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Crystallisation temperature control of stoichiometry and selectivity in host–guest compounds

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Correction for ‘Crystallisation temperature control of stoichiometry and selectivity in host–guest compounds’ by Nicole M. Sykes *et al.*, *CrystEngComm*, 2017, 19, 5892–5896.

The authors regret the incorrect space group labelling of structure 1 as monoclinic, instead of triclinic. The corrected table of crystallographic data for this paper is shown below.

Table 1 Crystallographic data parameters of the host–guest complexes studied

Compound	1	2	3	4	5	6
Structural formula	C ₉₆ H ₈₆ O ₁₀	C ₃₆ H ₃₈ O ₄	C ₉₈ H ₉₀ O ₁₀	C ₄₄ H ₅₈ O ₆	C ₆₆ H ₆₁ Cl ₃ O ₇	C ₉₆ H ₈₆ O ₁₀
Host : guest ratio	1 : 1½	1 : 2	1 : 1½	1 : 4	1 : 2	1 : 1½
Molecular mass(g mol ^{−1})	1399.74	534.66	1427.79	682.90	1072.50	1399.74
Data collection temp. (K)	153	153	153	153	153	153
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P</i> 1̄	<i>P</i> 1̄	<i>P</i> 1̄	<i>P</i> 1̄	<i>P</i> 1̄	<i>P</i> 1̄
<i>a</i> (Å)	10.314(2)	8.5974(17)	10.328(2)	9.4041(19)	9.6930(19)	10.150(2)
<i>b</i> (Å)	18.768(4)	9.1212(18)	11.176(2)	9.4706(19)	14.066(3)	10.397(2)
<i>c</i> (Å)	20.269(4)	11.602(2)	18.112(4)	12.423(3)	21.052(4)	18.780(4)
α (°)	83.06(3)	92.96(3)	75.76(3)	111.38(3)	83.94(3)	104.29(3)
β (°)	81.59(3)	102.02(3)	79.16(3)	96.88(3)	82.70(3)	94.58(3)
γ (°)	82.49(3)	117.04(3)	88.31(3)	95.54(3)	89.93(3)	96.70(3)
Volume (Å ³)	3827.2(13)	781.3(3)	1989.9(7)	1011.0(4)	2831.0(10)	1895.2(7)
<i>Z</i>	2	1	1	1	2	1
D _c , calc density(g cm ^{−3})	1.215	1.136	1.191	1.122	1.258	1.226
θ range	1.42–27.90	1.82–27.95	1.18–27.75	1.79–28.00	1.52–27.96	2.03–27.97
Reflections collected	55 397	12 457	26 269	13 319	68 486	34 826
No data <i>I</i> > 2 sigma (<i>I</i>)	11 137	3214	6986	3458	11 569	7144
Final <i>R</i> indices [<i>I</i> > 2 sigma (<i>I</i>)]	0.0576	0.0490	0.0476	0.0574	0.0449	0.0451
<i>R</i> indices (all data)	0.1313	0.1324	0.1181	0.1363	0.1118	0.1089
Goodness-of-fit on <i>F</i> ²	1.029	1.060	1.042	1.030	1.038	1.057
Host torsion angle (°)	0.8, 7.7, 175.2	180	2.4, 180	180	1.3, 8.7	180, 0.2
CCDC no.	1558129	1558130	1558131	1558132	1558133	1558134

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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