Table D. Cell dimensions (Å, deg.) for α-oxalic acid dihydrate. X, N refer to X-ray or neutron diffraction respectively. For convenience, all the measurements reported are included in the Table, although only those at room temperature (if not specified, then given as nominally 295* K) and 100 K are discussed in the text. The s.u.s (in round brackets) are those given by the original investigators.

T(K); X or N; sample number	*a*	*b*	*c*	β	Brief notes on methodology used	REFCODE or Reference
299 X	6.119(1)	3.607(1)	12.057(1)	106.32(2)	Cu Kα to 110°; all reflections by LS procedure	OXACDH11
295* X	6.119(4)	3.604(3)	12.051(5)	106.27(2)	"Straumanis method" (presumably Cu Kα)	OXACDH12
300 X	6.120(2)	3.6058(8)	12.057(3)	106.29(2)	Mo Kα, 24 reflections, 2θ = 50–60°.	OXACDH24
295* X	6.115(2)	3.601(1)	12.050(3)	106.31(2)	Mo Kα (Nb filter) 54 reflections	OXACDH26
225 X	6.109(1)	3.5595(4)	12.008(2)	106.02(2)	do.	do.
170 X	6.102(2)	3.5298(5)	11.978(2)	105.89(2)	do.	do.
130 X	6.102(2)	3.5190(4)	11.973(2)	105.84(2)	do	do.
100 X	6.102(2)	3.5011(5)	11.964(3)	105.79(2)	do.	do.
100(2) X2	6.0986(5)	3.4981(3)	11.952(1)	105.777(8)	Mo $K\alpha_1$, 38 reflections at high Bragg angles	OXACDH09
100(3) X1	6.103(3)	3.498(3)	11.978(8)	105.87(5)	Mo Kα	Coppens (1984)
100(1) X3	6.0968(7)	3.4975(4)	11.9462(15))	105.78(1)	Mo Kα	Coppens (1984)
103(0.5) X4	6.1108(9)	3.5109(4)	11.9780(8)	105.767(8)	Mo Kα	Coppens (1984)
100(1) N1	6.1016(1)	3.4972(1)	11.9549(3)	105.759(2)	0.862 Å; powder;	Coppens (1984)
100 (0.05) N4	6.102(3)	3.496(2)	11.949(5)	105.66(4)	0.8213(2) Å	Coppens (1984)

15(0.5) X	6.093(2)	3.469(1)	11.926(2)	105.69(2)	Mo Kα (Nb filter), 86 reflections	OXACDH26

OXACDH11: Delaplane, R. G. & Ibers, J. A. (1969), *Acta Cryst*. B**25**, 2423–2437.

OXACDH12: Ahmed, F. R. & Cruickshank, D. W. J. (1953). *Acta Cryst*. **6**, 385–392.

OXACDH24: Wang, Y., Tsai, C. J., Liu, W. L. & Calvert, L. D. (1985). *Acta Cryst.* B**41**, 131–135.

OXACDH09: Dam, J., Harkema, S. & Feil, D. (1983). *Acta Cryst*. B**39**, 760–768.

Coppens, P. *et al*. (1984). *Acta Cryst*. A**40**, 184–195.

OXACDH26: Zobel, D., Luger, P., Dreissig D. & Koritsanszky, T. (1992). *Acta Cryst*. B**48**, 837–848.

Table E. Cell dimensions (Å, deg.) of anthracene

T(K); X	*a*	*b*	*c*	β	Brief notes on methodology used	REFCODE or Reference
290 X	8.561(10)	6.036(10)	11.163(10)	124.70(8)	Cu Kα, "carefully calibrated oscillation and moving-film photographs."	ANTCEN02.
290 X	8.562(6)	6.038(8)	11.184(8)	124.70(10)	Calibrated Weissenberg photographs, using Cu $K\alpha_{1,2}$	ANTCEN.
295* X	8.554(4)	6.016(4)	11.174(4)	124.60(2)	Cu Kα, "inclined type diffractometer"	ANTCEN07.
295 X	8.5526(12)	6.0158(11)	11.1720(16)	124.596(15)	CAD-4 diffractometer, Mo Kα, 10 Friedel pairs, 20•2θ•38°.	ANTCEN14.
290 X	8.550(8)	6.028(8)	11.172(8)	124.67(8)		Ryzhenkov et al., 1969
100 X	8.407(3)	6.006(6)	11.092(4)	125.31(2)	Cu Kα, "inclined type diffractometer"	ANTCEN08.
95 X	8.443(6)	6.002(7)	11.124(8)	125.60(12)	Calibrated Weissenberg photographs,	ANTCEN01.

					using Cu $K\alpha_{1,2}$	
94 X crystal 3	8.4260(15)	5.9830(12)	11.0968(26)	125.328(19)	CAD-4 diffractometer, Mo Kα, 10 Friedel pairs, 20•2θ•38°.	ANTCEN09.
94 X crystal 4	8.4144(20)	5.9903(14)	11.0953(17)	125.293(18)	CAD-4 diffractometer, Mo Kα, 10 Friedel pairs, 20•2θ•38°.	ANTCEN09.
95 X	8.440(8)	5.994(8)	11.113(8)	125.08(8)		Ryzhenkov et al., 1969

ANTCEN09; ANTCEN14: Brock, C. P. & Dunitz, J. D. (1990). *Acta Cryst*. B**46**, 795–806.
ANTCEN; ANTCEN01: Mason, R. (1964). *Acta Cryst*. **17**, 547–555.
ANTCEN02: Mathieson, A. McL., Robertson, J. M. & Sinclair, V. C. (1950).*Acta Cryst*. **3**, 245–256.
ANTCEN07; ANTCEN08: Ponomarev, V. I. & Shilov, G. V. (1983). *Sov. Phys. Crystallogr*, **28**,397–399.
Ryzhenkov, A. I., Kozhin, V. M. & Myasnikova, R. M. (1969). *Sov. Phys. Crystallogr*, **13**, 896–898.

