Version 12h58 18th September 2010

Appendix A

'Practical applications of averages and differences of Friedel opposites'
by H. D. Flack, M. Sadki, A. L. Thompson and D. J. Watkin (2010).
Acta Cryst. A43, xxx-yyy.

Notes on structure determinations analysed in the above publication.

"Achiral molecule"

"Chiral molecule"

"Enantiopure"
The original report indicates that the stereochemistry and the enantiopurity were apparent from the original synthesis.

"Not necessarily enantiopure"
The original report does not provide sufficient information to establish the enantiopurity of the bulk compound. However it is clear from the crystal structure that the molecule is chiral.

CICXES
Cisnetti, F., Guillot, R., Therisod, M. & Policar, C. (2007). Acta Cryst. C63, m201–m203.
DOI: 10.1107/S0108270107013522
Space group: oP212121 ; Z' = 1
Enantiopure
Flack x: CIF x = 0.015(8), CRYSTALS x = 0.01(1)

CICYIX
V in Yasodha, V., Govindarajan, S., Low, J. N. & Glidewell, C. (2007). Acta Cryst. C63, m207–m215.
DOI: 10.1107/S010827010701459X
Space group: aP1 ; Z' = 1
Not necessarily enantiopure
Flack x: CIF x = -0.002(17), CRYSTALS x = 0.00(2)

CIJWUO
I in Blake, A. J., Lippolis, V., Pivetta, T. & Verani, G. (2007). Acta Cryst. C63, m364–m367.
DOI: 10.1107/S0108270107026753
Space group: oP212121 ; Z' = 1
Not necessarily enantiopure
Flack x: CIF x = 0.41(3)

CIJXAV

II in Blake, A. J., Lippolis, V., Pivetta, T. & Verani, G. (2007). Acta Cryst. C63, m364–m367.
DOI: 10.1107/S0108270107026753
Space group: oP212121 ; Z' = 1
Not necessarily enantiopure
3932 refs; 3205 > 3s(I); 1186 pairs
Flack x: CIF x = 0.00(3), CRYSTALS x = 0.017(29)

CIKCUV
Guzei, I. A., Keter, F. K., Spencer, L. C. & Darkwa, J. (2007). Acta Cryst. C63, o481–o483.
DOI: 10.1107/S0108270107031952
Space group: oPna21 ; Z' =1
Achiral molecule
Flack x: CIF x = -0.05(4), CRYSTALS x = -0.05(4)

DOPKID
Harvey, J. S., Malcolmson, S. J., Dunne, K. S., Meek, S. J., Thompson, A. L., Schrock, R. R., Hoveyda, A. H. & Gouverneur, V. (2009). Angew. Chem., Int. Ed., 48, 762-766.
DOI: 10.1002/anie.200805066
Space group: mP21 ; Z' =1
Enantiopure
Flack x: CRYSTALS x = -0.08(6)

EDUZOT
Zhang, C.-N. & Zheng, Y.-F. (2007). Acta Cryst. E63, o3310.
DOI: 10.1107/S1600536807030255
Space group: mP21 ; Z' = 1
Not necessarily enantiopure
1839 refs; 1734 > 3s(I); 854 pairs
Flack x: CIF x = 0.04(6), CRYSTALS x = 0.047(63)

EZEQAB
Chauvin, A.-S., Bernardinelli, G. & Alexakis, A. (2004). Tetrahedron Asymmetry, 15, 1857–1879.
DOI: 10.1016/j.tetasy.2004.04.031
Space group: oP212121 ; Z' = 1
Enantiopure
Flack x: CIF x = -0.03(11)
There are numerous typographical errors in this paper communicated to us by one of the authors (GB. HDF has a document containing rectifications to the crystallographic part of this paper.
Intensity data in an unsuitable format for use in CRYSTALS.

GIHDAD
Wang, B.-T., Luo, S.-P., Yue, H.-D., Wang, L.-P. & Xu, D.-Q. (2007). Acta Cryst. E63, o2786.
DOI: 10.1107/S1600536807020594
Space group: aP1 ; Z' = 1
Chiral molecule

Flack x: CIF x = 0.062(1), CRYSTALS x = 0.05(1)

GIHKEO
Gowda, B. T., Usha, K. M., Kozisek, J., Tokarcik, M. & Fuess, H. (2007). Acta Cryst. E63, m1739–m1740.
DOI: 10.1107/S1600536807025184
Space group: mC2 ; Z' = 1
Not necessarily enantiopure
Flack x: CIF x = -0.018(12), CRYSTALS x = -0.01(1)

KEXYOC
Ia in Wardell, S. M. S. V., de Souza, M. V. N., Wardell, J. L., Low, J. N. & Glidewell, C. (2007). Acta Cryst. B63, 101–110.
DOI: 10.1107/S0108768106041358
Space group: mCc ; Z' = 1
Not necessarily enantiopure
Flack x: CIF x= -0.05(5)
Intensity data do not appear to agree with the structure. Refinement of the intensity data against the published structure gives an R = 56%. Wrote to correspondence author C. Glidewell. Consequently the analysis of intensities in FB2008 and the current paper refer to the intensity data of the structure which has been deposited as being compound Ia, KEXYOC whereas it may be the data of some other compound. Of course structural information drawn from the paper and the cif do refer to Ia KEXYOC. The CIF and the intensity data may well refer to different compounds.

