

*Acta Cryst.* (1965). **19**, 869

**Crystal data (I) for some pregnane-related compounds\***. By JEAN M. OHRT, BARBARA A. HANER and DORITA A. NORTON, *Biophysics Department, Roswell Park Memorial Institute, Buffalo, New York, U.S.A.*

(Received 19 May 1965)

The lattice constants for 11 pregnane derivatives, on which no further work is anticipated at the present time, have been measured as described in earlier crystal data papers (Haner & Norton, 1964; Ohrt, Haner & Norton, 1964) with an estimated experimental error of 0.10%. The crystal data are listed in Table 1.

#### References

- HANER, B. & NORTON, D. A. (1964). *Acta Cryst.* **17**, 1610.  
OHRT, J. M., HANER, B. A. & NORTON, D. A. (1964). *Acta Cryst.* **17**, 1611.

\* This investigation was supported in part by Public Health Service Research Grant CA-06183 from the National Cancer Institute.

Table 1. *Crystal data (I) for some pregnane-related compounds*

	1	2	3	4	5	6
Formula	C <sub>21</sub> H <sub>32</sub> O <sub>2</sub>	C <sub>21</sub> H <sub>30</sub> O <sub>3</sub>	C <sub>21</sub> H <sub>34</sub> O <sub>3</sub>	C <sub>21</sub> H <sub>36</sub> O <sub>3</sub>	C <sub>21</sub> H <sub>36</sub> O <sub>4</sub>	C <sub>23</sub> H <sub>36</sub> O <sub>3</sub>
Mol. wt.	316.47	330.45	334.48	336.50	352.50	360.50
<i>D<sub>m</sub></i> (g.cm <sup>-3</sup> )	1.182	1.156	1.135	1.194	1.156	1.128
<i>D<sub>x</sub></i> (g.cm <sup>-3</sup> )	1.212	1.216	1.166	1.097	1.196	1.147
Space group	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	<i>P</i> 1	<i>P</i> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub>
<i>Z</i>	4	4	1	2	8	4
<i>a</i> (Å)*	12.233	9.836	6.510	13.587	14.347	27.347
<i>b</i> (Å)*	22.485	23.466	12.492	10.522	23.000	7.682
<i>c</i> (Å)*	6.440	7.819	6.365	7.319	11.860	9.938
α(°)	—	—	93.37	—	—	—
β(°)	—	—	107.72	103.25	—	91.61
γ(°)	—	—	103.64	—	—	—
<i>V</i> (Å <sup>3</sup> )	1771	1805	476	1018	3914	2088
Solvent	Ethyl acetate	Benzene	Unknown	Unknown	Unknown	Unknown

  

	7a	7b	8	9	10	11
Formula	C <sub>23</sub> H <sub>34</sub> O <sub>4</sub>	C <sub>23</sub> H <sub>34</sub> O <sub>4</sub>	C <sub>23</sub> H <sub>32</sub> O <sub>6</sub>	C <sub>25</sub> H <sub>40</sub> O <sub>4</sub>	C <sub>25</sub> H <sub>40</sub> O <sub>4</sub>	C <sub>27</sub> H <sub>42</sub> O <sub>8</sub>
Mol. wt.	374.50	374.50	404.50	404.50	404.50	494.50
<i>D<sub>m</sub></i> (g.cm <sup>-3</sup> )	1.190	1.165	1.041	1.145	1.166	1.222
<i>D<sub>x</sub></i> (g.cm <sup>-3</sup> )	1.212	1.208	1.074	1.139	1.158	1.233
Space group	<i>P</i> 2 <sub>1</sub>	<i>C</i> 2	<i>P</i> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub>
<i>Z</i>	2	4	2	8	4	2
<i>a</i> (Å)*	14.096	21.709	16.722	10.009	11.665	13.572
<i>b</i> (Å)*	7.601	7.608	7.663	61.486	29.071	13.755
<i>c</i> (Å)*	9.719	13.923	9.787	7.675	6.839	7.535
α(°)	—	—	—	—	—	—
β(°)	99.82	116.42	94.70	—	—	108.81
γ(°)	—	—	—	—	—	—
<i>V</i> (Å <sup>3</sup> )	1026	2059	1250	4723	2319	1332
Solvent	Ethanol	Ethanol	Unknown	Unknown	Pentane	Unknown

\* ± 0.008 Å

1. 5α-Pregnan-3,20-dione
2. 4-Pregnen-17α-ol-3,20-dione
3. 5α-Pregnan-3β,17α-diol-20-one
4. 5α-Pregnan-3β,17α,20β-triol
5. 5α-Pregnan-3β,11β,20β,21-tetrol
6. 5α-Pregnan-3β-ol-20-one 3-acetate
7. 5α-Pregnan-21-ol-3,20-dione 21-acetate
8. 5α-Pregnan-17α,21-diol-3,11,20-trione 21-acetate
9. 5α-Pregnan-3β,20α-diol diacetate
10. 5α-Pregnan-3β,20β-diol diacetate
11. 5α-Pregnan-3β,11β,17α,20β,21-pentol 3,20,21-triacetate