Supramolecular architectures sustained by delocalised C–I···π(arene) interactions in molecular crystals and the propensity of their formation

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ELECTRONIC SUPPLEMENTARY INFORMATION

The ESI Tables 1-8 present images of all aggregation patterns, values of *d* and θ for each contact along with full details of crystal composition and literature citation. In addition, geometric parameters characterising the additional and relevant C–I···π(arene) contacts but outside the specified search criteria are also included. The data are categorised in the following manner:

ESI Table 1. Zero-dimensional aggregates sustained by a single C–I···π(arene) interaction

ESI Table 2. Zero-dimensional aggregates sustained by two C–I···π(arene) interactions

ESI Table 3. Linear, one-dimensional chains sustained by C–I···π(arene) interactions

ESI Table 4. Zig-zag, one-dimensional chains sustained by C–I···π(arene) interactions

ESI Table 5. Helical, one-dimensional chains sustained by C–I···π(arene) interactions

ESI Table 6. Two-dimensional aggregates sustained by C–H···π(arene) interactions

ESI Table 7. Supramolecular aggregates in solvates sustained by C–H···π(arene) interactions

ESI Table 8. Supramolecular aggregates in co-crystals sustained by C–H···π(arene) interactions

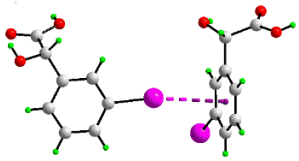
ESI Table 9. A survey of iodide analogues of **1**-**181** along with bromide, chloride and fluoride congeners, when known. Full composition, pertinent unit-cell data and literature citations are presented. When present in their crystals, geometric data for C–X···π(arene) interactions are included.

ESI Figure 1. A plot of θ (°) versus *d* (Å). Note the outlier, indicated with an asterisk, corresponds to **163**. When the data point for **163** is omitted, the value of $R^2 = 0.0088$ for $y = 3.4387x + 154.16$.

ESI Table 1. Zero-dimensional aggregates sustained by a single C–I···π(arene) interaction

1. POPKAI

Hydroxy(3-iodophenyl)acetic acid



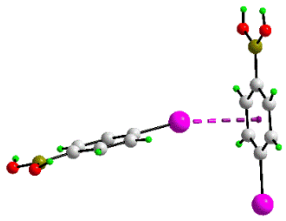
d = 3.521(3) Å; θ = 165.0(2)°

S. J. Coles, A. L. Ellis, K. Leung, J. Sarson, T. L. Threlfall and G. J. Tizzard, *CrystEngComm*, 2014, **16**, 10816-10823; DOI: 10.1039/C4CE01832J

{Three independent molecules comprise the asymmetric unit. One acts as a donor to another to form a two-molecule aggregate}

2. NIQZET

4-Iodophenylboronic acid hemihydrate



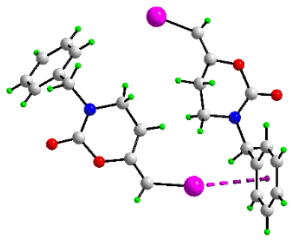
d = 3.523(5) Å; θ = 167.5(4)°

M. R. Shimpi, N. SeethaLekshmi and V. R. Pedireddi, *Cryst. Growth Des*., 2007, **7**, 1958-1963; DOI: 10.1021/cg060863p

{The two independent molecules, each with mirror symmetry bisecting the molecule along the IC_2B axis, are connected into a two-molecule aggregate}

3. DAVHIU

3-Benzyl-6-(iodomethylene)-1,3-oxazinan-2-one



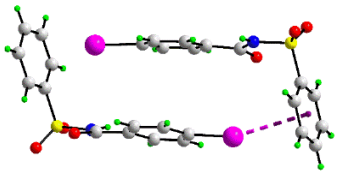
d = 3.5814(14) Å; θ = 160.62(9)°

P. Quinodoz, A. Quelhas, K. Wright, B. Drouillat, J. Marrot and F. Couty, *Eur. J. Org. Chem.*, 2017, 2621-2626; DOI: 10.1002/ejoc.201700231

{Two independent molecules – these associate to form a two-molecule aggregate. The second I atom also forms an interaction but, with geometric parameters beyond the specified search limits: *d* = 3.6730(16) Å; θ = 144.85(9)°}

4. SAJPIF

4-Iodo-N-(phenylsulfonyl)benzamide hemihydrate



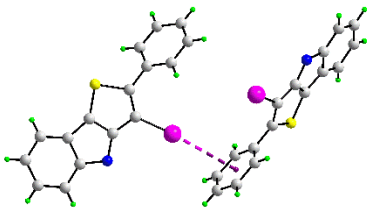
d = 3.5945(18) Å; θ = 160.90(11)°

P. A. Suchetan, A. G. Sudha, E. Suresha, N. K. Lokanath, S. Naveen and I. Warad, *IUCrData*, 2017, **2**, x170149; DOI: 10.1107/S2414314617001493

{The two independent molecules are connected into a two-molecule aggregate via one interaction. The second interaction has *d* = 3.6406(16) Å; θ = 146.42(12)°, i.e. outside the specified search criteria for delocalised interactions}

5. KUMSAP

3-Iodo-2-phenyl-4H-thieno[3,2-b]indole



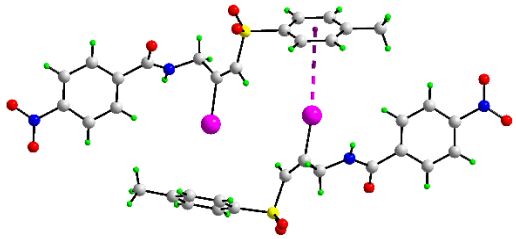
d = 3.770(3) Å; θ = 174.19(13)°

G. Leonel, D. F. Back and G. Zeni, Adv. Synth. Catal., 2020, 362, 585-593; DOI: 10.1002/adsc.201901213

{Two independent molecules comprise the asymmetric unit: these assembles into a two-molecule aggregate via a single interaction}

6. EVEFOC

N-(2-Iodo-3-((4-methylphenyl)sulfonyl)prop-2-en-1-yl)-4-nitrobenzamide



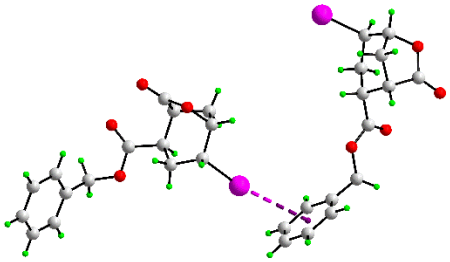
d = 3.829(4) Å; θ = 161.42(19)°

G. C. Senadi, B.-C. Guo, W.-P. Hu and J.-J. Wang, *Chem. Commun*., 2016, **52**, 11410-11413; DOI: 10.1039/C6CC05138C

{Two independent molecules – these associate to form a two-molecule aggregate via a single contact; the second I atom is aligned to form a similar contact but this lies outside the search parameters with *d* = 3.706(3) Å; θ = 155.37(19)°}

7. GUQRIV

(1S,2R,4R,5R)-benzyl 4-iodo-7-oxo-6-oxabicyclo[3.2.1]octane-2-carboxylate



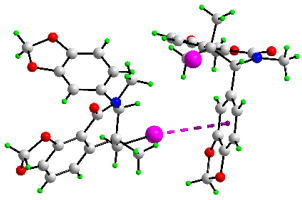
d = 3.854(3) Å; θ = 169.59(15)°

H. Wang and F. Chen, Private Communication to the Cambridge Structural Database, Refcode GUQRIV, 2015.

{Two independent molecules. These associate into a two-molecule aggregate via one interaction}

8. PONKUA

7-(1,3-Benzodioxol-5-yl)-6-(iodomethyl)-6,8-dimethyl-7,8-dihydro[1,3]dioxolo[4,5-h]isoquinolin-9(6H)-one



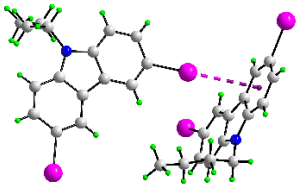
d = 3.8710(16) Å; θ = 166.73(12)°

D. A. Petrone, H. Yoon, H. Weinstabl and M. Lautens, *Angew.Chem., Int. Ed.*, 2014, **53**, 7908-7912; DOI: 10.1002/anie.201404007

{Two independent molecules. These are connected into a two-molecule aggregate via a single interaction}

9. CEYXAI

9-n-Butyl-3,6-diiodo-9H-carbazole



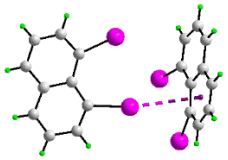
d = 3.526(2) Å; θ = 171.37(18)°

J. G. Malecki, Private Communication to the Cambridge Structural Database, Refcode CEYXAI, 2018.

{Four independent molecules – two of these associate to form a two-molecule aggregate}

10. PIPQUA

1,8-Di-iodonaphthalene



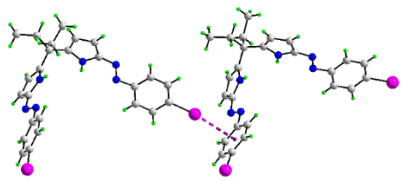
d = 3.570(3) Å; θ = 169.9(2)°

H. Bock, M. Sievert and Z. Havlas, *Chem. - Eur. J.*, 1998, **4**, 677-685; DOI: 10.1002/(SICI)1521-3765(19980416)4:4<677::AID-CHEM677>3.0.CO;2-P

{Six independent molecules comprise the asymmetric unit. One acts as a donor to another to form a two-molecule aggregate}

11. OGOXOY

2,2'-Pentane-3,3-diylbis(5-((4-iodophenyl)diazenyl)-1H-pyrrole) ethyl acetate solvate



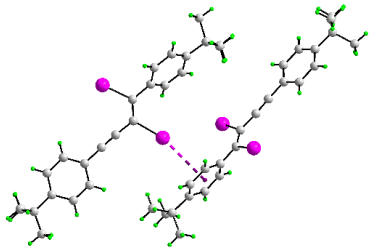
d = 3.578(3) Å; θ = 170.1(2)°

Z. Yin, W. Wang, M. Du, X. Wanga and J. Guo, *CrystEngComm*, 2009, **11**, 2441-2446; DOI: 10.1039/b905568a

{The two independent molecules are connected into a two-molecule aggregate}

12. RETRIR

1,4-bis(4-t-Butylphenyl)-1,2-di-iodo-but-1-en-3-yne



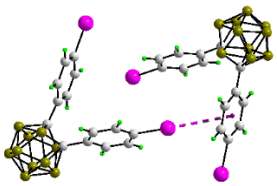
d = 3.767(3) Å; θ = 160.4(2)°

J. Barluenga, I. Llorente, L. J. Alvarez-García, J. M. González, P. J. Campos, M. R. Díaz and S. García-Granda, *J. Am. Chem. Soc*., 1997, **119**, 6933-6934; DOI: 10.1021/ja970108n

{Two independent molecules. These assemble into a two-molecule aggregate via one interaction}

13. GUTFOS

1,2-bis(4-Iodophenyl)-1,2-dicarba-closo-dodecaborane(10)



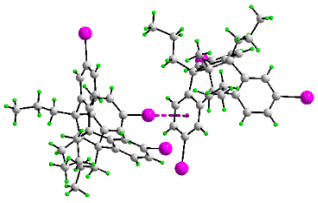
d = 3.8415(16) Å; θ = 174.19(10)°

K. Kokado and Y. Chujo, *Macromolecules*, 2009, **42**, 1418-1420; DOI: 10.1021/ma8027358

{Two independent molecules – these associate to form a two-molecule aggregate via a single contact; the second I atom is aligned to form a similar contact but lies outside the search parameters with *d* = 3.706(3) Å; θ = 155.37(19)°}

14. EWINEF

(+)-(M)-2,6,10-Triiodo-12d-methyl-4b,8b,12b-tripropyl-4b,8b,12b,12d-tetrahydrodibenzo-[2,3:4,5]pentaleno[1,6-ab]indene



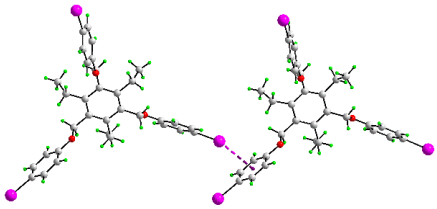
d = 3.583(3) Å; θ = 172.91(17)°

D. Beaudoin, F. Rominger and M. Mastalerz, *Eur. J. Org. Chem.*, 2016, 4470-4472; DOI: 10.1002/ejoc.201600890

{Four independent molecules – two associate to form a two-molecule aggregate. The remaining two molecules associate in a similar fashion but, with *d* = 3.924(3) Å; θ = 171.89(17)°, i.e. outside the search parameters}

15. YASQIU03

1,3,5-Triethyl-2,4,6-tris((4-iodophenoxy)methyl)benzene



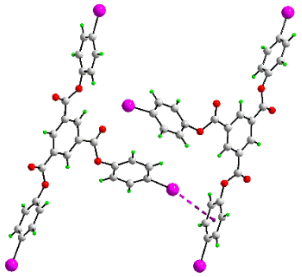
d = 3.657(2) Å; θ = 160.11(15)°

V. G. Saraswatula and B. K. Saha, *New J. Chem.*, 2014, **38**, 897-901; DOI: 10.1039/c3nj01395b

{Two independent molecules. These assemble to form a two-molecule aggregate via a single interaction. Another contact is noted with parameters *d* = 3.535(2) Å; θ = 152.9(2)°. When these interactions are taken into account, a twisted chain is evident. As the m-xylene solvate [**YASRAN**, No. **86**], molecules assemble into a linear chain}

16. WOHXAT

tris(4-Iodophenyl) benzene-1,3,5-tricarboxylate



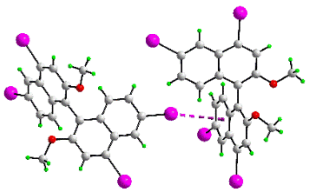
d = 3.766(2) Å; θ = 166.33(13)°

F. C. Pigge, V. R. Vangala, P. P. Kapadia, D. C. Swenson and N. P. Rath, *Chem. Commun*., 2008, 4726-4728; DOI: 10.1039/b809592b

{Two independent molecules. These assemble into a two-molecule aggregate via a single interaction. While there is no second interaction between the illustrated molecules, there are additional contacts noted, with parameters *d* = 3.535(2) Å; θ = 152.9(2)°, along with complementary I···O=C halogen bonding interactions which lead to a hexagonal array. This compound has also been co-crystallised with solvent chloroform, see **87**, **WOHXEX**, which assembles into a linear chain}

17. COPYEO

4,4',6,6'-Tetraiodo-2,2'-dimethoxy-1,1'-binaphthalene



d = 3.421(4) Å; θ = 164.2(3)°

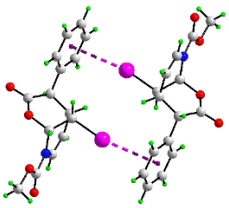
H. Nakazawa, M. Sako, Y. Masui, R. Kurosaki, S. Yamamoto, T. Kamei and T. Shimada, *Org. Lett*., 2019, **21**, 6466-6470; DOI: 10.1021/acs.orglett.9b02358

{Two independent molecules – these associate to form a two-molecule aggregate}

ESI Table 2. Zero-dimensional aggregates sustained by two C–I···π(arene) interactions

18. XIPWOI

4-Methoxycarbonyl-8-phenyl-9-iodo-4-aza-6-oxabicyclo(3.3.1)non-2-en-7-one



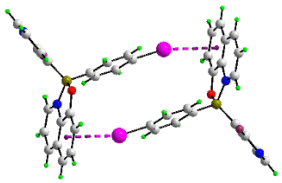
d = 3.500(3) Å; θ = 168.7(2)°

H. Rudler, B. Denise, A. Parlier and J.-C. Daran, *Chem. Commun*., 2002, 940-941; DOI: 10.1039/b201780f

{Molecules self-assemble about a centre of inversion to form a dimeric aggregate}

19. CITSOP

2-(2-Fluoropyridin-3-yl)-2-(4-iodophenyl)-2H-3l5,2l5-[1,3,2]oxazaborolo[5,4,3-ij]quinoline



d = 3.5251(7) Å; θ = 165.28(4)°

G. Wesela-Bauman, P. Ciećwierz, K. Durka, S. Luliński, J. Serwatowski and K.Woźniak *Inorg*. *Chem*. 2013, **52**, 10846-10859; DOI: 10.1021/ic400729t

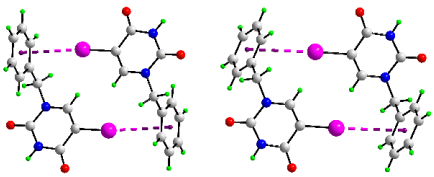
{Centrosymmetrically related molecules associate to form a dimeric aggregate

For variable pressure study, see:

G. Wesela-Bauman, S. Parsons, J. Serwatowski and K. Woźniak, *CrystEngComm*, 2014, **16**, 10780-10790; DOI: 10.1039/C4CE01730G}

20. VIXQUQ

1-Benzyl-5-iodopyrimidine-2,4(1H,3H)-dione



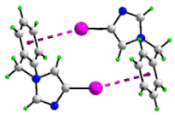
d = 3.566(4) Å; θ = 166.2(3)°; *d* = 3.791(5) Å; θ = 173.8(3)°

A. Valkonen, M. Chucklieb and K. Rissanen, *Cryst. Growth Des*., 2013, **13**, 4769-4775; DOI: 10.1021/cg400924n

{Two independent molecules. Each self-assembles about a centre of inversion into a dimeric aggregate}

21. YADSUU

1-Benzyl-4-iodo-1H-imidazole



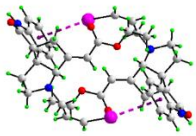
d = 3.5860(9) Å; θ = 161.82(5)°

C. I. Nwachukwu, N. P. Bowling and E. Bosch, *Acta Crystallogr., Sect. C: Cryst. Struct. Chem*., 2017, **73**, 2-8; DOI: 10.1107/S2053229616018702

{Molecules self-assemble about a centre of inversion to form a dimeric aggregate}

22. QOYJUK

(3aS*,5aS*,11bR*)-Ethyl (3-((Z)-3-iodo-2-propen-1-yl)-6-oxo-1,2,3,3a,5,5a,6,7-octahydro-4H-pyrrolo[3',2':2,3]cyclopenta[1,2-c]quinolin-4-ylidene)acetate



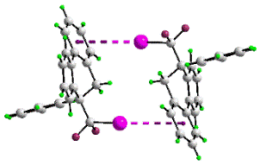
d = 3.6125(12) Å; θ = 161.80(9)°

P. Selig, E. Herdtweck and T. Bach, *Chem. - Eur. J*., 2009, **15**, 3509-3525; DOI: 10.1002/chem.200802383

{The molecules assemble about a centre of inversion into a two-molecule aggregate}

23. CEWCIT

9-[Difluoro(iodo)methyl]-9-phenyl-9,10-dihydrophenanthrene



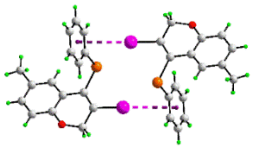
d = 3.621(2) Å; θ = 175.39(8)°

T. Fujita, R. Kinoshita, T. Takanohashi, N. Suzukia and J. Ichikawa, *Beilstein J. Org. Chem.*, 2017, **13**, 2682-2689; DOI: 10.3762/bjoc.13.266

{Two independent molecules. One self-associates about a centre of inversion to form a dimeric aggregate. The second molecule associates in a similar fashion but, the parameters are outside the specified search criteria: *d* = 3.939(2) Å; θ = 157.91(8)°}

24. OGOYEP

3-Iodo-6-methyl-4-(phenylselanyl)-2H-chromene



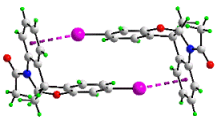
d = 3.626(2) Å; θ = 172.80(13)°

B. Godoi, A. Sperança, D. F. Back, R. Brandão, C. W. Nogueira and G. Zeni, *J. Org. Chem.*, 2009, **74**, 3469-3477; DOI: 10.1021/jo900307k

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

25. CONRUU

1-(3-Iodo-10b-methyl-5a,10b-dihydro-6H-[1]benzofuro[2,3-b]indol-6-yl)ethanone



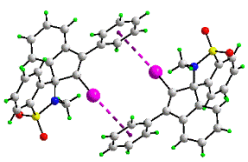
d = 3.6364(9) Å; θ = 160.85(6)°

T. Tomakinian, R. Guillot, C. Kouklovsky and G. Vincent, *Angew. Chem., Int. Ed.*, 2014, **53**, 11881-11885; DOI: 10.1002/anie.201404055

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

26. BOVRIP

2'-Iodo-2-methyl-3'-phenylspiro[1,2-benzothiazole-3,1'-indene] 1,1-dioxide



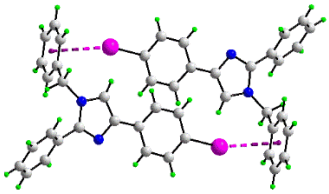
d = 3.6418(16) Å; θ = 161.27(10)°

L. Sun, Y. Zhu, J. Wang, P. Lu and Y. Wang, *Org. Lett*., 2015, **17**, 242-245; DOI: 10.1021/ol503316e

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

27. QAQDOE

1-Benzyl-4-(4-iodophenyl)-2-phenyl-1H-imidazole



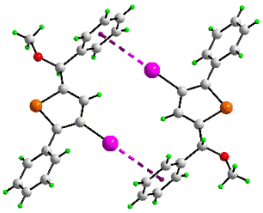
d = 3.656(3) Å; θ = 163.7(2)°

C.-K. Liu, Z. Yang, Y. Zeng, K. Guo, Z. Fang and B. Li, *Org. Chem. Front*., 2017, **4**, 1508-1512; DOI: 10.1039/C7QO00247E

{The molecules assemble about a centre of inversion into a two-molecule aggregate}

28. YACXIM

3-Iodo-5-(methoxy(phenyl)methyl)-2-phenylselenophene



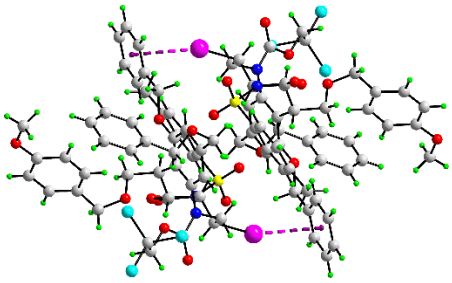
d = 3.662(3) Å; θ = 176.05(10)°

R. P. Pistoia, J. A. Roehrs, D. F. Back and G. Zeni, *Org. Chem. Front*., 2017, **4**, 277-282; DOI: 10.1039/C6QO00491A

{Molecules self-assemble about a centre of inversion to form a dimeric aggregate}

29. QEZGEH

(2R*,3S*,4S*,11S*)-4-Iodo-11-(4-methoxyphenylmethoxymethyl)-3-(p-tosyl)-2-oxo-10-(benzyloxy)-8-(benzyloxymethyl)-6-(2,2,2-trichloroethoxycarbonyl)-2,3,3a,4,5,6,11,11a-octahydro-oxazolo(4,5-d)(1)benzazocine



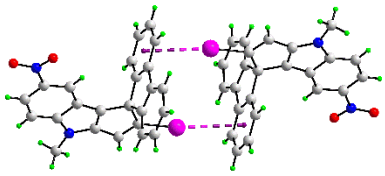
d = 3.6813(15) Å; θ = 161.08(8)°

I. M. Fellows, D. E. Kaelin and S. F. Martin, *J. Am. Chem. Soc*., 2000, **122**, 10781-10787; DOI: 10.1021/ja0013879

{Molecules self-associate about a centre of inversion to form a two-molecule aggregate}

30. TIHGOI

2-Iodo-4-methyl-7-nitro-4H-spiro[cyclopenta[b]indole-1,9'-fluorene]



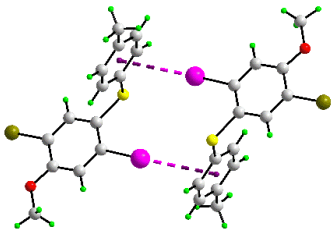
d = 3.687(2) Å; θ = 170.73(14)°

L. Zhang, Y. Zhu, G. Yin, P. Lu and Y. Wang, *J. Org. Chem*., 2012, **77**, 9510-9520; DOI: 10.1021/jo300339a

{Two independent molecules, one self-assembles into a centrosymmetric dimer}

31. BELLAI

1-Bromo-4-iodo-2-methoxy-5-((4-methylphenyl)sulfanyl)benzene



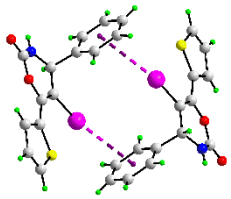
d = 3.7016(12) Å; θ = 168.68(8)°

P. Franzmann, S. B. Beil, P. M. Winterscheid, D. Schollmeyer and S. R. Waldvogel, *Synlett*, 2017, **28**, 957-961; DOI: 10.1055/s-0036-1588140

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

32. TIKRIQ

5-Iodo-4-phenyl-6-(2-thienyl)-3,4-dihydro-2H-1,3-oxazin-2-one



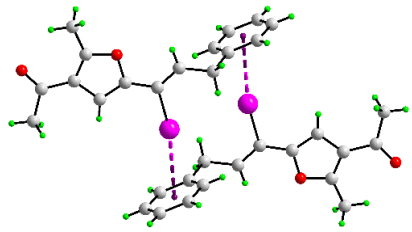
d = 3.7208(18) Å; θ = 161.78(8)°

A. Monleón, G. Blay, L. R. Domingo, M. Carmen Muñoz and J. R. Pedro, *Chem. - Eur. J.*, 2013, **19**, 14852-14860; DOI: 10.1002/chem.201302089

{Molecules self-assemble into a centrosymmetric dimer}

33. KOYJEQ

1-[5-(1-Iodo-3-phenylprop-1-en-1-yl)-2-methylfuran-3-yl]ethan-1-one



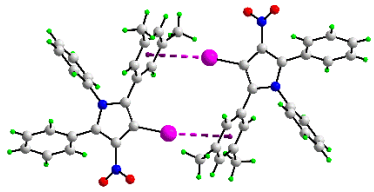
d = 3.7333(14) Å; θ = 165.47(9)°

M. Li, F. Yang, T. Yuan, H. Li, J. Li, Z.-S. Chen and K. Ji, *J. Org. Chem.*, 2019, **84**, 12617-12625; DOI: 10.1021/acs.joc.9b01852

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

34. LIPCEU

2-(3,5-Dimethylphenyl)-3-iodo-4-nitro-1,5-diphenyl-1H-pyrrole



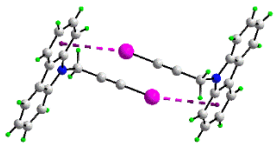
d = 3.735(2) Å; θ = 170.98(9)°

G. Bharathiraja, S. Sakthivel, M. Sengoden and T. Punniyamurthy, *Org. Lett.*, 2013, **15**, 4996-4999; DOI: 10.1021/ol402305b

{The molecules assemble into a centrosymmetric, two-molecule aggregate}

35. TADKAK

N-(3-Iodo-2-propynyl)-carbazole



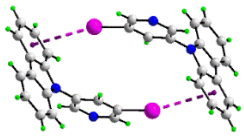
d = 3.735(3) Å; θ = 163.86(11)°

V. E. Shklover, V. A. Igonin, Yu. T. Struchkov, I. R. Golding, N. A. Vasnyova, I. V. Chernoglazova, O. L. Lazareva and A. N. Shchegolikhin, *Mol. Cryst. Liq. Cryst*., 1990, **180B**, 417-423; DOI: org/10.1080/00268949008042222

{Molecules self-assemble into a centrosymmetric dimer}

36. GOYMAL

9-(5-Iodopyridin-3-yl)-9H-carbazole



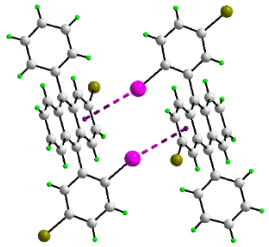
d = 3.741(3) Å; θ = 163.2(2)°

H. Sasabe, Y. Kato, Y. Watanabe, T. Ohsawa, N. Aizawa, W. Fujiwara, Y.-J. Pu, H. Katagiri and J. Kido, *Chem. - Eur. J*., 2019, **25**, 16294-16300; DOI: 10.1002/chem.201903100

{Two independent molecules. One self-associates to form a dimeric aggregate. The second molecule associates in the same way but, with parameters outside of the specified search criteria: *d* = 3.635(3) Å; θ = 145.6(2)°}

37. NICRAU

2-Bromo-10-(5-bromo-2-iodophenyl)-9-phenylanthracene



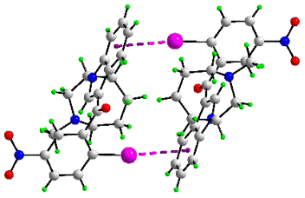
d = 3.762(2) Å; θ = 166.46(13)°

M. Xue, L. Ding, L. Lin, Y. Lu, B. He, Y. Deng, Y. Guo, Y. Hong, J. W. Y. Lam, H. Qiu, Z. Zhao and B. Z. Tang, *Asian J. Org. Chem*., 2012, **1**, 331-335; DOI: 10.1002/ajoc.201200111

{Centrosymmetrically related molecules assemble into a two-molecule aggregate}

38. MIMKUQ

(2-Iodo-5-nitrophenyl)(1-(1-methylazepan-3-yl)-1H-indol-3-yl)methanone



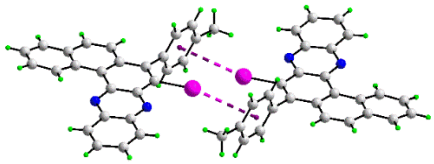
d = 3.766(2) Å; θ = 165.89(8)°

Z.-W. Li, J.-S. Li, S.-Y. Kang, W.-D. Liu, D.-X. Wua and Z. Cao, *Chin. J. Struct. Chem*., 2013, **32**, 1100-1104.

