X-ray powder diffraction data for letrozole ($C_{17}H_{11}N_5$)

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X-ray powder diffraction data, unit-cell parameters, and space group for letrozole, $C_{17}H_{11}N_5$, are reported [$a = 7.034(0)$ Å, $b = 16.177(5)$ Å, $c = 13.411(3)$ Å, $\alpha = \gamma = 90°$, $\beta = 105.71(9)°$, unit-cell volume $V = 1469.0(3)$ Å^3, $Z = 4$, and space-group $P2_1/c$]. All measured lines were indexed and are consistent with the $P2_1/c$ space group. No detectable impurity was observed. © *2015 International Centre for Diffraction Data*. [doi:10.1017/S088571561500069X]

Key words: X-ray powder diffraction, letrozole

I. INTRODUCTION

Letrozole (Figure 1), systematic name 4,4′-(H-1,2,4-triazol-1-ylmethylene)-dibenzonitrile, a non-steroidal aromatase inhibitor, which can inhibit the peripheral conversion of circulating androgens to estrogens and is approved for the treatment of advanced breast cancer in postmenopausal women. Letrozole is superior to tamoxifen and as well tolerated as tamoxifen (Cohen *et al.*, 2002). Besides, letrozole can improve clinical outcome effectively and is superior to anastrozole in suppressing breast cancer tissue and plasma estrogen levels (Geisler *et al.*, 2008).

The atomic structure based on single-crystal data of letrozole was reported by Xu *et al.* (2002) and Wang *et al.* (2004), the average values of cell parameters were $a = 7.030(0)$ Å, $b = 16.170(3)$ Å, $c = 13.360(3)$ Å, $\alpha = \gamma = 90°$, $\beta = 104.80(3)°$, unit-cell volume $V = 1468.3(5)$ Å^3, $Z = 4$, and space-group $P2_1/c$. Presently, the detailed X-ray powder diffraction data for letrozole have not been reported in the literature.

II. EXPERIMENTAL

A. Sample preparation

The title compound letrozole was obtained from DaLian MeiLun Biology Technology Co., Ltd. (DaLian, China), recrystallized in methanol and dried. Then it was ground into powder ($\rho = 1.31$ g cm^{-3}, $T_{melt} = 182$–184 °C), sieved through a 200-mesh screen and then mounted on a flat zero background plate. It has also been characterized by UV (Figure S1) and elemental analysis. The elemental analysis showed the content of C, N, and H were 70.64, 24.57, and 3.38%, respectively.

B. Diffraction data collection and reduction

The diffraction pattern for the title compound was collected using an X'Pert PRO diffractometer (PANalytical) with an X'celerator detector and Cu$K\alpha$ radiation (generator setting: 40 kV, 40 mA). The diffraction data were collected over the angular range from 5° to 50° 2θ with a step size of 0.013 13°2θ and a counting time of 60 ms step^{-1}. Data evaluation was executed using the software package Material Studio 4.2 (Accelrys Co., Ltd., California, USA). All data were collected at room temperature and a controlled relative humidity of 60%.

Indexing was carried out by the X-Cell method, and then the indexing result was refined using the Pawley method (Pan *et al.*, 2012) resulting in final R_{wp} of the structure was converged at 5.70%.

III. RESULTS

The experimental powder diffraction pattern is depicted in Figure 2. Indexing results show that letrozole is monoclinic with the space-group $P2_1/c$ and unit-cell parameters: $a = 7.034(0)$ Å, $b = 16.177(5)$ Å, $c = 13.411(3)$ Å, $\alpha = \gamma = 90°$, $\beta = 105.71(9)°$, unit-cell volume $V = 1469.0(3)$ Å^3, and $Z = 4$. The values of $2\theta_{obs}$, d_{obs}, I_{obs}, h, k, l, $2\theta_{cal}$, d_{cal}, I_{cal}, and $\Delta 2\theta$ are listed in Table I. All lines of powder and single-crystal data were indexed and are consistent with the $P2_1/c$ space group.

