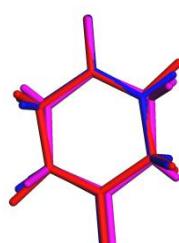


Piperazine-2,5-dione 2,5-dihydroxy-p-benzoquinone (AJAJEA, AJAJEA01)

Reference: Tzy-Jiun M.Luo, G.T.R.Palmore, *Cryst.Growth Des.* (2002), 2, 337.

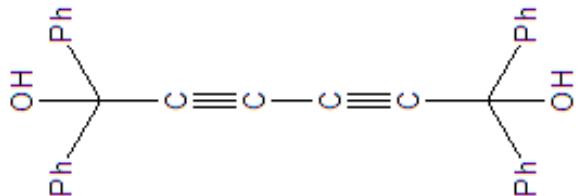
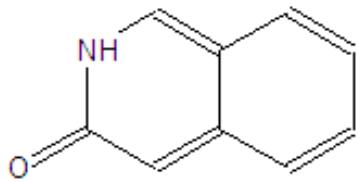


Piperazine-2,5-dione conformers



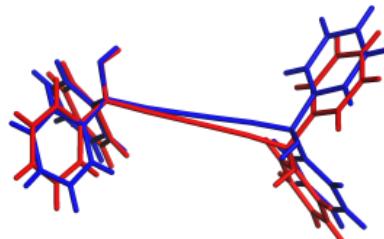
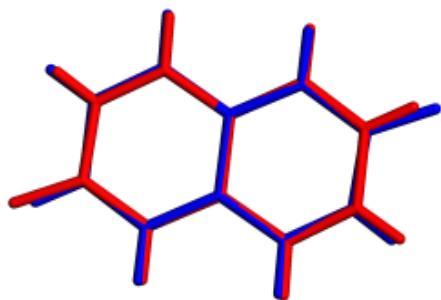
Piperazine-2,5-dione conformers

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1,1,6,6-Tetraphenyl-2,4-hexadiyne-1,6-diol bis(isoquinolin-3(2H)-one) (ANUMEC, ANUMEC01)

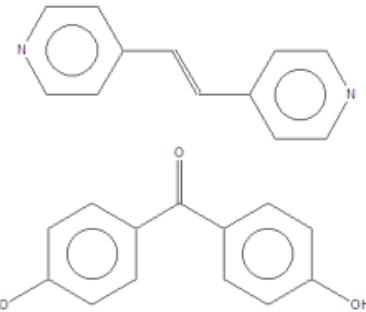
Reference: Deng-Ke Cao, T.V.Sreevidya, M.Botoshansky, G.Golden, J.B.Benedict, M.Kaftory, *CrystEngComm* (2011), 13, 3181.



1,1,6,6-Tetraphenyl-2,4-hexadiyne conformers

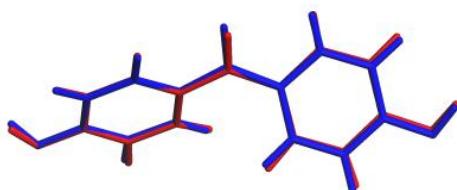
1,6-diol bis(isoquinolin-3(2H)-one) conformers

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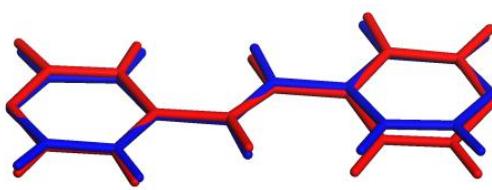


4,4'-Dihydroxybenzophenone 1,2-bis(4-pyridyl)ethylene (BIVSIJ, BIVSIJ01)

Reference: Jing Wang, Liyu Ding, Caiqin Yan, *CrystEngComm* (2007), 9, 591.

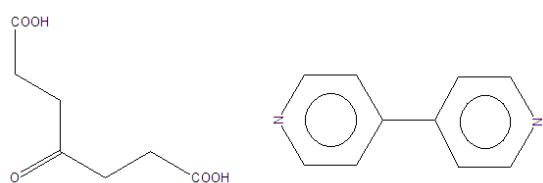


4,4'-Dihydroxybenzophenone conformers



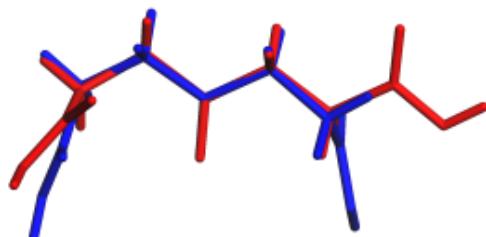
1,2-bis(4-pyridyl)ethylene conformers

27

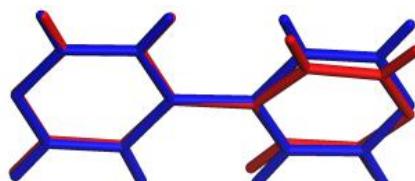


4-Oxo-heptane-1,7-dioic acid 4,4'-bipyridine (ELEGUY, ELEGUY01)

Reference: I.Halasz, M.Rubcic, K.Uzarevic, I.Dilovic, E.Mestrovic, *New J.Chem.* (2011), 35, 24

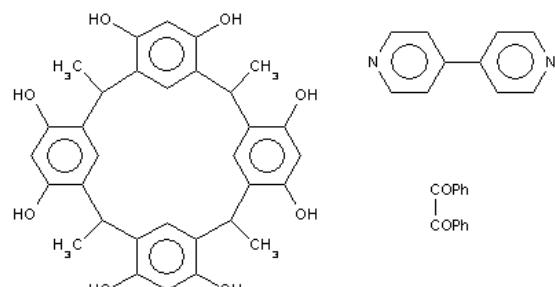


4-Oxo-heptane-1,7-dioic acid conformers



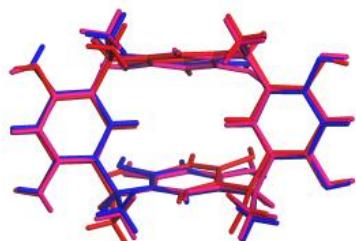
4,4'-bipyridine conformers

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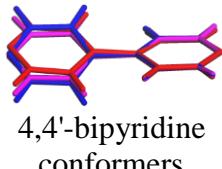


2,8,14,20-Tetramethyl-4,6,10,12,16,18,22,24-octahydroxycalix(4)arene 4,4'-bipyridine benzil clathrate (ENAZOI, ENAZOI01)

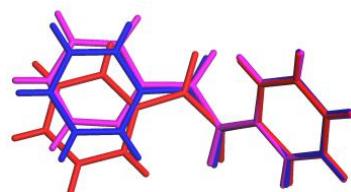
Reference: Bao-Qing Ma, Yuegang Zhang, P.Coppens, *J.Org.Chem.* (2003), 68, 9467.



2,8,14,20-Tetramethyl-4,6,10,12,16,18,22,24-octahydroxycalix(4)arene conformers

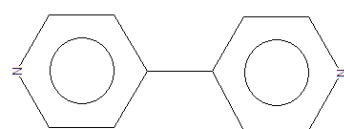
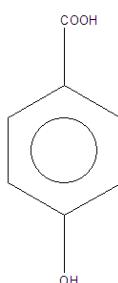


4,4'-bipyridine conformers



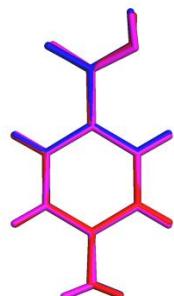
benzil clathrate conformers

29

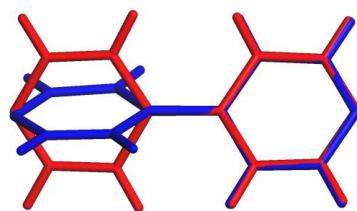


bis(4-Hydroxybenzoic acid) 4,4'-bipyridine (EPUPUB, EPUPUB01)

Reference: A.Mukherjee, G.R.Desiraju, *Chem.Commun.* (2011), 47, 4090.

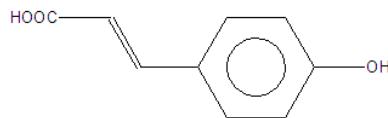
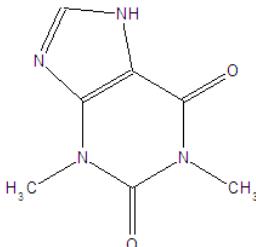


4-Hydroxybenzoic acid conformers



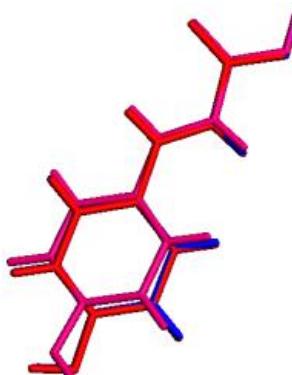
4,4'-bipyridine conformers

30

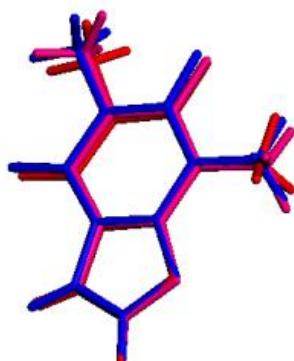


3-(4-Hydroxyphenyl)acrylic acid 1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione (IJIBEJ, IJIBEJ01)

Reference: N.Schultheiss, M.Roe, S.X.M.Boerrigter, *CrystEngComm* (2011), 13, 611.

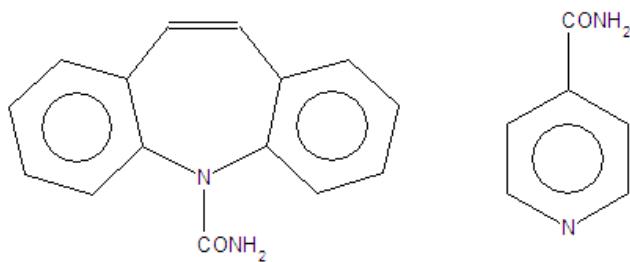


3-(4-Hydroxyphenyl)acrylic acid conformers



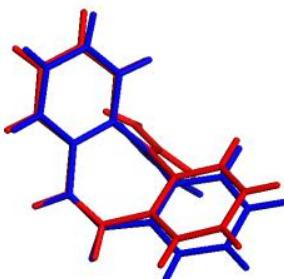
1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione conformers

31

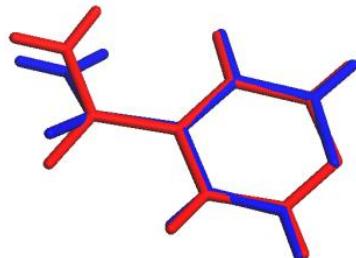


5H-Dibenzo[b,f]azepine-5-carboxamide isonicotinamide (LOFKIB, LOFKIB01)

Reference: (a) J.H.ter Horst, P.W.Cains, *Cryst.Growth Des.* (2008), 8, 2537; (b) M.Habgood, M.A.Deij, J.Mazurek, S.L.Price, J.H.ter Horst, *Cryst.Growth Des.* (2010), 10, 903.

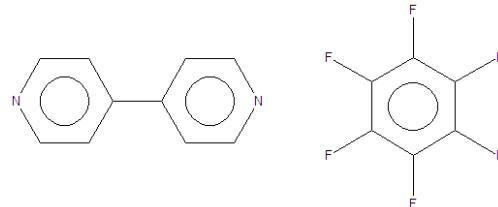


5H-Dibenzo[b,f]azepine-5-carboxamide conformers



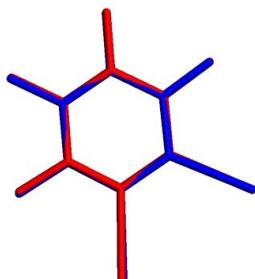
Isonicotinamide conformers

32

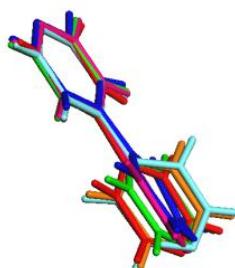


Tetrafluoro-1,2-diiodobenzene 4,4'-bipyridine (MIYKOU, MIYKOU01)

Reference: (a) R.Liantonio, P.Metrangolo, T.Pilati, G.Resnati, *Acta Crystallogr., Sect.E: Struct. Rep.Online* (2002), 58, o575; (b) M.B.Hursthouse, T.Gelbrich, M.J.Plater, *Private Communication* (2003).

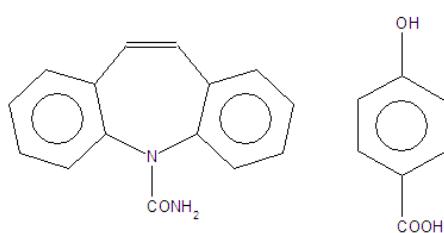


Tetrafluoro-1,2-diiodobenzene conformers



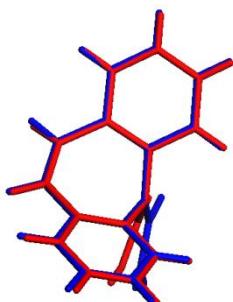
4,4'-bipyridine conformers

33

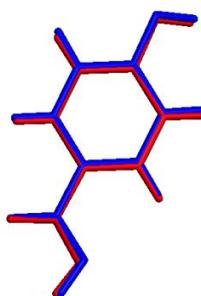


Carbamazepine 4-hydroxybenzoic acid (MOXVIF, MOXVIF01)

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

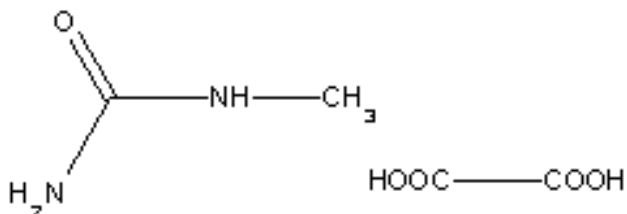


Carbamazepine conformers



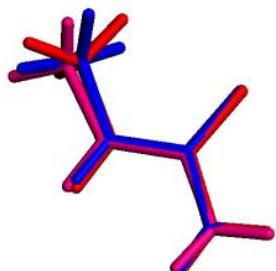
4-hydroxybenzoic acid conformers

34

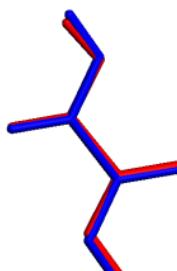


bis(N-Methyl-urea) oxalic acid (MUROXA, MUROXA01)

Reference: S.Harkema, J.H.M.ter Brake, H.J.G.Meutstege, *Acta Crystalogr., Sect.B: Struct.Crystallogr.Cryst.Chem.* (1979), 35, 2087

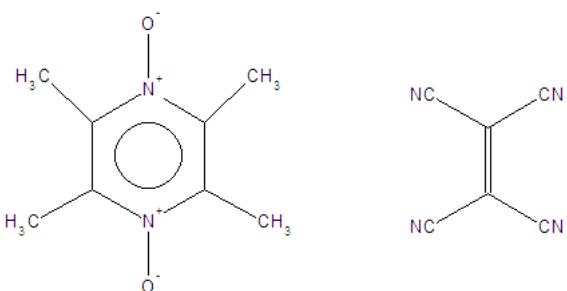


bis(N-Methyl-urea) conformers

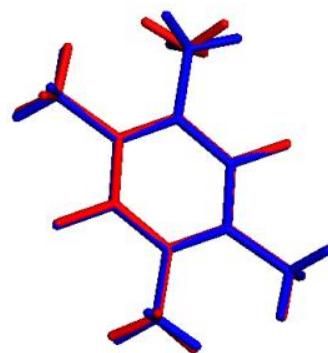
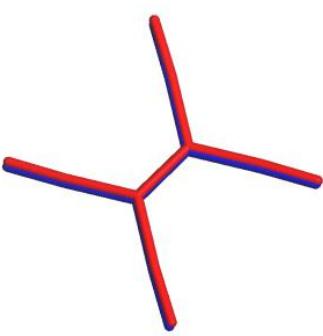


oxalic acid conformers

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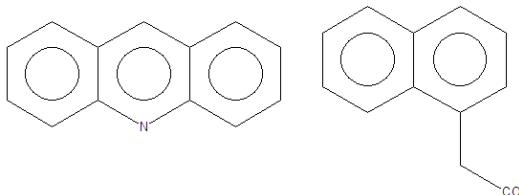


bis(2,3,5,6-Tetramethylpyrazine-N,N'-dioxide) tetracyanoethylene (NITRIR, NITRIR01)

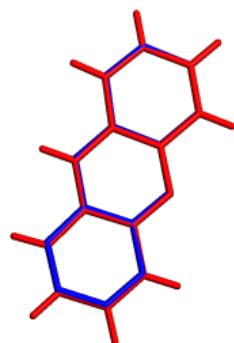
Reference: M.L.Greer, B.J.McGee, R.D.Rogers, S.C.Blackstock, *Angew.Chem.,Int.Ed.* (1997), 36, 1864.bis(2,3,5,6-Tetramethylpyrazine-N,N'-dioxide)
conformers

tetracyanoethylene conformers

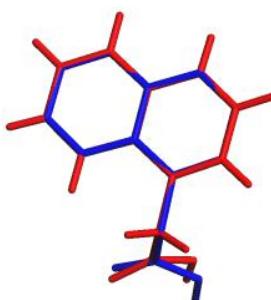
36



Acridine 1-(naphthyl)deuteroacetic acid (NOVSIA, NOVSIA01)

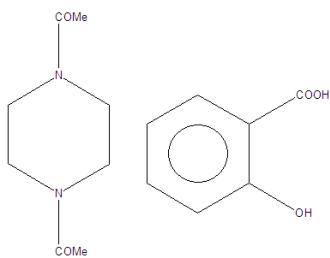
Reference: H.Koshima, K.Ding, Y.Chisaka, T.Matsuura, I.Miyahara, K.Hirotsu, *J.Am.Chem.Soc.* (1997), 119, 10317.