{The centrosymmetrically related molecules assemble into a two-molecule aggregate}

39. OTENUY

8-Iodo-7-(4-methylphenyl)naphtho[1,2-a]phenazine



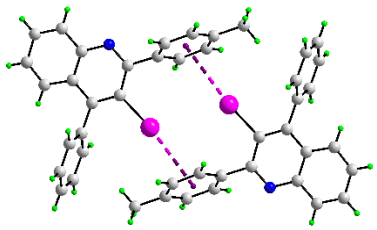
d = 3.7678(8) Å; θ = 166.82(4)°

A. V. Gulevskaya, *Eur. J. Org. Chem*., 2016, 4207-4214; DOI: 10.1002/ejoc.201600660

{The molecules assemble about a centre of inversion to form a two-molecule aggregate}

40. IVIMUW

3-Iodo-2-(4-methylphenyl)-4-phenylquinoline



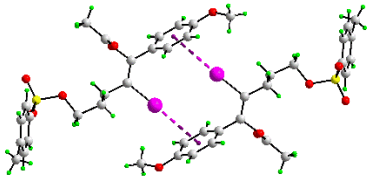
d = 3.776(2) Å; θ = 164.15(11)°

S. Ali, H.-T. Zhu, X.-F. Xia, K.-G. Ji, Y.-F. Yang, X.-R. Song and Y.-M. Liang, *Org. Lett*., 2011, **13**, 2598-2601; DOI: 10.1021/ol2007154

{Two molecules associate about a centre of inversion to form a two-molecule aggregate}

41. VALQOQ

2-Iodo-1-(4-methoxyphenyl)-5-(((4-methylphenyl)sulfonyl)oxy)pent-1-en-1-yl acetate



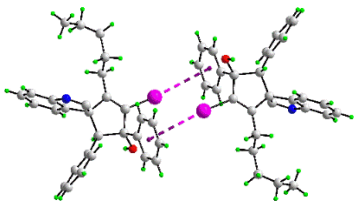
d = 3.787(4) Å; θ = 160.34(13)°

N. Okamoto, Y. Miwa, H. Minami, K. Takeda and R. Yanada, *J. Org. Chem*., 2011, **76**, 9133-9138; DOI: 10.1021/jo201609r

{Molecules associate about a centre of inversion to form a two-molecule aggregate}

42. GOZJEN

4-Iodo-5-pentyl-2,3-diphenylspiro[cyclopent-4-ene-1,3'-indol]-3-ol



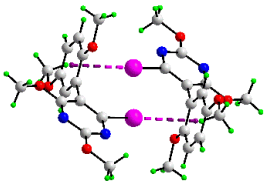
d = 3.820(3) Å; θ = 168.94(15)°

S. Yaragorla, D. Bag and R. Dada, *Eur. J. Org. Chem.*, 2019, **2019**, 6983-6988; DOI: 10.1002/ejoc.201901393

{Two independent molecules. One self-associates to form a dimeric aggregate about a centre of inversion}

43. TIPQAM

5-(2,5-Dimethoxyphenyl)-4-iodo-2,6-dimethoxypyrimidine



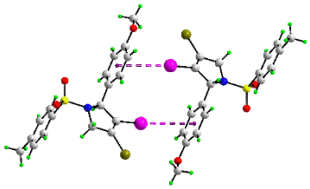
d = 3.833(2) Å; θ = 174.93(14)°

R. R. Kadiyala, D. Tilly, E. Nagaradja, T. Roisnel, V. E. Matulis, O. A. Ivashkevich, Y. S. Halauko, F. Chevallier, P. C. Gros and F. Mongin, *Chem. - Eur. J.*, 2013, **19**, 7944-7960; DOI: 10.1002/chem.201300552

{Molecules self-assemble into a centrosymmetric dimer}

44. LAKTIC

4-Bromo-3-iodo-2-(4-methoxyphenyl)-1-((4-methylphenyl)sulfonyl)-2,5-dihydro-1H-pyrrole



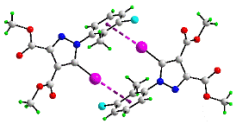
d = 3.835(3) Å; θ = 163.71(11)°

K.-G. Ji, H.-T. Zhu, F. Yang, A. Shaukat, X.-F. Xia, Y.-F. Yang, X.-Y. Liu and Y.-M. Liang, *J. Org. Chem.*, 2010, **75**, 5670-5678; DOI: 10.1021/jo101085f

{The molecules assemble into a centrosymmetric, two-molecule aggregate}

45. TOSCIQ

Dimethyl 1-(3-chloro-2-methylphenyl)-5-iodo-1H-pyrazole-3,4-dicarboxylate



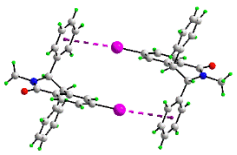
d = 3.837(3) Å; θ = 161.18(19)°

M. M. Popa, I. C. Man, C. Draghici, S. Shova, M. R. Caira, F. Dumitrascu and D. Dumitrescu, *CrystEngComm*, 2019, **21**, 7085-7093; DOI: 10.1039/C9CE01263J

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

46. CEXJUM

6-Iodo-2-methyl-trans-3,4-diphenyl-3,4-dihydroisoquinolin-1(2H)-one



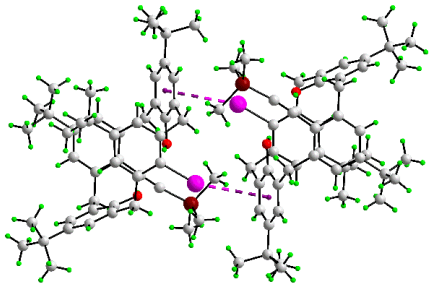
d = 3.857(3) Å; θ = 172.41(15)°

Q. Tang, D. Xia, X. Jin, Q. Zhang, X.-Q. Sun and C. Wang, *J. Am. Chem. Soc*., 2013, **135**, 4628-4631; DOI: 10.1021/ja400020e

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

47. CAZYIM

5,11,17,23-Tetra-t-butyl-25,27-dihydroxy-28-iodo-26-(2-(trimethylsilyl)ethynyl)calix(4)arene chloroform solvate



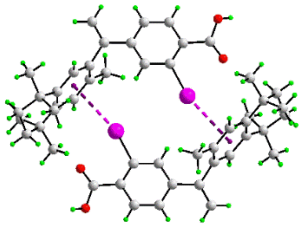
d = 3.857(2) Å; θ = 160.46(13)°

H. Al-Saraierh, D. O. Miller and P. E. Georghiou, *J. Org. Chem*., 2005, **70**, 8273-8280; DOI: 10.1021/jo050488s

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

48. DEGWUJ

2-Iodo-4-(1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)vinyl)benzoic acid



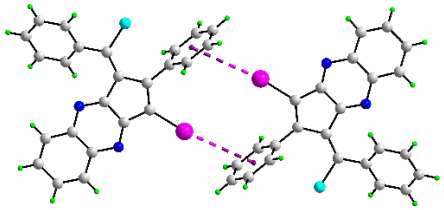
d = 3.862(2) Å; θ = 163.38(15)°

J. K. Furmick, I. Kaneko, A. N. Walsh, J. Yang, J. S. Bhogal, G. M. Gray, J. C. Baso, D. O. Browder, J. L. S. Prentice, L. A. Montano, C. C. Huynh, L. M. Marcus, D. G. Tsosie, J. S. Kwon, A. Quezada, N. M. Reyes, B. Lemming, P. Saini, A. van der Vaart, T. L. Groy, P. A. Marshall, P. W. Jurutka and C. E. Wagner, *ChemMedChem*, 2012, **7**, 1551-1556; DOI: 10.1002/cmdc.201290042

{Molecules associate about a centre of inversion to form a two-molecule aggregate}

49. XEYLEU

1-(Chloro(phenyl)methylene)-3-iodo-2-phenyl-1H-cyclopenta[b]quinoxaline



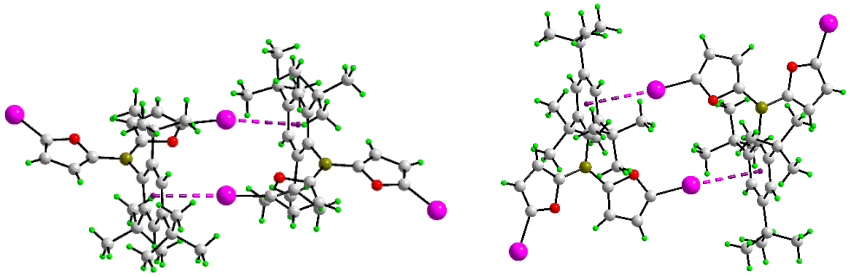
d = 3.8785(7) Å; θ = 168.70(5)°

A. V. Gulevskaya, R. Yu. Lazarevich and A. F. Pozharskii, *Tetrahedron*, 2013, **69**, 910-917; DOI: 10.1016/j.tet.2012.10.098

{Molecules self-assemble about a centre of inversion to form a dimeric aggregate}

50. QEYVOI

bis(5-Iodofuran-2-yl)(2,4,6-tri-t-butylphenyl)borane



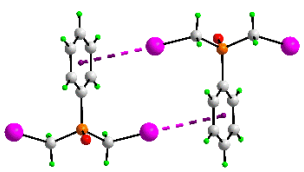
d = 3.4830(15) Å; θ = 174.67(12)° and *d* = 3.4948(14) Å; θ = 164.56(11)°; *d* = 3.6428(15) Å; θ = 172.29(11)°

N. A. Riensch, L. Fritze, T. Schindler, M. Kremer and H. Helten, *Dalton Trans*., 2018, **47**, 10399-10403; DOI: 10.1039/C8DT01716F

{Three independent molecules comprise the asymmetric unit. Two associate via two contacts to form a two-molecule aggregate, while the other self-associates (third entry; right-hand image) over a centre of inversion to form a two-molecule aggregate}

51. VIKHOP

bis(Iodomethyl)phenylphosphine oxide



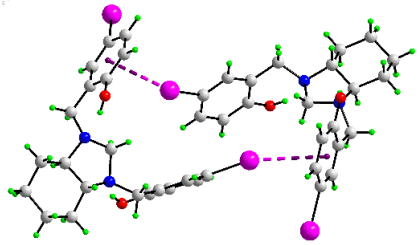
d = 3.6983(19) Å; θ = 170.77(12)°

M. A. Stevens, F. H. Hashim, E. S. H. Gwee, E. I. Izgorodina, R. E. Mulvey and V. L. Blair, *Chem. - Eur. J.*, 2018, **24**, 15669-15677; DOI: 10.1002/chem.201803477

{Molecules associate about a centre of inversion to form a two-molecule aggregate}

52. AYOVEQ

2-((3-[(2-Hydroxy-5-iodophenyl)methyl]-octahydro-1H-1,3-benzodiazol-1-yl)methyl)-4-iodophenol



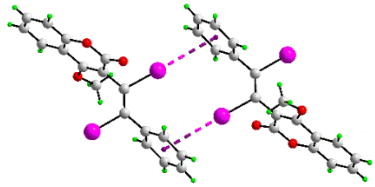
d = 3.710(3) Å; θ = 162.5(3)°

A. Rivera, D. Quiroga, J. Rios-Motta, K. Fejfarová and M.Dusek, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2011, **67**, o2256; DOI: 10.1107/S1600536811030054

{Molecules self-associate about a 2-fold axis to form a dimeric aggregate}

53. EMUZIW

3-(1,2-Diiodo-2-phenylvinyl)-4-methoxy-2H-chromen-2-one



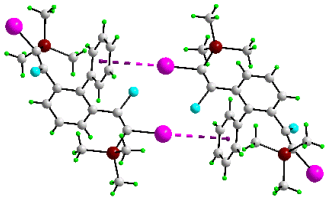
d = 3.737(2) Å; θ = 178.94(11)°

G. Raffa, S. Belot, G. Balme and N. Monteiro, *Org. Biomol. Chem.*, 2011, **9**, 1474-1478; DOI: 10.1039/c0ob00935k

{Two independent molecules. One self-associates about a centre of inversion to form a two-molecule aggregate; the other does not form analogous interactions}

54. OPUWED

(Biphenyl-2,6-diylbis(2-chloro-1-iodoethene-2,1-diyl))bis(trimethylsilane)



d = 3.8018(6) Å; θ = 174.44(4)°

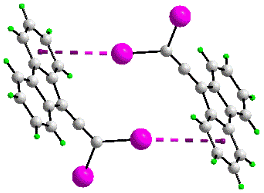
K. C. Sproul and W. A. Chalifoux, *Org. Lett*., 2015, **17**, 3334-3337; DOI:

10.1021/acs.orglett.5b01558

{The molecules assemble about a centre of inversion to form a two-molecule aggregate}

55. ZEFNIK

9-(Diiodoethenylidene)-9H-fluorene



d = 3.823(3) Å; θ = 173.0(2)°

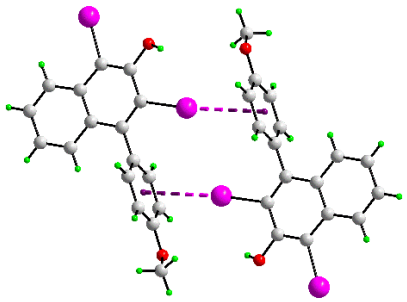
N. Gulia, B. Pigulski and S. Szafert, *Arkivoc*, 2017, **18**, 191-204; DOI:

10.3998/ark.5550190.p010.133

{Two independent molecules. One self-assembles about a centre of inversion to form a dimeric aggregate}

56. BUCTOK

1,3-Diiodo-4-(4-methoxyphenyl)-2-naphthol



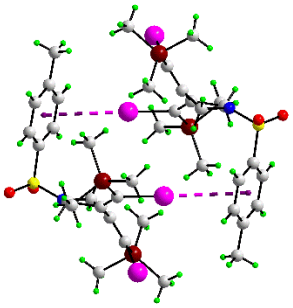
d = 3.8381(14) Å; θ = 169.42(8)°

P. B. Koswatta, J. Das, M. Yousufuddin and C. J. Lovely, *Eur. J. Org .Chem*., 2015, 2603-2613; DOI: 10.1002/ejoc.201403650

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

57. WUFLUE

3,4-bis(Trimethylsilyl(iodo)methylene)-N-tosylpyrrolidine



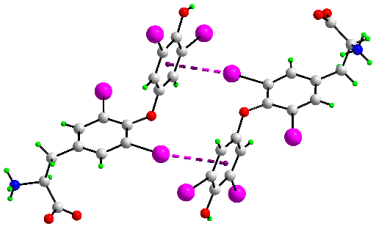
d = 3.8444(14) Å; θ = 166.57(10)°

N. Y. Yamamoto, T. Ohno and K. Itoh, *Chem. - Eur. J*., 2002, **8**, 4734-4741; DOI: 10.1002/1521-3765(20021018)8:20<4734::AID-CHEM4734>3.0.CO;2-B

{Molecules self-assemble about a 2-fold axis of symmetry to form a dimeric aggregate}

58. ZUQMIJ

2-Ammonio-3-(4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodophenyl)propanoate hydrate



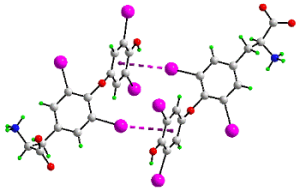
d = 3.443(3) Å; θ = 170.5(2)°; *d* = 3.457(3) Å; θ = 167.6(2)°

S. Mondal and G. Mugesh, *Angew. Chem., Int. Ed*., 2015, **54**, 10833-10837; DOI: 10.1002/anie.201505281

{Two independent iodo-molecules comprise the asymmetric unit and are connected into a non-symmetric, two-molecule aggregate, cf. **ZUQMOP**}

59. ZUQMOP

2-Ammonio-3-(4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodophenyl)propanoate tetrahydrate



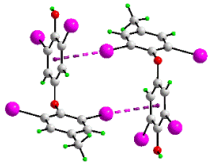
d = 3.476(3) Å; θ = 168.6(3)°; *d* = 3.489(3) Å; θ = 168.6(3)°

S. Mondal and G. Mugesh, *Angew. Chem., Int. Ed*., 2015, **54**, 10833-10837; DOI: 10.1002/anie.201505281

{Two independent iodo-molecules comprise the asymmetric unit and are connected into a non-symmetric, two-molecule aggregate, cf. **ZUQMIJ**}

60. GAPWUP

4'-Hydroxy-4-methyl-2,3',5',6-tetraiodophenol ether



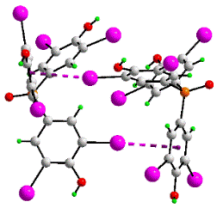
d = 3.634(3) Å; θ = 164.44(18)°

K. Prout, J. Fail, R. M. Jones, R. E. Warner and J. C. Emmett, *J. Chem. Soc., Perkin Trans. 2*, 1988, 265-284; DOI: 10.1039/p29880000265

{Molecules self-associate about a centre of inversion to form a dimeric aggregate}

61. WAMBOE

4,4',4''-Phosphoryltris(2,6-diiodophenol) dimethyl sulfoxide solvate



d = 3.522(3) Å; θ = 172.06(19)°

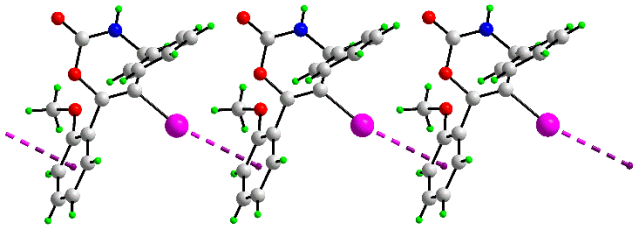
N. A. Bewick, A. Arendt, Y. Li, S. Szafert, T. Lis, K. A. Wheeler, J. Young, R. Dembinski and *Curr. Org. Chem*. 2015, **19**, 469-474; DOI: 10.2174/1385272819666141231000247

{Molecules self-assemble about a 2-fold axis of symmetry to form a dimeric aggregate}

ESI Table 3. Linear, one-dimensional chains sustained by C–I···π(arene) interactions

62. TIKREM

5-Iodo-6-(2-methoxyphenyl)-4-phenyl-3,4-dihydro-2H-1,3-oxazin-2-one



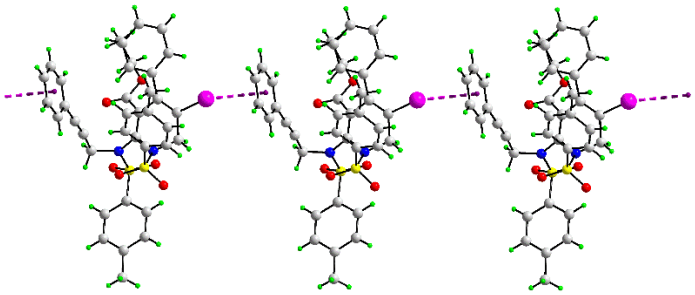
d = 3.513(2) Å; θ = 165.43(12)°

A. Monleón, G. Blay, L. R. Domingo, M. Carmen Muñoz and J. R. Pedro, *Chem. - Eur. J.*, 2013, **19**, 14852-14860; DOI: 10.1002/chem.201302089

{Molecules self-assemble into a linear chain}

63. HEWMUU

Ethyl 5-iodo-1-[(4-methylphenyl)sulfonyl]-2-{[(4-methylphenyl)sulfonyl](3-phenylprop-2-yn-1-yl)amino}-4-phenyl-1,6-dihydropyridine-3-carboxylate



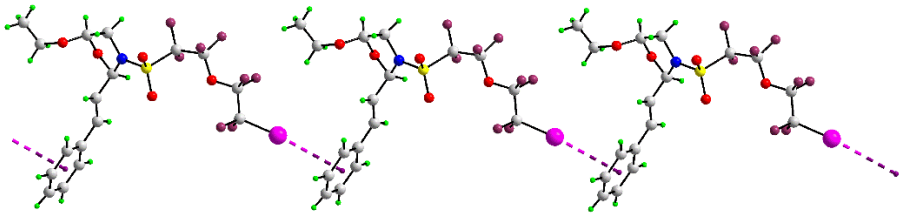
d = 3.5790(15) Å; θ = 161.35(9)°

S. Nayak, B. Prabagar, N. Ghosh, R. K. Mallick and A. K. Sahoo, *Synthesis*, 2017, **49**, 4261-4271; DOI: 10.1055/s-0036-1588841

{Molecules assemble to form a linear chain}

64. PARCUH

syn-5-Ethoxy-2-styryl-3-(1,1,2,2-tetrafluoro-2-(1,1,2,2-tetrafluoro-2-iodoethoxy)ethanesulfonyl)oxazolidine



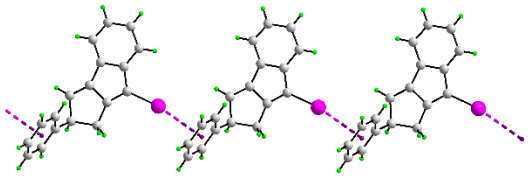
d = 3.609(3) Å; θ = 167.4(3)°

P. He and S. Zhu, *Tetrahedron*, 2005, **61**, 6088-6096; DOI: 10.1016/j.tet.2005.04.020

{Molecules are connected into a linear chain}

65. TIMDUQ

8-Iodo-2-phenyl-1,2-dihydrocyclopenta[a]indene



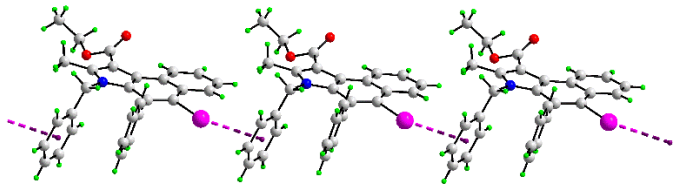
d = 3.6189(16) Å; θ = 160.33(11)°

P. Nösel, T. Lauterbach, M. Rudolph, F. Rominger and A. S. K. Hashmi, *Chem. - Eur. J.*, 2013, **19**, 8634-8641; DOI: 10.1002/chem.201300507

{Molecules self-assemble into a linear chain}

66. VUVVUF

Ethyl 3-benzyl-5-iodo-2-methyl-4-phenyl-3H-benzo[e]indole-1-carboxylate



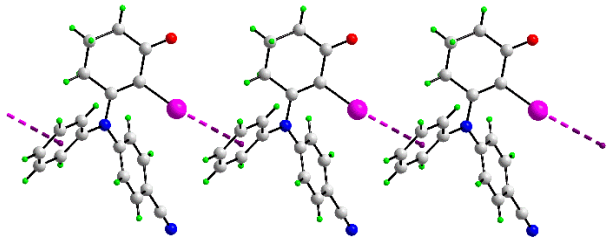
d = 3.626(2) Å; θ = 162.67(11)°

G. M. Martins, G. Zeni, D. F. Back, T. S. Kaufman and C. C. Silveira, *Adv. Synth. Catal.*, 2015, **357**, 3255-3261; DOI: 10.1002/adsc.201500275