SUPPLEMENTARY MATERIAL

The supplementary material for this article can be found at http://www.journals.cambridge.org/PDJ

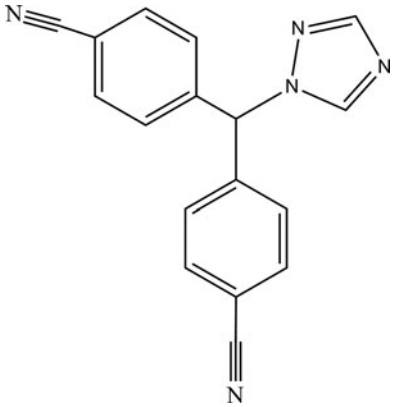

Figure 1. Structural formula of letrozole.

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TABLE I. Indexed X-ray powder diffraction data of letrozole. All measured lines were indexed and are consistent with the $P2_1/c$ space group. The d-values were calculated using Cu$K\alpha_1$ radiation ($\lambda = 1.540\,56$ Å).

$2\theta_{obs}$ (°)	d_{obs} (Å)	I_{obs}	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$
8.7597	10.0863	12	0	1	1	8.7560	10.0906	0.0037
10.9262	8.0908	16	0	2	0	10.9289	8.0888	−0.0027
13.0533	6.7767	78	1	0	0	13.0645	6.7709	−0.0112
13.7098	6.4536	15	0	0	2	13.7073	6.4549	0.0026
14.1169	6.2685	58	1	1	−1	14.1128	6.2703	0.0040
14.7471	6.0020	13	0	1	2	14.7637	5.9952	−0.0166
16.1652	5.4785	19	1	0	−2	16.1891	5.4705	−0.0239
17.0712	5.1897	100M	1	2	0	17.0637	5.1920	0.0075
17.0712	5.1897	M	1	1	−2	17.0962	5.1822	−0.0250
17.5570	5.0472	21	0	2	2	17.5637	5.0453	−0.0067
17.8065	4.9771	12	0	3	1	17.8108	4.9759	−0.0043
19.6973	4.5034	59	1	2	1	19.6944	4.5040	0.0028
21.0497	4.2170	28M	1	3	−1	21.0059	4.2257	0.0438
21.0497	4.2170	M	1	3	0	21.0435	4.2182	0.0062
21.4042	4.1479	73	1	0	2	21.4207	4.1448	−0.0165
21.9688	4.0426	21M	1	1	−3	21.9413	4.0476	0.0275
21.9688	4.0426	M	0	4	0	21.9589	4.0444	0.0099
22.1132	4.0165	16	1	1	2	22.1212	4.0151	−0.0079
23.0455	3.8561	15	0	4	1	23.0253	3.8594	0.0202
23.2687	3.8196	21	1	3	1	23.2441	3.8236	0.0246
23.9646	3.7102	14	1	2	−3	23.9409	3.7139	0.0237
24.1090	3.6883	8	1	2	2	24.1066	3.6887	0.0024
25.6321	3.4725	70M	1	4	−1	25.6038	3.4763	0.0284
25.6321	3.4725	M	1	4	0	25.6350	3.4721	−0.0028
25.9473	3.4311	17M	2	1	−1	25.9048	3.4366	0.0425
25.9473	3.4311	M	0	4	2	25.9768	3.4272	−0.0295
26.1836	3.4006	14	2	0	−2	26.1808	3.4010	0.0028
26.4725	3.3642	10	0	3	3	26.4774	3.3635	−0.0050
26.7876	3.3253	10	2	1	−2	26.7636	3.3282	0.0240
26.9583	3.3046	14	1	3	−3	26.9638	3.3040	−0.0055
27.4179	3.2503	20	1	4	−2	27.4020	3.2521	0.0158
27.4835	3.2427	20	1	4	1	27.4899	3.2419	−0.0063
27.6411	3.2245	18	2	2	−1	27.6352	3.2252	0.0059
28.1663	3.1656	24	0	1	4	28.1710	3.1651	−0.0048
28.4158	3.1384	13M	0	5	1	28.4150	3.1384	0.0008
28.4158	3.1384	M	2	2	−2	28.4456	3.1351	−0.0299
29.3743	3.0381	22	1	2	−4	29.3691	3.0386	0.0052
29.5450	3.0209	26M	2	1	1	29.5299	3.0224	0.0151
29.5450	3.0209	M	1	2	3	29.5611	3.0193	−0.0161
29.7944	2.9962	14	0	2	4	29.7799	2.9976	0.0145
30.3328	2.9442	10	0	4	3	30.3029	2.9471	0.0299
30.5823	2.9208	9M	1	5	−1	30.5714	2.9218	0.0109
30.5823	2.9208	M	1	5	0	30.5979	2.9193	−0.0157
30.8974	2.8917	10M	2	2	−3	30.8648	2.8947	0.0325
30.8974	2.8917	M	0	5	2	30.8890	2.8925	0.0084
31.1075	2.8727	10	2	2	1	31.0746	2.8756	0.0329
31.9084	2.8024	9	1	3	−4	31.9178	2.8015	−0.0094
33.5234	2.6709	7	2	3	1	33.5063	2.6723	0.0171
34.5476	2.5941	7M	2	4	0	34.5212	2.5960	0.0264
34.5476	2.5941	M	2	2	−4	34.5886	2.5911	−0.0410
35.2304	2.5453	7	1	4	−4	35.2077	2.5469	0.0227
35.6637	2.5154	9	1	2	4	35.6460	2.5166	0.0176
36.7010	2.4467	5	2	4	1	36.6703	2.4486	0.0307
36.8454	2.4374	5	2	3	−4	36.8146	2.4394	0.0308
38.4342	2.3402	7	2	5	0	38.4539	2.3391	−0.0197
40.1280	2.2453	7	3	1	−3	40.1259	2.2454	0.0021
40.3512	2.2334	8	1	0	−6	40.3660	2.2326	−0.0149
41.3228	2.1831	5	2	3	−5	41.3049	2.1840	0.0180
41.9793	2.1504	6	1	2	−6	41.9451	2.1521	0.0342
42.2026	2.1396	5	2	6	−1	42.1984	2.1398	0.0042
42.5308	2.1238	5	3	1	−4	42.5357	2.1236	−0.0049
42.8722	2.1077	6	2	6	0	42.8419	2.1091	0.0303
44.0802	2.0527	5	1	3	5	44.0672	2.0533	0.0129
44.5266	2.0331	5	2	6	−3	44.4972	2.0344	0.0294
47.0345	1.9304	4	0	8	2	47.0524	1.9297	−0.0179