Acridine conformers



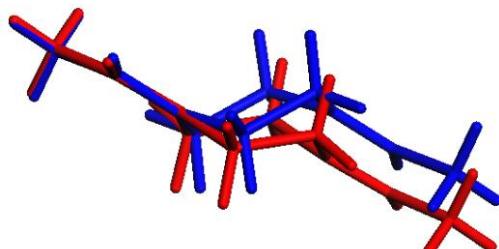
1-(naphthyl)deuteroacetic acid conformers

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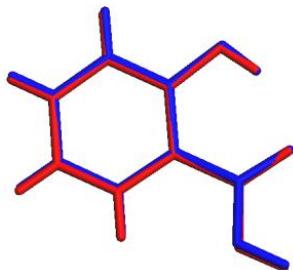


N,N'-Diacetyl piperazine bis(2-hydroxybenzoic acid) (NUKXEX, NUKXEX01)

Reference: S.Skovsgaard, A.D.Bond, *CrystEngComm* (2009), 11, 444.

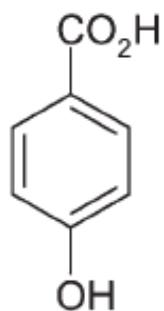


N,N'-Diacetyl piperazine conformers



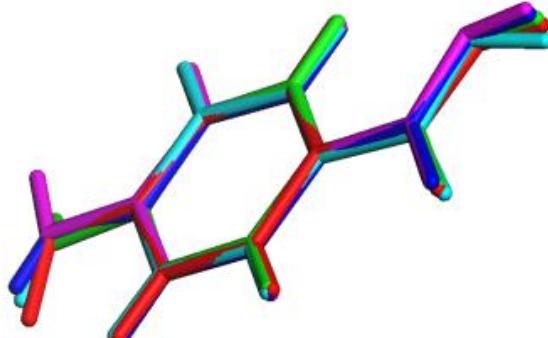
2-hydroxybenzoic acid conformers

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bis(4-Hydroxybenzoic acid) 2,3,5,6-tetramethylpyrazine (ODOBIT, ODOBIT01)

Reference: B.R.Sreekanth, P.Vishweshwar, K.Vyas, *Chem.Commun.* (2007), 2375.

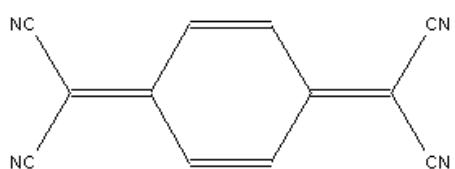
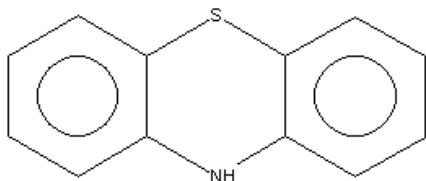


4-Hydroxybenzoic acid conformers

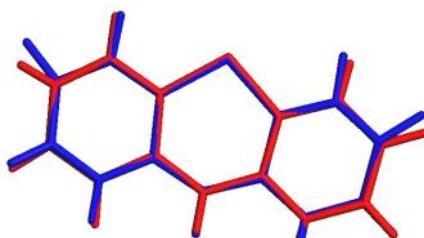


2,3,5,6-tetramethylpyrazine conformers

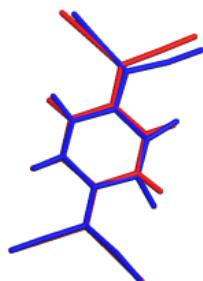
39



Reference: (a) H.Kobayashi, *Acta Crystallogr., Sect.B:Struct.Crystallogr.Cryst.Chem.* (1974), 30, 1010;
 (b) L.Toupet, N.Karl, *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.* (1995), 51, 249.

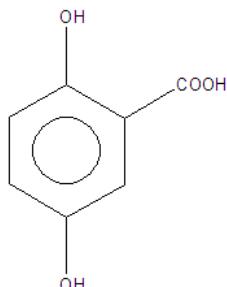
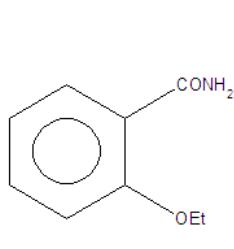


Phenothiazine conformers



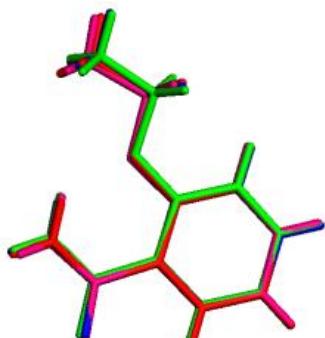
7,7,8,8-tetracyanoquinodimethane conformers

40

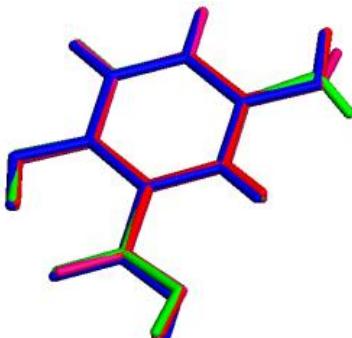


Ethenzamide-gentisic acid (QULLUF, QULLUF01, QULLUF02)

Reference: S.Aitipamula, Pui Shan Chow, R.B.H.Tan, *CrystEngComm* (2009), 11, 1823.

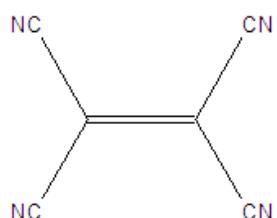
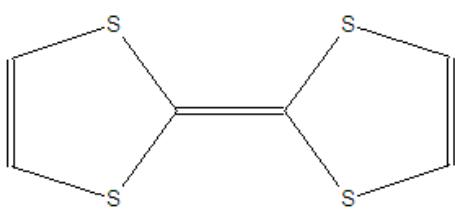


Ethenzamide conformers



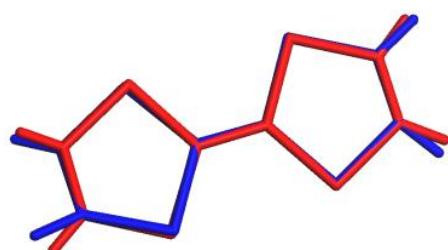
gentisic acid conformers

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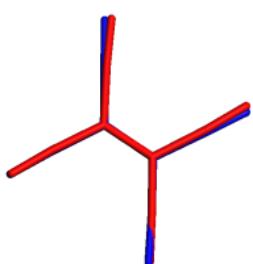


Tetrathiafulvalene tetracyanoethylene (RIFQAY, RIFQAY01)

Reference: D.A.Clemente, A.Marzotto, *J.Mater.Chem.* (1996), 6, 941.

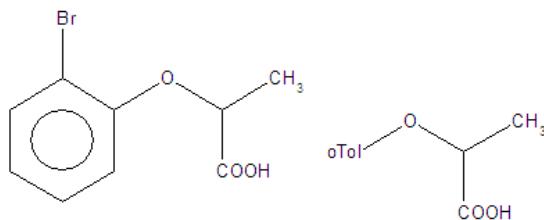


Tetrathiafulvalene conformers



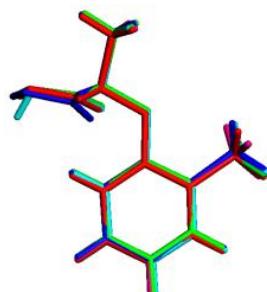
tetracyanoethylene conformers

42

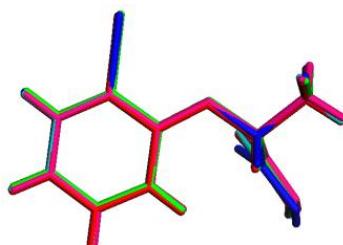


(R)-2-(2-Bromophenoxy)propionic acid (S)-2-(2-methylphenoxy)propionic acid (RIWWEA, RIWWEA01)

Reference: A.M.Lineberry, E.T.Benjamin, R.E.Davis, W.S.Kassel, K.A.Wheeler, *Cryst.Growth Des.* (2008), 8, 612.

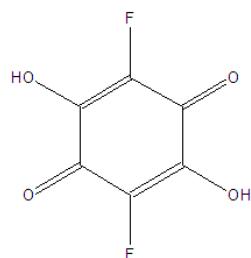
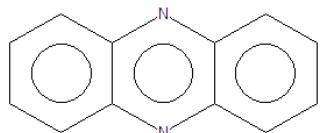


(R)-2-(2-Bromophenoxy)propionic acid conformers



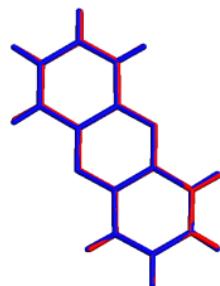
(S)-2-(2-methylphenoxy)propionic acid conformers

43

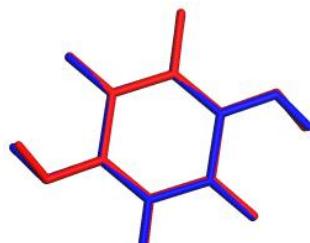


2,5-Difluoro-3,6-dihydroxy-1,4-benzoquinone phenazine (RURROM, RURROM01)

Reference: S.Horiuchi, R.Kumai, Y.Tokura, *J.Mater.Chem.* (2009), 19, 4421.

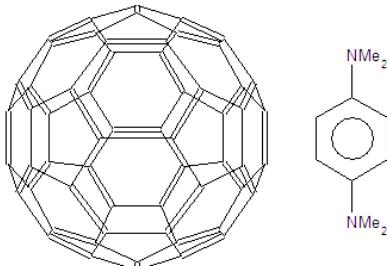


phenazine conformers



2,5-Difluoro-3,6-dihydroxy-1,4-benzoquinone conformers

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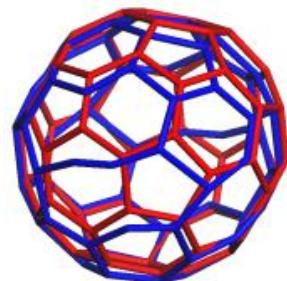


N,N,N',N'-Tetramethyl-p-phenylenediamine-C60fullerene (TONDUV, TONDUV02)

Reference: (a) V.A.Nadtochenko, V.V.Gritsenko, O.A.Dyachenko, G.V.Shilov, A.P.Moravsky, *Izv.Akad.Nauk SSSR,Ser.Khim.(Russ.)(Russ.Chem.Bull.)* (1996), 1285; (b) D.V.Konarev, A.Yu.Kovalevsky, A.L.Litvinov, N.V.Drichko, B.P.Tarasov, P.Coppens, R.N.Lyubovskaya, *J.Solid State Chem.* (2002), 168, 474.

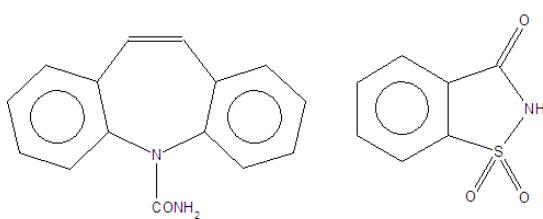


N,N,N',N'-Tetramethyl-p-phenylenediamine conformers



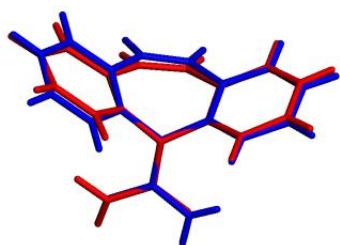
C60fullerene conformers

45

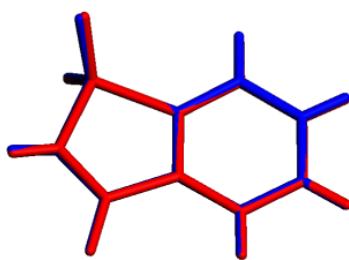


5H-Dibenz(b,f)azepine-5-carboxamide (UNEZAO, UNEZAO01)

Reference: (a) S.G.Fleischman, S.S.Kuduva, J.A.McMahon, B.Moulton, R.D.B.Walsh, N.Rodriguez-Hornedo, M.J.Zaworotko, *Cryst.Growth Des.* (2003), 3, 909; (b) W.W.Porter III, S.C.Elie, A.J.Matzger, *Cryst.Growth Des.* (2008), 8, 14.

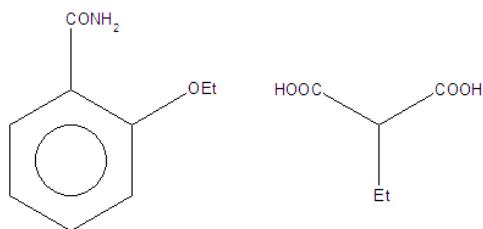


5H-Dibenz(b,f)azepine-5-carboxamide conformers



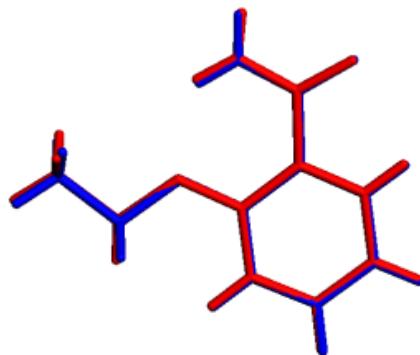
saccharin conformers

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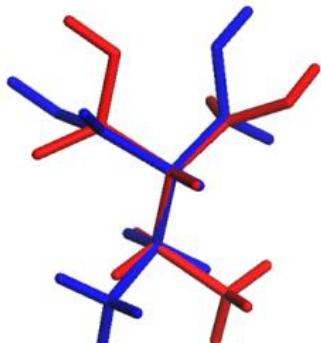


2-Ethoxybenzamide ethylmalonic acid (VAKTOS, VAKTOS01)

Reference: S.Aitipamula, Pui Shan Chow, R.B.H.Tan, *CrystEngComm* (2010), 12, 3691.

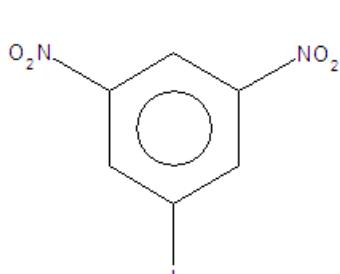
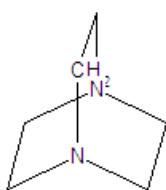


2-Ethoxybenzamide conformers



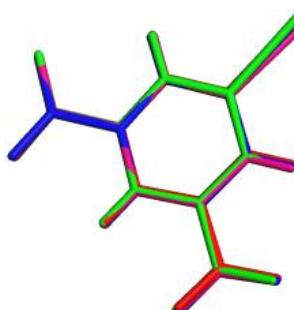
ethylmalonic acid conformers

47

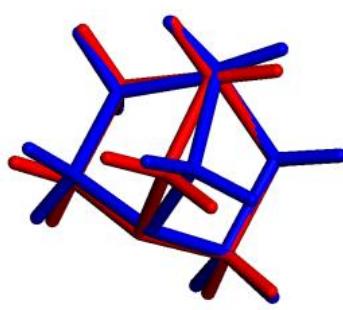


bis(1-Iodo-3,5-dinitrobenzene) 1,4-diazabicyclo[2.2.2]octane (VUJSOJ, VUJSOJ01)

Reference: K.Raatikainen, K.Rissanen, *CrystEngComm* (2009), 11, 750.