{Two independent molecules. One associates into a linear chain. The second molecule does the same but with parameters outside the search limits: *d* = 3.7618(17) Å; θ = 153.37(10)°}

67. FAVYAF

4-[(2-Iodo-3-oxocyclohex-1-en-1-yl)(phenyl)amino]benzonitrile



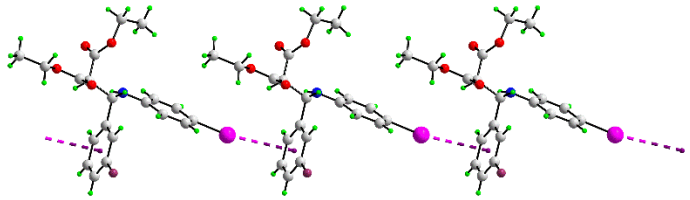
d = 3.6363(14) Å; θ = 165.48(6)°

D. Bhattacherjee, V. Thakur, A. Shil and P. Das, *Adv. Synth. Catal*., 2017, **359**, 2202-2208; DOI: 10.1002/adsc.201700004

{Molecules associate to form a linear chain}

68. ZIMKOY

Diethyl {(3-fluorophenyl)[(4-iodophenyl)amino]methyl}propanedioate



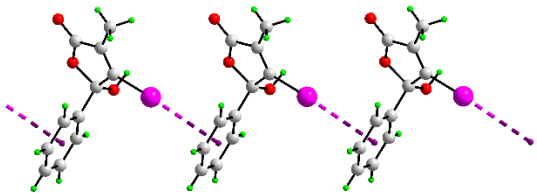
d = 3.6473(11) Å; θ = 163.29(6)°

M. Hussain, J. Liu, Z. Zhang, M. Hu, Y. Li and X. Min, *Chem. Sel*., 2018, **3**, 8787-8792; DOI: 10.1002/slct.201801064

{Molecules self-assemble to form a linear chain}

69. AVAKIR

3-Methyl-4-iodo-5-phenyl-5-hydroxy-2(5H)-furanone



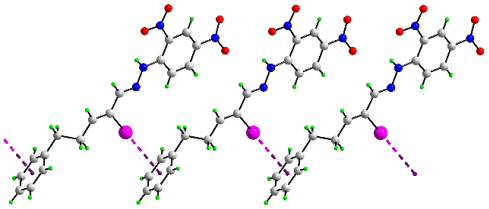
d = 3.661(3) Å; θ = 172.66(15)°

S. Ma, B. Wu and Z. Shi, *J. Org. Chem*., 2004, **69**, 1429-1431; DOI: 10.1021/jo0355698

{Molecules self-associate to form a linear chain}

70. WELWIV

1-(2,4-Dinitrophenyl)-2-(2-iodo-5-phenylpent-2-en-1-ylidene)hydrazine



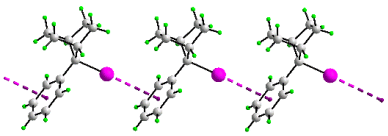
d = 3.6701(18) Å; θ = 161.01(8)°

M. Wang, C. Fu and S. Ma, *Chem. Sci*., 2013, **4**, 1016-1022; DOI: 10.1039/c2sc21920d

{Molecules self-assemble into a linear chain}

71. TUFXEZ

7-iodo-7-phenylbicyclo[2.2.1]heptane



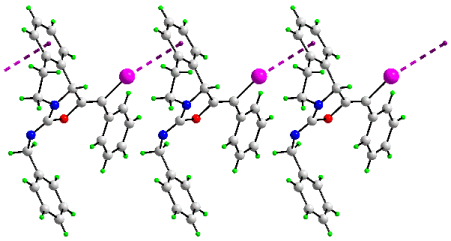
d = 3.681(5) Å; θ = 178.27(14)°

T. Montoro, G. Tardajos, A. Guerrero, M. del R. Torres, C. Salgado, I. Fernández and J. O. Barcina, *Org. Biomol. Chem*., 2015, **13**, 6194-6202; DOI: 10.1039/C5OB00366K

{Molecules self-assemble into a linear chain}

72. CAJZUL

N-Benzyl-1-(iodo(phenyl)methylene)-1,5,6,10b-tetrahydro[1,3]oxazolo[4,3-a]isoquinolin-3-imine



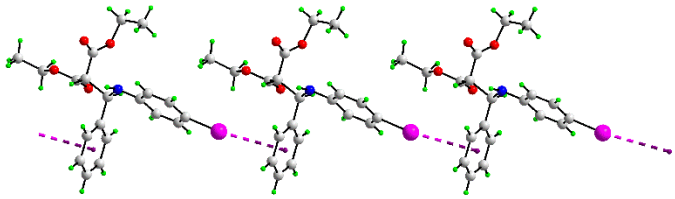
d = 3.6967(10) Å; θ = 167.42(6)°

C. Madaan, S. Saraf, G. Priyadarshani, P. P. Reddy, S. K. Guchhait, A. C. Kunwar and B. Sridhar, *Synlett*, 2012, **23**, 1955-1959; DOI: 10.1055/s-0032-1316606

{Molecules self-associate into a linear chain}

73. ZIMKUE

Diethyl {[(4-iodophenyl)amino](phenyl)methyl}propanedioate



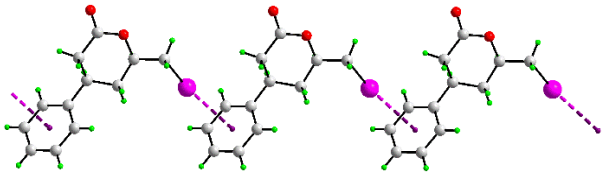
d = 3.7031(12) Å; θ = 161.27(6)°

M. Hussain, J. Liu, Z. Zhang, M. Hu, Y. Li and X. Min, *Chem. Sel*., 2018, **3**, 8787-8792; DOI: 10.1002/slct.201801064

{Molecules self-assemble to form a linear chain}

74. YAKXOY

cis-(4R,6R)-6-Iodomethyl-4-phenyltetrahydro-2H-pyran-2-one



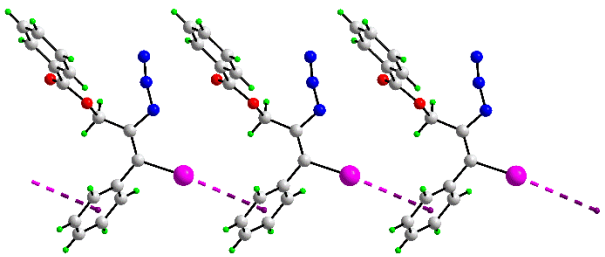
d = 3.7316(9) Å; θ = 172.86(6)°

S. M. Allin, M. Essat, C. H. Pita, R. D. Baird, V. McKee, M. Elsegood, M. Edgar, D. M. Andrews, P. Shah and I. Aspinall, *Org. Biomol. Chem*., 2005, **3**, 809-815; DOI: 10.1039/b416179c

{Molecules self-assemble to form a linear chain}

75. JOYXAY

(Z)-2-Azido-3-iodo-3-phenylprop-2-en-1-yl benzoate



d = 3.785(2) Å; θ = 172.87(11)°

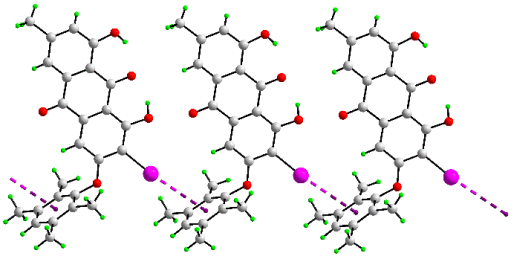
N. Okamoto, T. Sueda, H. Minami, Y. Miwa and R. Yanada, *Org. Lett*., 2015, **17**, 1336-1339;

DOI: 10.1021/acs.orglett.5b00395

{Molecules associate into a linear chain}

76. ATEQIZ

1,8-Dihydroxy-2-iodo-6-methyl-3-(2,3,5,6-tetramethylphenoxy)anthraquinone



d = 3.8431(18) Å; θ = 161.49(12)°

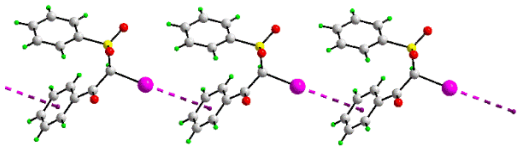
K. S. Daub, B. Habermann, T. Hahn, L. Teich and K. Eger, *Eur. J. Org. Chem*., 2004, 894-898;

DOI: 10.1002/ejoc.200300317

{Molecules self-associate to form a linear chain}

77. DUKWIP

2-Iodo-2-phenylsulfonyl-1-phenylethanone



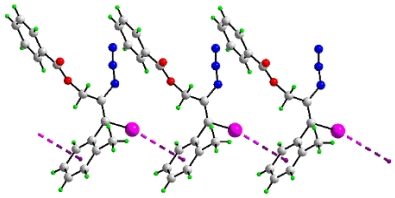
d = 3.857(4) Å; θ = 175.71(18)°

S. C. Kokkou and C. J. Cheer, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun*., 1986, **42**, 1074-1076; DOI: 10.1107/S0108270186093423

{Molecules associate into a linear chain}

78. JOYWUR

(Z)-2-Azido-3-iodo-3-(2-methylphenyl)prop-2-en-1-yl benzoate



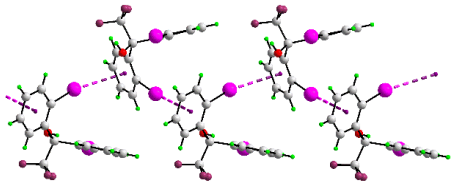
d = 3.869(6) Å; θ = 160.94(14)°

N. Okamoto, T. Sueda, H. Minami, Y. Miwa and R. Yanada, *Org. Lett*., 2015, **17**, 1336-1339; DOI: 10.1021/acs.orglett.5b00395

{Molecules associate into a linear chain}

79. YOYLAA

2,2,2-Trifluoro-1,1-bis(2-iodophenyl)ethanol



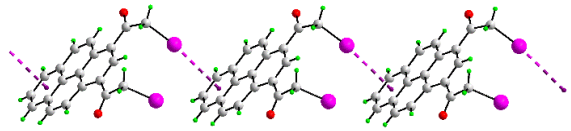
d = 3.516(4) Å; θ = 161.0(2)°; *d* = 3.620(4) Å; θ = 174.0(2)°

S. Matsukawa, H. Yamamichi, Y. Yamamoto and K. Ando, *J. Am. Chem. Soc*., 2009, **131**, 3418-3419; DOI: 10.1021/ja808113q

{Two independent molecules each form an acceptor and a donor contact to assemble into a linear, supramolecular chain}

80. UVECEF

1,1'-Pyrene-1,3-diylbis(2-iodoethanone)



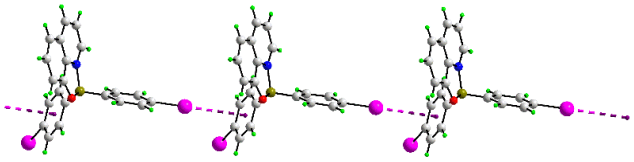
d = 3.647(3) Å; θ = 165.41(19)°

P. S. Salini, S. K. Rajagopal and M. Hariharan, *Cryst. Growth Des*., 2016, **16**, 5822-5830; DOI: 10.1021/acs.cgd.6b00919

{Molecules self-assemble into a linear chain}

81. KOLGUO

bis(4-Iodophenyl)-(8-quinolinolato-N)-boron



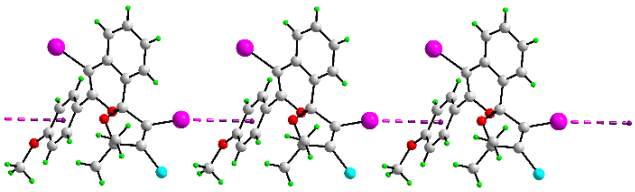
d = 3.665(3) Å; θ = 168.76(16)°

Y. Nagata and Y. Chujo, *Macromolecules*, 2008, **41**, 2809-2813; DOI: 10.1021/ma7025918

{Two independent molecules comprise the asymmetric unit. One of these assembles into a linear chain}

82. JODVAB

4-Chloro-3,4'-diiodo-3'-(4-methoxyphenyl)-5,5-dimethyl-5H-spiro[furan-2,1'-isochromene]



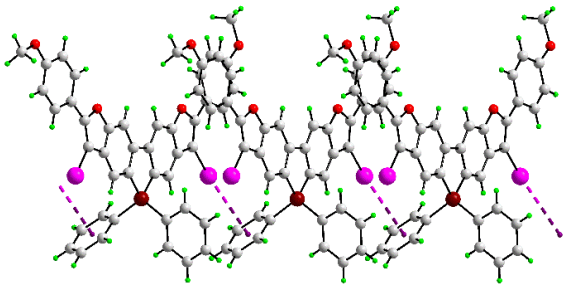
d = 3.796(3) Å; θ = 165.15(18)°

J. Wang, H.-T. Zhu, Y.-X. Li, L.-J. Wang, Y.-F. Qiu, Z.-H. Qiu, M. Zhong, X.-Y. Liu and Y.-M. Liang, *Org. Lett*., 2014, **16**, 2236-2239; DOI: 10.1021/ol500741a

{Molecules associate into a linear chain}

83. WIYPEB

3,7-Diiodo-2,8-bis(4-methoxyphenyl)-5,5-diphenyl-5H-furo[2',3':5,6][1]benzosilolo[2,3-f][1]benzofuran chloroform solvate



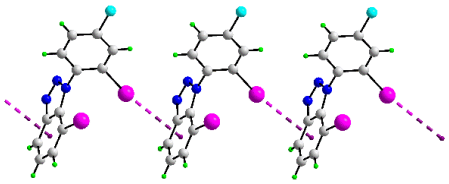
d = 3.8008 Å; θ = 162.08(7)°

L. Li, S. Li, C.-H. Zhao and C. Xu, *Eur. J. Inorg. Chem*., 2014, 1880-1885; DOI: 10.1002/ejic.201400061

{Molecules self-assemble into a linear chain}

84. XIZSAC

1-(4-Chloro-2-iodophenyl)-7-iodo-1H-benzotriazole



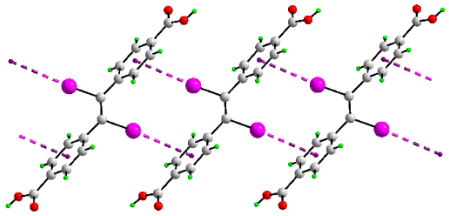
d = 3.824(3) Å; θ = 160.26(19) °

E. Nagaradja, F. Chevallier, T. Roisnel, V. Dorcet, Y. S. Halauko, O. A. Ivashkevich, V. E. Matulis and F. Mongin, *Org. Biomol. Chem*., 2014, **12**, 1475-1487; DOI: 10.1039/C3OB42380H

{Molecules self-assemble into a linear chain}

85. RUKFUA

4,4'-(1,2-Di-iodoethene-1,2-diyl)dibenzoic acid dimethyl sulfoxide solvate



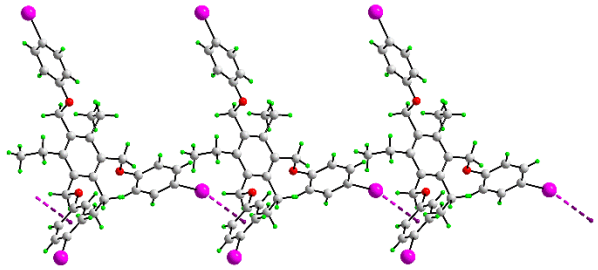
d = 3.7195(16) Å; θ = 167.13(11)°

R. J. Marshall, S. L. Griffin, C. Wilson and R. S. Forgan, *J. Am. Chem. Soc*., 2015, **137**, 9527-9530; DOI: 10.1021/jacs.5b05434

{The molecule is disposed about a centre of inversion. Each of the iodide participates in a connection to form a linear chain}

86. YASRAN

1,3,5-Triethyl-2,4,6-tris((4-iodophenoxy)methyl)benzene m-xylene solvate



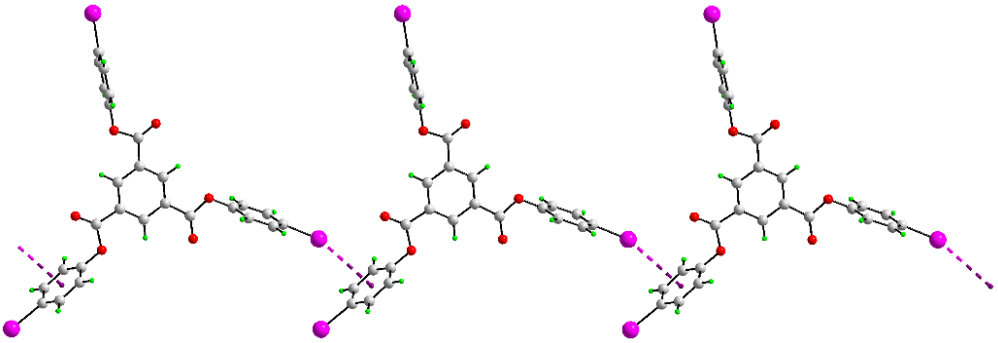
d = 3.664(4) Å; θ = 161.4(3)°

S. Bhattacharya and B. K. Saha, *Cryst. Growth Des*., 2012, **12**, 169-178; DOI: 10.1021/cg2009144

{Molecules self-assemble to form a linear chain. In the solvent-free form [**YASQIU03**, No. **15**], a two-molecule aggregate via a single interaction is observed}

87. WOHXEX

tris(4-Iodophenyl) benzene-1,3,5-tricarboxylate tris(chloroform) clathrate



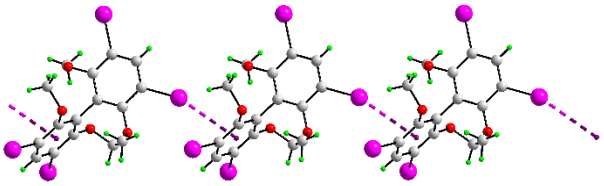
d = 3.717(4) Å; θ = 160.82(15)°

F. C. Pigge, V. R. Vangala, P. P. Kapadia, D. C. Swenson and N. P. Rath, *Chem. Commun*., 2008, 4726-4728; DOI: 10.1039/b809592b

{Molecules self-assemble into a linear chain. Each of the remaining two iodide atoms also form contacts but, outside the specified geometric criteria: *d* = 3.745(3) Å; θ = 157.46(16)°; *d* = 3.776(3) Å; θ = 158.3(2)°. When these extra interactions are taken into account, a flat, two-dimensional array is realised. See **16**, **WOHHAT** for a two-molecule aggregate sustained by a single interaction}

88. RALDOY

3,3',5,5'-Tetraiodo-2,2',6,6'-tetramethoxy-1,1'-biphenyl



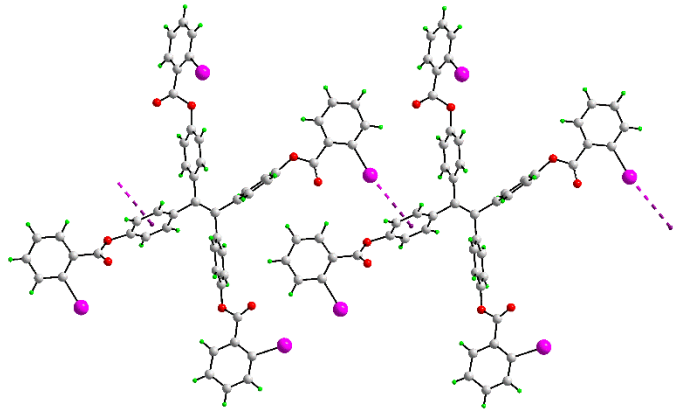
d = 3.680(3) Å; θ = 160.82(15)°

T. Zimmermann, R. Gompper, K. Polborn, J. G. Malecki, Private Communication to the Cambridge Structural Database, Refcode RALDOY, 2005.

{Molecules are connected into a linear chain}

89. DAVXAB

Ethene-1,1,2,2-tetrayltetra-4,1-phenylene tetrakis(2-iodobenzoate)



d = 3.837(4) Å; θ = 169.4(2)°

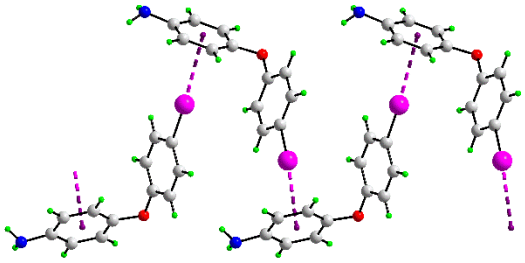
P. P .Kapadia, D. C. Swenson and F. C. Pigge, *Cryst. Growth Des*., 2012, **12**, 698-706; DOI: 10.1021/cg200986v

{Two independent molecules. One of these self-associate to form a linear chain. Analogous interactions are noted for the second molecule but, with parameters outside the search criteria: *d* = 3.976(4) Å; θ = 134.9(2)°}

ESI Table 4. Zig-zag, one-dimensional chains sustained by C–I···π(arene) interactions

90. FANYOJ

4-(4-(Iodo)phenoxy)aniline



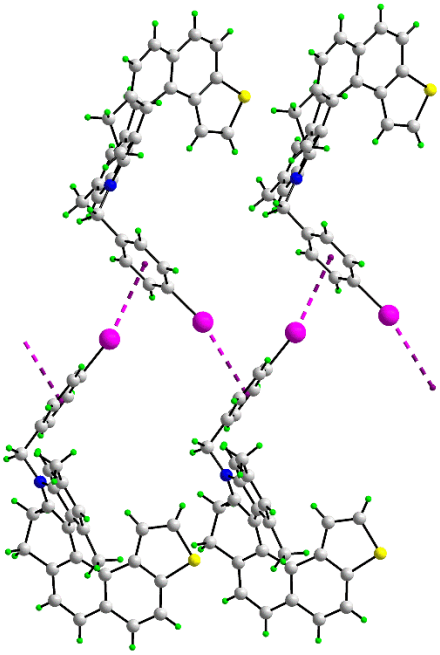
d = 3.5100(16) Å; θ = 171.39(12)°

A. Dey and G. R. Desiraju, *CrystEngComm*, 2004, **6**, 642-646; DOI: 10.1039/b416962j

{Molecules associate to form a zig-zag (glide-symmetry) chain}

91. GULLEG

(M)-7-(4-Iodobenzyl)-9,11-dimethyl-6,7-dihydro-5H-thieno[2',3':7,8]naphtho[2,1-c]carbazole



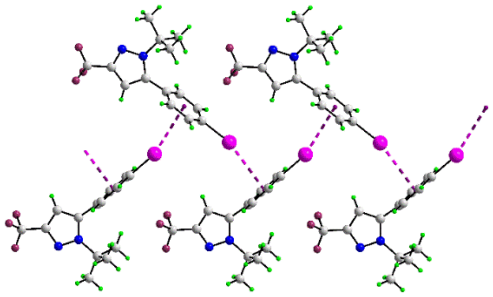
d = 3.5752(16) Å; θ = 165.91(9)°

L. Kötzner, M. J. Webber, A. Martińez, C. De Fusco and B. List, *Angew. Chem., Int. Ed.*, 2014, **53**, 5202-5205; DOI: 10.1002/anie.201400474

{Molecules associate to form a zig-zag (glide-symmetry) chain}

92. DOJDEN

1-t-Butyl-5-(4-iodophenyl)-3-(trifluoromethyl)-1H-pyrazole



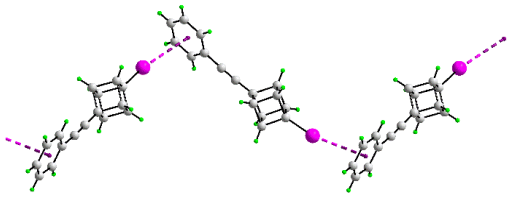
d = 3.5787(15) Å; θ = 163.74(11)°

M. A. P. Martins, C. P. Frizzo, A. C. L. Martins, A. Z. Tier, I. M. Gindri, A. R. Meyer, H. G. Bonacorso and N. Zanatta, *RSC Adv.*, 2014, **4**, 44337-44349; DOI: 10.1039/C4RA06040G

{The molecule has mirror symmetry. Molecules associate to form a zig-zag (glide-symmetry) chain}

93. QOCTIO

1-Iodo-4-(phenylethynyl)cubane



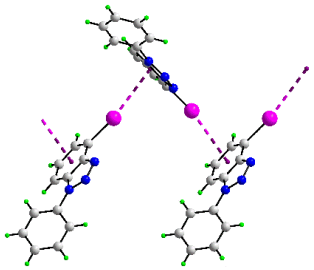
d = 3.6497(8) Å; θ = 167.29(4)°

K. Flanagan, S. S. R. Bernhard, S. Plunkett and M. O. Senge, *Chem. - Eur. J.*, 2019, **25**, 6941-6954; DOI: 10.1002/chem.201806432

{The molecules assemble into a zig-zag (glide-symmetry) chain}

94. XOBJEF

4-Iodo-1-phenyl-1H-benzotriazole



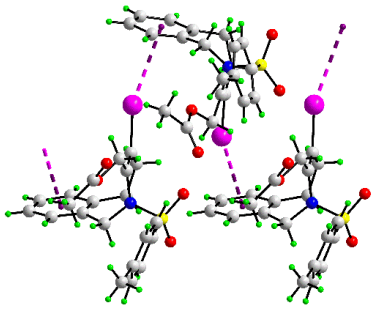
d = 3.6589(9) Å; θ = 169.09(6)°

E. Nagaradja, F. Chevallier, T. Roisnel, V. Dorcet, Y. S. Halauko, O. A. Ivashkevich, V. E. Matulis and F. Mongin, *Org. Biomol. Chem*., 2014, **12**, 1475-1487; DOI: 10.1039/C3OB42380H

{Molecules self-assemble into a zig-zag (glide-symmetry) chain}

95. FIQHEU

(4-Iodo-2-((4-methylphenyl)sulfonyl)-1,2,5,6-tetrahydro-2-benzazocin-3-yl)methyl acetate



