Supplementary Material for

**Crystal structure of palbociclib form A, C24H29N7O2**

Petr Buikin,1,2 Alexander Korlyukov,1 Ivan Ushakov,1 Alexander Goloveshkin,1 Elizaveta Kulikova,3 and Anna Vologzhanina1

*1 A. N. Nesmeyanov Institute of Organoelement Compounds RAS, Vavilova str. 28, 119334 Moscow, Russia*

*2 Institute of General and Inorganic Chemistry RAS, Leninsky Prosp. 31,119991, Moscow, Russia.*

*3 Kurchatov Institute, National Research Center, Pl. Akad. Kurchatova 1, 123182 Moscow, Russia*

**Figure S1.** Theoretical XRD pattern for palbociclib form A for CuKα-radiation.

**Table S1.** Characteristic peak positions and intensities for palbociclib (λ = 0.7500 Å)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| H | K | L | *d*obs (Å) | *d*calc (Å) | *∆d* | *2θ*obs (°) | *2θ*calc (°) | *∆2θ* | *I/I*o |
| 0 | 0 | 2 | 17.61274 | 17.56806 | -0.0447 | 2.445 | 2.446 | 0.001 | 0.36 |
| 1 | 0 | 0 | 11.07733 | 11.06238 | -0.015 | 3.885 | 3.885 | 0.000 | 0.23 |
| 0 | 0 | 4 | 8.7904 | 8.7840 | -0.0064 | 4.890 | 4.894 | 0.004 | 0.39 |
| 1 | 0 | 2 | 8.6134 | 8.6177 | 0.0043 | 4.980 | 4.998 | 0.018 | 0.53 |
| 1 | 0 | -4 | 7.6629 | 7.6641 | 0.0012 | 5.605 | 5.609 | 0.004 | 0.34 |
| 2 | 0 | 0 | 5.5347 | 5.5312 | -0.0035 | 7.755 | 7.775 | 0.020 | 0.15 |
| 2 | 0 | -4 | 5.1756 | 5.1687 | -0.0069 | 8.310 | 8.321 | 0.011 | 0.42 |
| 0 | 1 | 3 | 5.0661 | 5.0630 | -0.0031 | 8.485 | 8.495 | 0.010 | 0.13 |
| 0 | 1 | 4 | 4.7357 | 4.7309 | -0.0048 | 9.080 | 9.093 | 0.013 | 0.38 |
| 2 | 0 | -6 | 4.5002 | 4.4935 | -0.0067 | 9.565 | 9.574 | 0.009 | 0.38 |
| 1 | 1 | 4 | 4.1939 | 4.1900 | -0.0039 | 10.265 | 10.270 | 0.005 | 0.16 |
| 0 | 1 | 6 | 4.0559 | 4.0528 | -0.0031 | 10.605 | 10.618 | 0.013 | 0.11 |
| 2 | -1 | -1 | 3.9848 | 3.9790 | -0.0058 | 10.805 | 10.819 | 0.014 | 0.32 |
| 2 | 1 | 0 | 3.9447 | 3.9404 | -0.0043 | 10.910 | 10.922 | 0.012 | 1.00 |
| 2 | 1 | 1 | 3.8601 | 3.8556 | -0.0045 | 11.150 | 11.163 | 0.013 | 0.33 |
| 3 | 0 | -2 | 3.7462 | 3.7629 | 0.0167 | 11.490 | 11.439 | -0.051 | 0.09 |
| 3 | -1 | -2 | 3.1192 | 3.1259 | 0.0067 | 13.805 | 13.780 | -0.025 | 0.15 |
| 3 | 1 | 0 | 3.0858 | 3.0822 | -0.0036 | 13.960 | 13.977 | 0.017 | 0.11 |
| 3 | -1 | -5 | 3.01703 | 3.0136 | -0.0034 | 14.275 | 14.297 | 0.021 | 0.06 |
| 3 | 1 | 2 | 2.9573 | 2.9531 | -0.0042 | 14.570 | 14.591 | 0.021 | 0.09 |
| 3 | 0 | 6 | 2.8692 | 2.8726 | 0.0034 | 15.020 | 15.002 | -0.018 | 0.07 |

Atomic coordinates of the optimized model

CELL 0.71073 11.3249 5.6315 35.9681 90 101.51 90

LATT 1

SYMM 0.5-X,0.5+Y,0.5-Z

 O1 0.6457 0.40195 0.13914

 O5 0.57219 -0.10485 0.06614

 N1 1.28085 1.68049 0.16829

 N5 1.44953 1.91006 0.22889

 H113 1.47685 2.06175 0.24456

 N9 1.15084 1.40188 0.07563

 N13 0.92427 0.8083 0.08677

 N17 0.92404 0.78132 0.01969

 N21 0.80337 0.559 0.11527

 N25 1.0352 1.07024 0.05588

 H85 1.04935 1.12257 0.02921

 C1 1.4497 1.96414 0.1883

 H1 1.54201 2.00692 0.18536

 H5 1.39157 2.118 0.17793

 C5 1.40493 1.74737 0.16367

 H9 1.40331 1.78939 0.13385

 H13 1.46762 1.59675 0.17162

 C9 1.27615 1.63904 0.20859

 H17 1.18183 1.60966 0.21067

 H21 1.32855 1.47962 0.21998

 C13 1.32402 1.85688 0.23269

 H25 1.26257 2.00837 0.22363

 H29 1.32334 1.81972 0.26265

 C17 1.09126 1.21386 0.08634

 C21 1.09032 1.16927 0.12475

 H33 1.0423 1.01657 0.13259

 C25 1.15429 1.32062 0.1522

 H37 1.15635 1.2805 0.18193

 C29 1.21778 1.51753 0.14185

 C33 1.21028 1.54665 0.10222

 H41 1.25493 1.69728 0.09168

 C37 0.84497 0.62899 0.08332

 C41 0.80167 0.51142 0.04812

 C45 0.84849 0.59958 0.01722

 H45 0.82279 0.52265 -0.01117

 C49 0.95931 0.8807 0.0551

 C53 0.69772 0.41562 0.11217

 C57 0.66252 0.28112 0.07646

 C61 0.71411 0.32389 0.04546

 C65 0.85865 0.66719 0.15259

 H49 0.94597 0.73208 0.14815

 C69 0.88317 0.49808 0.18721

 H53 0.80259 0.39427 0.18875

 H57 0.95825 0.37673 0.18629

 C73 0.90894 0.67823 0.22025

 H61 0.90678 0.59742 0.24788

 H65 0.99905 0.75682 0.22222

 C77 0.81028 0.87116 0.20861

 H69 0.72794 0.81859 0.21831

 H73 0.83847 1.04409 0.22141

 C81 0.7861 0.87938 0.16437

 H77 0.81652 1.04573 0.15362

 H81 0.69008 0.85954 0.15207

 C85 0.56042 0.10313 0.07452

 C89 0.44197 0.20053 0.08196

 H89 0.45463 0.25616 0.11175

 H93 0.41615 0.36099 0.06489

 H97 0.37093 0.06626 0.07532

 C93 0.67619 0.19551 0.00792

 H101 0.6237 0.31392 -0.01354

 H105 0.75567 0.13752 -0.00284

 H109 0.62153 0.03916 0.01061