Table F. Cell dimensions of naphthalene (rejected because of insufficient information).

T(K); X	*a*	*b*	*c*	β	Brief notes on methodology used	Reference
295* X	8.235(5)	6.003(10)	8.658(10)	122.92(8)	Cu Kα, "carefully calibrated oscillation and moving-film photographs."	NAPHTA.
298 X	8.259(8)	5.980(2)	8.668(6)	122.60(10)	Cu Kα	NAPHTA05.
295* N	8.272	5.980	8.671	122.7	Neutron λ • 2.46 Å, calibrated to 0.001 Å.	El Hamamsy *et al.*, 1977

NAPHTA: Abrahams, S. C., Robertson, J. M. & White, J. G. (1949). *Acta Cryst*. **2**, 233–238.
NAPHTA05: Chanh, N. B. & Haget-Bouillaud, Y. (1972). *Acta Cryst*. B**28**, 3400–3404.
El Hamamsy, M., Elnahwy, S., Damask, A. C., Taub, H. & Daniels, W. B.(1977). *J. Chem. Phys*. **67**, 5501–5504.

Table G. Cell dimensions of acetamide (rejected because of insufficient information).

T(K); X or N	*a*	*c*	Brief notes on methodology used	Reference
299 X	11.526(5)	13.589(5)	Cu Kα ("LS fit of θ values")	Denne & Small, 1971
295* X	11.493(2)	13.547(2)	Mo Kα (Nb filter)	Zobel, Luger, Dreissig & Koritsanszky, 1992.
173 X	11.536(5)	13.194(5)	Cu Kα ("LS fit of θ values")	Denne & Small, 1971
100 X	11.490(2)	13.045(2)	Mo Kα (Nb filter)	Zobel, Luger, Dreissig & Koritsanszky, 1992.
85(0.2) X	11.504(6)	12.986(7)	LS fit of angular coordinates of 9 Mo $K\alpha_1$ reflections with 70•2θ•80°.	Ottersen, Almlöf & Hope, 1980
23 X	11.492(2)	12.892(2)	Mo Kα (Nb filter)	Zobel, Luger, Dreissig & Koritsanszky, 1992.
22.6(5) N	11.513(3)	12.883(4)	λ=1.0445(2) Å; LS fit of $\sin^2\theta$ values with 46•2θ•49°	Jeffrey, Ruble, McMullan, DeFrees, Binkley & Pople, 1980.

Denne, W. A. & Small, R. W. H. (1971). *Acta Cryst*. B**27**, 1094–1098.
Jeffrey, G. A., Ruble, J. R., McMullan, R. K., DeFrees, D. J., Binkley, J. S. & Pople, J. A. (1980). *Acta Cryst*. B**36**, 2292–2299.
Mathieson, A. McL., Robertson, J. M. & Sinclair, V. C. (1950).*Acta Cryst*. **3**, 245–256.
Ottersen, T., Almlöf, J. & Hope, H. (1980). *Acta Cryst*. B**36**, 1147–1154.
Zobel, D., Luger, P., Dreissig D. & Koritsanszky, T. (1992). *Acta Cryst*. B**48**, 837–848.

Table H. Cell dimensions of organometallic and organic crystals measured by area detector methods and reported in *Acta Cryst*., C**53**, nos. 10 and 11 (1997). All measurements were made using Mo Kα radiation, with λ given sometimes as 0.71069 and sometimes as 0.71073 Å. The standard uncertainties are those taken from the papers and averaged over *a*, *b*, *c* (given as parts in 10^5), and averaged over α, β, γ (given in units of 10^{-3} degrees). SS denotes Siemens SMART CCD System

Area detector system	No. of reflections used for cell parameter determination	θ range (deg.)	Averaged u(length) (parts in 10^5)	Averaged u(angle) (10^{-3} degrees).	Starting page of paper

SS	4605	3–20	23	10	1385
Nonius Kappa	94916	4.64–25.65	20	-	1383
SS	4149(I>10σ(I))	1.6–26.0	3	1	1436
SS	3751 (220 K)	2.07–23.26	10	2	1438
SS	4175 (220 K)	2.17–23.28	8	40	1439
SS	3385 (220 K)	2.27–23.28	11	2	1442
SS	8192	2.0–18.0	1	1	1473 (Compd. 2a)
SS	5784	1.4–26	5	1	1549
SS	3103	2–23	5	-	1555
Stoe IP	397	9.5–56.3	130	80	1572
SS	512	1.38–23.42	10	-	1653
R-axis 2CS	3934	θ_{max} =27.70	24	13	1692
FAST	250	1.77–24.97	11	-	1701
P4 SMART	27	22–30	4	2	1707 (“crystals not of high quality”)
SS	1497	2.50–23.24	12	2	1720