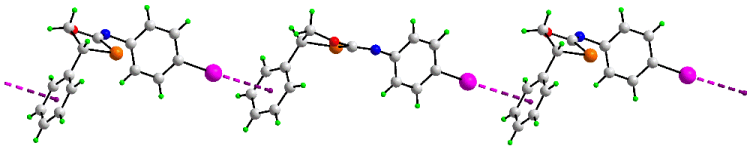
d = 3.665(3) Å; θ = 162.0(2)°

K. Igawa, T. Kawabata, R. Ni and K. Tomooka, *Chem. Lett*., 2013, **42**, 1374-1376; DOI: 10.1246/cl.130735

{Molecules associate to form a zig-zag (glide-symmetry) chain}

96. FEBZIX

(Z)-4-Iodo-N-(4-phenyl-1,3-oxaselenolan-2-ylidene)aniline



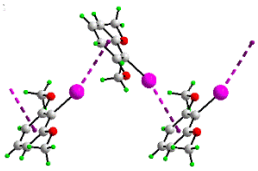
d = 3.682(4) Å; θ = 170.7(3)°

M. Sengoden and T. Punniyamurthy, *RSC Adv*., 2012, **2**, 2736-2738; DOI: 10.1039/c2ra00042c

{Molecules associate to form a zig-zag (glide-symmetry) chain}

97. MUBQUW

2-Iodo-1,3-dimethoxybenzene



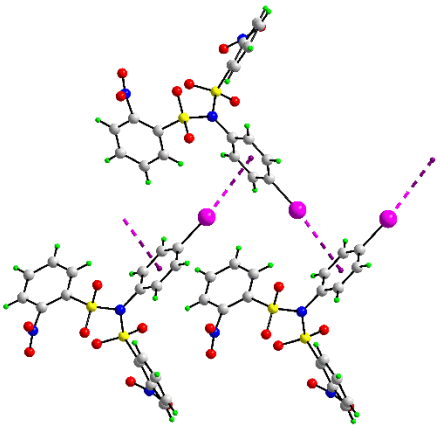
d = 3.695(2) Å; θ = 164.17(14)°

L.-P. Xue and J.-H. Qin, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2009, **65**, o1790; DOI: 10.1107/S1600536809025264

{The molecule has mirror symmetry with the plane bisecting the phenyl ring and containing the iodide atom. Molecules assemble into a zig-zag (glide-symmetry) chain}

98. CELMOW

4-Iodophenyliminobis(2-nitrobenzenesulfinate)



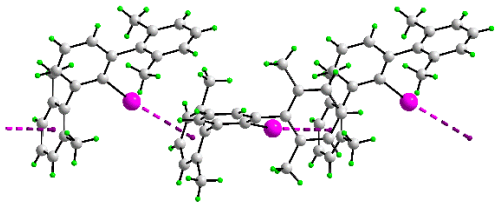
d = 3.7071(10) Å; θ = 168.71(7)°

J. N. Low, J. M. S. Skakle, J. L. Wardell and C. Glidewell, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2006, **62**, o423-o425; DOI: 10.1107/S0108270106019408

{Molecules self-associate into a zig-zag (glide-symmetry) chain}

99. CIYQUY01

2^{2}-Iodo-1^{2},1^{6},3^{2},3^{6}-tetramethyl-1^{1},2^{1}:2^{3},3^{1}-terphenyl



d = 3.7152(12) Å; θ = 169.07(7)°

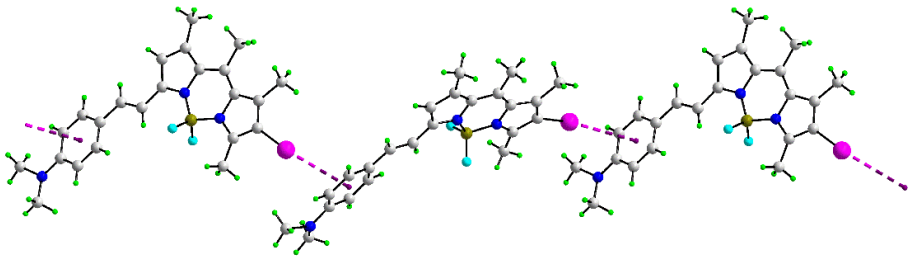
A. Linden, S. Duttwyler and J. S. Siegel, Private Communication to the Cambridge Structural Database, Refcode CIYQUY01, 2018.

{Molecules self-associate to form a zig-zag (glide-symmetry) chain. A monoclinic (*C*2/*c*) polymorph compliments the *Pbca* polymorph above. No equivalent interactions are noted. T.

J. Blundell, F. R. Hastings, B. M. Gridley, G. J. Moxey, W. Lewis, A. J. Blake and D. L. Kays, *Dalton Trans*., 2014, **43**, 14257-14264; DOI: 10.1039/C4DT00647J}

100. DANCAY

4-(2-(5,5-Difluoro-8-iodo-1,7,9,10-tetramethyl-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-3-yl)vinyl)-N,N-dimethylaniline



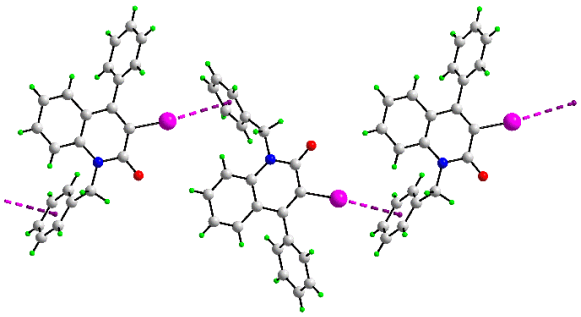
d = 3.730(5) Å; θ = 162.3(3)°

S. Niu, G. Ulrich, P. Retailleau and R. Ziessel, *Org. Lett.*, 2011, **13**, 4996-4999; DOI: 10.1021/ol201600s

{Molecules assemble into a zig-zag (glide-symmetry) chain}

101. RIPCEA

1-Benzyl-3-iodo-4-phenylquinolin-2(1H)-one



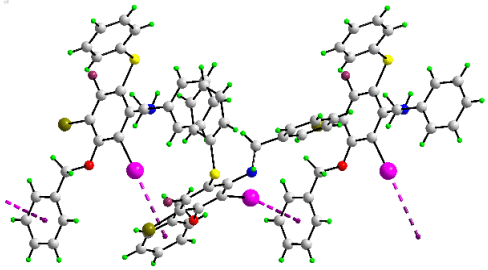
d = 3.746(3) Å; θ = 170.0(2)°

L.-J. Wang, H.-T. Zhu, Y.-F. Qiu, X.-Y. Liu and Y.-M. Liang, *Org. Biomol. Chem*., 2014, **12**, 643-650; DOI: 10.1039/C3OB42020E

{Molecules assemble into a zig-zag (glide-symmetry) chain}

102. OVOCOS

N-Benzyl-3-(benzyloxy)-4-bromo-5-fluoro-2-iodo-6-(phenylsulfanyl)aniline



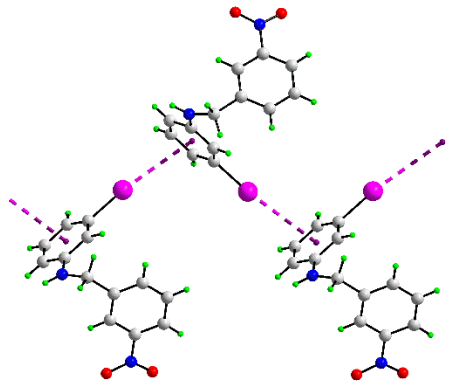
d = 3.751(3) Å; θ = 164.93(12)°

H. Seo, K. Ohmori and K. Suzuki, *Chem. Lett*., 2011, **40**, 744-746; DOI: 10.1246/cl.2011.744

{Molecules are connected into a zig-zag (glide-symmetry) chain}

103. XOSCEN

3-Iodo-N-(3-nitrobenzyl)aniline



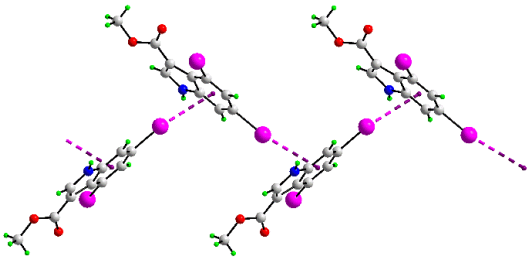
d = 3.8236(9) Å; θ = 166.57(7)°

C. Glidewell, J. N. Low, J. M. S. Skakle, S. M. S. V. Wardell and J. L. Wardell, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun*., 2002, **58**, o487-o490; DOI: 10.1107/S010827010201140X

{Molecules self-assemble into a zig-zag (glide-symmetry) chain}

104. OSOSUL

Methyl 4,6-di-iodo-1H-indole-3-carboxylate



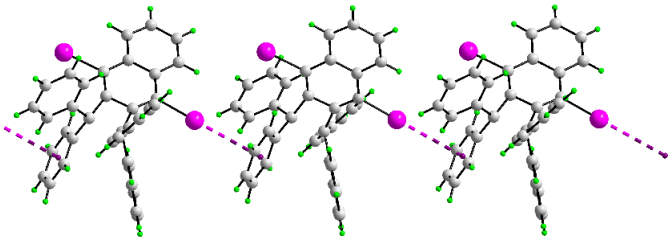
d = 3.492(2) Å; θ = 169.42(16)°

T. Honda, H. Nagahara, H. Mogi, M. Ban and H. Aono, *Bioorg. Med. Chem. Lett*., 2011, **21**, 1782-1785; DOI: 10.1016/j.bmcl.2011.01.063

{Molecules are connected into a zig-zag (glide-symmetry) chain}

105. QOMYOG

1,1,2,2-Tetraphenyl-3,8-diiodocyclobuta(b)naphthalene



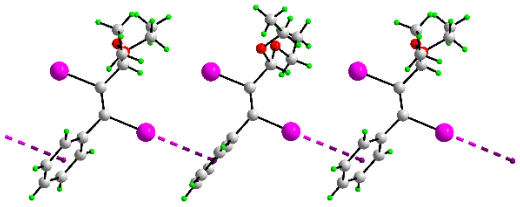
d = 3.577(3) Å; θ = 170.81(13)°

K. Tanaka, N. Takamoto, Y. Tezuka, M. Kato and F. Toda, *Tetrahedron*, 2001, **57**, 3761-3767; DOI: 10.1016/S0040-4020(01)00249-6

{Molecules assemble into a zig-zag (glide-symmetry) chain}

106. ZULNIF

(E)-(3,3-Diethoxy-1,2-di-iodoprop-1-en-1-yl)benzene



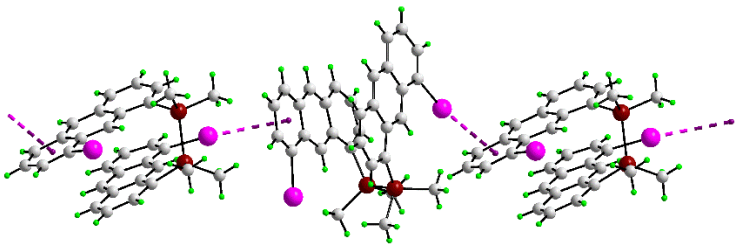
d = 3.6612(18) Å; θ = 166.57(11)°

C. Hettstedt, P. Mayer and K. Karaghiosoff, *New J. Chem*., 2015, **39**, 8522-8533; DOI: 10.1039/C5NJ00821B

{Molecules self-assemble to form a zig-zag (glide-symmetry) chain}

107. INIWAE

1,2-bis(8-Iodo-1-anthryl)-1,1,2,2-tetramethyldisilane



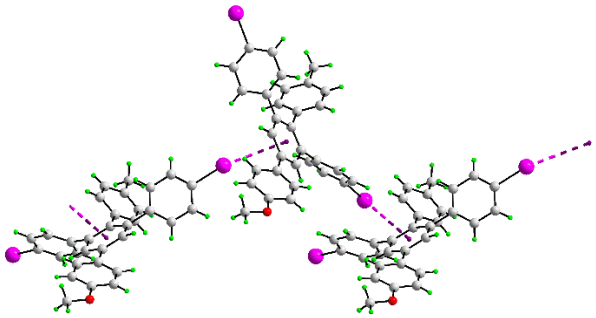
d = 3.746(2) Å; θ = 171.16(6)°

W. Nakanishi, S. Hitosugi, Y. Shimada and H. Isobe, *Chem. Asian J*., 2011, **6**, 554-559; DOI: 10.1002/asia.201000543

{Molecules assemble to form a zig-zag (glide-symmetry) chain}

108. LUNDIH

2,6-bis(4-Iodophenyl)-4-(4-methoxyphenyl)-1-p-tolylbenzene



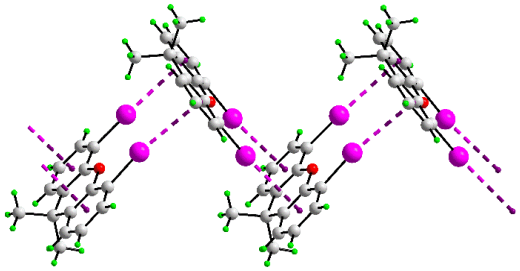
d = 3.804(5) Å; θ = 166.8(3)°

S. Höger, S. Rosselli, A.-D. Ramminger and V. Enkelmann, *Org. Lett*., 2002, **4**, 4269-4272; DOI: 10.1021/ol026870y

{The molecules assemble into a zig-zag (glide-symmetry) chain}

109. MIWWIB

4,5-Diiodo-9,9-dimethyl-9H-xanthene



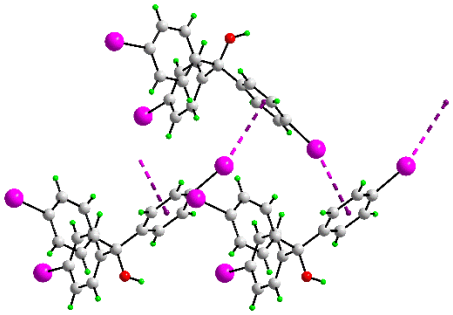
d = 3.5508(14) Å; θ = 170.45(9)°

L. Wang, D. Deng, K. Škoch, C. G. Daniliuc, G. Kehr and G. Erker, *Organometallics*, 2019, **38**, 1897-1902; DOI: 10.1021/acs.organomet.9b00002

{The molecule has mirror symmetry and forms two acceptor and two donor contacts to form a chain with a zig-zag topology}

110. GIZTIT

tris(4-Iodophenyl)methanol dichloromethane solvate



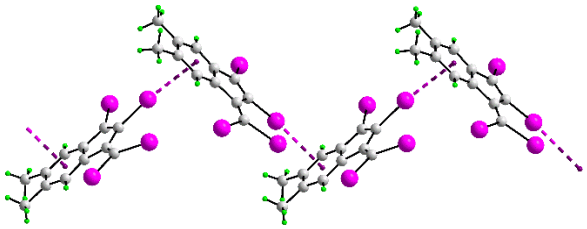
d = 3.617(2) Å; θ = 161.79(17)°

D. Schollmeyer, O. V. Shishkin, T. Rühl and M. O. Vysotsky, *CrystEngComm*, 2008, **10**, 715-723; DOI: 10.1039/b716442d

{The molecule has mirror symmetry. One iodide forms an interaction resulting in a zig-zag chain with mirror symmetry; the rings related across the mirror plane also form I···π contacts but, these also participate in bifurcated O–H···π contacts. For unsolvated form, see **156**, **GIZTEP**: a helical chain}

111. FUDQEC

1-(Di-iodomethylene)-2,3-bis(iodo)-5,6-dimethyl-1H-indene



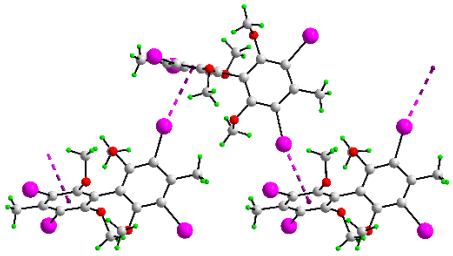
d = 3.416(3) Å; θ = 163.4(2)°

P. Nösel, V. Müller, S. Mader, S. Moghimi, M. Rudolph, I. Braun, F. Rominger, A. Stephen and K. Hashmi, *Adv. Synth. Catal.*, 2015, **357**, 500-506; DOI: 10.1002/adsc.201400749

{Molecules associate to form a zig-zag (glide-symmetry) chain}

112. YOZLUW

3,3',5,5'-Tetraiodo-2,2',6,6'-tetramethoxy-4,4'-dimethylbiphenyl



d = 3.598(3) Å; θ = 167.14(19)°

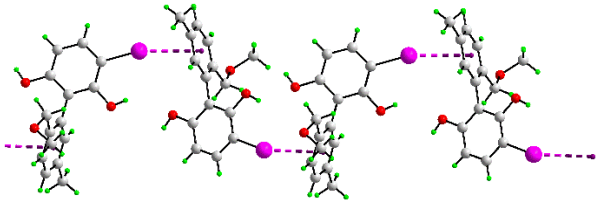
W. Lu, Z. Wei, D. Yuan, J. Tian, S. Fordham and H.-C. Zhou, *Chem. Mater.*, 2014, **26**, 4589-4598; DOI: 10.1021/cm501922h

{Molecules are connected into a zig-zag (glide-symmetry) chain}

ESI Table 5. Helical, one-dimensional chains sustained by C–I···π(arene) interactions

113. DOZLOV

3-Iodo-2'-(methoxymethyl)-5'-methylbiphenyl-2,6-diol



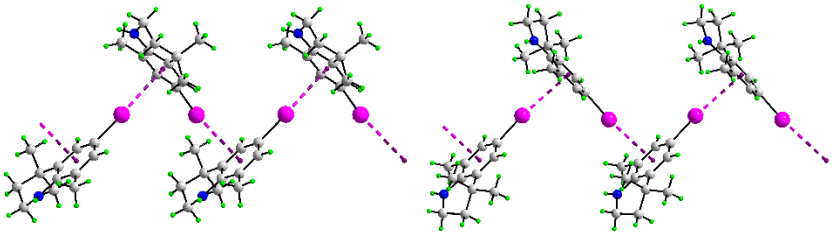
d = 3.4326(9) Å; θ = 161.02(5)°

K. Mori, M. Kobayashi, T. Itakura and T. Akiyama, *Adv. Synth. Catal.*, 2015, **357**, 35-40; DOI: 10.1002/adsc.201400611

{The molecules associate to form a helical (2_1-screw axis) chain}

114. YAKLII

6-Iodo-4,4,8-trimethyl-1,2,3,4-tetrahydroquinoline



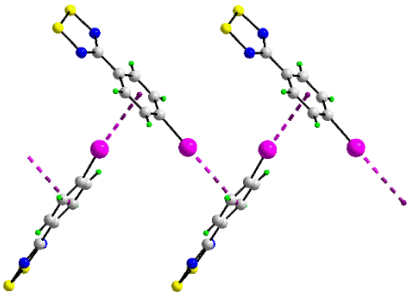
d = 3.4676(9) Å; θ = 174.26(6)°; *d* = 3.5319(8) Å; θ = 166.55(6)°

D. R. Chisholm, G.-L. Zhou, E. Pohl, R. Valentine and A. Whiting, *Beilstein J. Org. Chem.*, 2016, **12**, 1851-1862; DOI: 10.3762/bjoc.12.174

{Two independent molecules. Each self-associates into a helical (2_1-screw axis) chain}

115. DOQYUD

4-(4-Iodophenyl)-1,2,3,5-dithiadiazolyl radical



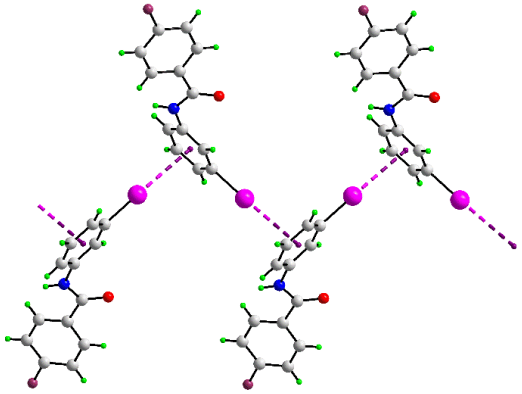
d = 3.514(2) Å; θ = 169.73(15)°

N. Bricklebank, S. Hargreaves and S. E. Spey, *Polyhedron*, 2000, **19**, 1163-1166; DOI: 10.1016/S0277-5387(00)00384-3

{The molecules associate to form a helical (2_1-screw axis) chain}

116. IWARII

4-Fluoro-N-(3-iodophenyl)benzamide



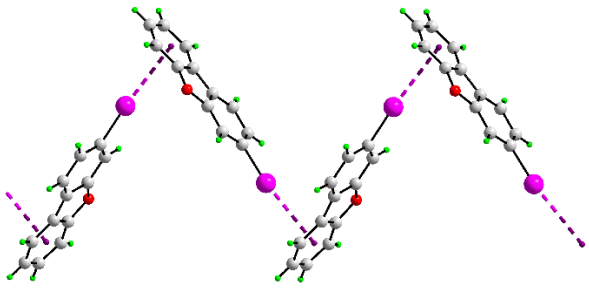
d = 3.545(2) Å; θ = 168.56(16)°

S. K. Nayak, M. K. Reddy, T. N. G. Row and D. Chopra, *Cryst. Growth Des.*, 2011, **11**, 1578-1596; DOI: 10.1021/cg101544z

{Molecules assemble to form a helical (2_1-screw symmetry) chain}

117. ZIKYOH

3-Iododibenzofuran



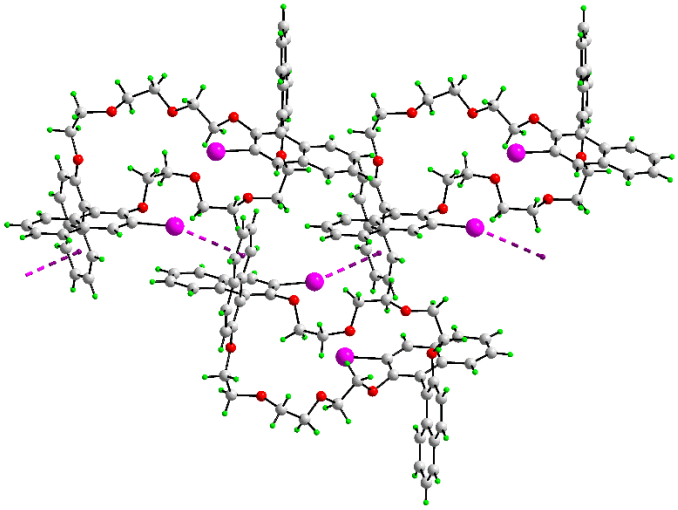
d = 3.554(3) Å; θ = 173.05(16)°

P. A. Chaloner, P. B. Hitchcock and P. G. Sutton, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 1995, **51**, 2680-2683; DOI: 10.1107/S0108270194013338

{Molecules are connected into a helical (2_1-screw axis) chain}

118. NUGSAK

6,28-Di-iodo-8,9,11,12,14,15,30,31,33,34,36,37-dodecahydrotetranaphtho[2,1-k:1',2'-m:2'',1''-y:1''',2'''-a1][1,4,7,10,15,18,21,24]octaoxacyclo-octacosine



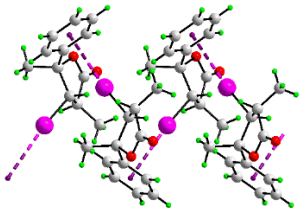
d = 3.558(3) Å; θ = 161.87(16)°

H. Kawai, A. Kusuda, S. Mizuta, S. Nakamura, Y. Funahashi, H. Masuda and N. Shibata, *J. Fluorine Chem*., 2009, **130**, 762-765; DOI: 10.1016/j.jfluchem.2009.06.004

{The molecules are connected into a helical (2_1-screw axis) chain}

119. DIFTUI

(3S,4R,5S)-4-Iodo-3,5-dimethyl-5-phenyldihydrofuran-2(3H)-one



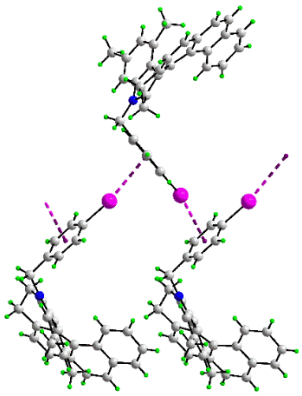
d = 3.5922(10) Å; θ = 174.63(5)°

J.-M. Garnier, S. Robin, R. Guillot and G. Rousseau, *Tetrahedron: Asymm*., 2007, **18**, 1434-1442; DOI: 10.1016/j.tetasy.2007.05.028

{The molecules associate to form a helical (2_1-screw axis) chain}

120. GULLAC

(M)-7-(4-Iodobenzyl)-9,11-dimethyl-6,7-dihydro-5H-phenanthro[3,4-c]carbazole



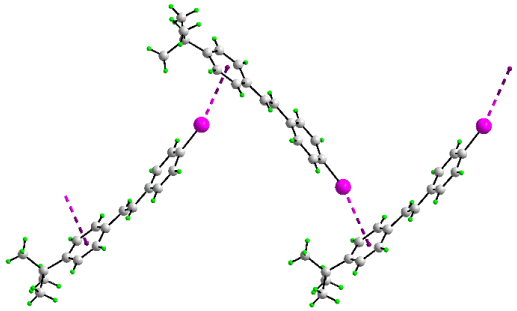
d = 3.606(2) Å; θ = 167.66(12)°

L. Kötzner, M. J. Webber, A. Martínez, C. De Fusco and B. List, *Angew. Chem., Int. Ed*., 2014, **53**, 5202-5205; DOI: 10.1002/anie.201400474

{Molecules assembles into a helical (2_1-screw symmetry) chain}

121. KUKTIV

1-t-butyl-4-(2-(4-iodophenyl)vinyl)benzene



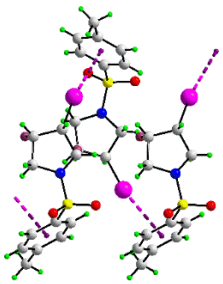
d = 3.628(4) Å; θ = 165.5(3)°

Z. Chen and G. J. Moxey, *Acta Crystallogr., Sect. E: Cryst. Commun*., 2015, **71**, o309-o310; DOI: 10.1107/S2056989015007185

{Two independent molecules. One assembles into a helical (2_1-screw) chain. The other does the same but, outside the specified parameters: *d* = 3.567(4) Å; θ = 153.6(3)°}

