

SUPPLEMENTARY MATERIAL

Reduced atomic coordinates for form I of phenobarbital.

	x	y	z
Na1	0.1857 (14)	0.2446 (2)	0.641 (3)
Ca2	0.2828 (15)	0.2292 (2)	0.734 (4)
Na3	0.3803 (12)	0.2452 (2)	0.822 (3)
Ca4	0.3793 (15)	0.2741 (2)	0.848 (3)
Ca5	0.2698 (8)	0.2908 (2)	0.745 (1)
Ca6	0.1656 (12)	0.2732 (2)	0.638 (4)
Oa2	0.2944 (16)	0.2036 (2)	0.718 (3)
Oa4	0.4677 (12)	0.2842 (4)	0.946 (2)
Oa6	0.0678 (11)	0.2850 (3)	0.587 (2)
Ca7	0.2162 (20)	0.3090 (2)	0.908 (2)
Ca8	0.1644 (18)	0.2902 (4)	1.064 (2)
Ca9	0.3208 (16)	0.3115 (3)	0.592 (3)
Ca10	0.2625 (16)	0.3368 (3)	0.530 (3)
Ca11	0.3064 (15)	0.3570 (3)	0.403 (3)
Ca12	0.4130 (15)	0.3482 (3)	0.318 (3)
Ca13	0.4724 (18)	0.3226 (3)	0.365 (3)
Ca14	0.4293 (14)	0.3036 (3)	0.501 (3)
Ha1	0.1182 (14)	0.2328 (2)	0.563 (3)
Ha3	0.4604 (12)	0.2345 (2)	0.872 (3)
Ha7a	0.1474 (20)	0.3216 (2)	0.849 (2)
Ha7b	0.2846 (20)	0.3215 (2)	0.972 (2)
Ha8a	0.1983 (18)	0.2704 (4)	1.047 (2)
Ha8b	0.0699 (18)	0.2904 (4)	1.043 (2)
Ha8c	0.1931 (18)	0.2982 (4)	1.198 (2)
Ha10	0.1782 (16)	0.3407 (3)	0.582 (3)
Ha11	0.2652 (15)	0.3761 (3)	0.376 (3)
Ha12	0.4493 (15)	0.3609 (3)	0.217 (3)
Ha13	0.5505 (18)	0.3176 (3)	0.297 (3)
Ha14	0.4736 (14)	0.2851 (3)	0.533 (3)
Nb1	0.1362 (12)	0.0048 (3)	0.218 (2)
Cb2	0.2128 (12)	0.0174 (3)	0.366 (3)
Nb3	0.3298 (11)	0.0047 (3)	0.385 (3)
Cb4	0.3719 (9)	-0.0202 (3)	0.311 (4)
Cb5	0.2703 (8)	-0.0373 (2)	0.191 (1)
Cb6	0.1623 (13)	-0.0184 (3)	0.104 (2)

Ob2	0.1814 (14)	0.0402 (2)	0.430 (2)
Ob4	0.4818 (9)	-0.0268 (4)	0.330 (2)
Ob6	0.0840 (12)	-0.0294 (4)	-0.007 (2)
Cb7	0.3261 (19)	-0.0532 (2)	0.019 (2)
Cb8	0.3651 (19)	-0.0309 (4)	-0.127 (3)
Cb9	0.2250 (13)	-0.0587 (4)	0.343 (3)
Cb10	0.1079 (12)	-0.0586 (4)	0.426 (3)
Cb11	0.0786 (15)	-0.0783 (4)	0.568 (3)
Cb12	0.1604 (10)	-0.1010 (3)	0.615 (3)
Cb13	0.2800 (11)	-0.1002 (4)	0.547 (3)
Cb14	0.3050 (16)	-0.0817 (4)	0.393 (3)
Hb1	0.0491 (12)	0.0139 (3)	0.189 (3)
Hb3	0.3966 (11)	0.0160 (4)	0.469 (3)
Hb7a	0.2617 (19)	-0.0665 (2)	-0.046 (2)
Hb7b	0.4009 (19)	-0.0649 (2)	0.070 (2)
Hb8a	0.2937 (19)	-0.0285 (4)	-0.231 (3)
Hb8b	0.4428 (19)	-0.0381 (4)	-0.187 (3)
Hb8c	0.3827 (19)	-0.0127 (4)	-0.052 (3)
Hb10	0.0438 (12)	-0.0437 (4)	0.382 (3)
Hb11	-0.0014 (15)	-0.0763 (4)	0.637 (3)
Hb12	0.1331 (10)	-0.1175 (3)	0.696 (3)
Hb13	0.3482 (11)	-0.1130 (4)	0.607 (3)
Hb14	0.3819 (16)	-0.0848 (4)	0.318 (3)
Nc1	0.1612 (12)	0.1747 (3)	0.324 (3)
Cc2	0.2530 (14)	0.1887 (3)	0.230 (4)
Nc3	0.3661 (12)	0.1757 (2)	0.209 (3)
Cc4	0.4012 (11)	0.1485 (3)	0.256 (4)
Cc5	0.2996 (8)	0.1309 (2)	0.347 (1)
Cc6	0.1854 (14)	0.1481 (3)	0.401 (4)
Oc2	0.2398 (17)	0.2137 (2)	0.186 (3)
Oc4	0.5066 (9)	0.1400 (4)	0.234 (3)
Oc6	0.1015 (13)	0.1365 (4)	0.483 (2)
Cc7	0.3597 (21)	0.1160 (3)	0.535 (2)
Cc8	0.4114 (18)	0.1342 (4)	0.707 (2)
Cc9	0.2606 (14)	0.1081 (4)	0.192 (3)
Cc10	0.3408 (15)	0.0870 (4)	0.134 (3)
Cc11	0.3196 (13)	0.0666 (4)	-0.013 (3)
Cc12	0.2014 (11)	0.0682 (4)	-0.114 (3)
Cc13	0.1137 (12)	0.0875 (4)	-0.054 (3)
Cc14	0.1512 (15)	0.1097 (4)	0.069 (3)