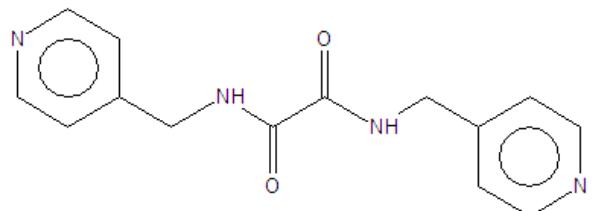


1-Iodo-3,5-dinitrobenzene conformers



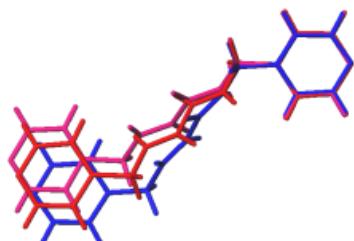
1,4-diazabicyclo[2.2.2]octane conformers

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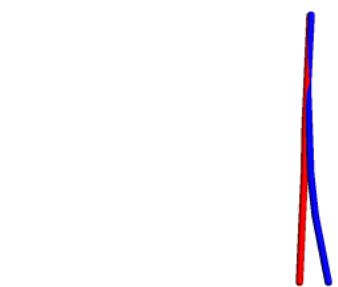


bis(4-Pyridylmethyl)oxalamide 1,4-di-iodobuta-1,3-diyne clathrate (WANNUV, WANNUV01)

Reference: (a) N.S.Goroff, S.M.Curtis, J.A.Webb, F.W.Fowler, J.W.Lauher, *Org.Lett.* (2005), 7, 1891; (b) C.Wilhelm, S.A.Boyd, S.Chawda, F.W.Fowler, N.S.Goroff, G.P.Halada, C.P.Grey, J.W.Lauher, Liang Luo, C.D.Martin, J.B.Parise, C.Tarabrella, J.A.Webb, *J.Am.Chem.Soc.* (2008), 130, 4415.



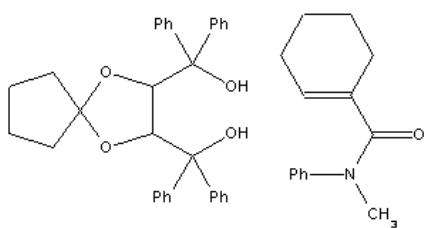
4-Pyridylmethylloxalamide conformers



1,4-di-iodobuta-1,3-diyne clathrate conformers

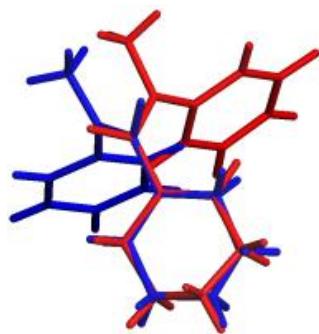
49	<p>2,3,5,6-Tetramethylpyrazine 2,5-dichloro-3,6-bis(deuteroxy)-1,4-benzoquinone (WATREP, WATREP01, WATREP02)</p> <p>Reference: M.Prager, A.Pietraszko, L.Sobczyk, A.Pawlukojc, E.Grech, T.Seydel, A.Wischnewski, M.Zamponi, <i>J.Chem.Phys.</i> (2006), 125, 194525.</p> <table border="1"> <tr> <td data-bbox="169 958 812 967"></td><td data-bbox="812 958 1516 967"></td></tr> <tr> <td data-bbox="169 967 812 975">2,3,5,6-Tetramethylpyrazine conformers</td><td data-bbox="812 967 1516 975">2,5-dichloro-3,6-bis(deuteroxy)-1,4-benzoquinone conformers</td></tr> </table>			2,3,5,6-Tetramethylpyrazine conformers	2,5-dichloro-3,6-bis(deuteroxy)-1,4-benzoquinone conformers
2,3,5,6-Tetramethylpyrazine conformers	2,5-dichloro-3,6-bis(deuteroxy)-1,4-benzoquinone conformers				
50	<p>8-Carbamoyl-3-methylimidazo(5,1-d)-1,2,3,5-tetrazin-4(3H)-one hemikis(4,4'-bipyridine-N,N'-dioxide) (WOBQEK, WOBQEK01)</p> <p>Reference: N.J.Babu, L.S.Reddy, S.Aitipamula, A.Nangia, <i>Chem.Asian J.</i> (2008), 3, 1122.</p> <table border="1"> <tr> <td data-bbox="169 1381 812 1879"></td><td data-bbox="812 1381 1516 1879"></td></tr> <tr> <td data-bbox="169 1879 812 1888">8-Carbamoyl-3-methylimidazo(5,1-d)-1,2,3,5-tetrazin-4(3H)-one hemikis conformers</td><td data-bbox="812 1879 1516 1888">4,4'-bipyridine-N,N'-dioxide conformers</td></tr> </table>			8-Carbamoyl-3-methylimidazo(5,1-d)-1,2,3,5-tetrazin-4(3H)-one hemikis conformers	4,4'-bipyridine-N,N'-dioxide conformers
8-Carbamoyl-3-methylimidazo(5,1-d)-1,2,3,5-tetrazin-4(3H)-one hemikis conformers	4,4'-bipyridine-N,N'-dioxide conformers				

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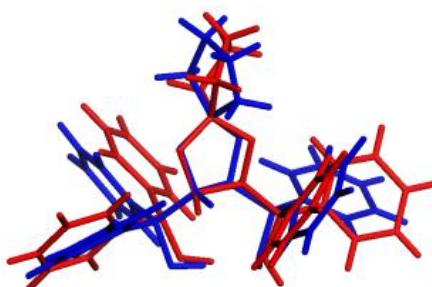


(R,R)-(-)-trans-2,3-bis(Hydroxydiphenylmethyl)-1,4-dioxaspiro(4.4)nonane N-methyl-N-phenylcyclohexene-1-carboxamide clathrate (WOTZAG, WOTZAG01)

Reference: S.Ohba, H.Hosomi, K.Tanaka, H.Miyamoto, F.Toda, *Bull.Chem.Soc.Jpn.* (2000), 73, 2075.

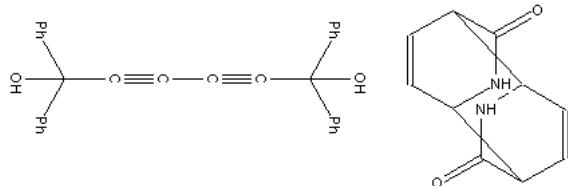


N-methyl-N-phenylcyclohexene-1-carboxamide clathrate conformers



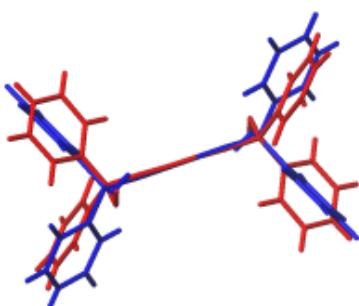
(R,R)-(-)-trans-2,3-bis(Hydroxydiphenylmethyl)-1,4-dioxaspiro(4.4)nonane conformers

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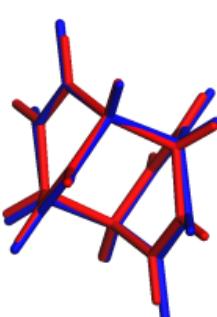


1,1,6,6-Tetraphenyl-2,4-hexadiyne-1,6-diol 3,7-diazatricyclo(4.2.2.22,5)dodeca-9,11-diene-4,8-dione clathrate (XETZIG, XETZIG01)

Reference: T.Lavy, M.Kaftory, *CrystEngComm* (2007), 9, 123.

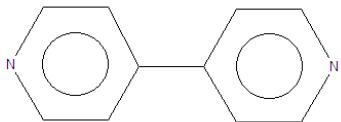
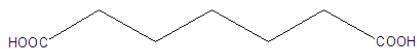


1,1,6,6-Tetraphenyl-2,4-hexadiyne-1,6-diol conformers



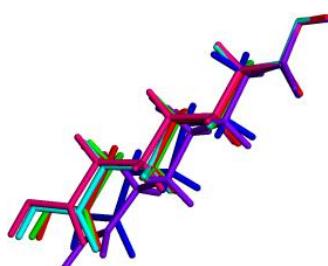
3,7-diazatricyclo(4.2.2.22,5)dodeca-9,11-diene-4,8-dione clathrate conformers

53

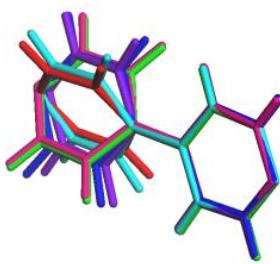


Heptane-1,7-dioic acid 4,4'-bipyridine (XOLHUC, XOLHUC01, XOLHUC02)

Reference: D.Braga, G.Palladino, M.Polito, K.Rubini, F.Grepioni, M.R.Chierotti, R.Gobetto, *Chem.-Eur.J.* (2008), 14, 10149

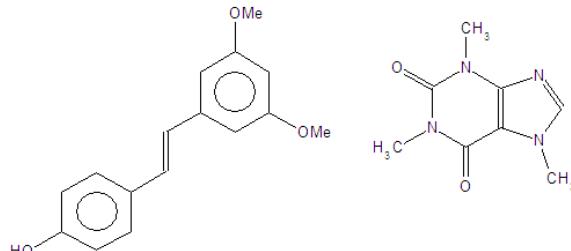


Heptane-1,7-dioic acid conformers



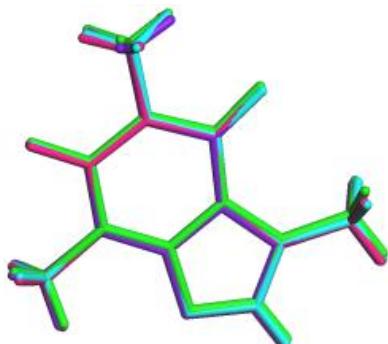
4,4'-bipyridine conformers

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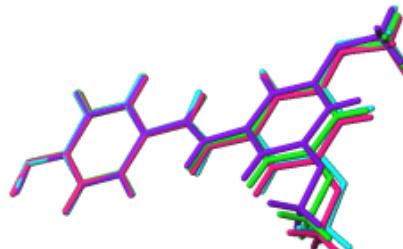


Caffeine-pterostilbene (YABHAM, YABHAM01)

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

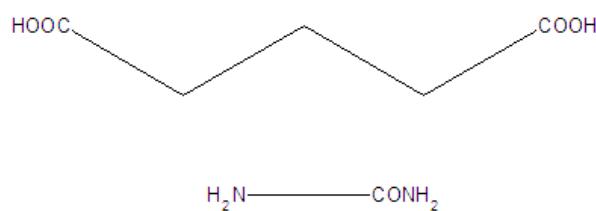


Caffeine conformers



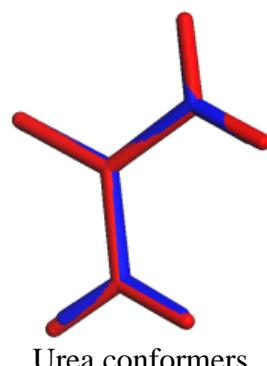
pterostilbene conformers

55

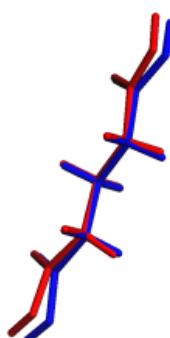


Urea glutaric acid (ZODWIY, ZODWIY01)

Reference: (a) V.Videnova-Adrabinska, *J.Mater.Chem.* (1995), 5, 2309; (b) K.Chadwick, R.Davey, G.Sadiq, W.Cross, R.Pritchard, *CrystEngComm* (2009), 11, 412.

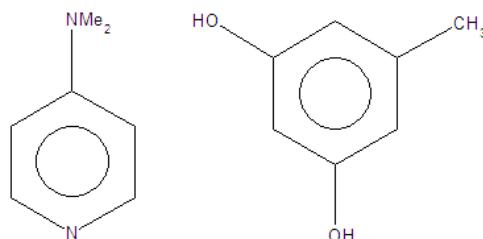


Urea conformers



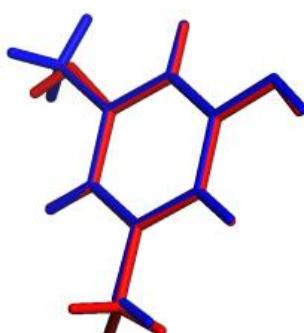
Glutaric acid conformers

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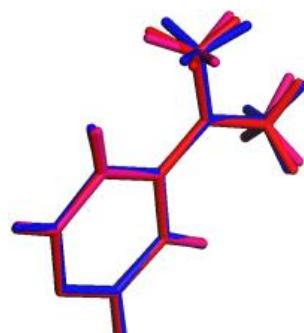


5-Methylbenzene-1,3-diol + bis(N,N-dimethylpyridin-4-amine) (EWAPAU, EWAPAU01)

Reference: A.Mukherjee, P.Grobelny, T.S.Thakur, G.R.Desiraju, *Cryst.Growth Des.* (2011), 11, 2637.

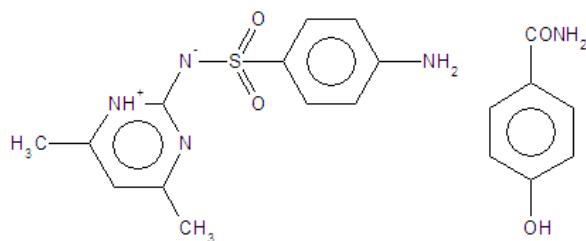


5-Methylbenzene-1,3-diol conformers



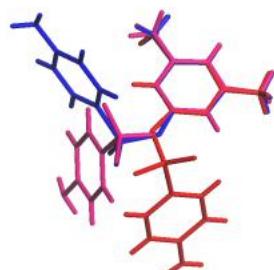
N,N-dimethylpyridin-4-amine conformers

57

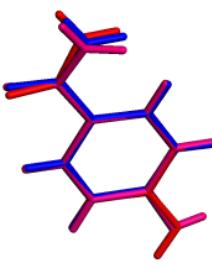


4-amino-N-(4,6-dimethylpyrimidinium-2-yl)benzenesulfonamide 4-hydroxybenzamide (EXAPID, EXAPID01)

Reference: S.Ghosh, P.P.Bag, C.M.Reddy, *Cryst.Growth Des.* (2011), 11, 3489.

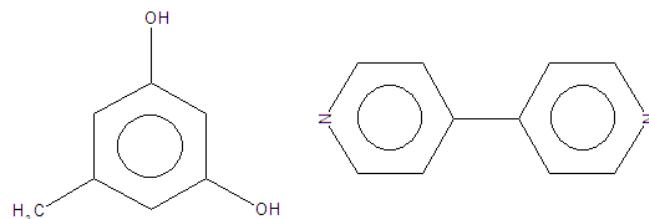


4-amino-N-(4,6-dimethylpyrimidinium-2-yl)benzenesulfonamide conformers



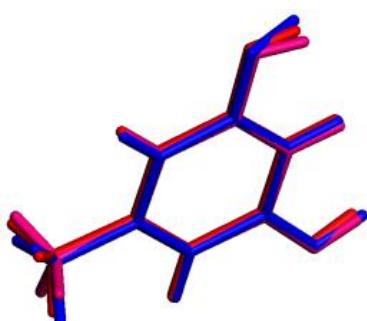
4-hydroxybenzamide conformers

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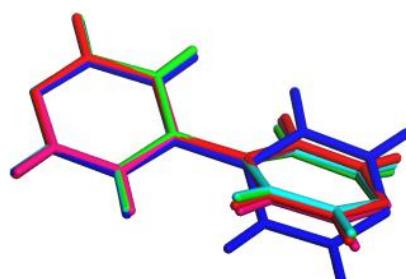


5-Methylbenzene-1,3-diol sesquikis(4,4'-bipyridine) (UBUJIM, UBUJIM01)

Reference: (a) S.Tothadi, A.Mukherjee, G.R.Desiraju, *Chem.Commun.* (2011), 47, 12080; (b) R. Dubey, M. S. Pavan, T. N. G. Row and G. R. Desiraju, *IUCrJ*, 2014, 1, 8.