METSIO
Tooke, D. M., Zijp, E. J., van der Vlugt, J. I., Vogt, D. & Spek, A. L. (2007). Acta Cryst. E63, m86–m88.
DOI: 10.1107/S1600536806052044
Space group: mP21 ; Z' = 4
Enantiopure
Flack x: CIF x = -0.021(3)
Structure fails to refine easily.

METWIS
Li, H.-Y., Huang, F.-P., Jiang, Y.-M. & Ng, S. W. (2007). Acta Cryst. E63, m219–m220.
DOI: 10.1107/S1600536806053529
Space group: aP1 ; Z' = 1
Enantiopure
Flack x: CIF x = 0.010(10), CRYSTALS x = 0.04(2)

MOKXEQ02
Thompson, A. L., Watkin, D. J., Gal, Z. A., Jones, L., Hollinshead, J., Jenkinson, S. F., Fleet, G. W. J. & Nash, R. J. (2008). Acta Cryst., C64, o649-o652.
DOI: 10.1107/S0108270108037086
Space group: mC2 ; Z' = 1
Enantiopure
Flack x: CRYSTALS x = -0.017(17)

PEFXII
Kuendig, E. P., Datta Chaudhuri, P., House, D. & Bernardinelli, G. (2006). Angew. Chem. Int. Ed. 45, 1092–1095.
DOI: 10.1002/anie.200502688
Space group oP212121 ; Z' = 2
Not necessarily enantiopure
Flack x: CIF x = -0.01(2)
Intensity data in an unsuitable format for use in CRYSTALS.

PIFDOY
Fu, D.-W. & Zhao, H. (2007). Acta Cryst. E63, m1630.
DOI: 10.1107/S1600536807021654
Space group: oP212121 ; Z' = 4
Not necessarily enantiopure
Flack x: CIF x = 0.011(19), CRYSTALS x = 0.04(2)

RIGHEV
Gainsford, G. J., Lensink, C. & Falshaw, A. F. (2007). Acta Cryst. C63, m331–m334.
DOI: 10.1107/S0108270107026170
Space group: mP21 ; Z' = 2
Enantiopure
Flack x: CIF x = 0.05(3), CRYSTALS x = 0.07(3)
Structure is disordered and the disorder is incompletely modelled.

RIGMAW
Cunico, W., Gomes, C. R. B., Wardell, S. M. S. V., Low, J. N. & Glidewell, C. (2007). Acta Cryst. C63, o411–o414.
DOI: 10.1107/S0108270107022913
Space group: oP212121 ; Z' = 2 (one enantiomer S, the other R)
Chiral racemate
Flack x: CIF x = -0.02(6)

RIHMUR
Abbasi, A., Habibian, M. & Sandstrom, M. (2007). Acta Cryst. E63, m1904.
DOI: 10.1107/S1600536807027912
Space group: oP212121 ; Z' = 1
Not necessarily enantiopure
Flack x: CIF : x = -0.02(3), CRYSTALS x = -0.02(3)

SEZPUJ
Moskalev, N. V., Gribble, G. W. & Jasinski, J. P. (2007). Acta Cryst. E63, o1279–o1281.
DOI: 10.1107/S1600536807005764
Space group: aP1 ; Z'=3
Not necessarily enantiopure
7146 refs; 2530 > 3s(I); 335 pairs all h0l
Flack x: CIF x = 0.12(11), CRYSTALS x = 0.483(235)
Structure is disordered.