122. ZECMIF

3-Fluoro-4-iodo-1-((4-methylphenyl)sulfonyl)pyrrolidine



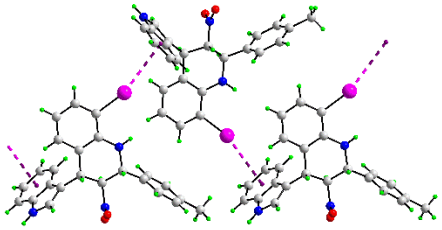
d = 3.629(3) Å; θ = 169.5(2)°

L. E. Combettes, P. Clausen-Thue, M. A. King, B. Odell, A. L. Thompson, V. Gouverneur and T. D. W. Claridge, *Chem. - Eur. J.*, 2012, **18**, 13133-13141; DOI: 10.1002/chem.201201577

{Molecules are connected into a helical (2_1-screw axis) chain}

123. CUCQOI

4-(1H-Indol-3-yl)-8-iodo-2-(4-methylphenyl)-3-nitro-1,2,3,4-tetrahydroquinoline



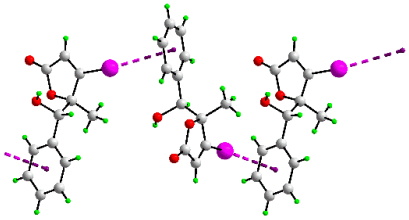
d = 3.6402(15) Å; θ = 162.92(8)°

M. R. Zanwar, S. D. Gawande, V. Kavala, C.-W. Kuo and C.-F. Yao, *Adv. Synth. Catal.*, 2014, **356**, 3849-3860; DOI: 10.1002/adsc.201400424

{The molecules associate to form a helical (2_1-screw axis) chain}

124. KUHWUI

5-[Hydroxy(phenyl)methyl]-4-iodo-5-methylfuran-2(5H)-one



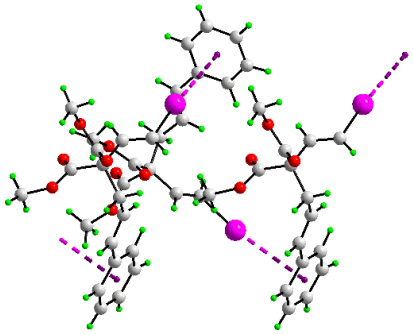
d = 3.645(2) Å; θ = 160.24(13)°

F. Z., Q.-Y. Xue and L. Yin, *Angew. Chem., Int. Ed*., 2020, **59**, 1562-1566; DOI: 10.1002/anie.201912140

{Molecules self-associate to form a helical (2_1-screw symmetry) chain}

125. BEHHUS

(E,E)-2-(2'-Iodovinyl)-2-(3''-phenyl-2''-propenyl)malonic acid dimethyl ester



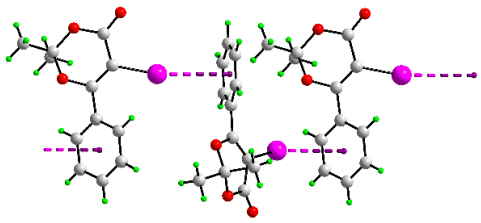
d = 3.6542(19) Å; θ = 171.14(9)°

S. Ma, J. Zhang, Y. Cai and L. Lu, *J. Am. Chem. Soc*., 2003, **125**, 13954-13955; DOI: 10.1021/ja038131y

{Molecules self-associate to form a helical (2_1-screw symmetry) chain}

126. NAWDUL

5-Iodo-2,2-dimethyl-6-phenyl-4H-1,3-dioxan-4-one



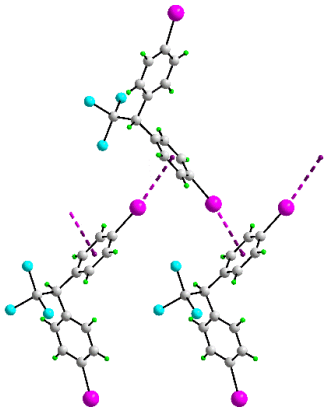
d = 3.6578(19) Å; θ = 161.11(10)°

V.-A. Vu, P. Knochel and K. Polborn, Private Communication to the Cambridge Structural Database, Refcode NAWDUL, 2005.

{Molecules assemble into a helical (2_1-screw symmetry) chain}

127. ZZZQAC01

1,1,1-Trichloro-2,2-bis(4-iodophenyl)ethane



d = 3.665(4) Å; θ = 162.5(3)°

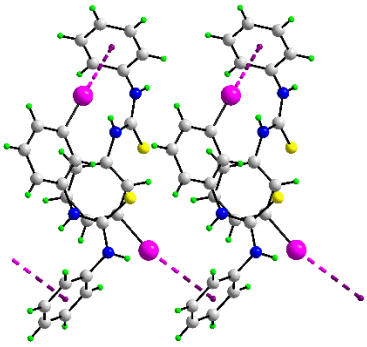
G. Smith, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2012, **68**, o2504; DOI:

10.1107/S1600536812032254

{Molecules self-assemble to form a helical (2_1-screw symmetry) chain}

128. AVACOR

1-(3-Iodophenyl)-3-phenylthiourea



d = 3.684(2) Å; θ = 162.08(11)°

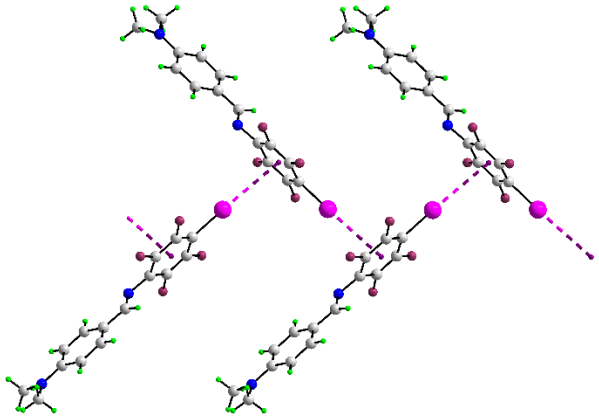
V. S. Koshti, S. H. Thorat, R. P. Gote, S. H. Chikkali and R. G. Gonnade, *CrystEngComm*,

2016, **18**, 7078-7093; DOI: 10.1039/C6CE01324D

{Molecules self-associate to form a helical (2_1-screw symmetry) chain}

129. SAYNIS

N,N-Dimethyl-4-{[(2,3,5,6-tetrafluoro-4-iodophenyl)imino]methyl}aniline



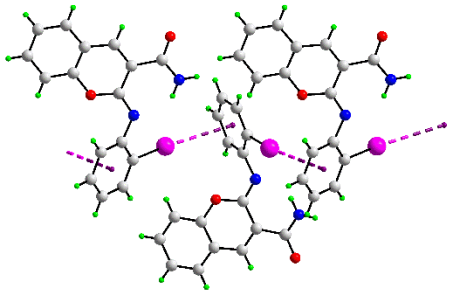
d = 3.685(3) Å; θ = 178.0(2)°

Y. Wang, H. Shang, B. Li, H. Zhang and S. Jiang, *CrystEngComm*, 2017, **19**, 3801-3807; DOI: 10.1039/C7CE00805H

{Two independent molecules. One self-associates into a helical (2_1-screw symmetry) chain. The second independent molecule assembles in the same manner but, has *d* = 3.908(3) Å; θ = 137.2(2)°, i.e. outside the specified search criteria for delocalised interactions}

130. FOYMIS

2-[(2-Iodophenyl)imino]-2H-1-benzopyran-3-carboxamide



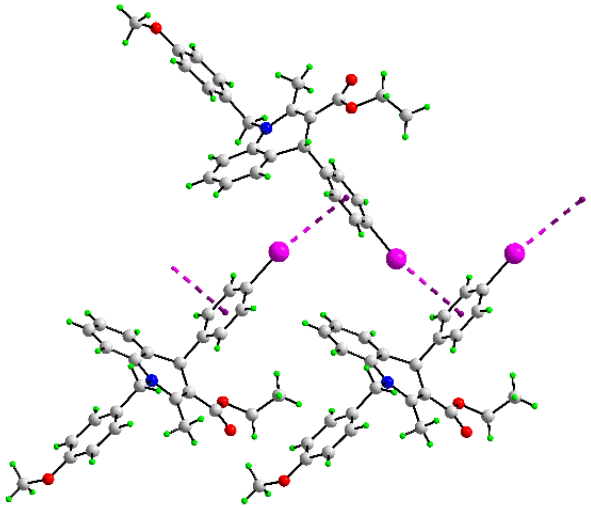
d = 3.6899(19) Å; θ = 166.72(13)°

S. V. Shishkina, I. S. Konovalova, S. M. Kovalenko, P. V. Trostianko, A. O. Geleverya, L. L. Nikolayeva and N. D. Bunyatyan, *Acta Crystallogr., Sect. B: Struct. Sci., Cryst. Eng. Mat.*, 2019, **75**, 887-902; DOI: 10.1107/S2052520619010485

{Molecules self-associate to form a helical (2_1-screw symmetry) chain}

131. WAQNIO

(R)-Ethyl 4-(4-iodophenyl)-1-(4-methoxybenzyl)-2-methyl-1,4-dihydroquinoline-3-carboxylate



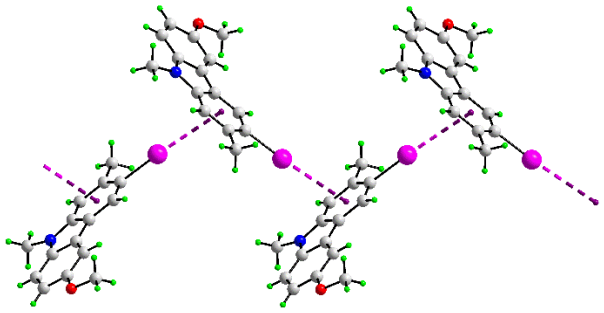
d = 3.6980(14) Å; θ = 169.21(9)°

T. Hodík and C. Schneider, *Org. Biomol. Chem*., 2017, **15**, 3706-3716; DOI: 10.1039/C7OB00488E

{Molecules self-assemble into a helical (2_1-screw symmetry) chain}

132. PILQAE

3-Iodo-6-methoxy-2,9-dimethyl-9H-carbazole



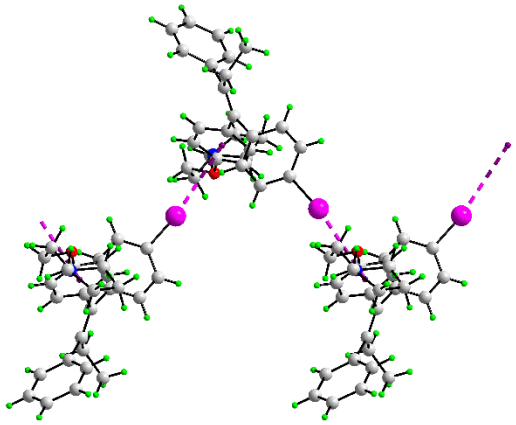
d = 3.698(2) Å; θ = 165.19(14)°

B. Alcaide, P. Almendros, J. M. Alonso, S. Cembellin, I. Fernandez, T. M. del Campo, M. Rosario Torres, *Chem. Commun*., 2013, **49**, 7779-7781; DOI: 10.1039/C3CC44073G

{Molecules are connected into a helical (2_1-screw symmetry) chain}

133. WIKPAH

trans-1-(4-Iodophenyl)-1-(4-(2-pyrrolidinylethoxy)phenyl)-2-phenylbutene



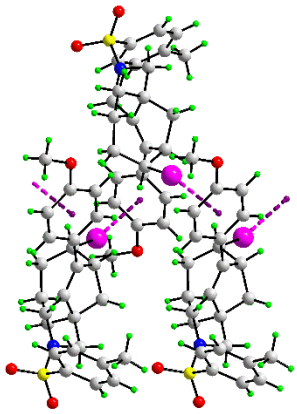
d = 3.7120(17) Å; θ = 162.79(7)°

C. M. Nunn and E. J. Parker, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 1994, **50**, 2043-2045; DOI: 10.1107/S0108270194008309

{Molecules self-assemble into a helical (2_1-screw symmetry) chain}

134. TIHJUR

8-Iodo-6-(4-methoxyphenyl)-3-((4-methylphenyl)sulfonyl)-3-azatricyclo[5.4.1.01,5]dodec-5-ene



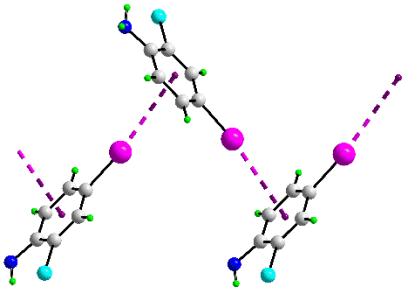
d = 3.739(4) Å; θ = 163.9(2)°

M.-C. P. Yeh, C.-J. Liang, C.-W. Fan, W.-H. Chiu and J.-Y. Lo, *J. Org. Chem.*, 2012, **77**, 9707-9717; DOI: 10.1021/jo301764g

{Molecules self-assemble into a helical (2_1-screw symmetry) chain}

135. VOJBAY

2-Chloro-4-iodoaniline



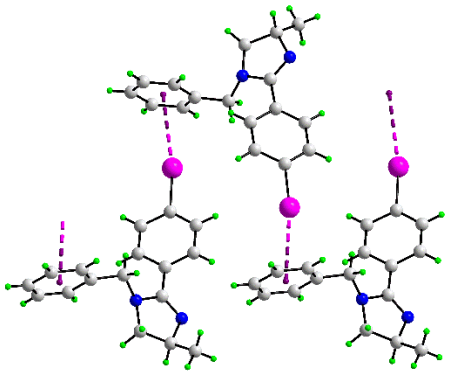
d = 3.7399(15) Å; θ = 171.08(9)°

Y.-H. Xu, C. Wang and F. Qu, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2008, **64**, o2300; DOI: 10.1107/S1600536808036076

{Molecules assemble into a helical (2_1-screw axis) supramolecular chain}

136. ZAGVOV

1-Benzyl-2-(4-iodophenyl)-4-methyl-4,5-dihydro-1H-imidazole



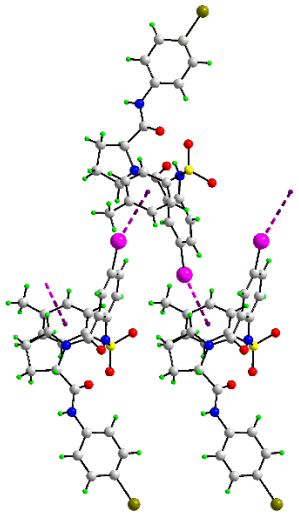
d = 3.743(4) Å; θ = 169.9(2)°

S. Huang, Y. Shao, L. Zhang and X. Zhou, *Angew.Chem., Int. Ed.*, 2015, **54**, 14452-14456; DOI: 10.1002/anie.201508442

{Molecules are connected into a helical (2_1-screw axis) chain}

137. LIDGAI

N-(4-Bromophenyl)-1-(5-iodo-2-(((4-methylphenyl)sulfonyl)amino)benzoyl)prolinamide



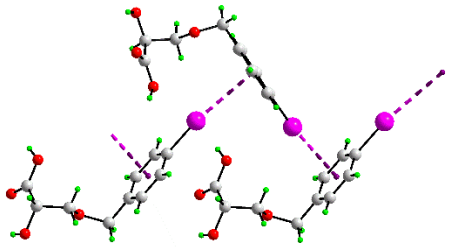
d = 3.770(5) Å; θ = 163.7(2)°

V. H. Thorat, T. S. Ingole, K. N. Vijayadas, R. V. Nair, S. S. Kale, V. V. E. Ramesh, H. C. Davis, P. Prabhakaran, R. G. Gonnade, R. L. Gawade, V. G. Puranik, P. R. Rajamohanan and G. J. Sanjayan, *Eur. J. Org. Chem*., 2013, 3529-3542; DOI: 10.1002/ejoc.201201739

{The molecules assemble into a helical (2_1-screw symmetry) chain}

138. OBEKAK

2-Hydroxy-3-((4-iodobenzyl)oxy)propanoic acid



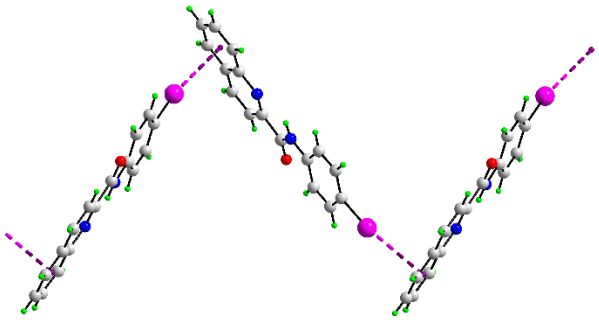
d = 3.7746(6) Å; θ = 169.65(4)°

Y. Wang, N. M. S. van den Akker, D. G. M. Molin, M. Gagliardi, C. van der Marel, M. Lutz, M. L. W. Knetsch and L. H. Koole, *Adv. Healthcare Mater*., 2013, **3**, 290-299; DOI: 10.1002/adhm.201300215

{The molecules are connected into a helical (2_1-screw axis) chain}

139. BANWIX

N-(4-Iodophenyl)quinoline-2-carboxamide



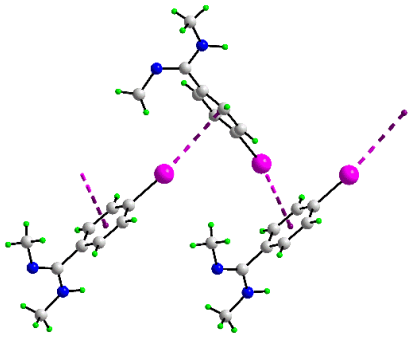
d = 3.7804(14) Å; θ = 171.57(8)°

J. Y. Qi, L. Q. Qiu, Q. Y. Yang, Z. Y. Zhou and A. S. C. Chan, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2003, **59**, o104-o105; DOI: 10.1107/S1600536802022419

{Molecules self-associate to form a helical (2_1-screw symmetry) chain}

140. VIZLEW

4-Iodo-N,N'-dimethylbenzamidine



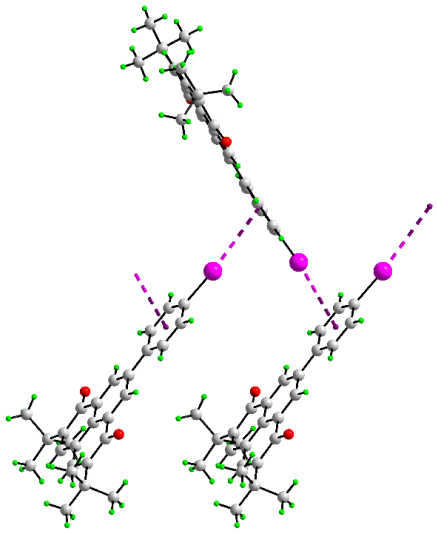
d = 3.792(3) Å; θ = 167.48(16)°

W. Chen and T. Ren, *J. Cluster Sci*., 2008, **19**, 99-108; DOI: 10.1007/s10876-007-0155-4

{Molecules assemble into a helical (2_1-screw axis) supramolecular chain}

141. IFUCAP

2,5-Di-t-butyl-6-hydroxy-8-(4-iodophenyl)-1H-phenalen-1-one acetonitrile solvate



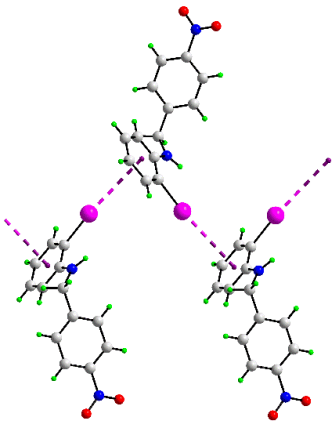
d = 3.8221(19) Å; θ = 174.49(12)°

S. Nishida, J. Kawai, M. Moriguchi, T. Ohba, N. Haneda, K. Fukui, A. Fuyuhiro, D. Shiomi, K. Sato, T. Takui, K. Nakasuji and Y. Morita, *Chem. - Eur. J.*, 2013, **19**, 11904-11915; DOI: 10.1002/chem.201301783

{Molecules assemble to form a helical (2_1-screw symmetry) chain}

142. EYOFAZ

2-Iodo-N-(4-nitrobenzyl)aniline



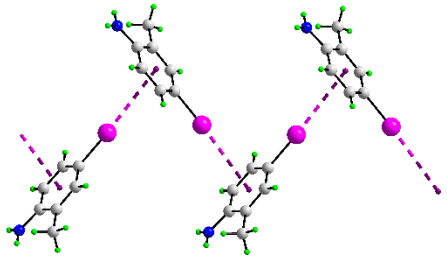
d = 3.8232(12) Å; θ = 165.50(7)°

C. Glidewell, J. N. Low, J. M. S. Skakle, S. M. S. V. Wardell and J. L. Wardell, *Acta Crystallogr., Sect. B: Struct. Sci.*, 2004, **60**, 472-480; DOI: 10.1107/S0108768104012017

{The molecules associate to form a helical (2_1-screw axis) chain}

143. TITZUS

4-Iodo-2-methylaniline



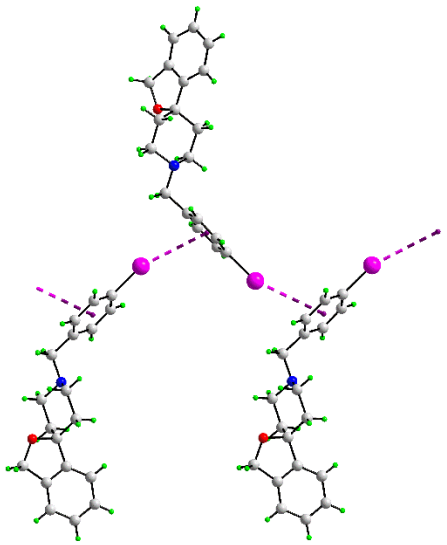
d = 3.831(5) Å; θ = 176.6(3)°

W. Luo, R. Liu, Y.-H. Li, W. Chen and H.-J. Zhu, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2008, **64**, o591; DOI: 10.1107/S1600536808004145

{Molecules self-assemble into a helical (2_1-screw symmetry) chain}

144. QIFHET

1'-(4-Iodobenzyl)spiro(isobenzofuran-1(3H),4'-piperidine)



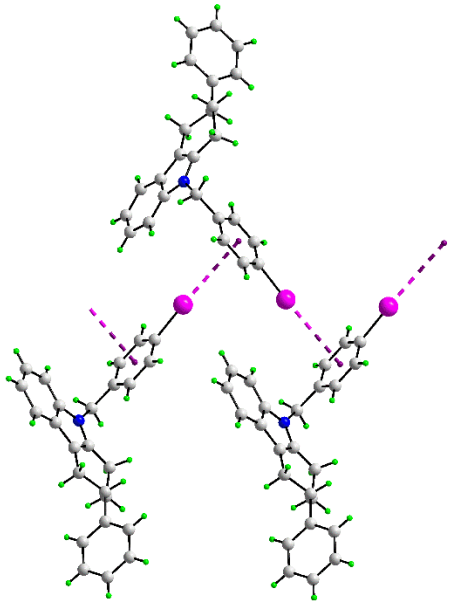
d = 3.8454(9) Å; θ = 161.22(5)°

Q.-Y. Zhang, Y. Li, H.-M. Jia and B.-L. Liu, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2007, **63**, o2418-o2419; DOI: 10.1107/S1600536807015966

{Molecules are connected into a helical (2_1-screw symmetry) chain}

145. BAGJAW

9-(4-Iodobenzyl)-3-phenyl-2,3,4,9-tetrahydro-1H-carbazole



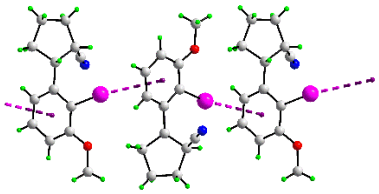
d = 3.8492(11) Å; θ = 172.32(6)°

S. Müller, M. J. Webber and B. List, *J. Am. Chem. Soc*., 2011, **133**, 18534-18537; DOI: 10.1021/ja2092163

{Two independent molecules. One self-associates to form a helical (2_1-screw symmetry) chain. The second molecule does the same but, outside the specific geometric criteria: *d* = 3.9595(11) Å; θ = 172.16(6)°}

146. VIVNAP

cis-1-Cyano-2-(2-iodo-3-methoxy)phenylcyclopentane



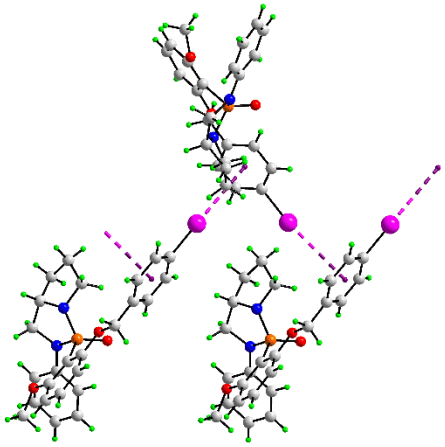
d = 3.8548(18) Å; θ = 168.45(10)°

G. D. Cuny, A. Gutierrez and S. L. Buchwald, *Organometallics*, 1991, **10**, 537-539; DOI: 10.1021/om00049a006

{Molecules assemble into a helical (2_1-screw axis) supramolecular chain}

147. ALACAS

1-(2-((4-Iodobenzyl)oxy)-6-methoxyphenyl)-2-phenylhexahydro-1H-pyrrolo[1,2-c][1,3,2]diazaphosphole 1-oxide



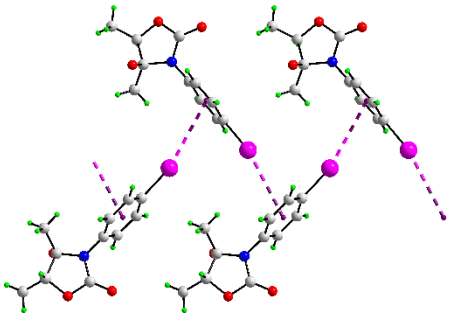
d = 3.856(2) Å; θ = 168.04(13)°

G. Cheng, A. M. Z. Slawin, N. R. Vautravers, P. André, R. E. Morris, I. D. W. Samuel and D. Cole-Hamilton, *Org. Biomol. Chem*., 2011, **9**, 1189-1200; DOI: 10.1039/c0ob00297f