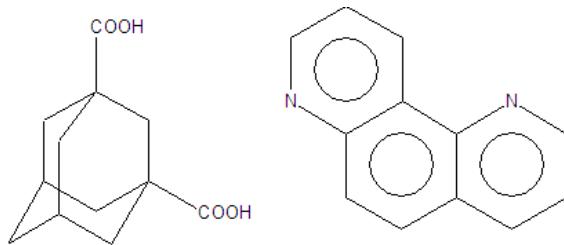


5-Methylbenzene-1,3-diol conformers



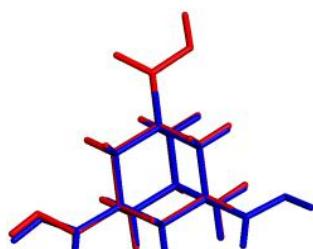
4,4'-bipyridine conformers

59

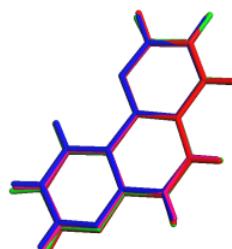


1,3-Adamantanedicarboxylic acid bis(1,7-phenanthroline) (PANQUS, PANQUS01)

Reference: Y.Manjare, V.R.Pedireddi, *Cryst.Growth Des.* (2011), 11, 5079.

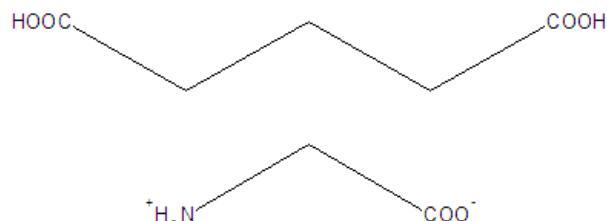


1,3-Adamantanedicarboxylic acid conformers



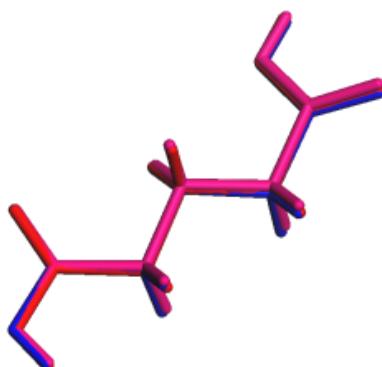
1,7-phenanthroline conformers

60

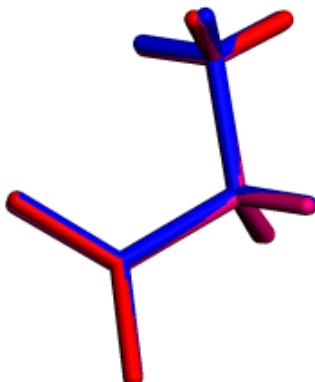


glutaric acid glycine (AWIHOE02-AWIHOE10)

Reference: (a) E.A.Losev, B.A.Zakharov, T.N.Drebushchak, E.V.Boldyreva, *Acta Crystallogr., Sect.C: Cryst.Struct.Commun.* (2011), 67, o297; (b) B.A.Zakharov, E.A.Losev, B.A.Kolesov, V.A.Drebushchak, E.V.Boldyreva, *Acta Crystallogr., Sect.B: Struct.Sci.* (2012), 68, 287

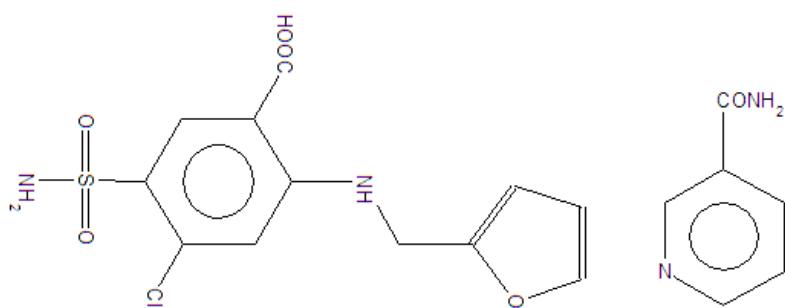


Glutaric acid conformers



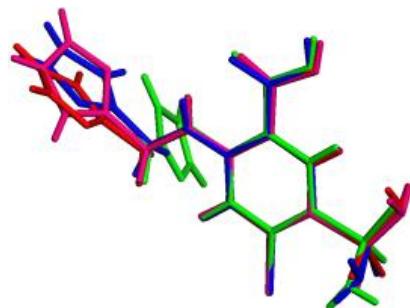
Glycine conformers

61



4-Chloro-2-((2-furylmethyl)amino)-5-sulfamoylbenzoic acid nicotinamide (YASGOQ, YASGOQ01, YASGOQ02, YASGOQ03)

Reference: T.Ueto, N.Takata, N.Muroyama, A.Nedu, A.Sasaki, S.Tanida, K.Terada, *Cryst.Growth Des.* (2012), 12, 485

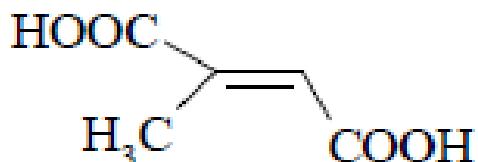
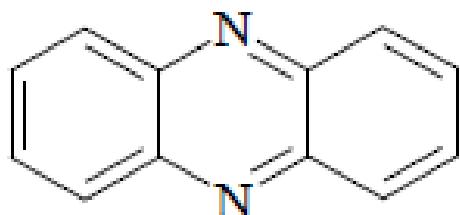


4-Chloro-2-((2-furylmethyl)amino)-5-sulfamoylbenzoic acid conformers



nicotinamide conformers

62

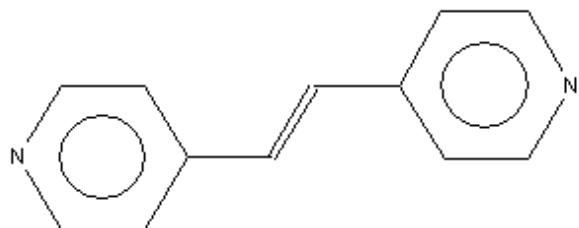
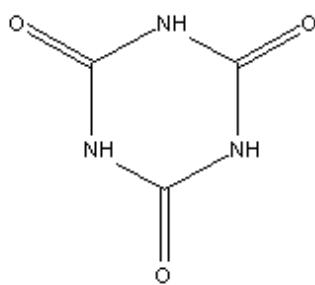


Dibenzopyrazine trans-2-methylbut-2-ene-1,4-dioic acid (WOQBAF, WOQBAF01)

Reference: (a) E.Batchelor, J.Klinowski, W.Jones, *J.Mater.Chem.* (2000), 10, 839; (b) E.Batchelor, J.Klinowski, W.Jones, *Mol.Cryst.Liq.Cryst.Sci.Technol.,Sect.A* (2001), 356, 263.

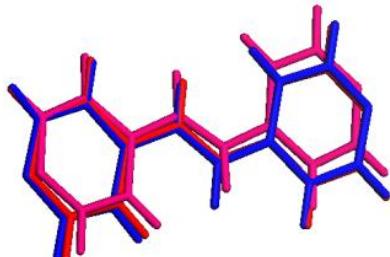
3D coordinates are not available for one of the polymorphs.

63

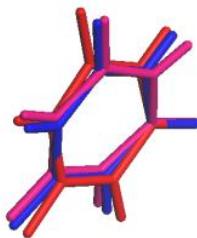


trans-1,2-bis(Pyrid-4-yl)ethylene cyanuric acid (HADKUT, HADKUT01)

Reference: S.A.Barnett, A.J.Blake, N.R.Champness, *CrystEngComm* (2003), 5, 134.

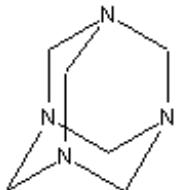


trans-1,2-bis(Pyrid-4-yl)ethylene conformers



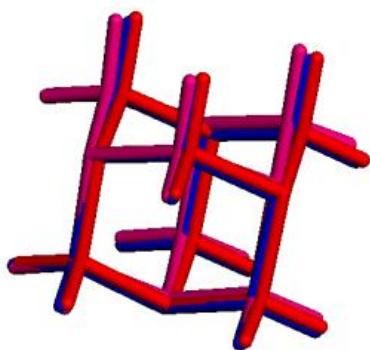
cyanuric acid conformers

64



Hexamethylenetetramine pimelic acid (IJETOG, IJETOG02)

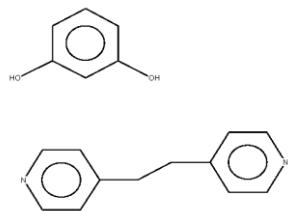
Reference: M.Gardon, C.B.Pinheiro, G.Chipuis, *Acta Crystallogr., Sect.B: Struct.Sci.* (2003), 59, 527.



Hexamethylenetetramine conformers

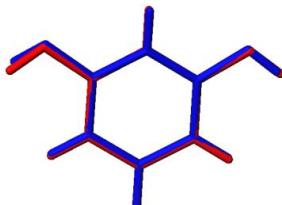
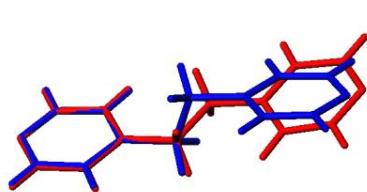
Crystal structure of one of the polymorphs contains disordered pimelic acid conformers, and hence not overlayed.

65



trans-1,2-bis(4-pyridyl)ethylene resorcinol (ACOYOG, ACOYOG01)

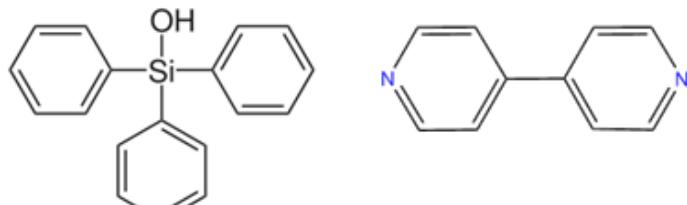
Reference: (a) G.S.Papaefstathiou, L.R.MacGillivray, Org.Lett. (2001), 3, 3835; (b) M.Khan, V.Enkelmann, G.Brunklaus, J.Org.Chem. (2009), 74, 2261.



Resorcinol conformers

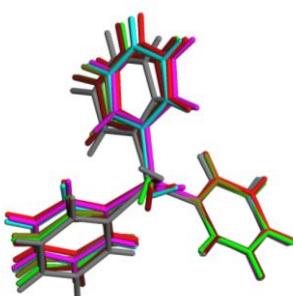
trans-1,2-bis(4-pyridyl)ethylene conformers

66

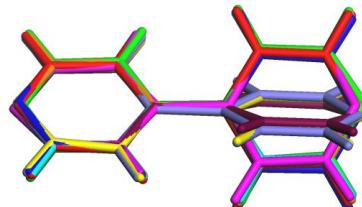


Triphenylsilanol+4,4'-Bipyridine

Reference: K. F. Bowes, G. Ferguson, A. J. Lough and C. Glidewell, *Acta Cryst.*, 2003, B59, 277.

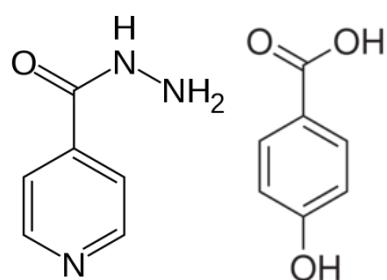


Triphenylsilanol conformers (Disordered conformers were not overlayed)



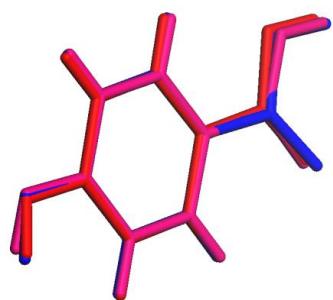
4,4'-Bipyridine conformers

67

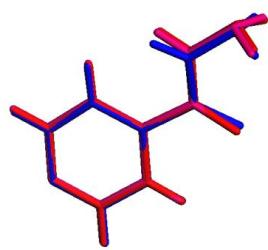


Isoniazid+4-hydroxybenzoic acid+water

Reference: S. Aitipamula, A. B. H. Wong, P. S. Chow and R. B. H. Tan, *CrystEngComm*, 2013, 15, 5877.

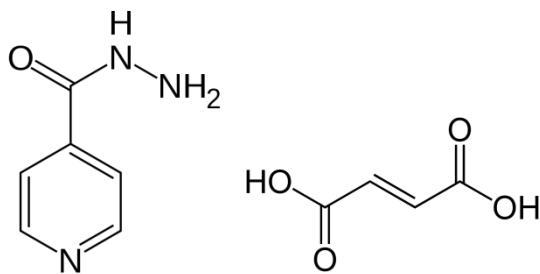


4-hydroxybenzoic acid conformers



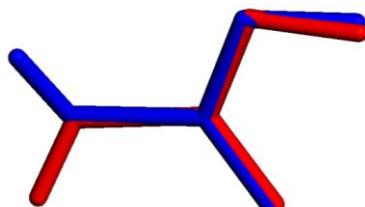
Isoniazid conformers

68

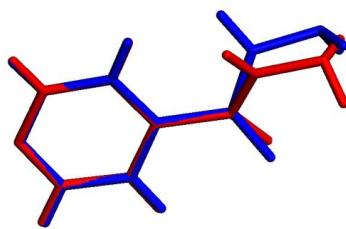


Isoniazid+Fumaric acid

Reference: S. Aitipamula, A. B. H. Wong, P. S. Chow and R. B. H. Tan, *CrystEngComm*, 2013, 15, 5877.

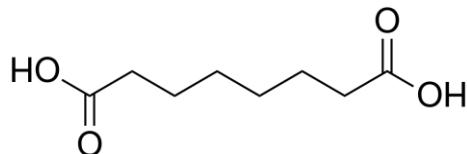
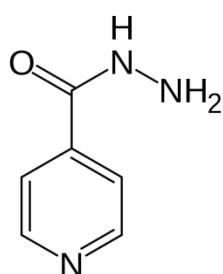


Fumaric acid conformers



Isoniazid conformers

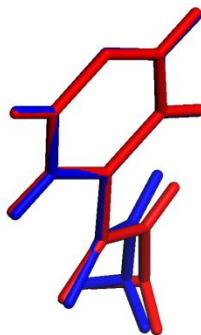
69



Isoniazid+Suberic acid

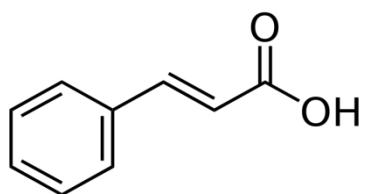
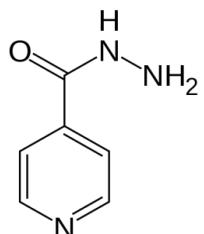
Reference: I. Sarcevica, L. Orola, M. V. Veidis, A. Podjava and S. Belyakov, *Cryst. Growth Des.*, 2013, **13**, 1082.

Crystal structure of only one of the polymorphs has been reported.



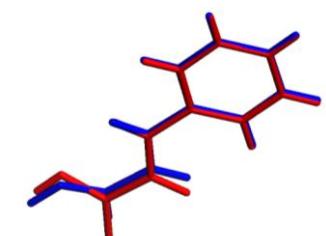
Isoniazid conformers

70

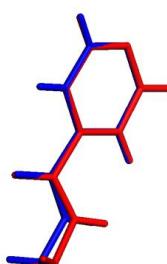


Isoniazid + Cinnamic acid

Reference: I. Sarcevica, L. Orola, M. V. Veidis, A. Podjava and S. Belyakov, *Cryst. Growth Des.*, 2013, **13**, 1082.

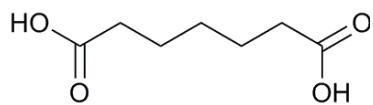
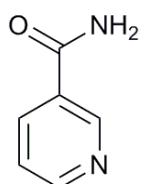


Cinnamic acid conformers



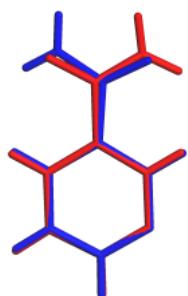
Isoniazid conformers

71

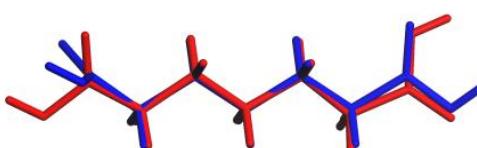


Nicotinamide+Pimelic acid

Reference: S. Aitipamula, A. B. H. Wong, P. S. Chow and R. B. H. Tan, *CrystEngComm*, 2012, 14, 8193; (b) S. Karki, T. Friscic and W. Jones, *CrystEngComm*, 2009, 11, 470.