SIHDET
King, G., Bergin, E., Muller-Bunz, H. & Gilheany, D. G. (2007). Acta Cryst. E63, o3278.
DOI: 10.1107/S1600536807029479
Space group: oP212121 ; Z' = 1
Enantiopure
6693 refs; 5390 > 3s(I); 2860 pairs
Flack x: CIF x = -0.02(8), CRYSTALS x = -0.033(79)

TIBCAJ
Scharwitz, M., Schafer, S., van Almsick, T. & Sheldrick, W. S. (2007). Acta Cryst. E63, m1111–m1113.
DOI: 10.1107/S1600536807011750
Space group: oP212121 ; Z' =1
Bulk compound is a racemate from a non-enantiospecific synthesis.
Flack x: CIF x = -0.039(14), CRYSTALS x = 0.03(2), Hooft y = 0.5

TIBFIU
Ma, A.-Q. (2007). Acta Cryst. E63, m1073–m1075.
DOI: 10.1107/S1600536807011865
Space group: mP21 ; Z'= 1
Achiral molecule
Flack x: CIF x = 0.01(1), CRYSTALS x = 0.45(2), Hooft y = ~0.5
In the author's intensity data file, F**2(hkl)model = F**2(-h-k-l)model for all reflections.

TICFIV
Cymborowski, M., Chruszcz, M., Dauter, Z. & Minor,W. (2007). Acta Cryst. E63, o1557–o1559.
DOI: 10.1107/S1600536807009129
Space group: mC2 ; Z' = 1
Enantiopure
Flack x: CIF x = -0.01(2), CRYSTALS x = -0.01(2)

UDUSIW
Ghadimi, S., Valmoozi, A. A. E. & Pourayoubi, M. (2007). Acta Cryst. E63, o3260.
DOI: 10.1107/S1600536807028838
Space group: aP1 ; Z' = 1
Not necessarily enantiopure
2791 refs; 2622 > 3s(I); 1328 pairs
Flack x: CIF x = -0.03(7), CRYSTALS x = -0.006(72)

UNEVAK01
Zhu, H.-Y. & Jiang, S.-D. (2007). Acta Cryst. E63, o2833.
DOI: 10.1107/S1600536807019770
Space group: aP1 ; Z'=2
Enantiopure
4322 refs; 3228 > 3s(I); 678 pairs

Flack x: CIF x = -0.03(7), CRYSTALS x = -0.049(153)
Disorder was not modelled. Strong correlations within the disorder.

WIGWUF
Bekaert, A., Lemoine, P., Brion, J. D. & Viossat, B. (2007). Acta Cryst. E63, o3187–o3189.
DOI: 10.1107/S1600536807027158
Space group: aP1 ; Z' = 1
Chiral molecule
Flack x: CIF x = -0.016(10), CRYSTALS x = 0.01(1)

XICNED
Chantrapromma, S., Jindawong, B., Fun, H.-K. & Patil, P. S. (2007). Acta Cryst. E63, o2321–o2323.
DOI: 10.1107/S1600536807016078
Space group: aP1 ; Z' = 1
Not necessarily enantiopure
Flack x: CIF x = 0.012(7), CRYSTALS x = 0.02(1)

XIFSIP
Xia, C.-N., Li, B.-W., Hu, W. & Zhou, W. (2007). Acta Cryst. E63, o3107.
DOI: 10.1107/S1600536807026803
Space group: aP1 ; Z'=2
Enantiopure
4861 refs; 4133 > 3s(I); 1048 pairs
Flack x: CIF x = 0.00(5), CRYSTALS x = 0.051(62)

XORXEH
II in Breydo, L., Barnes, C.L., & Gates, K.S. (2002). Acta Cryst. C58, o447.
DOI: 10.1107/S0108270102007503
Space group: aP1 ; Z' = 1
Enantiopure
2820 refs; 2651 > 3s(I); 908 pairs
Flack x: CIF x = 0.07(7), CRYSTALS x = 0.10(7)

YIDJIF
Chartrand, D., Theobald, I. & Hanan, G. S. (2007). Acta Cryst. E63, m1561.
DOI: 10.1107/S1600536807020259
Space group: aP1 ; Z' = 1
Not necessarily enantiopure
Flack x: CIF x = 0.041(5), CRYSTALS x = 0.048(4)

YIFZAP
Gowda, B. T., Nayak, R., Kozisek, J., Tokarcik, M. & Fuess, H. (2007). Acta Cryst. E63, o2967.
DOI: 10.1107/S1600536807024221
Space group: mPc ; Z' = 1
Achiral molecule
Room temperature data collection
Flack x: CIF x = -0.1(3)

YINLEM
Larsonneur, A.-M., Turpin, R., Castan, P. & Bernardinelli, G. (1994).
Inorganica Chimica Acta 227, 85-90.
DOI: N/A
Space group: oFdd2 ; Z' = 0.5
Flack x: CIF x = 0.01(1)
In entry in the CSD, there are two errors:
  (1) The Cl atom is in the wrong position, inverted with respect to the Au atom
  (2) There is more than one asymmetric unit in the atom list
Intensity data in an unsuitable format for use in CRYSTALS.