Continued

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TABLE I. Continued

$2\theta_{obs}$ (°)	d_{obs} (Å)	I_{obs}	h	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$
47.2709	1.9213	4	2	5	−5	47.2610	1.9217	0.0099
47.5728	1.9098	4	2	5	3	47.5542	1.9105	0.0187
49.0697	1.8550	5	1	2	6	49.0411	1.8560	0.0286

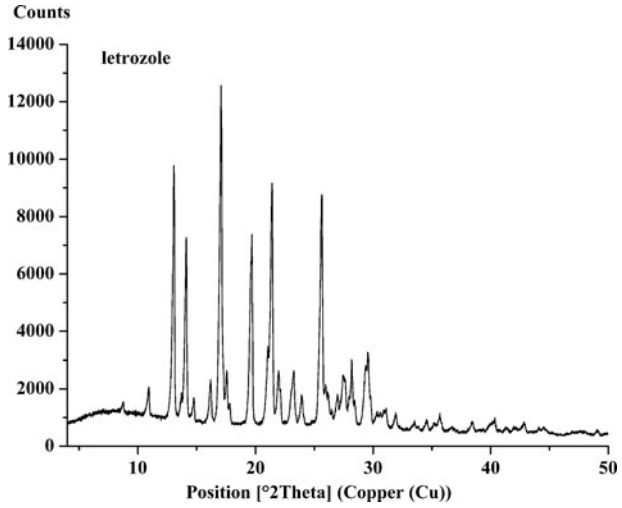

Figure 2. X-ray powder diffraction pattern of letrozole, using Cu$K\alpha_1$ radiation ($\lambda = 1.540\,56$ Å).

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