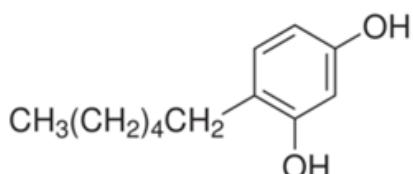
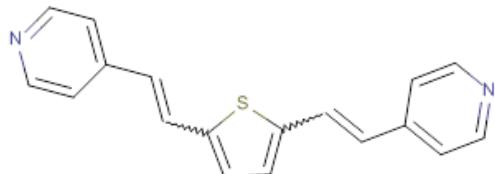


Nicotinamide conformers



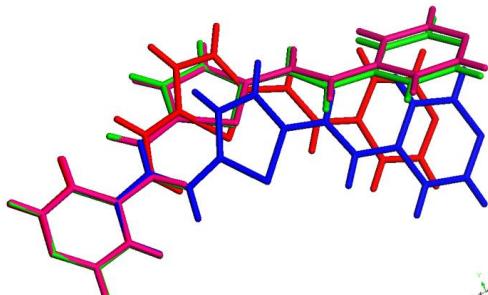
Pimelic acid conformers

72

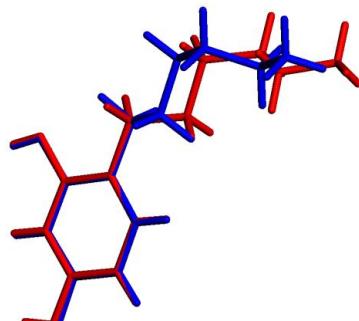


all-trans-2,5-bis(2-(4-Pyridyl)ethenyl)thiophene 4-hexylresorcinol
MacGillivray example

Reference: A. N. Sokolov, D. C. Swenson and L. R. MacGillivray, *Proc. Nat. Acad. Sci.*, 2008, 105, 1794.

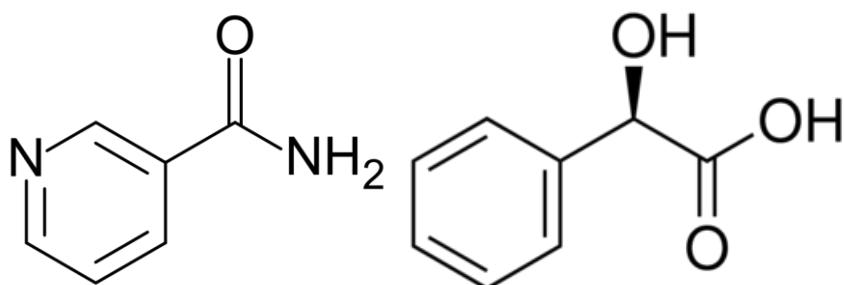


all-trans-2,5-bis(2-(4-Pyridyl)ethenyl)thiophene conformers



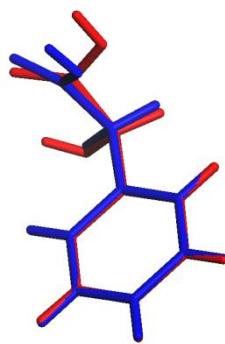
4-hexylresorcinol conformers

73

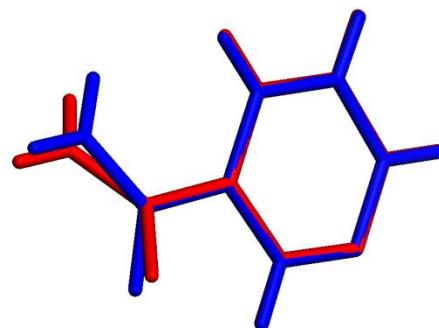


Nicotinamide+R-mandelic acid

Reference: S. Zhang, I. A. Guzei, M. M. de Villiers, L. Yu and J. F. Krzyzaniak, *Cryst. Growth Des.*, 2012, 12, 4090.

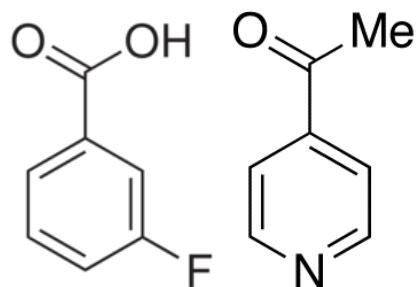


Nicotinamide conformers



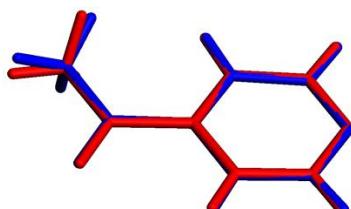
R-mandelic acid conformers

74

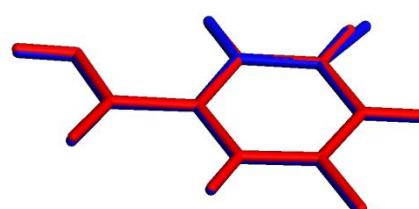


3-Fluorobenzoic acid+4-Acetylpyridine (HOLJAU, HOLJAU01, HOLJAU02, HOLJAU03)

Reference: L. H. Thoma, G. A. Craig, M. J. Gutmann, A. Parkin, K. Shankland and C. C. Wilson, *CrystEngComm*, 2011, 13, 3349.

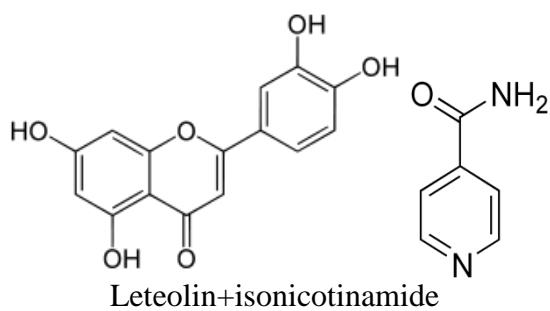


3-Fluorobenzoic acid conformers

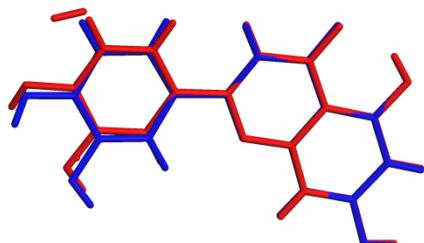


4-Acetylpyridine conformers

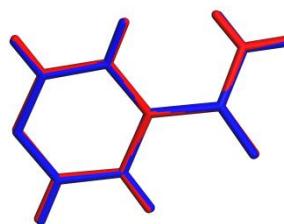
75



Reference: M. Sowa, K. Ślepokura, E. Matczak-Jon, *CrystEngComm*, 2013, 15, 7696.

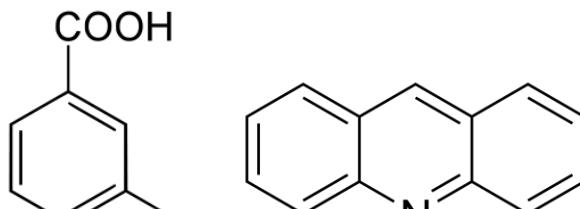


Leteolin conformers



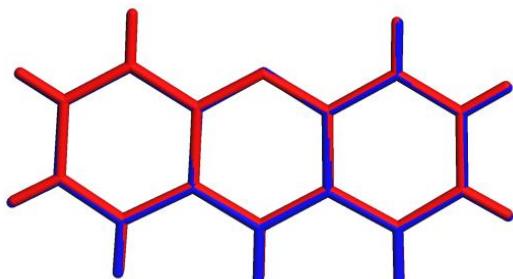
Isonicotinamide conformers

76

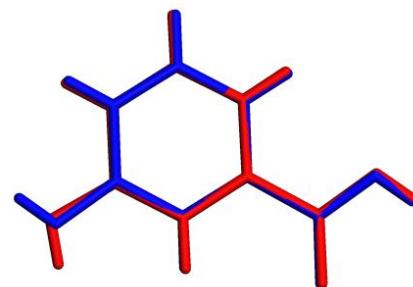


3-Hydroxybenzoic acid+acridine

Reference: A. Lammerer, A. Adsmond, C. Esterhuysen and J. Bernstein, *Cryst. Growth Des.*, 2013, 13, 3935.

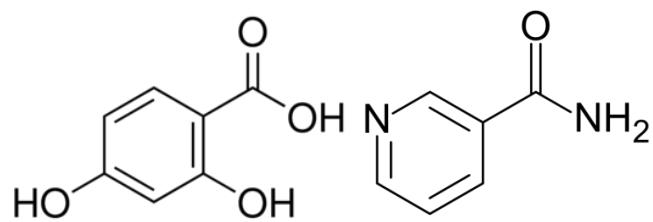


Acridine conformers



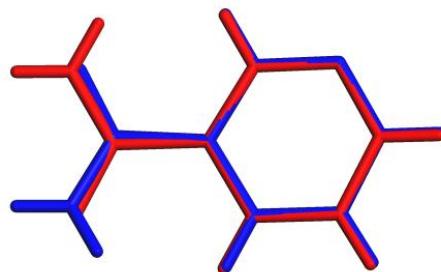
3-Hydroxybenzoic acid conformers

77

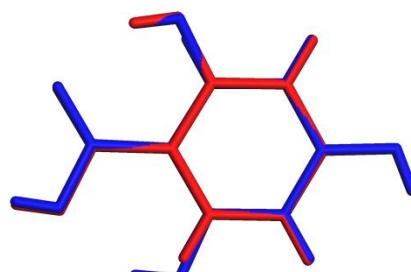


2,4-dihydroxybenzoic acid+nicotinamide

Reference: A. Lammerer, A. Adsmond, C. Esterhuysen and J. Bernstein, *Cryst. Growth Des.*, 2013, **13**, 3935.

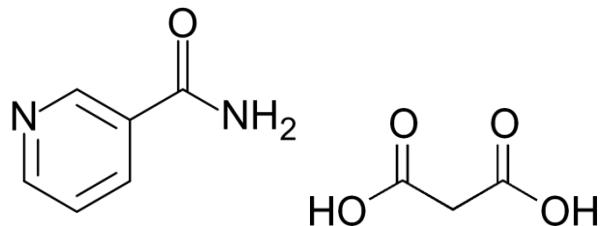


Nicotinamide conformers



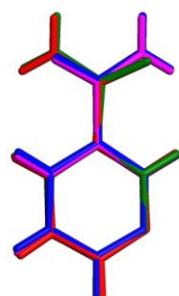
2,4-Dihydroxybenzoic acid conformers

78

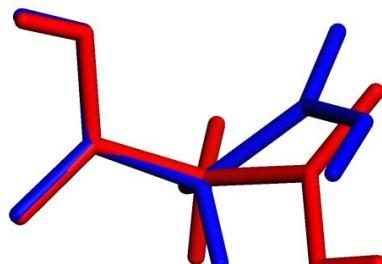


Malonic acid + nicotinamide

Reference: A. Lammerer, A. Adsmond, C. Esterhuysen and J. Bernstein, *Cryst. Growth Des.*, 2013, **13**, 3935.

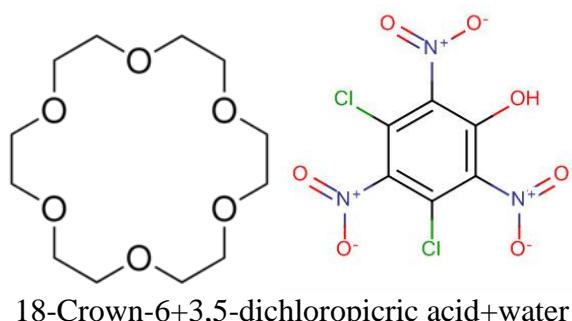


Nicotinamide conformers



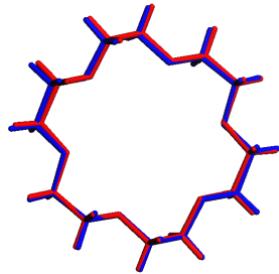
Malonic acid conformers

79

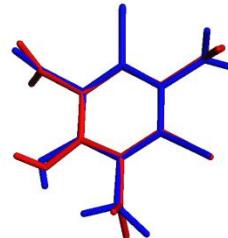


18-Crown-6+3,5-dichloropicric acid+water

Reference: D. Britton, M. K. Chantoni Jr., I. M. Kolthoff, *Acta Cryst.* 1988, C44, 303.

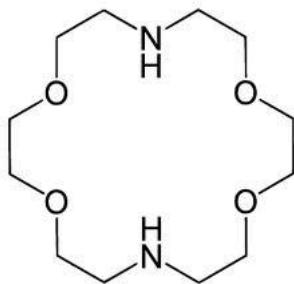
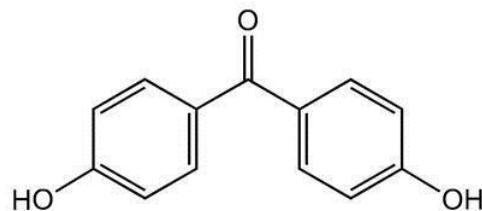


18-Crown-6 conformers



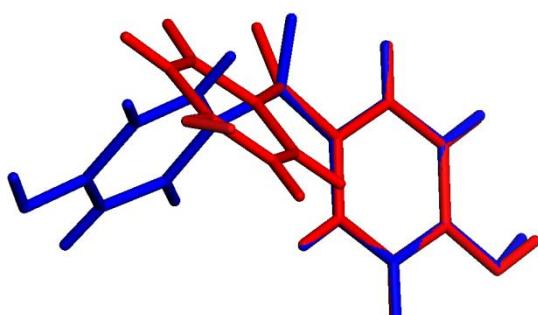
3,5-dichloropicric acid conformers

80

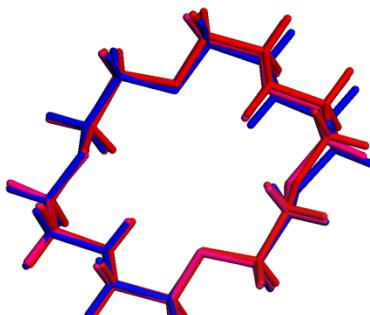


4,4'-Dihydroxybenzophenone + 4,13-diaza-18-crown-6 (KAXWAJ01, KAXWAJ02)

Reference: Y. Zhang, G. Wu, B. R. Wenner, F. V. Bright and P. Coppens, *Crystal Engineering*, 1999, 2, 1.

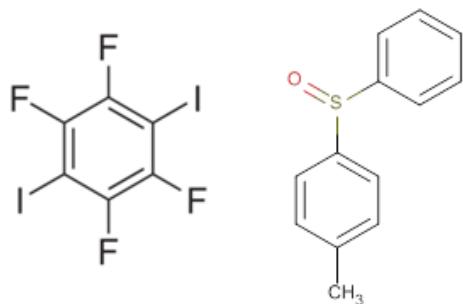


4,4'-Dihydroxybenzophenone conformers



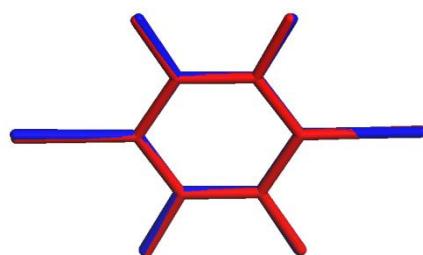
4,13-diaza-18-crown-6 conformers

81

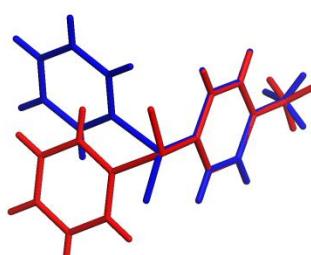


1,4-Diiodotetrafluorobenzene + (\pm)-Phenyl 4-Tolyl Sulfoxide (PEFNIZ, PEFNIZ01)

Reference: K. S. Eccles, R. E. Morrison, S. P. Stokes, G. E. O'Mahony, J. A. Hayes, D. M. Kelly, N. M. O'Boyle, L. Fábián, H. A. Moynihan, A. R. Maguire and S. E. Lawrence, *Cryst. Growth Des.*, 2012, 12, 2969.