{Molecules self-associate to form a helical (2_1-screw symmetry) chain}

148. RAKWEH

4-Hydroxy-3-(4-iodophenyl)-4,5-dimethyl-1,3-oxazolidin-2-one



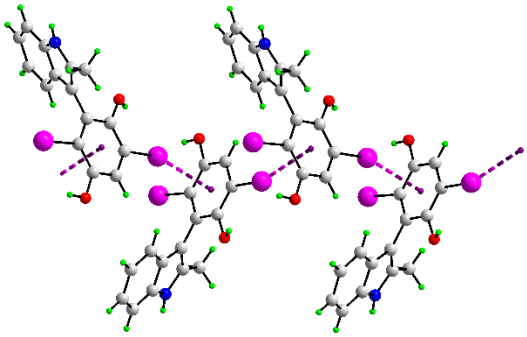
d = 3.876(2) Å; θ = 163.50(16)°

R. Kojima, S. Sawamoto, A. Okamura, H. Takahashi, S. Tsunoi and I. Shibata, *Eur. J. Org. Chem*., 2011, 7255-7258; DOI: 10.1002/ejoc.201101465

{Molecules are connected into a helical (2_1-screw symmetry) chain}

149. HOMSOU

2,5-Diiodo-3-(2-methyl-1H-indol-3-yl)benzene-1,4-diol



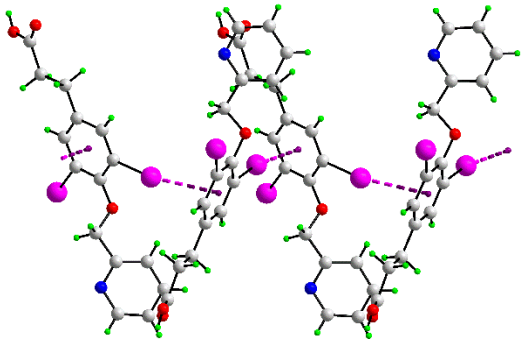
d = 3.3854(18) Å; θ = 160.43(13)°

D.-L. Lu, Y.-H. Chen, S.-H. Xiang, P. Yu, B. Tan and S. Li, *Org. Lett.*, 2019, **21**, 6000-6004; DOI: 10.1021/acs.orglett.9b02143

{Molecules assemble to form a helical (2_1-screw symmetry) chain}

150. DEXZEN

3-(3,5-Diiodo-4-(pyridin-2-ylmethoxy)phenyl)propanoic acid monohydrate



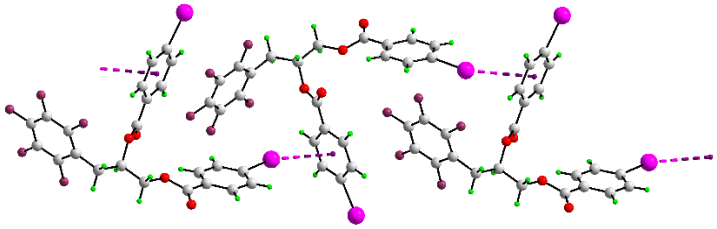
d = 3.5547(13) Å; θ = 170.36(9)°

A. Balamurugan, A. K. Gupta, R. Boomishankar, M. L. Reddy and M. Jayakannan, *ChemPlusChem*, 2013, **78**, 737-745; DOI: 10.1002/cplu.201300121

{The molecules associate to form a helical (2_1-screw axis) chain. The solvent water molecules link chains via OH···O hydrogen bonding}

151. GILKAO

3-(Perfluorophenyl)propane-1,2-diyl bis(4-iodobenzoate)



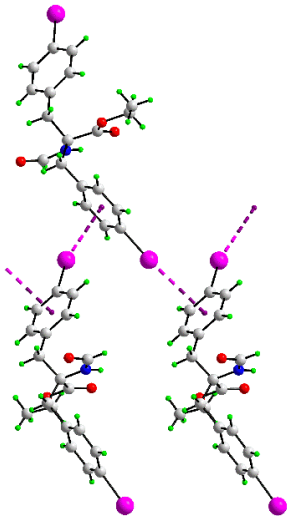
d = 3.693(4) Å; θ = 161.9(2)°

K. Sakakibara, K. Nakano and K. Nozaki, *Macromolecules*, 2007, **40**, 6136-6142; DOI: 10.1021/ma070428j

{Molecules associate to form a helical (2_1-screw symmetry) chain}

152. MACMEJ

Ethyl 2-formamido-2-(4-iodobenzyl)-3-(4-iodophenyl)propionate



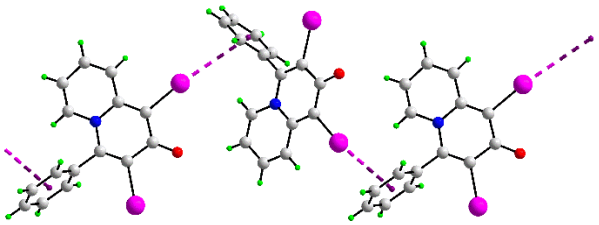
d = 3.810(3) Å; θ = 165.21(14)°

L. Damodharan, V. Pattabhi, M. Behera and S. Kotha, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2003, **59**, o216-o218; DOI: 10.1107/S0108270103005183

{The molecules assemble into a helical (2_1-screw symmetry) chain}

153. KUHNOT

1,3-Diiodo-4-phenyl-2H-quinolizin-2-one



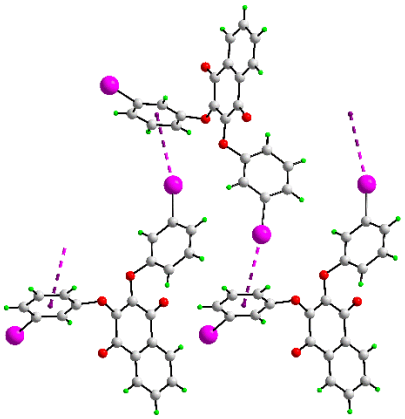
d = 3.8339(15) Å; θ = 172.52(8)°

W.-W. Yang, J.-W. Zhang, L.-L. Chen, J.-Y. Fu, J.-Y. Zhu and Y.-B. Wang, *Chem. Commun.*, 2019, **55**, 12607-12610; DOI: 10.1039/C9CC06250E

{The molecules assemble into a helical (2_1-screw) chain}

154. XETRUM

2,3-bis(3-Iodophenoxy)-1,4-naphthoquinone



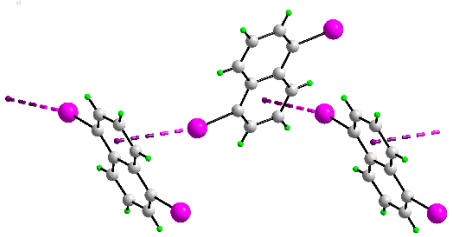
d = 3.859(6) Å; θ = 160.3(3)°

J. Milić, M. Zalibera, D. Talaat, J .Nomrowski, N. Trapp, L. Ruhlmann, C. Boudon, O. S. Wenger, A. Savitsky, W. Lubitz and F. Diederich, *Chem. - Eur. J.*, 2018, **24**, 1431-1440; DOI: 10.1002/chem.201704788

{Molecules self-assemble into a helical (2_1-screw symmetry) chain}

155. NIFHAM

1,5-Diiodonaphthalene



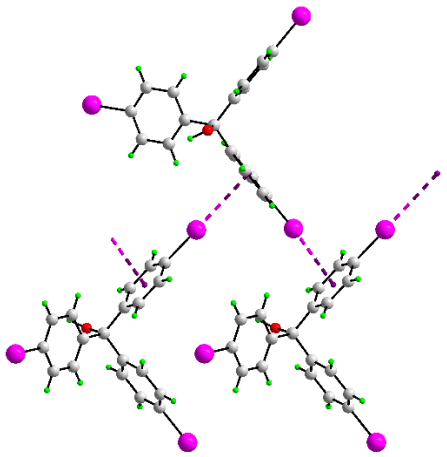
d = 3.8680(19) Å; θ = 166.79(10)°

I. Novak, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2007, **63**, o2726; DOI: 10.1107/S1600536807020508

{The molecules assemble into a helical (2_1-screw symmetry) chain}

156. GIZTEP

tris(4-Iodophenyl)methanol



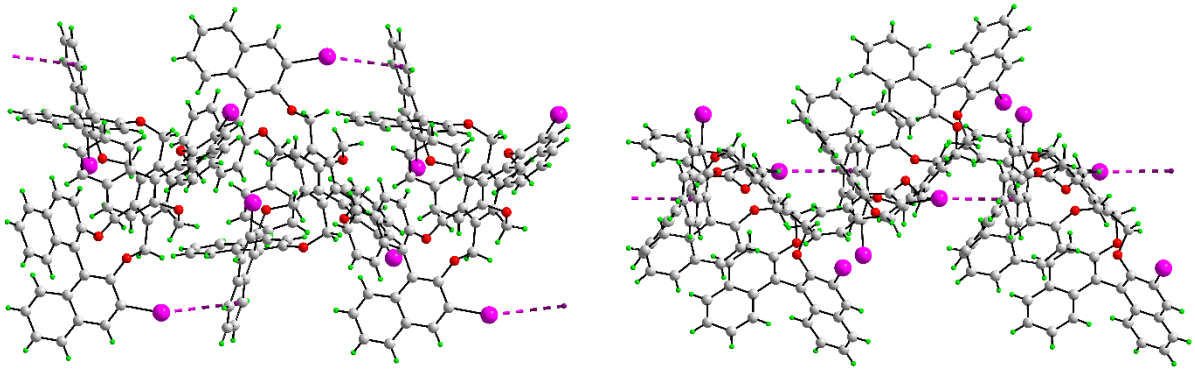
d = 3.6600(18) Å; θ = 169.77(15)°

D. Schollmeyer, O. V. Shishkin, T. Rühl and M. O. Vysotsky, *CrystEngComm*, 2008, **10**, 715-723; DOI: 10.1039/b716442d

{Molecules associate to form a helical (2_1-screw symmetry) chain. For solvated form, see **110**, **GIZTIT**, a zig-zag chain}

157. TENPUA

6,11,36-Triiodo-8,9,22,23,38,39-hexahydrobenzo[g]hexanaphtho[2,3-g:2,3-g':2,3-g'':2,3-i:2,3-i':2,3-i'']benzo[1,6-c:2,3-c':4,5-c'']tris[1,6]dioxecine



d = 3.714(6) Å; θ = 165.8(3)°; *d* = 3.855(5) Å; θ = 162.6(3)°

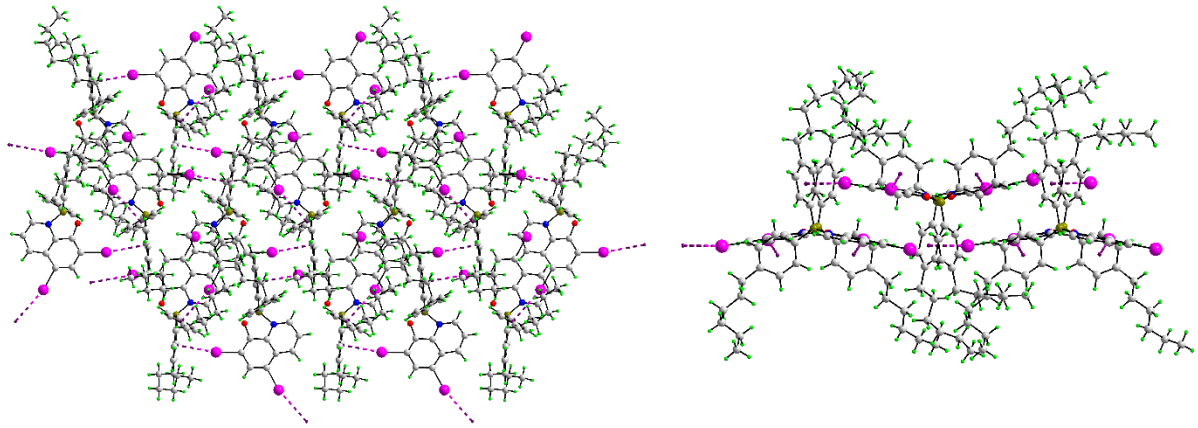
D. Mosca, A. Stopin, J. Wouters, N. Demitri and D. Bonifazi, *Chem. - Eur. J.*, 2017, **23**, 15348-15354; DOI: 10.1002/chem.201702032

{Two independent molecules and each self-assembles into a helical (2_1-screw symmetry) chain}

ESI Table 6. Two-dimensional aggregates sustained by C–H···π(arene) interactions

158. VELTOY

(5,7-Diiodoquinolin-8-olato)bis(4-hexylphenyl)boron



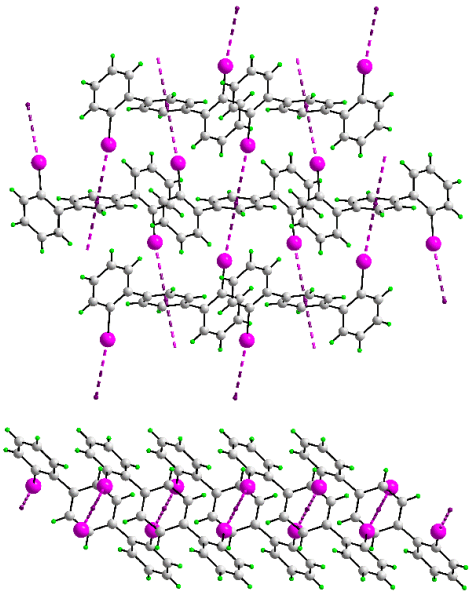
d = 3.487(5) Å; θ = 165.0(3)°; *d* = 3.558(5) Å; θ = 162.4(3)° and *d* = 3.587(5) Å; θ = 160.0(3)°; *d* = 3.605(5) Å; θ = 162.4(3)°

Y. Qi, W. Xu, R. Kang, N. Ding, Y. Wang, G. He and Y. Fang, *Chem. Sci*., 2018, **9**, 1892-1901; DOI: 10.1039/C7SC05243J

{Two independent molecules. Each accepts two and donates two interactions. The molecules aggregate into a two-dimensional array, two molecules thick}

159. LITBIA

2,2''-bis(Iodo)-(1,1':4',1'')terphenyl



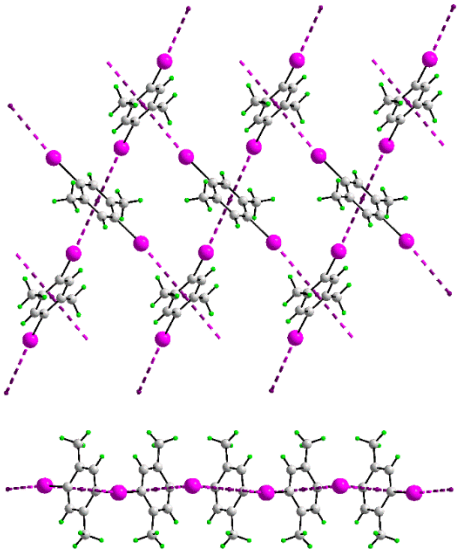
d = 3.606(3) Å; θ = 171.50(16)°

C. Poriel, J.-J. Liang, J. Rault-Berthelot, F. Barrière, N. Cocherel, A. M. Z. Slawin, D. Horhant, M. Virboul, G. Alcaraz, N. Audebrand, L. Vignau, N. Huby, G. Wantz and L. Hirsch, *Chem. - Eur. J.*, 2007, **13**, 10055-10069; DOI: 10.1002/chem.200701036

{The molecule is disposed about an inversion centre. The central ring accepts two interactions and each I atom participates in one so that a two-dimensional array is generated, with a flat topology}

160. IBILEN

1,4-bis(Iodo)-2,5-dimethylbenzene



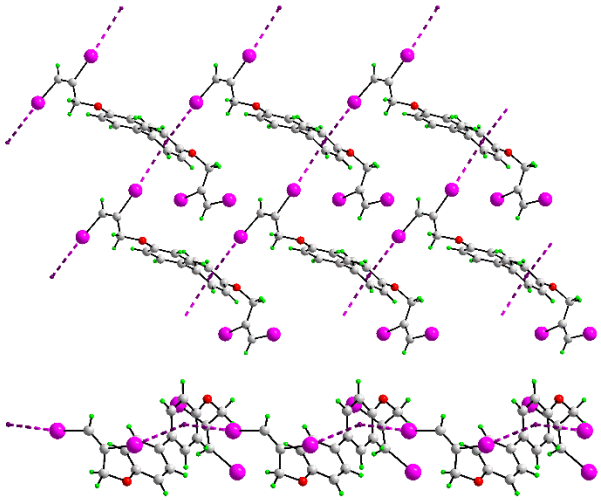
d = 3.849(3) Å; θ = 173.66(8)°

E. Albright, J. Cann, A. Decken and S. Eisler, *CrystEngComm*, 2017, **19**, 1024-1027; DOI: 10.1039/C6CE02339H

{Molecule is situated about a centre of inversion. Each I atom interacts with the ring to generate a two-dimensional array with a slight undulating topology}

161. ULEFUN

4,4'-bis[(E)-(2,3-Di-iodoprop-2-en-1-yl)oxy]biphenyl



d = 3.569(2) Å; θ = 171.54(15)°; *d* = 3.604(2) Å; θ = 167.74(12)°

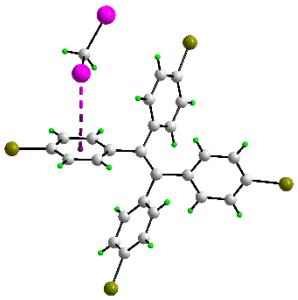
K. Shah, M. R. Shah and S. W. Ng, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2011, **67**, o568; DOI: 10.1107/S1600536811003874

{Molecules self-assemble into a flat two-dimensional array where one ring accepts two interactions}

ESI Table 7. Supramolecular aggregates in solvates sustained by C–H···π(arene) interactions

162. KUWYOS

Tetrakis(4-bromophenyl)ethylene sesquikis(diiodomethane)



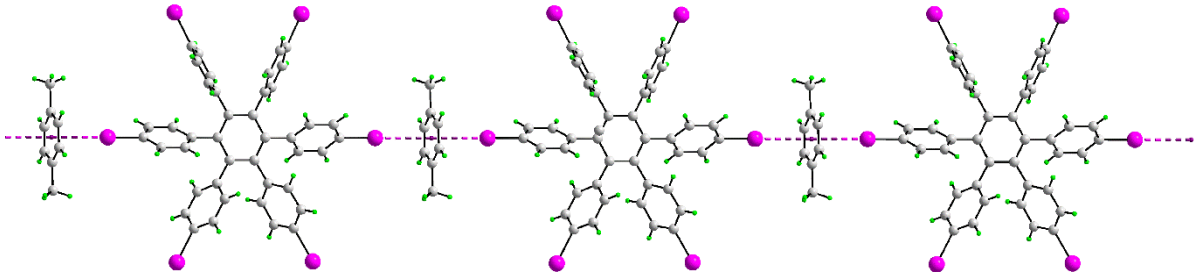
d = 3.853(2) Å; θ = 170.7(2)°

F. M. A. Noa, S. A. Bourne and L. R. Nassimbeni, *Cryst. Growth Des*., 2015, **15**, 3271-3279; DOI: 10.1021/acs.cgd.5b00402

{In the 2:3 CH_2I_2 solvate, one of each different component assembles into a two-molecule aggregate}

163. FELMUF

Hexakis(4-iodophenyl)benzene p-xylene solvate



d = 3.272(5) Å; θ = 180°

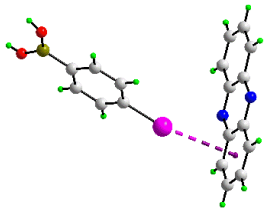
K. Kobayashi, N. Kobayashi, M. Ikuta, B. Therrien, S. Sakamoto and K. Yamaguchi, *J. Org. Chem*., 2005, **70**, 749-752; DOI: 10.1021/jo048521i

{Each molecule has 2-fold symmetry. The iodide atoms lying on the 2-fold axis form I···π(arene) rings to form a twisted chain}

ESI Table 8. Supramolecular aggregates in co-crystals sustained by C–H···π(arene) interactions

164. RORPEV

(4-Iodophenyl)boronic acid phenazine



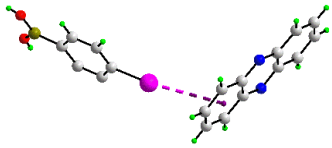
d = 3.678(2) Å; θ = 166.45(12)°

S. SeethaLekshmi, S. Varughese, L. Giri and V. R. Pedireddi, *Cryst. Growth Des*., 2014, **14**, 4143-4154; DOI: 10.1021/cg500750p

{The co-crystal co-formers (two independent molecules each) assemble into a two-molecule aggregate via a single interaction}

165. RORPAR

(4-Iodophenyl)boronic acid bis(phenazine) monohydrate



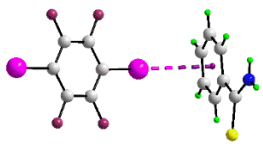
d = 3.839(3) Å; θ = 169.36(10)°

S. SeethaLekshmi, S. Varughese, L. Giri and V. R. Pedireddi, *Cryst. Growth Des*., 2014, **14**, 4143-4154; DOI: 10.1021/cg500750p

{The co-crystal co-formers assemble into a two-molecule aggregate via a single interaction}

166. VULLEV

Thiobenzamide 1,4-di-iodotetrafluorobenzene



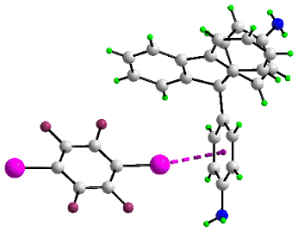
d = 3.429(3) Å; θ = 160.21(9)°

K. S. Eccles, R. E. Morrison, A. S. Sinha, A. R. Maguire and S. E .Lawrence, *Cryst. Growth Des*., 2015, **15**, 3442-3451; DOI: 10.1021/acs.cgd.5b00513

{The two co-crystal co-formers are connected into a two-molecule aggregate}

167. MOCGET

9,9-bis(4-Aminophenyl)fluorene 1,4-diiodotetrafluorobenzene



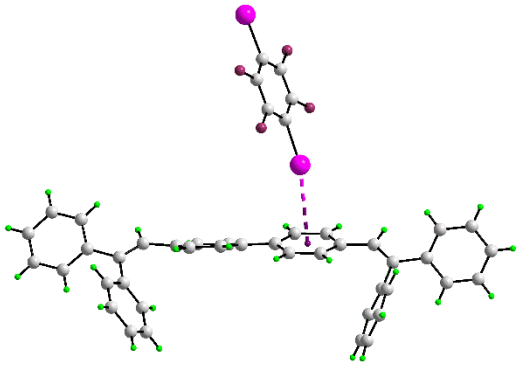
d = 3.4573(11) Å; θ = 164.94(10)°

R. Bhowal, S. Biswas, D. P. A. Saseendran, A. L. Konera and D. Chopra, *CrystEngComm*, 2019, **21**, 1940-1947; DOI: 10.1039/C8CE02118J

{The two co-crystal co-formers are connected into a two-molecule aggregate. The second iodide atom forms an analogous interaction with the same ring but, with parameters () outside the search criteria, i.e. *d* = 3.4738(11) Å; θ = 155.35(10)°. If take into consideration, a linear chain eventuates}

168. MOCFUI

4,4'-bis(2,2-Diphenylethenyl)-1,1'-biphenyl 1,2,4,5-tetrafluoro-3,6-diiodobenzene



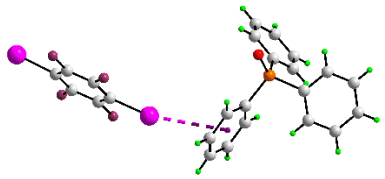
d = 3.4655(10) Å; θ = 166.51(7)°

R. Bhowal, S. Biswas, D. P. A. Saseendran, A. L. Konera and D. Chopra, *CrystEngComm*, 2019, **21**, 1940-1947; DOI: 10.1039/C8CE02118J

{The two molecules are connected into a two-molecule aggregate}

169. JUZRUT

Triphenylphosphine oxide bis(1,2,4,5-tetrafluoro-3,6-di-iodobenzene)



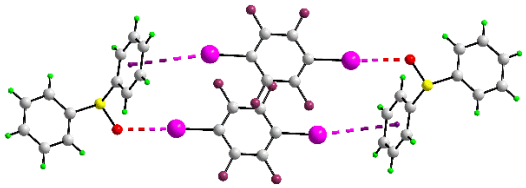
d = 3.7369(15) Å; θ = 165.65(8) °

Y. Xu, J. Viger-Gravel, I. Korobkov and D. L. Bryce, *J. Phys. Chem. C*, 2015, **119**, 27104-27117; DOI: 10.1021/acs.jpcc.5b09737

{Molecules associate into a zero-dimensional aggregate}

170. PEFNEV

1,4-Di-iodotetrafluorobenzene diphenylsulfoxide



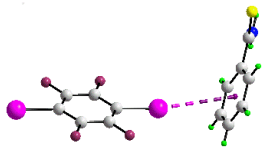
d = 3.848(2) Å; θ = 165.58(12)°

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**, 2969-2977; DOI: 10.1021/cg300189v

{The co-crystal co-formers assemble into a two-molecule aggregate. These are connected into a four-molecule aggregate via I···O [2.848(3) Å] secondary bonding interactions occurring about a centre of inversion}

171. KUWPEZ

bis(Benzenecarbothioamide) tris(1,2,4,5-tetrafluoro-3,6-diiodobenzene)



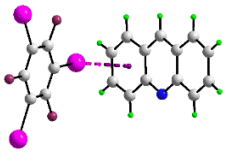
d = 3.868(2) Å; θ = 171.55(15)°

K. S. Eccles, R. E. Morrison, A. S. Sinha, A. R. Maguire and S. E. Lawrence, *Cryst. Growth Des*., 2015, **15**, 3442-3451; DOI: 10.1021/acs.cgd.5b00513

{One of the $C_6F_4I_2$ molecules is disposed about a centre of inversion. The co-crystal co-formers in the general positions assemble into a two-molecule aggregate}

172. SAJDAL

Acridine 1,3,5-trifluoro-2,4,6-triiodobenzene



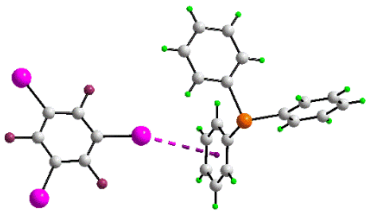
d = 3.4499(14) Å; θ = 161.51(7)°

P. M. J. Szell, S. A. Gabriel, R. D. D. Gill, S. Y. H. Wan, B. Gabidullin and D. L. Bryce, *Acta Crystallogr., Sect. C: Cryst. Struct. Chem*., 2017, **73**, 157-167; DOI: 10.1107/S2053229616015023