ZAYWIJ
3 in Clegg, W., Dunbar, J.M., Elsegood, M.R.J., Jackson, R.F.W. & Palmer, N.J. (1995). Acta Cryst., C51, 1950.
DOI: 10.1107/S0108270195004276
Space group: aP1 ; Z' = 2
Enantiopure
1601 refs; 1483 > 3s(I); 245 pairs
Flack x: CIF x = -0.03(14), CRYSTALS x = 0.16(23)

ZUHWEE
Bratovanov, . Linden, A. & Bienz S. (1996). Acta Cryst. C52, 1045.
DOI: 10.1107/S0108270195014338
Space group: aP1 ; Z'=2
Enantiopure
13158 refs; 9082 > 3s(I); 5646 pairs
Flack x: CIF x = -0.02(7), CRYSTALS x = 0.01(8)

9BER01
Bernardinelli, G. Private communication. K H (2R,3R) tartrate
Space group: oP212121 ; Z' = 1
Intensity data in an unsuitable format for use in CRYSTALS.

9YAN01
Yang, H., Costin, G., Keogh, J., Lu, R. & Downs, R. T. (2007). Acta Cryst. E63, i53–i55.
DOI: 10.1107/S1600536807003029
Space group: oP212121 ; Z' = 1
Achiral "molecule"
Not in CSD (It is a mineral structure)
Flack x: CIF x = -0.01(3)

Table of various values for compounds with near zero value of the Flack parameter, usable intensity data and untroubled refinement. All refinements and calculations were carried out with CRYSTALS.

REFCODE	RA%	RD%	Friedif	Flack	su	Hooft	su	Number of reflections Total	Unpaired Pairs	Unpaired Centric
CICXES	4.0	56.0	386	0.01	0.01	0.01	0.01	9372	3880	599	1013
CICYIX	3.1	71.0	314	0.00	0.02	0.01	0.01	2104	1005	94	0
CIJXAV	6.6	86.1	501	0.02	0.03	-0.02	0.02	3932	1186	916	644
CIKCUV	3.7	77.7	119	-0.05	0.04	0.00	0.02	2446	1151	2	142
DOPKID	3.5	89.8	76	-0.08	0.06	-0.06	0.03	2440	1047	100	246
EDUZOT	2.8	97.4	108	0.05	0.06	-0.06	0.04	1839	854	78	53
GIHDAD	3.8	70.3	802	0.05	0.01	0.09	0.01	2423	1078	267	0
GIHKEO	4.2	52.6	949	-0.01	0.01	0.00	0.01	1880	789	129	173
METWIS	3.5	65.6	570	0.04	0.02	0.08	0.01	5011	1171	2669	0
MOKXEQ02	4.2	97.5	36	-0.01	0.17	-0.03	0.09	1476	650	50	126
PIFDOY	4.4	81.5	531	0.04	0.02	0.02	0.01	1879	746	1	386
RIGHEV	7.4	94.4	253	0.07	0.03	0.06	0.01	15770	7511	466	282
RIHMUR	2.0	72.6	198	-0.02	0.03	-0.06	0.02	3032	1283	8	458
SEZPUJ	5.9	100.5	81	0.48	0.24	0.44	0.19	7146	335	6476	0
SIHDET	7.6	97.1	75	-0.03	0.08	-0.04	0.04	6693	2860	21	952
TIBCAJ	4.0	63.4	1259	-0.03	0.02	0.50	0.01	2980	544	1279	613
TIBFIU	5.0	169.6	481	0.45	0.02	0.45	0.01	3337	1522	197	96
TICFIV	3.0	54.1	370	-0.01	0.02	-0.02	0.01	4678	2142	26	368
UDUSIW	4.6	96.6	74	-0.03	0.08	0.03	0.05	2791	1328	135	0
UNEVAK01	4.9	97.6	70	0.01	0.12	0.06	0.08	4322	678	2966	0
WIGWUF	5.1	47.8	937	-0.01	0.01	-0.01	0.01	1461	658	145	0
XICNED	2.7	52.6	421	0.02	0.01	0.01	0.00	7236	3382	472	0
XIFSIP	4.0	93.9	104	0.04	0.06	0.05	0.04	4861	1048	2765	0
XORXEH	4.6	98.4	84	0.10	0.07	0.11	0.05	2809	903	1003	0
YIDJIF	4.4	47.2	700	0.05	0.00	0.06	0.00	6965	3117	731	0
YIFZAP	10.0	100.9	100	-0.49	0.40	-0.67	0.11	1053	378	292	5
ZAYWIJ	6.3	98.2	79	-0.16	0.23	-0.49	0.25	1601	245	1111	0
ZUHWEE	7.2	98.4	77	-0.01	0.08	-0.04	0.04	13115	5624	1867	0
9YAN01	6.7	87.1	617	0.08	0.06	-0.02	0.03	1343	488	91	276