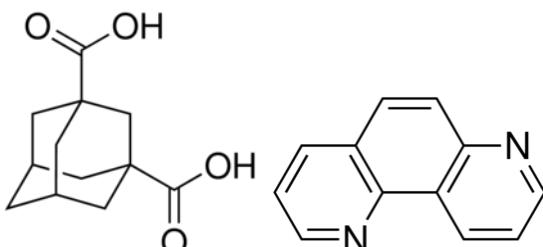


1,4-Diiodotetrafluorobenzene conformers



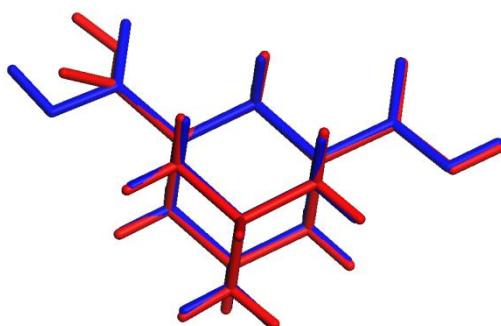
(\pm)-Phenyl 4-Tolyl Sulfoxide conformers

82

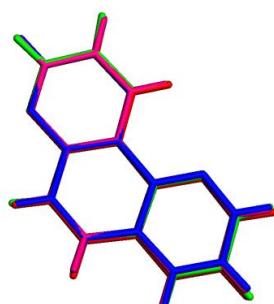


1,3-Adamantanedicarboxylic Acid+1,7-phenanthroline

Reference: Y. Manjare and V. R. Pedireddi, *Cryst. Growth Des.*, 2011, 11, 5079.

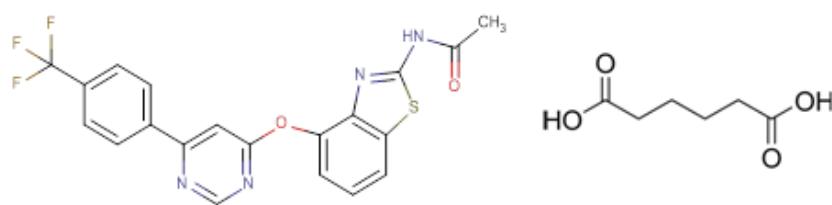


1,3-Adamantanedicarboxylic Acid conformers



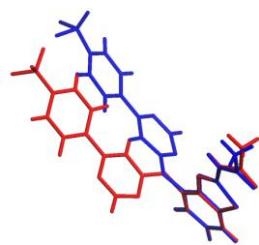
1,7-phenanthroline conformers

83

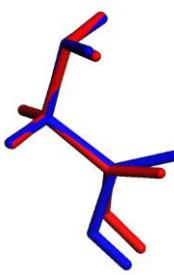


N-(4-(6-(4-(trifluoromethyl)phenyl)pyrimidin-4-yloxy)benzo[d]thiazol-2-yl)acetamide + Adipic acid

Reference: M. L. Peterson, M. K. Stanton, R. C. Kelly, R. Staples and A. Cheng, *CrystEngComm*, 2011, 13, 1170.

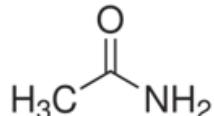
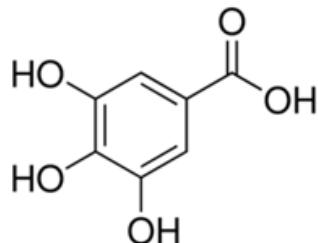


N-(4-(6-(4-(trifluoromethyl)phenyl)pyrimidin-4-yloxy)benzo[d]thiazol-2-yl)acetamide conformers



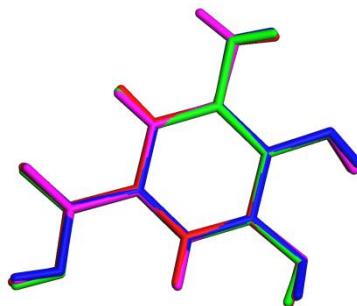
Adipic acid conformers

84

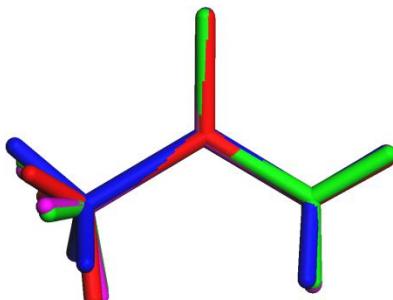


Gallic acid + Acetamide (1:1) (PEFGEO, PEFGEO01, PEFGEO02, PEFGEO03)

Reference: R. Kaur and T. N. G. Row, *Cryst. Growth Des.*, 2012, **12**, 2744.

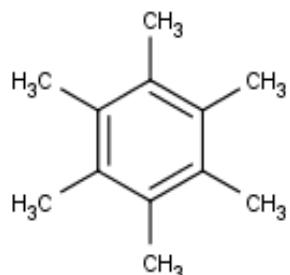
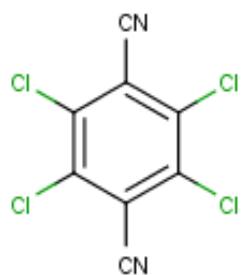


Gallic acid conformers



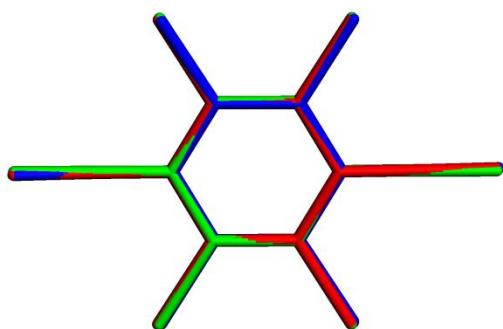
Acetamide conformers

85

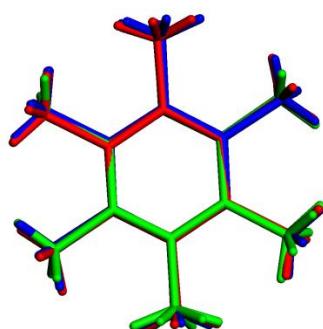


p-Tetrachlorodicyanobenzene + hexamethylbenzene (ADULEQ)

Reference: D.Britton, Acta Crystallogr.,Sect.B:Struct.Sci. (2002), 58, 553.

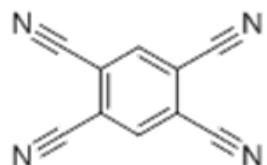
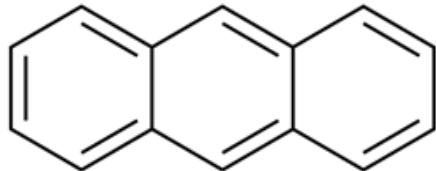


p-Tetrachlorodicyanobenzene conformers



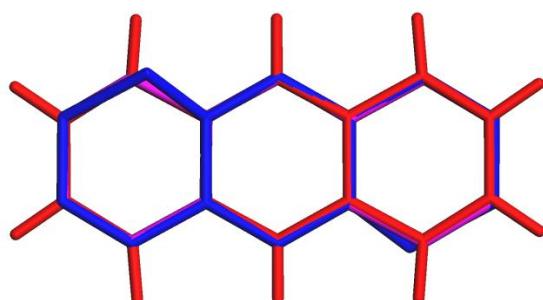
Hexamethylbenzene conformers

86

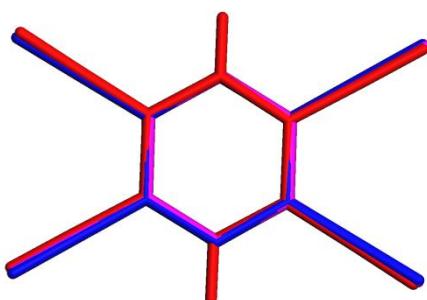


Anthracene 1,2,4,5-tetracyanobenzene (ANTCYB)

Reference: H.Tsuchiya, F.Marumo, Y.Saito, Acta Crystallogr.,Sect.B:Struct.Crystallogr.Cryst.Chem. (1972), 28, 1935; J.J.Stezowski, J.Chem.Phys. (1980), 73, 538.

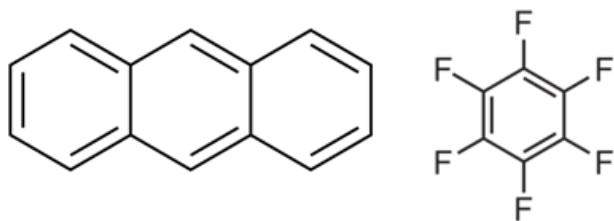


Anthracene conformers



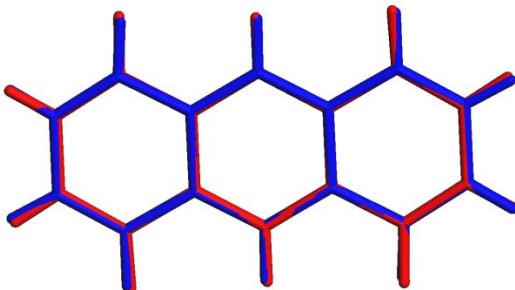
1,2,4,5-tetracyanobenzene conformers

87

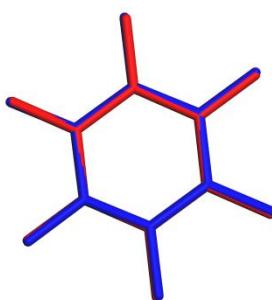


Anthracene + Hexafluorobenzene (ZZZGMW01, ZZZGMW02)

Reference: M.W.Day, A.J.Matzger, R.H.Grubbs, Private Communication (2001); J.C.Collings, K.P.Roscoe, E.G.Robins, A.S.Batsanov, L.M.Stimson, J.A.K.Howard, S.J.Clark, T.B.Marder, New J.Chem. (2002), 26, 1740

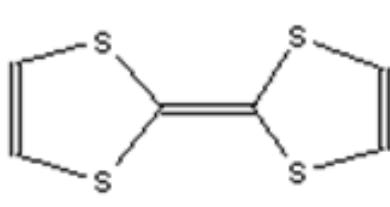


Anthracene conformers



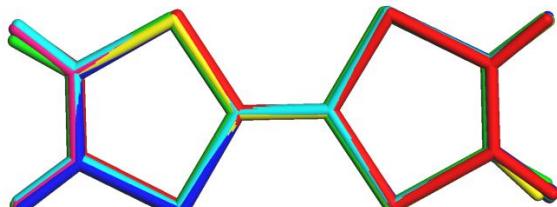
Hexafluorobenzene conformers

88

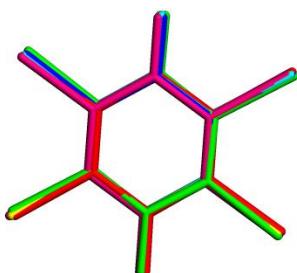


1,1',3,3'-Tetrathiafulvalene + 2,3,5,6-tetrabromo-p-benzoquinone (CAZLAR, CAZLAR01, CAZLAR02)

Reference: P.Garcia, S.Dahaoui, P.Fertey, E.Wenger, C.Lecomte, Phys.Rev.B,Condens.Mat. (2005), 72, 104115.

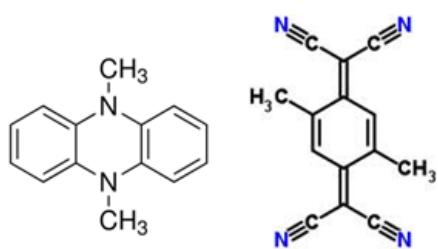


1,1',3,3'-Tetrathiafulvalene conformers



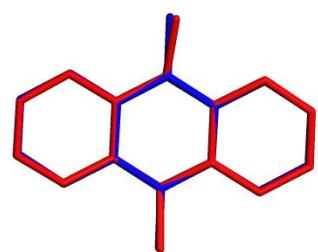
2,3,5,6-tetrabromo-p-benzoquinone conformers

89

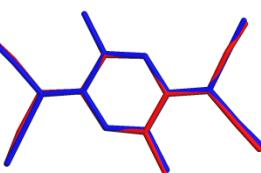


5,10-Dihydro-5,10-dimethylphenazine + 2,5-dimethyl-7,7,8,8-tetracyano-p-quinodimethane
(LOCVOO, LOCVOO01)

Reference: S.Horiuchi, R.Kumai, Y.Okimoto, Y.Tokura, J.Am.Chem.Soc. (1999), 121, 6757.

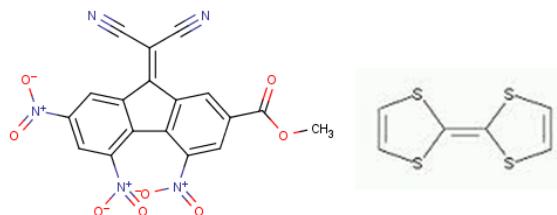


5,10-Dihydro-5,10-dimethylphenazine
conformers



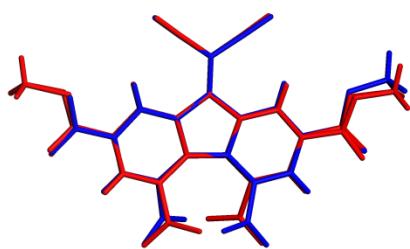
2,5-dimethyl-7,7,8,8-tetracyano-p-quinodimethane
conformers

90

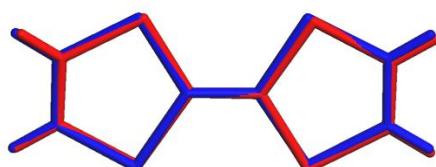


2,2'-bis(1,3-Dithiole) (9-dicyanomethylene-4,5,7-trinitro-fluorene-2-carboxylic acid methyl ester)
(IJETEW, IJETEW01)

Reference: A.Salmeron-Valverde, S.Bernes, J.G.Robles-Martinez, Acta Crystallogr., Sect.B:Struct.Sci.
(2003), 59, 505.