{The two co-crystal co-formers are connected into a two-molecule aggregate}

173. FIYZUL

1,3,5-Trifluoro-2,4,6-tri-iodobenzene triphenylarsine



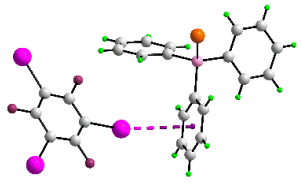
d = 3.5610(10) Å; θ = 163.17(6)°

K. Lisac, F. Topić, M. Arhangelskis, S. Cepić, P. A. Julien, C. W. Nickels, A. J. Morris, T. Friščić and D. Cinčić, *Nat. Commun*., 2019, **10**, 61; DOI: 10.1038/s41467-018-07957-6

{The co-crystal co-formers associate to form a two-molecule aggregate}

174. COFFIO

Triphenylphosphane selenide 1,3,5-trifluoro-2,4,6-tri-iodobenzene



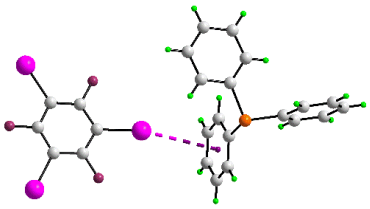
d = 3.5746(12) Å; θ = 160.25(10)°

J. Viger-Gravel, J. E. Meyer, I. Korobkov and D. L. Bryce, *CrystEngComm*, 2014, **16**, 7285-7297; DOI: 10.1039/C4CE00345D

{Two pairs of independent molecules in the co-crystal – one pair associates to form a two-molecule aggregate. The second molecule forms two similar contacts to link a pair of $Ph_3P{=}Se$ molecules but with parameters outside the specified search criteria: *d* = 3.9132(12) Å; θ = 124.38(8)°; *d* = 3.9231(13) Å; θ = 78.76(7)°}

175. KIPCOE01

1,3,5-Trifluoro-2,4,6-tri-iodobenzene triphenylphosphane



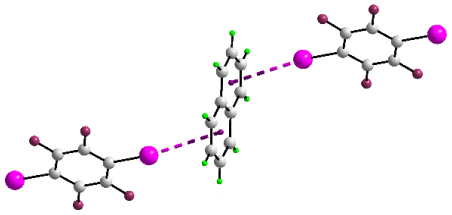
d = 3.5930(8) Å; θ = 166.19(5)°

K. Lisac, F. Topić, M. Arhangelskis, S. Cepić, P. A. Julien, C. W. Nickels, A. J. Morris, T. Friščić and D. Cinčić, *Nat. Commun.*, 2019, **10**, 61; DOI: 10.1038/s41467-018-07957-6

{The co-crystal co-formers assemble into a two-molecule aggregate}

176. NICTAW

bis(1,2,4,5-Tetrafluoro-3,6-diiodobenzene) naphthalene



d = 3.737(3) Å; θ = 171.75(18)°

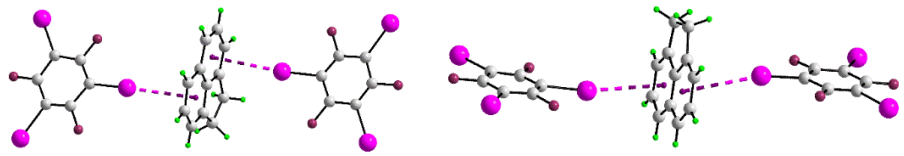
Q. J. Shen, X. Pang, X. R. Zhao, H. Y. Gao, H.-L. Sun and W. J. Jin, *CrystEngComm*, 2012, **14**, 5027-5034; DOI: 10.1039/C2CE25338K

{The naphthalene molecule is disposed about a centre of inversion. The co-crystal co-formers assemble into a three-molecule aggregate. Additional interactions but, outside the search

criteria are noted for the second iodide atom (d = 3.578(3) Å; θ = 149.78(18)°) – of included, the result is a supramolecular tape}

177. YIRFAJ

1,2-Dihydroacenaphthylene 1,3,5-trifluoro-2,4,6-tri-iodobenzene (1/2)



d = 3.520(7) Å; θ = 160.8(5)° & d = 3.450(7) Å; θ = 163.2(5)°

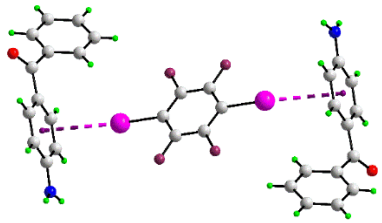
d = 3.476(7) Å; θ = 166.7(5)° & d = 3.610(6) Å; θ = 163.2(5)°; right-hand image

L. Li, Z. F. Liu, W. X. Wu and W. J. Jin, *Acta Crystallogr., Sect. B: Struct. Sci., Cryst. Eng. Mat.*, 2018, **74**, 610-617; DOI: 10.1107/S2052520618013483

{Two independent 1,2-dihydroacenaphthylene molecules and four independent 1,3,5-trifluoro-2,4,6-tri-iodobenzene molecules comprise the asymmetric unit. Each 1,2-dihydroacenaphthylene molecule co-former forms two interactions, one per ring, and each iodo co-former donates a single contact. The result is a pair of three-molecule aggregates. If the criteria are relaxed {d = 3.555(7) Å; θ = 158.5(5)°; d = 3.561(6) Å; θ = 154.4(4)°; d = 3.536(7) Å; θ = 157.9(5)° & d = 3.608(8) Å; θ = 159.1(5)°} each 1,2-dihydroacenaphthylene molecule co-former forms four interactions, two per ring and iodo co-former donates two contacts with the result a two-dimensional array with an undulating topology is formed}

178. JEJBUY

bis((4-Aminophenyl)(phenyl)methanone) 1,2,4,5-tetrafluoro-3,6-diiodobenzene



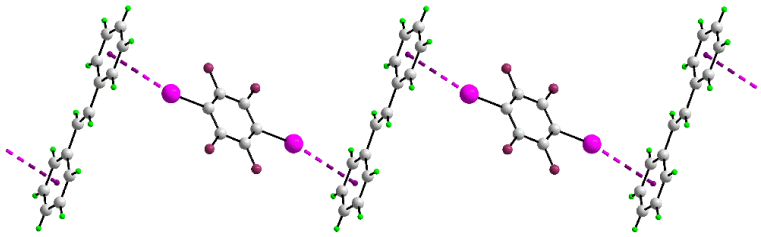
d = 3.5283(19) Å; θ = 167.63(13)°

V. Nemec and D. Cinčić, *CrystEngComm*, 2016, **18**, 7425-7429; DOI: 10.1039/C6CE01703G

{The CF_4I_2 molecule is disposed about a centre of inversion in this 2:1 co-crystal. The molecules assemble into a three-molecule aggregate}

179. GUFNOM

1,1'-Ethene-1,2-diyldibenzene 1,2,4,5-tetrafluoro-3,6-di-iodobenzene



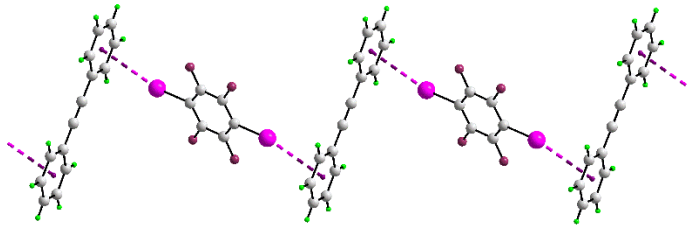
d = 3.580(6) Å; θ = 166.7(4)°

S. d'Agostino, F. Grepioni, D. Braga and B. Ventura, *Cryst. Growth Des.*, 2015, **15**, 2039-2045; DOI: 10.1021/acs.cgd.5b00226

{Each co-crystal co-former is situated about a centre of symmetry. Molecules assemble into a linear chain with a step-ladder topology}

180. GUFNEC

1,1'-Ethyne-1,2-diyldibenzene 1,2,4,5-tetrafluoro-3,6-di-iodobenzene



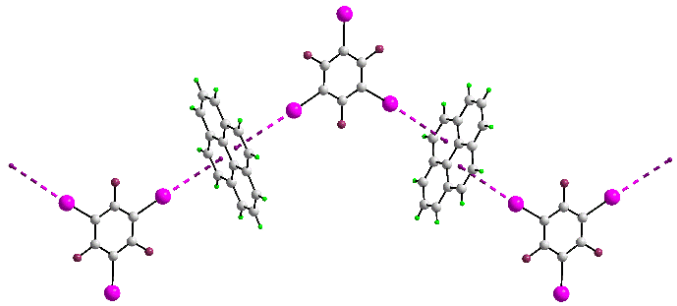
d = 3.6043(18) Å; θ = 165.83(11)°

S. d'Agostino, F. Grepioni, D. Braga and B. Ventura, *Cryst. Growth Des.*, 2015, **15**, 2039-2045; DOI: 10.1021/acs.cgd.5b00226

{Each co-crystal co-former is situated about a centre of symmetry. Molecules assemble into a linear chain with a step-ladder topology}

181. QEVWEW

Pyrene 1,3,5-trifluoro-2,4,6-triiodobenzene



d = 3.792(3) Å; θ = 162.86(15)°

L. Li, W. X. Wu, Z. F. Liu and W. J. Jin, *New J. Chem*., 2018, **42**, 10633-10641; DOI: 10.1039/C7NJ04536K

{The pyrene molecule is situated about a centre of inversion, and the 2,4,6-triiodobenzene molecule has 2-fold symmetry. The co-crystal co-formers assemble into a zig-zag chain (glide-symmetry)}

ESI Table 9. A survey of iodide analogues of **1**-**181** along with bromide, chloride and fluoride congeners, when known. Full composition, pertinent unit-cell data and literature citations are presented. When present in their crystals, geometric data for C–X···π(arene) interactions are included.

1 POPKAI hydroxy(3-iodophenyl)acetic acid; $P\bar{1}$, $Z' = 3$ **1**

{d = 3.521(3) Å; θ = 165.0(2)°: two-molecule aggregate sustained by a single interaction}

Congeners:

POPJEL **Br_1** $P2_1/c$ polymorph, $Z' = 1$ **1**

{no C–Br···π(arene) interactions}

POPJEL01 **Br_2** $P\bar{1}$ polymorph, $Z' = 2$ **1**

{Side-on connection with d = 3.7763(19) Å and θ = 112.95(13)°}

FIZPEL02 **Cl_1** $P2_1/c$ polymorph, $Z' = 1$ **1**

{no C–Cl···π(arene) interactions}

FIZPEL **Cl_2** $P\bar{1}$ polymorph, $Z' = 2$ **2**

{Side-on connection with d = 3.8225(10) Å and θ = 110.20(7)°}

WESBIF01 **F_1** $P2_1/a$ polymorph, $Z' = 1$ **1**

{no C–F···π(arene) interactions}

WESBIF **F_2** $P\bar{1}$ polymorph, $Z' = 2$ **3**

{Side-on, bifurcated connections with d = 3.5961(12) Å and θ = 132.46(7)° & d = 3.7691(12) Å and θ = 78.84(8)°}

{No isomorphous relationship between **1** and congeners}

1 S. J. Coles, A. L. Ellis, K. Leung, J. Sarson, T. L. Threlfall and G. J. Tizzard, *CrystEngComm*, 2014, **16**, 10816-10823; DOI: 10.1039/C4CE01832J

2 S. J. Coles, T. L. Threlfall and G. J. Tizzard, *Cryst. Growth Des*., 2014, **2**, 1623-1628; DOI: 10.1021/cg401655h

3 S. Larsen and K. Marthi, *Acta Crystallogr., Sect. B: Struct. Sci*., 1994, **50**, 373-381; DOI: 10.1107/S0108768193010766

2 NIQZET 4-Iodophenylboronic acid hemihydrate; $Z' = 1$; *Ibam* **1**

{d = 3.523(5) Å; θ = 167.5(4)°: two-molecule aggregate sustained by a single interaction}

Analogues:

LOXDAF **2**.isonicotinamide **2**

LOXDEJ **2**.nicotinamide **2**

RORLUH **2**.4,4'-bipyridine monohydrate **3**

RORMAO **2**.sesquikis(trans-1,2-bis(4-pyridyl)ethene) **3**

RORMES **2**.hemikis(4,7-phenanthroline) **3**

164 RORPEV **2**.phenazine **3**

{*d* = 3.678(2) Å; θ = 166.45(12)°}

165 RORPAR **2**.bis(phenazine) monohydrate **3**

{*d* = 3.839(3) Å; θ = 169.36(10)°}

ULURAW **2**.1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione **4**

1 M. R. Shimpi, N. SeethaLekshmi and V. R. Pedireddi, *Cryst. Growth Des*., 2007, **7**, 1958-1963; DOI: 10.1021/cg060863p

2 J. Hernández-Paredes, A. L. Olvera-Tapia, J. I. Arenas-García, H. Höpfl, H. Morales-Rojas, D. Herrera-Ruiz, A. I. Gonzaga-Morales, L. Rodríguez-Fragoso, *CrystEngComm*, 2015, **17**, 5166-5186; DOI: 10.1039/C4CE01934B

3 S. SeethaLekshmi, S. Varughese, L. Giri and V. R. Pedireddi, *Cryst. Growth Des*., 2014, **14**, 4143-4154; DOI: 10.1021/cg500750p

4 M. TalwelkarShimpi, S. Oberg, L. Giri and V. R. Pedireddi, *RSC Adv*., 2016, **6**, 43060-43068; DOI: 10.1039/C6RA04100K

4 SAJPIF 4-Iodo-N-(phenylsulfonyl)benzamide hemihydrate; $P\bar{1}$, $Z' = 2$ **1**

{*d* = 3.5945(18) Å; θ = 160.90(11)°}

Congeners:

The X = Br, Cl and F compounds are unsolvated and are isostructural with each other

QEVSES **Br**: $P\bar{1}$, $Z' = 1$ **2**

{*d* = 3.533(3) Å; θ = 142.0(2)°}

DUJKAV **Cl**: $P\bar{1}$, $Z' = 1$ **3**

{*d* = 3.6417(15) Å; θ = 139.78(8)°}

PURBAH **F**: $P\bar{1}$, $Z' = 1$ **4**

{no C–F···π(arene) interactions}

1 P. A. Suchetan, A. G. Sudha, E. Suresha, N. K. Lokanath, S. Naveen and I. Warad, *IUCrData*, 2017, **2**, x170149; DOI: 10.1107/S2414314617001493

2 S. Naveen, A. G. Sudha, E. Suresha, N. K. Lokanath and P. A. Suchetan, *Z. Kristallogr. - Cryst. Mater.*, 2017, **232**, 767-780; DOI: 10.1515/zkri-2016-2008

3 P. A. Suchetan, B. T. Gowda, S. Foro and H. Fuess, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2009, **65**, o3156-;DOI: 10.1107/S1600536809048399

4 P. A. Suchetan, S. Sreenivasa, K. S. Srivishnu, H. N. Lakshmikantha, G. M. Supriya, S. Naveen and N. K. Lokanath, *Z. Kristallogr. - Cryst. Mater.*, 2015, **230**, 543-550; DOI: 10.1515/zkri-2014-1832

15 YASQIU03 1,3,5-Triethyl-2,4,6-tris((4-iodophenoxy)methyl)benzene; $P2_1/n$, $Z' = 2$, a = 19.548(<1), b = 13.351(<1), c = 26.323(<1) Å, β = 108.85(<1)° (190 K) **1**

{d = 3.657(2) Å; θ = 160.11(15)°: Two independent molecules assemble to form a two-molecule aggregate via a single interaction. A second interaction, d = 3.535(2) Å; θ = 152.9(2)°, connects molecules into a twisted chain}

Analogues:

86 YASRAN **15**.m-xylene **2**

{d = 3.664(4) Å; θ = 161.4(3)°: molecules assemble into a linear chain}

YASSIW **15**.chloroform **2**

{isostructural to YASRAN but parameters outside the range: d = 3.806(3) Å; θ = 157.5(3)° to give a linear chain}

YASTAP **15**.1,2-dichloroethane **2**

{parameters outside the range: d = 3.829(3) Å; θ = 156.1(3)° but, form a linear chain}

Congeners:

YASTOD **Br**: $P2_1/c$, $Z' = 2$, a = 19.267(<1), b = 13.448(<1), c = 25.303(1) Å, β = 109.81(<1)° (226 K) **1**

{isostructural; d = 3.5123(17) Å; θ = 157.64(14)° & d = 3.6204(17) Å; θ = 156.04(14)°: molecules assemble into a twisted chain}

YASXIB01 **Cl**: $P2_1/c$, $Z' = 2$, a = 19.091(<1), b = 13.396(<1), c = 24.803(1) Å, β = 110.35(<1)° (190 K) **2**

{isostructural; d = 3.5139(9) Å; θ = 159.70(8)° & d = 3.6901(9) Å; θ = 155.59(8)°: molecules assemble into a twisted chain}

1 V. G. Saraswatula and B. K. Saha, *New J. Chem.*, 2014, **38**, 897-901; DOI: 10.1039/c3nj01395b

2 S. Bhattacharya and B. K. Saha, *Cryst. Growth Des.*, 2012, **12**, 169-178; DOI: 10.1021/cg2009144

16. WOHXAT tris(4-Iodophenyl) benzene-1,3,5-tricarboxylate **1**

{d = 3.766(2) Å; θ = 166.33(13)°: two-molecule aggregate sustained by a single contact}

Analogue:

87 WOHXEX **16**.chloroform trisolvate **1**

{d = 3.717(4) Å; θ = 160.82(15)°: linear chain}

1 F. C. Pigge, V. R. Vangala, P. P. Kapadia, D. C. Swenson and N. P. Rath, *Chem. Commun.*, 2008, 4726-4728; DOI: 10.1039/b809592b

29. QEZGEH (2R*,3S*,4S*,11S*)-4-Iodo-11-(4-methoxyphenylmethoxymethyl)-3-(p-tosyl)-2-oxo-10-(benzyloxy)-8-(benzyloxymethyl)-6-(2,2,2-trichloroethoxycarbonyl)-2,3,3a,4,5,6,11,11a-octahydro-oxazolo(4,5-d)(1)benzazocine **1**

{d = 3.6813(15) Å; θ = 161.08(8)°: centrosymmetric dimer}

Analogue:

QEZGIL **29**.$CHCl_3$ **1**

{no contact}

1 I. M. Fellows, D. E. Kaelin and S. F. Martin, *J. Am. Chem. Soc.*, 2000, **122**, 10781-10787; DOI: 10.1021/ja0013879

36. GOYMAL 9-(5-Iodopyridin-3-yl)-9H-carbazole: $P\bar{1}$, Z' = 2, a = 6.189(<1), b = 13.246(<1), c = 18.312(1) Å, α = 74.52(<1), β = 89.92(<1), γ = 89.38(<1)° (room temp.) **1**

{*d* = 3.741(3) Å; θ = 163.2(2)°: centrosymmetric dimer; also the second independent molecule but, outside the specified criteria: *d* = 3.635(3) Å; θ = 145.6(2)°}

Congeners:

GOYLUE **Br**: $P\bar{1}$, Z' = 2, *a* = 6.147(<1), *b* = 13.083(<1), *c* = 18.222(1) Å, α = 105.33(<1), β = 90.86(<1), γ = 90.29(<1)° (room temp.) **1**

{isostructural: *d* = 3.646(3) Å; θ = 149.74(17)° & *d* = 3.738(3) Å; θ = 162.96(17)°}

GOYLIS **Cl**: $P2_1/c$, Z' = 1, *a* = 11.675(<1), *b* = 4.058(<1), *c* = 28.332(1) Å, β = 99.53(<1)° (room temp.) **1**

{*d* = 3.6753(12) Å; θ = 72.73(8)°: side-on interactions lead to a linear chain}

GOYMEP **F**: $Pna2_1$, Z' = 2, *a* = 17.480(<1), *b* = 25.382(<1), *c* = 6.187(<1) Å (room temp.) {no analogous interactions} **1**

1 H. Sasabe, Y. Kato, Y. Watanabe, T. Ohsawa, N. Aizawa, W. Fujiwara, Y.-J. Pu, H. Katagiri and J. Kido, *Chem. - Eur. J.*, 2019, **25**, 16294-16300; DOI: 10.1002/chem.201903100

37. NICRAU 2-Bromo-10-(5-bromo-2-iodophenyl)-9-phenylanthracene; $P\bar{1}$, Z' = 1, *a* = 8.119(1), *b* = 11.049(1), *c* = 13.905(2) Å, α = 96.92(<1), β = 105.38(<1), γ = 110.02(<1)° (room temp) **1**

{*d* = 3.762(2) Å; θ = 166.46(13)°: centrosymmetric dimer}

Congeners:

NICREY **Br**: $P\bar{1}$, Z' = 1, *a* = 8.252(1), *b* = 11.043(1), *c* = 13.100(1) Å, α = 74.59(<1), β = 80.48(<1), γ = 69.19(<1)° (room temp) **1**

{isostructural: *d* = 3.4926(17) Å; θ = 150.20(13)°: centrosymmetric dimer but, involving the central ring rather than a flanking ring}

KETXOY **Cl**: $P\bar{1}$, Z' = 1, *a* = 8.222(<1), *b* = 11.010(<1), *c* = 13.002(<1) Å, α = 96.92(<1), β = 105.38(<1), γ = 110.02(<1)° (room temp) **1**

{isostructural: *d* = 3.4912(17) Å; θ = 150.23(13)°: centrosymmetric dimer but, involving the central ring rather than a flanking ring}

1 M. Xue, L. Ding, L. Lin, Y. Lu, B. He, Y. Deng, Y. Guo, Y. Hong, J. W. Y. Lam, H. Qiu, Z. Zhao and B. Z. Tang, *Asian J. Org. Chem.*, 2012, **1**, 331-335; DOI: 10.1002/ajoc.201200111

48. DEGWUJ 2-Iodo-4-(1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)vinyl)benzoic acid; Z' = 1; $P2_1/n$ **1**

{d = 3.862(2) Å; θ = 163.38(15)°: centrosymmetric dimer}

Congeners:

DEGWOD **Br** **1**

{not isostructural: no interaction}

DEGWIX **Cl** **1**

{not isostructural: no interaction}

1 J. K. Furmick, I. Kaneko, A. N. Walsh, J. Yang, J. S. Bhogal, G. M. Gray, J. C. Baso, D. O. Browder, J. L. S. Prentice, L. A. Montano, C. C. Huynh, L. M. Marcus, D. G. Tsosie, J. S. Kwon, A. Quezada, N. M. Reyes, B. Lemming, P. Saini, A. van der Vaart, T. L. Groy, P. A. Marshall, P. W. Jurutka and C. E. Wagner, *ChemMedChem*, 2012, **7**, 1551-1556; DOI: 10.1002/cmdc.201290042

51. VIKHOP bis(Iodomethyl)phenylphosphine oxide; $P2_1/n$, Z' = 1; **1**

{d = 3.6983(19) Å; θ = 170.77(12)°: centrosymmetric dimer}

Congeners:

ODUMUX **Cl** **2**

{not isostructural; d = 3.447(3) Å; θ = 132.84(19)°: linear chain}

1 M. A. Stevens, F. H. Hashim, E. S. H. Gwee, E. I. Izgorodina, R. E. Mulvey and V. L. Blair, *Chem. - Eur. J.*, 2018, **24**, 15669-15677; DOI: 10.1002/chem.201803477

2 L. R. Almazahreh, U.-P. Apfel, W. Imhof, M. Rudolph, H. Görls, J. Talarmin, P. Schollhammer, M. El-khateeb, W, Weigand, *Organometallics*, 2013, **32**, 4523-4530; DOI: 10.1021/om4003544

58. ZUQMIJ 2-Ammonio-3-(4-(4-hydroxy-3,5-diiodophenoxy)-3,5-diiodophenyl)propanoate hydrate, **59**.H_2O **1**

{*d* = 3.443(3) Å; θ = 170.5(2)°; *d* = 3.457(3) Å; θ = 167.6(2)°: Two independent iodo-molecules comprise the asymmetric unit which are connected into a non-symmetric, two-molecule aggregate}

Analogue:

59. ZUQMOP **59**.4H_2O **1**

d = 3.476(3) Å; θ = 168.6(3)°; *d* = 3.489(3) Å; θ = 168.6(3)°: same non-symmetric dimer}

1 S. Mondal and G. Mugesh, *Angew. Chem., Int. Ed*., 2015, **54**, 10833-10837; DOI: 10.1002/anie.201505281

71. TUFXEZ 7-iodo-7-phenylbicyclo[2.2.1]heptane; $P2_1/n$, Z' = 1, *a* = 6.350(5), *b* = 31.010(30), *c* = 6.458(5) Å, β = 112.53(1)° (room temp.) **1**

{*d* = 3.681(5) Å; θ = 178.27(14)°: linear chain}

Congeners:

TUFXID **Br**: $P2_1/n$, Z' = 1, *a* = 6.201(5), *b* = 30.714(5), *c* = 6.350(5) Å, β = 114.35(<1)° (room temp.) **1**

{isostructural: *d* = 3.589(3) Å; θ = 176.62(9)°: linear chain}

TUFXOJ **Cl**: $P2_1/n$, Z' = 1, *a* = 6.392(<1), *b* = 6.858(<1), *c* = 24.607(1) Å, β = 94.26(<1)° (room temp.) **1**

{no analogous contact}

1 T. Montoro, G. Tardajos, A. Guerrero, M. del R. Torres, C. Salgado, I. Fernández and J. O. Barcina, *Org. Biomol. Chem*., 2015, **13**, 6194-6202; DOI: 10.1039/C5OB00366K

80. UVECEF 1,1'-Pyrene-1,3-diylbis(2-iodoethanone); $P\bar{1}$, Z' = 1, *a* = 8.638(5), *b* = 9.748(5), *c* = 10.406(5) Å, α = 103.30(<1), β = 94.98(<1), γ = 100.16(<1)° (room temp) **1**

{*d* = 3.647(3) Å; θ = 165.41(19)°: linear chain}

Congeners:

UVECAB **Br**: $P\bar{1}$, Z' = 1, *a* = 7.589(1), *b* = 8.043(1), *c* = 13.943(2) Å, α = 74.49(<1), β = 75.26(<1), γ = 89.92(<1)° (room temp) **1**

{isostructural: no analogous contact}

UVEBUU **Cl**: *P*$\bar{1}$, *Z*′ = 1, *a* = 7.784(1), *b* = 8.541(1), *c* = 12.007(1) Å, α = 98.13(<1), β = 101.83(<1), γ = 94.94(<1)° (room temp) **1**

{isostructural: no analogous contact}

UVEBOO **F**: *Pbca*, *Z* = 1, *a* = 7.485(1), *b* = 15.768(2), *c* = 24.344(3) Å (room temp)

{no analogous contact} **1**

1 P. S. Salini, S. K. Rajagopal and M. Hariharan, *Cryst. Growth Des*., 2016, **16**, 5822-5830; DOI: 10.1021/acs.cgd.6b00919

90. FANYOJ 4-(4-(Iodo)phenoxy)aniline; *Pna*2$_1$, *Z*′ =1, *a* = 7.724(1), *b* = 23.377(4), *c* = 6.115(<1) Å (100 K) **1**

{*d* = 3.5100(16) Å; θ = 171.39(12)°: zig-zag (glide-symmetry) chain}

Congeners:

FANYID Br: *Pna*2$_1$, *Z*′ =1, *a* = 7.697(<1), *b* = 23.105(3), *c* = 5.873(<1) Å (100 K) **1**

{isostructural: *d* = 3.4299(10) Å; θ = 169.66(7)°: zig-zag (glide-symmetry) chain}

FANYEZ Cl: *Pna*2$_1$, *Z*′ =1, *a* = 7.711(1), *b* = 22.935(4), *c* = 5.744(1) Å (100 K) **1**

{isostructural: *d* = 3.4288(11) Å; θ = 168.01(7)°: zig-zag (glide-symmetry) chain}

1 A. Dey and G. R. Desiraju, *CrystEngComm*, 2004, **6**, 642-646; DOI: 10.1039/b416962j

{Molecules associate to form a }

99. CIYQUY01 2^2-Iodo-1^2,1^6,3^2,3^6-tetramethyl-1^1,2^1:2^3,3^1-terphenyl: *Pbca*, *Z*′ = 1: *a* = 8.562(<1), *b* = 13.674(<1), *c* = 31.838(<1) Å **1**

{*d* = 3.7152(12) Å; θ = 169.07(7)°: zig-zag chain}

Analogue:

CIYQUY **99** polymorph: *C*2/*c*, *Z*′ = 0.5: *a* = 14.222(<1), *b* = 8.842(<1), *c* = 16.067(1) Å, β = 112.90(<1)° **2**

{no analogous interactions}

1 A. Linden, S. Duttwyler and J. S. Siegel, Private Communication to the Cambridge Structural Database, Refcode CIYQUY01, 2018.