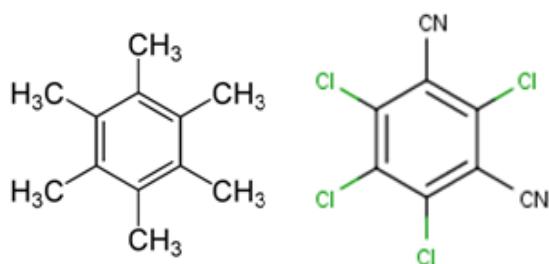


9-dicyanomethylene-4,5,7-trinitro-fluorene-2-
carboxylic acid methyl ester conformers



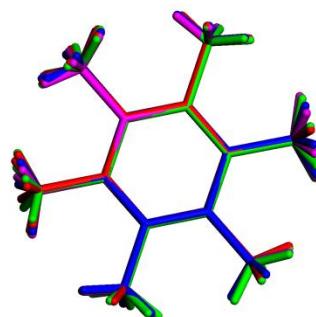
2,2'-bis(1,3-Dithiole) conformers

91

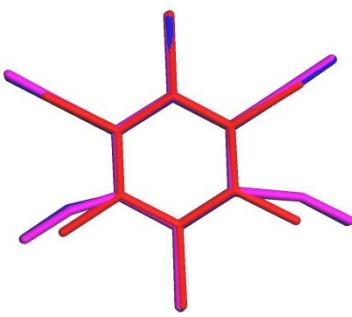


m-Tetrachlorodicyanobenzene + Hexamethylbenzene (MOCCOW, MOCCOW01)

Reference: D.Britton, Acta Crystallogr., Sect.B:Struct.Sci. (2002), 58, 553

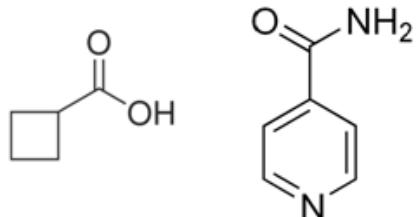


Hexamethylbenzene conformers



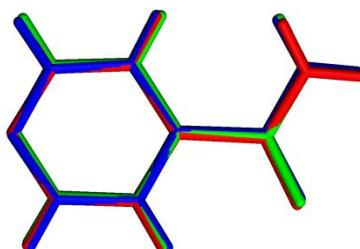
m-Tetrachlorodicyanobenzene conformers

92

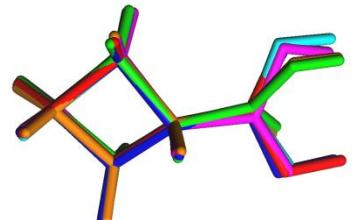


bis(Cyclobutanecarboxylic acid) + Isonicotinamide (ACOMUC, ACOMUC01)

Reference: A.Lemmerer, M.A.Fernandes, New J.Chem. (2012), 36, 2242

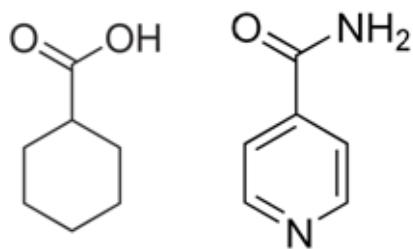


Isonicotinamide conformers



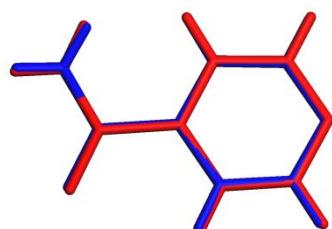
Cyclobutanecarboxylic acid conformers

93

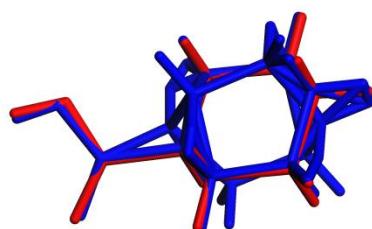


Cyclohexanecarboxylic acid + Isonicotinamide (ACONIR, ACONIR01)

Reference: A.Lemmerer, M.A.Fernandes, New J.Chem. (2012), 36, 2242

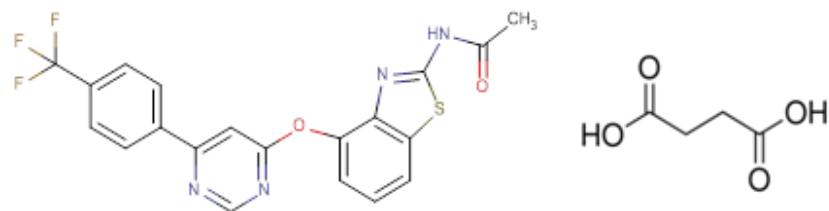


Isonicotinamide conformers



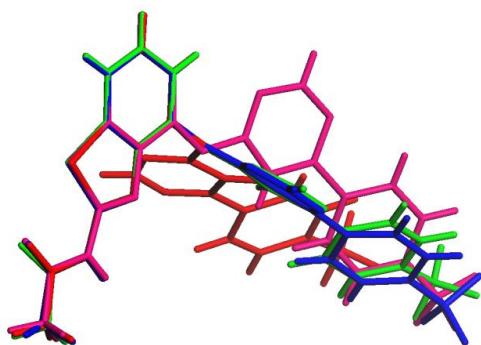
Cyclohexanecarboxylic acid conformers

94

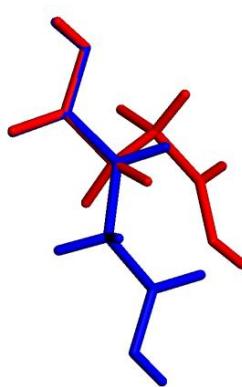


N-(4-(6-(4-(trifluoromethyl)phenyl)pyrimidin-4-yloxy)benzo[d]thiazol-2-yl)acetamide + succinic acid

Reference: M. L. Peterson, M. K. Stanton, R. C. Kelly, R. Staples and A. Cheng, *CrystEngComm*, 2011, 13, 1170.

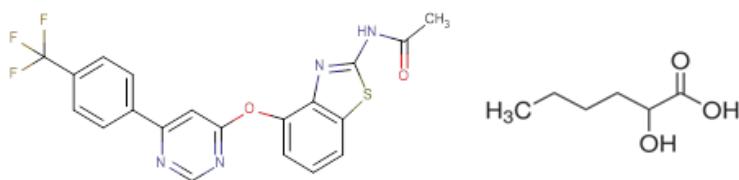


N-(4-(6-(4-(trifluoromethyl)phenyl)pyrimidin-4-yloxy)benzo[d]thiazol-2-yl)acetamide conformers



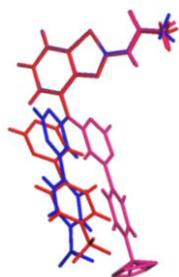
succinic acid conformers

95

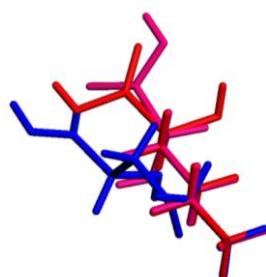


N-(4-(6-(4-(trifluoromethyl)phenyl)pyrimidin-4-yloxy)benzo[d]thiazol-2-yl)acetamide + 2-hydroxycaproic acid

Reference: M. L. Peterson, M. K. Stanton, R. C. Kelly, R. Staples and A. Cheng, *CrystEngComm*, 2011, 13, 1170.

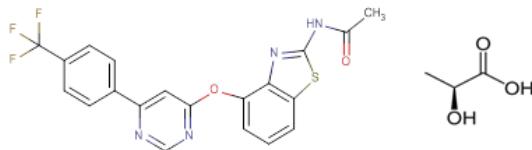


N-(4-(6-(4-(trifluoromethyl)phenyl)pyrimidin-4-yloxy)benzo[d]thiazol-2-yl)acetamide conformers



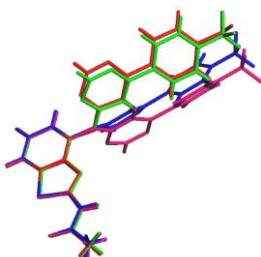
2-hydroxycaproic acid conformers

96

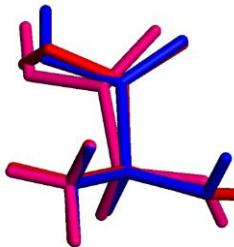


N-(4-(6-(4-(trifluoromethyl)phenyl)pyrimidin-4-yloxy)benzo[d]thiazol-2-yl)acetamide + (+)-lactic acid

Reference: M. L. Peterson, M. K. Stanton, R. C. Kelly, R. Staples and A. Cheng, *CrystEngComm*, 2011, 13, 1170.

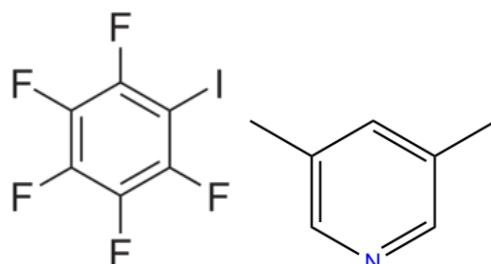


N-(4-(6-(4-(trifluoromethyl)phenyl)pyrimidin-4-yloxy)benzo[d]thiazol-2-yl)acetamide conformers

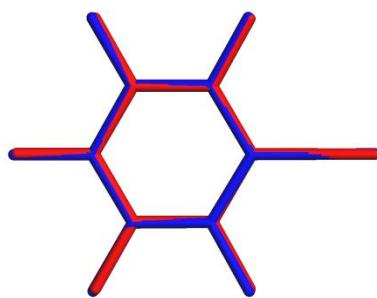


(+)-lactic acid conformers

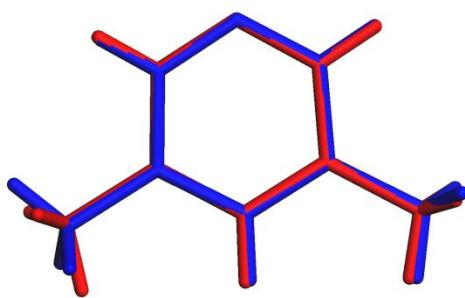
97



Iodopentafluorobenzene + 3,5-dimethylpyridine

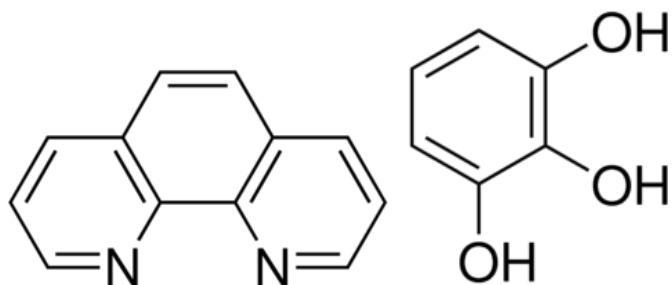
Reference: A. Wasilewska, M. Gdaniec and T. Polonski, *CrystEngComm*, 2007, 9, 203.

Iodopentafluorobenzene conformers

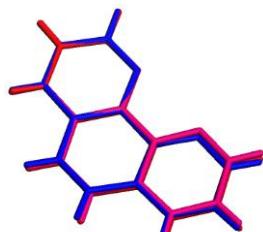


3,5-dimethylpyridine conformers

98



1,10-phenanthroline–pyrogallol (CEKKOU, CEKKOU01)

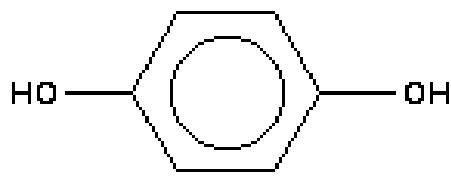
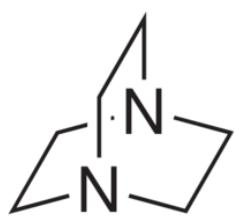
Reference: M. V. Veidis, L. Orola and I. Mutikainen and I. Sarcevica, *CrystEngComm*, 2012, 14, 7253.

1,10-phenanthroline conformers



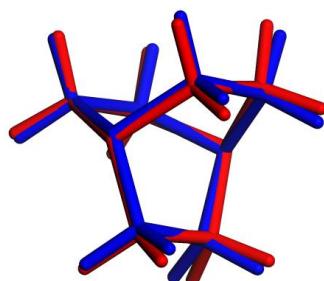
Pyrogallol conformers

99

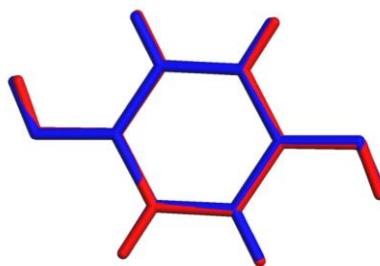


1,4-diazabicyclo-[2.2.2]octane + hydroquinone

Reference: H.-Y. Ye, J.-Z. Ge, F. Chen, R.-G. Xiong, *CrystEngComm*, 2010, 12, 1705.

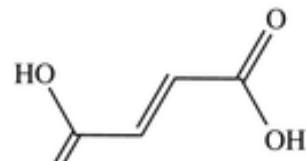
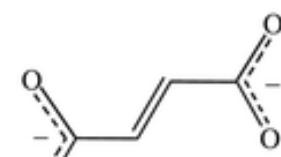
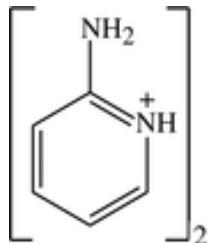


1,4-diazabicyclo-[2.2.2]octane conformers



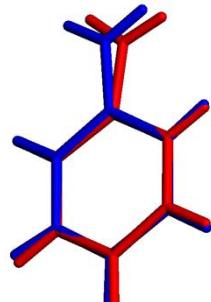
Hydroquinone conformers

100

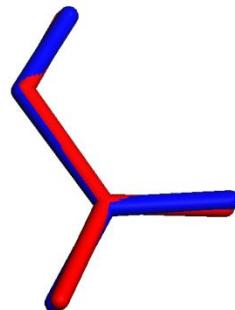


2-Aminopyridinium fumarate + Fumaric acid

Reference: S. Dong, Y. Tao, X. Shen and Z. Pan, *Acta Cryst.* 2013, C69, 896.

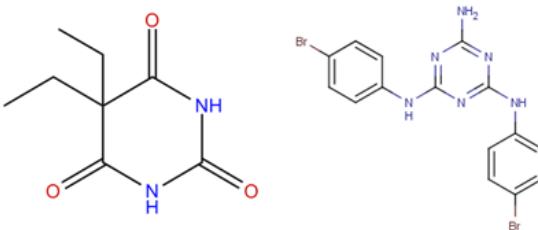


2-Aminopyridinium conformers



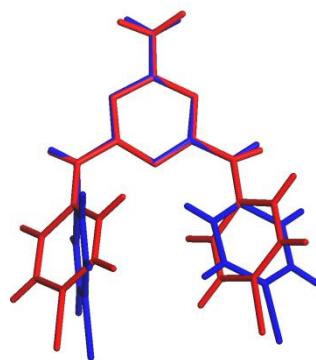
Fumaric acid conformers

101

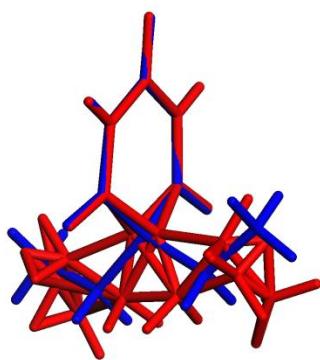


N,N'-bis(4-Bromophenyl)melamine 5,5-diethylbarbituric acid (JICTUK01, JICTUK10)

Reference: J.A.Zerkowski, J.C.MacDonald, C.T.Seto, D.A.Wierda, G.M.Whitesides, J.Am.Chem.Soc. (1994), 116, 2382.

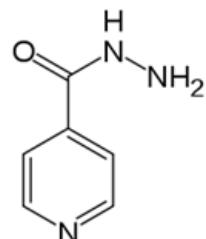


N,N'-bis(4-Bromophenyl)melamine conformers



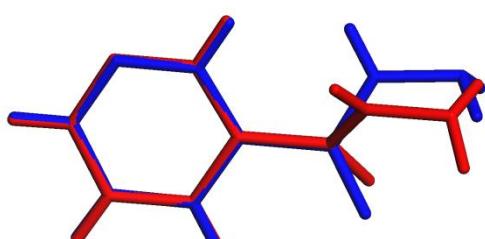
5,5-diethylbarbituric acid conformers

102

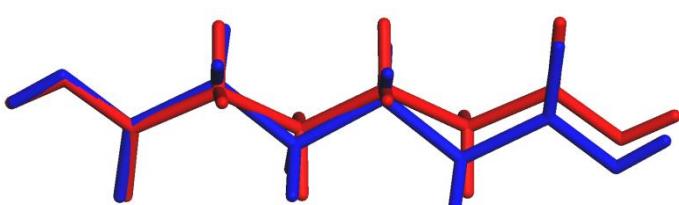


Isoniazid + Adipic acid (UKOSAP, UKOSAP01)

Reference: A.Lemmerer, J.Bernstein, V.Kahlenberg, CrystEngComm (2011), 13, 55; A.Lemmerer, J.Bernstein, V.Kahlenberg, Acta Crystallogr., Sect.E:Struct.Rep.Online (2012), 68, o190

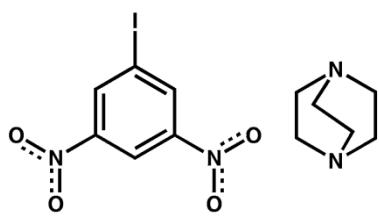


Isoniazid conformers



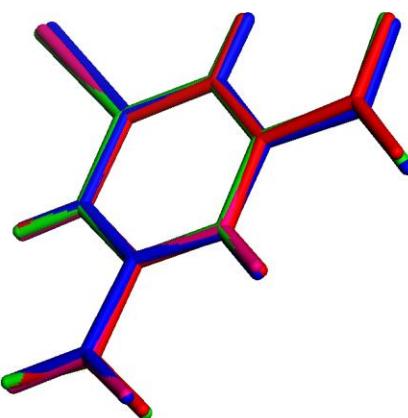
Adipic acid conformers

103

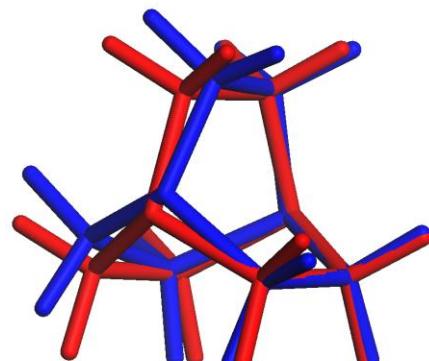


1-Iodo-3,5-dinitrobezoic acid + DABCO (1:1)

Reference: K. Raatikainen and K. Rissanen, *CrystEngComm*, 2009, 11, 750.