2 J. Blundell, F. R. Hastings, B. M. Gridley, G. J. Moxey, W. Lewis, A. J. Blake and D. L. Kays, *Dalton Trans*., 2014, **43**, 14257-14264; DOI: 10.1039/C4DT00647J}

105. QOMYOG 1,1,2,2-Tetraphenyl-3,8-diiodocyclobuta(b)naphthalene; $P2_1/n$, $Z' = 1$, a = 16.332(3), b = 9.217(5), c = 19.212(2) Å, β = 94.45(1)° (room temp.) **1**

{d = 3.577(3) Å; θ = 170.81(13)°: zig-zag (glide-symmetry) chain}

Congeners:

QOMYIA **Br**: $P2_1/n$, $Z' = 1$, a = 9.000(4), b = 17.027(4), c = 17.680(4) Å, β = 96.29(3)° (room temp.)

{no analogous interaction} **1**

ZIVLIZ **Cl**: $P2_1/n$, $Z' = 1$, a = 8.988(6), b = 16.861(4), c = 17.737(2) Å, β = 96.48(3)° (room temp.)

{no analogous interaction} **2**

1 K. Tanaka, N. Takamoto, Y. Tezuka, M. Kato and F. Toda, *Tetrahedron*, 2001, **57**, 3761-3767; DOI: 10.1016/S0040-4020(01)00249-6

2 F. Toda, K. Tanaka, Z. Stein and I. Goldberg, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun*., 1996, **52**, 177-180; DOI: 10.1107/S0108270195011097

110. GIZTIT tris(4-Iodophenyl)methanol dichloromethane solvate **1**

{d = 3.617(2) Å; θ = 161.79(17)°: zig-zag chain with mirror symmetry}

Analogues:

156. GIZTEP **110**.unsolvated

{d = 3.6600(18) Å; θ = 169.77(15)°: helical chain} **1**

GIZTOZ **110**.benzene hemi-solvate **1**

{no analogous interaction}

1 D. Schollmeyer, O. V. Shishkin, T. Rühl and M. O. Vysotsky, *CrystEngComm*, 2008, **10**, 715-723; DOI: 10.1039/b716442d

127. ZZZQAC01 1,1,1-Trichloro-2,2-bis(4-iodophenyl)ethane; *Pca*2$_1$, *Z*′ = 1, *a* = 9.812(<1), *b* = 20.345(<1), *c* = 8.049(<1) Å (200 K) **1**

{*d* = 3.665(4) Å; θ = 162.5(3)°: helical chain}

Congeners:

ZZZQUDU01 **Br**: *Pca*2$_1$, *Z*′ = 1, *a* = 9.832(<1), *b* = 19.562(<1), *c* = 7.868(<1) Å (173 K) **2**

{isostructural: *d* = 3.529(2) Å; θ = 162.34(18)°: helical chain}

CPTCET12 **Cl**: *Pca*2$_1$, *Z*′ = 1, *a* = 9.815(<1), *b* = 19.012(1), *c* = 7.799(<1) Å (100 K) **3**, **4**

{isostructural: data from ref. **4**: *d* = 3.4487(10) Å; θ = 161.56(7)°: helical chain}

GOXCUU **F**: *P*2$_1$/*c*, *Z*′ = 4, *a* = 7.871(1), *b* = 34.698(6), *c* = 20.060(3) Å, β = 99.45(<1)° (100 K) **5**

{Four independent molecules, one pair associates via a single interaction: *d* = 3.413(2) Å; θ = 159.70(19)°, many other C–F/Cl···π(arene) contacts}

GOXCUU01 **F**: *P*2$_1$/*c*, *Z*′ = 1, *a* = 9.302(1), *b* = 13.294(1), *c* = 10.935(1) Å, β = 97.41(<1)° (100 K) **5**

{long, side-on interaction with *d* = 3.9303(15) Å; θ = 83.78(9)°, leading to a dimeric aggregate}

1 G. Smith, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2012, **68**, o2504; DOI: 10.1107/S1600536812032254

2 G. Smith, *Private Communication to the Cambridge Structural Database*, Refcode ZZZQUDU01, 2013.

3 T. P. DeLacy, C. H. L. Kennard, *J. Chem. Soc., Perkin Trans. 2*, 1972, 2148-2153; DOI: 10.1039/p29720002148

4 J. Yang, C. T. Hu, X. Zhu, Q. Zhu, M. D. Ward and B. Kahr, *Angew. Chem., Int. Ed.*, 2017, **56**, 10165-10169; DOI: 10.1002/anie.201703028

5 X. Zhu, C. T. Hu, J. Yang, L. A. Joyce, M. Qiu, M. D. Ward and B. Kahr, *J. Am. Chem. Soc.*, 2019, **141**, 16858-16884; DOI: 10.1021/jacs.9b08125

129. SAYNIS N,N-Dimethyl-4-{[(2,3,5,6-tetrafluoro-4-iodophenyl)imino]methyl}aniline **1**

{*d* = 3.685(3) Å; θ = 178.0(2)°: helical (2$_1$-screw symmetry) chain}

Analogue:

SAYNOY **129**.4,4'-bipyridine

{no analogous interaction}

1 Y. Wang, H. Shang, B. Li, H. Zhang and S. Jiang, *CrystEngComm*, 2017, **19**, 3801-3807; DOI: 10.1039/C7CE00805H

130. FOYMIS 2-[(2-Iodophenyl)imino]-2H-1-benzopyran-3-carboxamide: $P2_1/c$, Z' = 1, a = 6.940(<1), b = 10.258(<1), c = 20.761(<1) Å, β = 96.93(<1)° (room temp.)

{d = 3.6899(19) Å; θ = 166.72(13)°: helical chain} **1**

Congeners:

FOYMAK01 **Br**: $P2_1/c$, Z' = 1, a = 6.940(<1), b = 10.261(<1), c = 20.764(1) Å, β = 96.92(<1)° (293 K) **1**

{isostructural: d = 3.683(5) Å; θ = 166.8(3)°: helical chain}

FOYLUD **Cl**: $P2_1/c$, Z' = 1, a = 4.375(<1), b = 30.823(5), c = 9.855(3) Å, β = 93.23(1)° (room temp.) **1**

{no analogous interaction}

FOYLIR01 **F**: $P2_1/c$, Z' = 1, a = 4.700(1), b = 30.579(8), c = 8.853(3) Å, β = 92.70(2)° (room temp.) **1**

{no analogous interaction}

1 S. V. Shishkina, I. S. Konovalova, S. M. Kovalenko, P. V. Trostianko, A. O. Geleverya, L. L. Nikolayeva and N. D. Bunyatyan, *Acta Crystallogr., Sect. B: Struct. Sci., Cryst. Eng. Mat.*, 2019, **75**, 887-902; DOI: 10.1107/S2052520619010485

134. TIHJUR 8-Iodo-6-(4-methoxyphenyl)-3-((4-methylphenyl)sulfonyl)-3-azatricyclo[5.4.1.01,5]dodec-5-ene: $P2_1$, Z' = 1, a = 12.813(4), b = 6.246(2), c = 15.497(5) Å, β = 110.30(<1)° (200 K) **1**

{d = 3.739(4) Å; θ = 163.9(2)°: helical chain}

Congener:

TIHKOM **Cl**: $P2_1$, Z' = 1, a = 12.578(5), b = 6.194(2), c = 14.866(6) Å, β = 108.50(1)° (200 K) **1**

{isostructural: d = 3.727(3) Å; θ = 165.7(2)°: helical chain}

1 M.-C. P. Yeh, C.-J. Liang, C.-W. Fan, W.-H. Chiu and J.-Y. Lo, *J. Org. Chem.*, 2012, **77**, 9707-9717; DOI: 10.1021/jo301764g

135. VOJBAY 2-Chloro-4-iodoaniline: $P2_12_12_1$, Z' = 1, a = 5.628(<1), b = 8.786(<1), c = 14.922(<1) Å (90 K) **1**

{d = 3.7399(15) Å; θ = 171.08(9)°: helical chain}

Congeners:

HUGSAE **Br**: $P2_12_12_1$, Z' = 1, a = 10.965(4), b = 15.814(6), c = 4.023(1) Å (90 K) **2**

{no analogous interaction}

WEMDIB **Cl**: $P2_12_12_1$, Z' = 1, a = 15.536(6), b = 11.255(4), c = 3.934(2) Å (room temp. **3**

{no analogous interaction}

1 Y.-H. Xu, C. Wang and F. Qu, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2008, **64**, o2300; DOI: 10.1107/S1600536808036076

2 Z.-B. Wei, Z.-H. Liu, J.-L. Ye and H.-K. Zhang, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2010, **66**, o250; DOI: 10.1107/S1600536809054944

3 S.-Q. Dou, N. Weiden and A. Weiss, *Acta Chim. Hung.*, 1993, **130**, 497-522.

139. BANWIX N-(4-Iodophenyl)quinoline-2-carboxamide: $P2_1/n$, Z' = 1, a = 6.539(1), b = 17.036(3), c = 12.702(2) Å, β = 102.38(<1)° (room temp.) **1**

{d = 3.7804(14) Å; θ = 171.57(8)°: helical chain}

Congeners:

NAZDOJ **Br**: $P2_1/c$, Z' = 1, a = 6.362(<1), b = 16.997(<1), c = 12.600(1) Å, β = 105.89(<1)° (150 K) **2**

{isostructural: d = 3.6072(13) Å; θ = 172.46(10)°: helical chain}

RIXHUD **Cl**: $P2_1/n$, Z' = 1, a = 14.176(3), b = 6.025(1), c = 15.551(4) Å, β = 98.31(1)° (room temp.) **3**

{no analogous interaction}

RIXJAL **F**: $P2_12_12_1$, Z' = 1, a = 4.951(<1), b = 14.593(1), c = 17.678(1) Å (room temp.) **3**

{side-on interaction: d = 3.619(3) Å; θ = 123.97(18)°: helical chain}

1 J. Y. Qi, L. Q. Qiu, Q. Y. Yang, Z. Y. Zhou and A. S. C. Chan, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2003, **59**, o104-o105; DOI: 10.1107/S1600536802022419

2 P. Bobal, J. Sujan, J. Otevrel, A. Imramovsky, Z. Padelkova and J. Jampilek, *Molecules*, 2012, **17**, 1292-1306; DOI: 10.3390/molecules17021292

3 H. R. Khavasi, A. Ghanbarpour and A. A. Tehrani, *CrystEngComm*, 2014, **16**, 749-752; DOI: 10.1039/C3CE41853G

140. VIZLEW 4-Iodo-N,N'-dimethylbenzamidine; Z' = 1, *Pbca*, a = 8.828(1), b = 12.070(1), c = 19.196(3) Å (room temp.) **1**

{d = 3.792(3) Å; θ = 167.48(16)°: supramolecular chain}

Congener:

VIZLAS Br; Z' = 1, *Pbca*, a = 8.810(1), b = 11.666(1), c = 19.196(3) Å (room temp.) **1**

{isostructural: d = 3.7316(14) Å; θ = 169.48(9)°: supramolecular chain}

1 W. Chen and T. Ren, *J. Cluster Sci*., 2008, **19**, 99-108; DOI: 10.1007/s10876-007-0155-4

143. TITZUS 2-Iodo-N-(4-nitrobenzyl)aniline; $P2_12_12_1$, Z' = 1: a = 5.591(1), b = 8.941(1), c = 15.674(3) Å (120 K) **1**

{d = 3.8232(12) Å; θ = 165.50(7)°: helical chain}

Analogue:

YIVHUI01 **142**.3,5-dinitrobenzoic acid **2**

Congeners:

ABRTOL **Br**: $P2_12_12_1$, Z' = 1: a = 15.265(3), b = 8.756(3), c = 5.578(1) Å (room temp.) **3**

{isostructural: d = 3.83 Å; θ = 178.9°: helical chain}

1 C. Glidewell, J. N. Low, J. M. S. Skakle, S. M. S. V. Wardell and J. L. Wardell, *Acta Crystallogr., Sect. B: Struct. Sci.*, 2004, **60**, 472-480; DOI: 10.1107/S0108768104012017

2 C. L. Jones, C. C. Wilson and L. H. Thomas, *CrystEngComm*, 2014, **16**, 5849-5858; DOI: 10.1039/C4CE00229F

3 H. van der Meer, *Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.*, 1972, **28**, 3098; DOI: 10.1107/S0567740872007484

155. NIFHAM 1,5-Diiodonaphthalene: $P2_12_12_1$, Z' = 1: a = 7.021(<1), b = 11.537(<1), c = 12.187(<1) Å **1**

{d = 3.8680(19) Å; θ = 166.79(10)°: helical chain}

Analogue:

NIFHAM01 **155** polymorph: $P2_1/n$, Z' = 1: a = 4.312(<1), b = 12.487(1), c = 17.981(1) Å, β = 93.17(<1)° **2**

{no analogous interaction}

Congeners:

COXLOQ **Br**: $C2/c$, Z' = 0.5: a = 14.576(5), b = 4.049(1), c = 15.046(6) Å, β = 92.18(3)°

{no analogous contact} **3**

DFNAPH10 **F**: $P2_1/c$, Z' = 0.5: a = 7.593(3), b = 3.912(3), c = 14.005(5) Å, β = 115.41(10)°

{no analogous contact} **4**

1 I. Novak, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2007, **63**, o2726; DOI: 10.1107/S1600536807020508

2 M. Bolte and N.-W. Liu, Private Communication to the Cambridge Structural Database, Refcode NIFHAM01, 2020

3 R. C. Haltiwanger, P. T. Beurskens, J. M. J. Vankan and W. S. Veeman, *J. Crystallogr. Spectrosc. Res.*, 1984, **14**, 589-597; DOI: 10.1007/BF01182146

4 A. Meresse, C. Courseille, F. Leroy and N. B. Chanh, *Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.*, 1975, **31**, 1236-1241; DOI: 10.1107/S0567740875004979

156. GIZTEP tris(4-Iodophenyl)methanol: $P2_12_12_1$, Z' = 1: a = 8.830(<1), b = 11.283(<1), c = 19.161(<1) Å (T = 193 K) **1**

{*d* = 3.6600(18) Å; θ = 169.77(15)°: helical chain}

Analogue:

110. **GIZTIT** **156**.Dichloromethane (T: 193 K)

{*d* = 3.5428(14) Å; θ = 161.79(17)°: zig-zag chain with mirror symmetry} **1**

GIZTOZ **156**.Benzene hemi-solvate **1**

{*d* = 3.6846(13) Å; θ = 151.63(11)°: dimer}

Congeners:

GIZTAL **Br**: $P2_12_12_1$, *Z′* = 1: *a* = 8.767(<1), *b* = 10.911(<1), *c* = 18.319(<1) Å (T = 193 K)

{isostructural: *d* = 3.5428(14) Å; θ = 172.21(11)°: helical chain} **1**

1 D. Schollmeyer, O. V. Shishkin, T. Rühl and M. O. Vysotsky, *CrystEngComm*, 2008, **10**, 715-723; DOI: 10.1039/b716442d

159. LITBIA 2,2''-bis(Iodo)-(1,1':4',1'')terphenyl: *Pbca*, *Z′* = 0.5, *a* = 11.222(1), *b* = 8.015(1), *c* = 16.796(3) Å (T = 93 K)

{*d* = 3.606(3) Å; θ = 171.50(16)°: two-dimensional array} **1**

Congener:

PORRAQ Br: *Pbca*, *Z′* = 0.5, *a* = 10.908(<1), *b* = 7.711(<1), *c* = 17.175(<1) Å (T = 100 K)

{ isostructural: *d* = 3.4877(11) Å; θ = 166.81(7)°: two-dimensional array} **2**

1 C. Poriel, J.-J. Liang, J. Rault-Berthelot, F. Barrière, N. Cocherel, A. M. Z. Slawin, D. Horhant, M. Virboul, G. Alcaraz, N. Audebrand, L. Vignau, N. Huby, G. Wantz and L. Hirsch, *Chem. - Eur. J.*, 2007, **13**, 10055-10069; DOI: 10.1002/chem.200701036

2 P. Debroy, S. V. Lindeman and R. Rathore, *J. Org. Chem.*, 2009, **74**, 2080-2087; DOI: 10.1021/jo802579f

160. IBILEN 1,4-bis(Iodo)-2,5-dimethylbenzene: *C*2/*c*, *Z′* = 0.5: *a* = 9.572(5), *b* = 8.414(5), *c* = 11.973(6) Å, β = 105.34(<1)° (T = 198 K)

{*d* = 3.849(3) Å; θ = 173.66(8)°: two-dimensional array} **1**

Congeners:

JAQJAN **Br**: $P2_1/n$, Z' = 1: a = 6.284(<1), b = 7.719(<1), c = 17.396(<1) Å, β = 95.37(<1)° (T = 143 K) **2**

{no analogous interactions}

JAQJAN01 **Br**: $P2_1/n$, Z' = 0.5: a = 6.260(<1), b = 10.482(1), c = 6.428(<1) Å, β = 98.13(<1)° (T = 133 K) **3**

{d = 3.5691(8) Å; θ = 157.13(5)°: similar two-dimensional array as for **160**}

1 E. Albright, J. Cann, A. Decken and S. Eisler, *CrystEngComm*, 2017, **19**, 1024-1027; DOI: 10.1039/C6CE02339H

2 S. A. Reiter, S. D. Nogai and H. Schmidbaur, *Z. Naturforsch., B: Chem. Sci.*, 2005, **60**, 511-519.

3 P. G. Jones and P. Kus, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2011, **67**, o131-o133; DOI: 10.1107/S0108270111008742

164. RORPEV (4-Iodophenyl)boronic acid phenazine: $P2_1/c$, Z' = 2: a = 19.700(8), b = 7.072(3), c = 25.731(10) Å, β = 107.70(<1)° (room temp.) **1**

{d = 3.678(2) Å; θ = 166.45(12)°: two-molecule aggregate via a single interaction}

Analogue:

165. RORPAR **164**.H_2O **1**

{d = 3.839(3) Å; θ = 169.36(10)°: two-molecule aggregate via a single interaction}

Congener:

RORNOD **Cl**: $P\bar{1}$, Z' = 1, a = 6.939(4), b = 9.959(5), c = 12.125(7) Å, α = 80.17(1)°, β = 87.69(1)°, γ = 83.07(1)° (room temp.) **1**

{no analogous contact}

1 S. SeethaLekshmi, S. Varughese, L. Giri and V. R. Pedireddi, *Cryst. Growth Des.*, 2014, **14**, 4143-4154; DOI: 10.1021/cg500750p

165. RORPAR (4-Iodophenyl)boronic acid bis(phenazine) monohydrate: $P\bar{1}$, Z' = 1, a = 8.996(5), b = 12.502(6), c = 14.051(7) Å, α = 109.40(<1), β = 94.07(<1), γ = 110.19(<1)° (room temp.) **1**

{*d* = 3.839(3) Å; θ = 169.36(10)°: two-molecule aggregate via a single interaction}

Analogue:

164. RORPEV unsolvated: (room temp.) **1**

{*d* = 3.678(2) Å; θ = 166.45(12)°: two-molecule aggregate via a single interaction}

Congener:

RORNUJ **Br**: *P*$\bar{1}$, *Z′* = 1, *a* = 8.982(6), *b* = 12.482(8), *c* = 13.945(8) Å, α = 109.23(<1), β = 95.72(<1), γ = 110.22(<1)° (room temp.) **1**

{isostructural: *d* = 3.756(3) Å; θ = 167.93(13)°: two-molecule aggregate via a single interaction}

1 S. SeethaLekshmi, S. Varughese, L. Giri and V. R. Pedireddi, *Cryst. Growth Des*., 2014, **14**, 4143-4154; DOI: 10.1021/cg500750p

166. VULLEV Thiobenzamide 1,4-di-iodotetrafluorobenzene **1**

{*d* = 3.429(3) Å; θ = 160.21(9)°: two-molecule aggregate}

Analogue:

171. KUWPEZ **166**.thiobenzamide **1**

{*d* = 3.868(2) Å; θ = 171.55(15)° : two-molecule aggregate}

1 K. S. Eccles, R. E. Morrison, A. S. Sinha, A. R. Maguire and S. E .Lawrence, *Cryst. Growth Des*., 2015, **15**, 3442-3451; DOI: 10.1021/acs.cgd.5b00513

179. GUFNOM 1,1'-Ethene-1,2-diyldibenzene 1,2,4,5-tetrafluoro-3,6-di-iodobenzene: $P2_1/c$, *Z′* = 0.5: *a* = 13.250(1), *b* = 5.759(<1), *c* = 12.691(1) Å, β = 101.30(1)° (room temp.) **1**

{*d* = 3.580(6) Å; θ = 166.7(4)°: linear chain}

Congener:

TIJTUB 1,1'-Ethene-1,2-diyldibenzene $\mathbf{C_6F_6}$: $P2_1/c$, *Z′* = 0.5: *a* = 11.401(3), *b* = 6.118(2), *c* = 12.262(4) Å, β = 107.09(2)° (120 K) **2**

{*d* = 3.635(4) Å; θ = 71.6(2)°: linear chain of alternating co-formers}

1 S. d'Agostino, F. Grepioni, D. Braga and B. Ventura, *Cryst. Growth Des*., 2015, **15**, 2039-2045; DOI: 10.1021/acs.cgd.5b00226

2 A. S. Batsanov, J. A. K. Howard, T. B. Marder and E. G. Robins, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2001, **57**, 1303-1305; DOI: 10.1107/S0108270101013294

180. GUFNEC 1,1'-Ethyne-1,2-diyldibenzene 1,2,4,5-tetrafluoro-3,6-di-iodobenzene

{d = 3.6043(18) Å; θ = 165.83(11)°: linear chain}

Analogue:

GUFNIG **180**.1,2,4,5-tetrafluoro-3,6-di-iodobenzene (1:2 co-crystal)

{d = 3.5671(19) Å; θ = 155.99(13)° & d = 3.821(2) Å; θ = 151.64(13)°: linear chain}

1 S. d'Agostino, F. Grepioni, D. Braga and B. Ventura, *Cryst. Growth Des.*, 2015, **15**, 2039-2045; DOI: 10.1021/acs.cgd.5b00226

181. QEVWEW Pyrene 1,3,5-trifluoro-2,4,6-triiodobenzene: *Pbcn*, Z' = 0.5: a = 5.122(<1), b = 17.608(<1), c = 22.790(<1) Å (room temp.) **1**

{d = 3.792(3) Å; θ = 162.86(15)°: zig-zag chain + plus many contacts outside the range}

Congeners:

QEVXOH **Br**: $P2_1/c$, Z' = 1: a = 7.840(<1), b = 14.708(<1), c = 17.297(<1) Å, β = 102.13(<1)° (room temp.) **1**

{side-on interactions only, with shortest contact: d = 3.597(4) Å; θ = 88.2(2)°}

ZZZGKE01 **F**: $P2_1/c$, Z' = 0.5: a = 6.947(1), b = 13.331(3), c = 9.301(1) Å, β = 106.67(3)° (200 K) **2**

{side-on interactions only, with shortest contact: d = 3.4918(16) Å; θ = 90.82(11)°}

1 L. Li, W. X. Wu, Z. F. Liu and W. J. Jin, *New J. Chem.*, 2018, **42**, 10633-10641; DOI: 10.1039/C7NJ04536K

2 J. C. Collings, K. P. Roscoe, E. G. Robins, A. S. Batsanov, L. M. Stimson, J. A. K. Howard, S. J. Clark and T. B. Marder, *New J. Chem.*, 2002, **26**, 1740-1746; DOI: 10.1039/b207102a

ESI Figure 1. A plot of θ (°) versus *d* (Å). Note the outlier, indicated with an asterisk, corresponds to **163**. When the data point for **163** is omitted, the value of $R^2 = 0.0088$ for $y = 3.4387x + 154.16$.