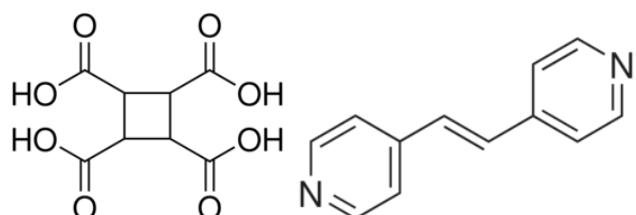


1-Iodo-3,5-dinitrobezoic acid conformers



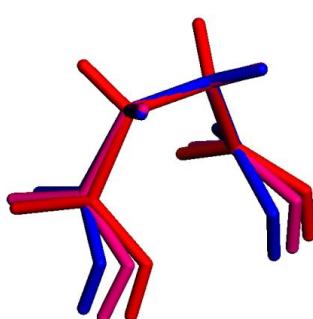
DABCO conformers

104

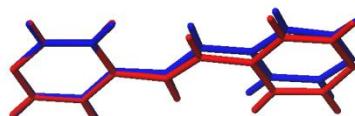


rctt-cyclobutanetetracarboxylic acid + *trans*-1,2-bis(4-pyridyl)ethylene (1:2)

Reference: S. Bhattacharya, J. Stojakovic, B. K. Saha and L. R. MacGillivray, *Org. Lett.*, 2013, 15, 744.

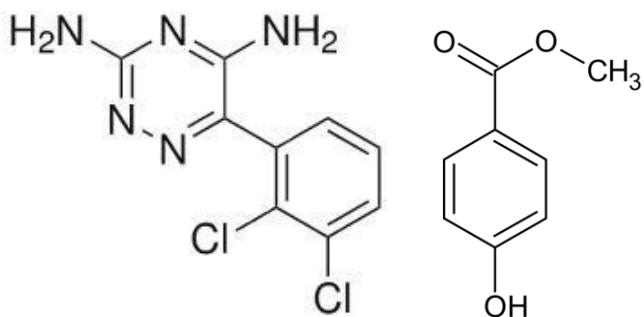


rctt-cyclobutanetetracarboxylic acid conformers
(symmetry independent half molecules)



trans-1,2-bis(4-pyridyl)ethylene conformers

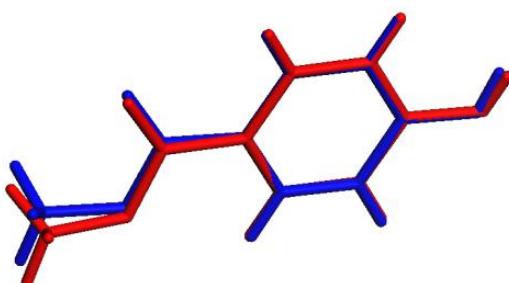
105



Lamotrigine + Methylparaben (1:1) (WUVKEE, WUVKEE01, WUVKEE02)

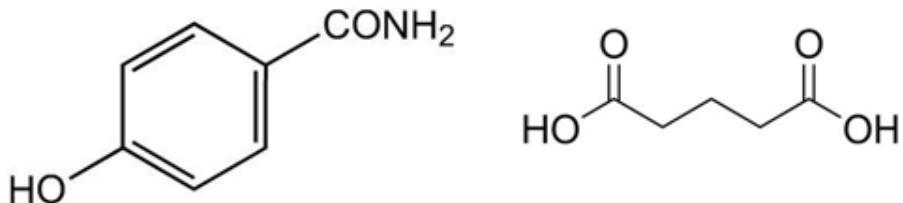
Reference: M. L. Cheney, N. Shan, E. R. Healey, M. Hanna, L. Wojtas, M. J. Zaworotko, V. Sava, S. Song and J. R. Sanchez-Ramos, *Cryst. Growth Des.*, 2010, 10, 394.

One of the polymorphs contain disordered lamotrigine molecule in the crystal structure, and hence not overlayed.



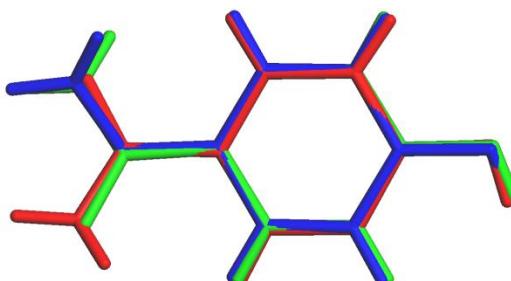
Methylparaben conformers

106

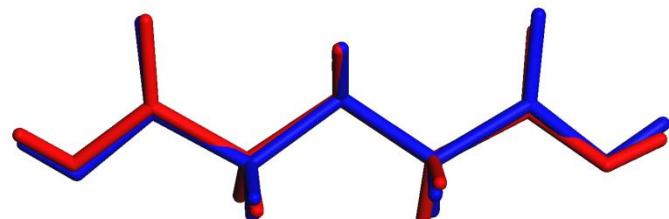


4-Hydroxybenzamide + Glutaric acid (2:1) (GESBIR, GESBIR01)

Reference: S. Tothadi, G.R. Desiraju, *Cryst. Growth Des.* (2012), 12, 6188

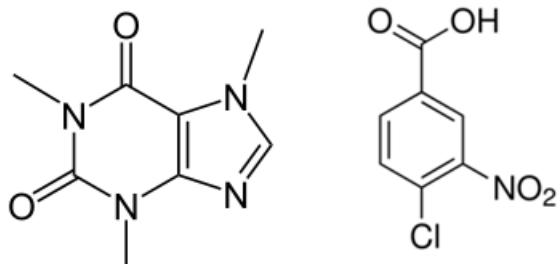


4-Hydroxybenzamide conformers



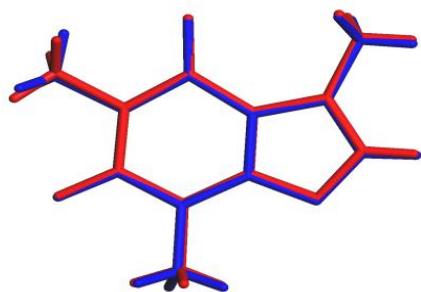
Glutaric acid conformers

107

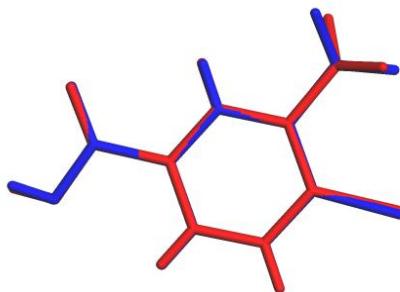


caffeine + 4-chloro-3-nitrobenzoic acid

Reference: S. Ghosh, A. Mondal, M. S. R. N. Kiran, U. Ramamurty and C. M. Reddy, *Cryst. Growth Des.*, 2013, 13, 4435.

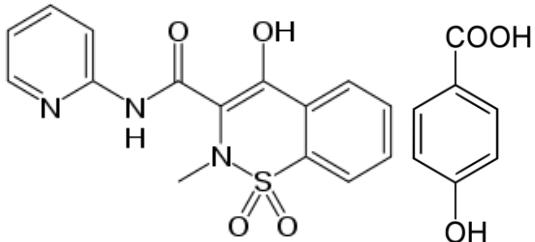


Caffeine conformers



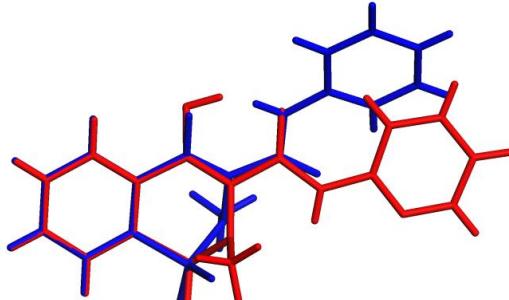
4-chloro-3-nitrobenzoic acid conformers

108

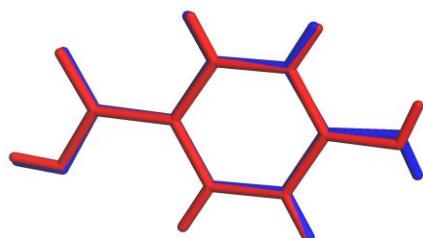


Piroxicam + 4-hydroxybenzoic acid (1:1)

Reference: S. L. Childs and K. I. Hardcastle, *Cryst. Growth Des.*, 2007, 7, 1291.

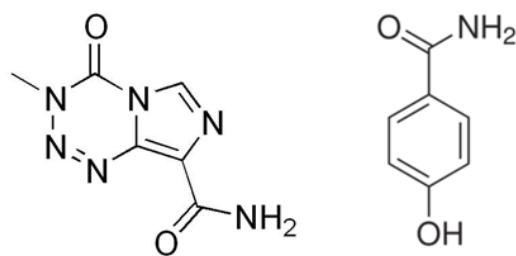


Piroxicam conformers

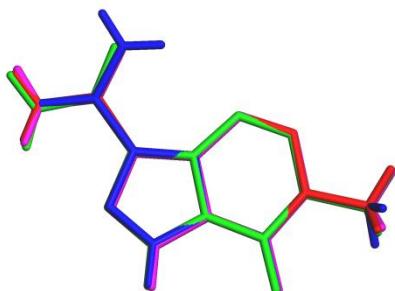


4-Hydroxybenzoic acid conformers

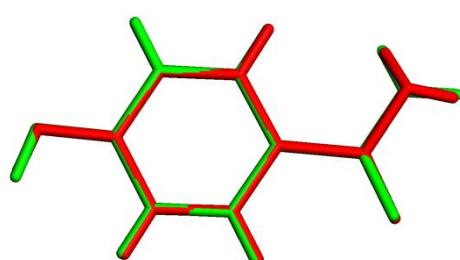
109



Temozolamide + 4-Hydroxybenzamide (2:1)

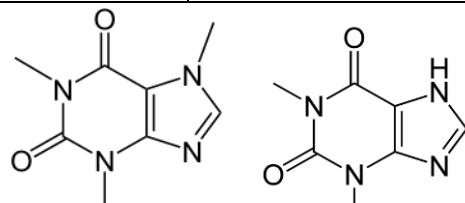
Reference: P. Sanphui, N. J. Babu and A. Nangia, *Cryst. Growth Des.*, 2013, **13**, 2208.

Temozolamide conformers

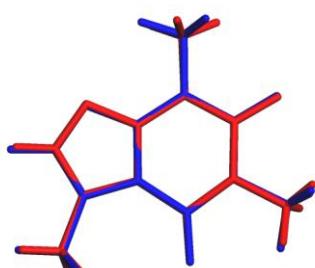


4-Hydroxybenzamide conformers

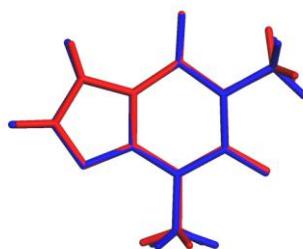
110



Caffeine + Theophylline (1:1)

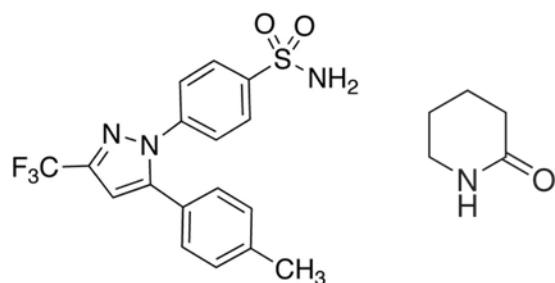
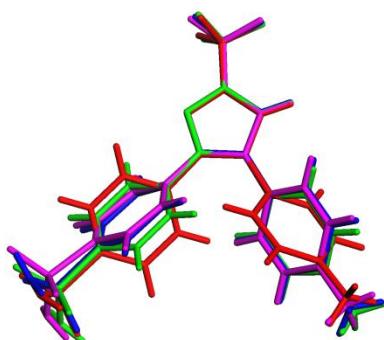
Reference: M. D. Eddleston, B. Patel, G. M. Day and W. Jones, *Cryst. Growth Des.*, 2013, **13**, 4599.

Caffeine conformers

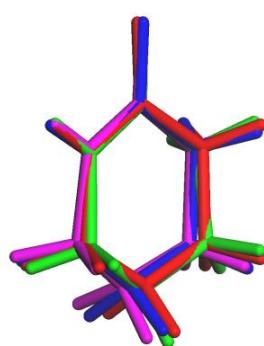


Theophylline conformers

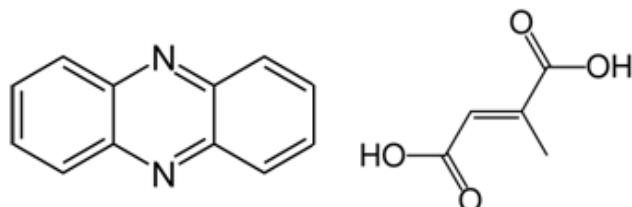
111

Celecoxib + δ -valerolactam (1:1)Reference: G. Bolla, S. Mittapalli and A. Nangia, *CrystEngComm*, 2014, 16, 24.

Celecoxib conformers

 δ -valerolactam conformers

112

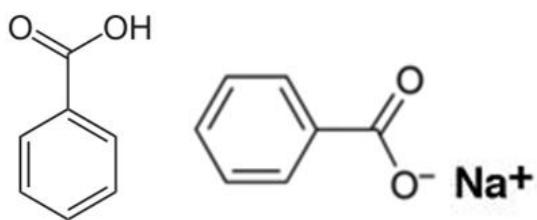


Phenazine + Mesaconic acid (WOQBAF02)

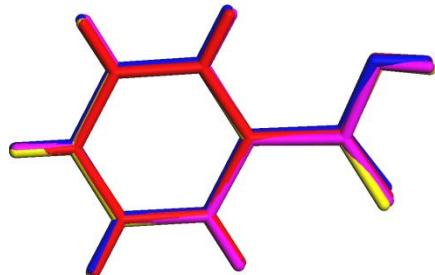
Reference: M.D.Eddleston, S.Sivachelvam, W.Jones, *CrystEngComm* (2013), 15, 175.

The cocrystal exists in three polymorphic forms (Form I-III). Crystal structure of only Form II has been reported. All other forms were characterized by powder X-ray diffraction and thermal methods.

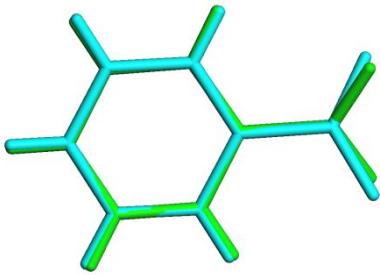
113



Ionic cocrystal of Benzoic acid + sodium Benzoate (2:1)

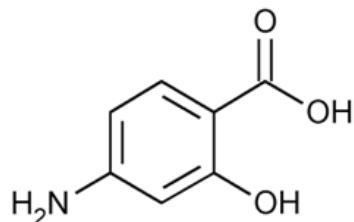
Reference: C. Butterhof, K. Bärwinkel, J. Senker and J. Breu, *CrystEngComm*, 2012, 14, 6744.

Benzoic acid conformers

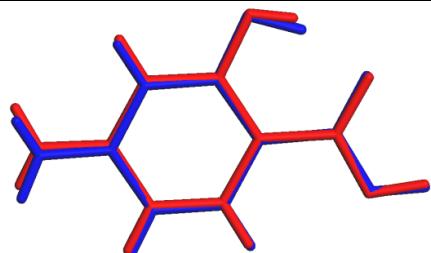


Benzoate conformers

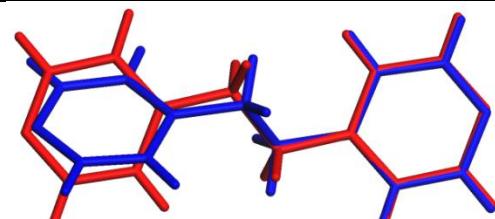
114



4-Aminosalicylic acid + 1,2-bis(4-pyridyl)ethane (1:1)

Reference: (a) P. K. Goswami, R. Thaimattam and A. Ramanan, *Cryst. Growth Des.*, 2013, 13, 360; (b) H. C. Garcia, R. T. Cunha, R. Diniz, L. Fernando and C. de Oliveira, *J. Mol. Struct.*, 2012, 1010, 104.

4-Aminosalicylic acid conformers



1,2-bis(4-pyridyl)ethane conformers