Hc1	0.0751 (12)	0.1841 (3)	0.337 (3)
Hc3	0.4334 (12)	0.1880 (2)	0.150 (3)
Hc7a	0.2941 (20)	0.1030 (3)	0.586 (2)
Hc7b	0.4309 (20)	0.1038 (3)	0.493 (2)
Hc8a	0.4229 (18)	0.1541 (4)	0.657 (2)
Hc8b	0.3489 (18)	0.1338 (4)	0.812 (2)
Hc8c	0.4944 (18)	0.1258 (4)	0.759 (2)
Hc10	0.4262 (15)	0.0865 (4)	0.207 (3)
Hc11	0.3839 (13)	0.0518 (4)	-0.043 (3)
Hc12	0.1798 (11)	0.0554 (4)	-0.231 (3)
Hc13	0.0223 (12)	0.0852 (4)	-0.100 (3)
Hc14	0.0984 (15)	0.1275 (4)	0.069 (3)

Bond lengths (Å) of form I of phenobarbital.

	Molecule 1	Molecule 2	Molecule 3
Ni1–Ci2	1.382 (22)	1.384 (22)	1.379 (25)
Ni1–Ci6	1.366 (13)	1.381 (20)	1.374 (21)
Ni1–Hi1	1.030	1.030	1.031
Ci2–Ni3	1.388 (21)	1.384 (18)	1.372 (20)
Ci2–Oi2	1.216 (13)	1.215 (21)	1.222 (17)
Ni3–Ci4	1.370 (13)	1.365 (22)	1.366 (18)
Ni3–Hi3	1.030	1.029	1.029
Ci4–Ci5	1.539 (18)	1.538 (18)	1.531 (18)
Ci4–Oi4	1.213 (22)	1.213 (14)	1.215 (17)
Ci5–Ci6	1.527 (17)	1.540 (16)	1.533 (18)
Ci5–Ci7	1.546 (17)	1.544 (16)	1.558 (16)
Ci5–Ci9	1.551 (21)	1.549 (21)	1.539 (22)
Ci6–Oi6	1.210 (18)	1.205 (20)	1.218 (24)
Ci7–Ci8	1.514 (23)	1.524 (22)	1.524 (22)
Ci7–Hi7a	1.009	1.010	1.010
Ci7–Hi7b	1.011	1.010	1.010
Ci8–Hi8a	1.010	1.010	1.009
Ci8–Hi8b	1.010	1.010	1.010
Ci8–Hi8c	1.011	1.009	1.011
Ci9–Ci10	1.397 (23)	1.411 (22)	1.390 (26)
Ci9–Ci14	1.401 (25)	1.405 (23)	1.388 (24)
Ci10–Ci11	1.392 (25)	1.392 (26)	1.395 (26)
Ci10–Hi10	1.010	1.009	1.010
Ci11–Ci12	1.377 (25)	1.402 (21)	1.394 (19)
Ci11–Hi11	1.008	1.010	1.011
Ci12–Ci13	1.394 (22)	1.391 (18)	1.387 (24)
Ci12–Hi12	1.009	1.010	1.012
Ci13–Ci14	1.390 (25)	1.400 (26)	1.384 (26)
Ci13–Hi13	1.009	1.009	1.010
Ci14–Hi14	1.009	1.011	1.009

Bond angles ($^{\circ}$) of form I of phenobarbital.

	Molecule 1	Molecule 2	Molecule 3
Ci2–Ni1–Ci6	129.8 (10)	127.9 (14)	119.4 (13)
Ci2–Ni1–Hi1	115.1	116.0	120.3
Ci6–Ni1–Hi1	115.0	116.1	120.3
Ni1–Ci2–Ni3	115.0 (15)	111.4 (12)	119.8 (13)
Ni1–Ci2–Oi2	124.1 (10)	118.4 (16)	120.1 (13)
Ni3–Ci2–Oi2	120.0 (9)	128.3 (14)	119.6 (12)
Ci2–Ni3–Ci4	125.8 (9)	131.1 (12)	128.6 (12)
Ci2–Ni3–Hi3	117.0	114.5	115.4
Ci4–Ni3–Hi3	117.2	114.4	115.7
Ni3–Ci4–Ci5	117.5 (8)	114.0 (13)	114.3 (10)
Ni3–Ci4–Oi4	116.6 (12)	121.8 (12)	121.3 (12)
Ci5–Ci4–Oi4	125.9 (15)	124.1 (10)	124.4 (11)
Ci4–Ci5–Ci6	116.2 (10)	112.4 (8)	114.3 (9)
Ci4–Ci5–Ci7	105.4 (9)	111.1 (10)	108.2 (10)
Ci4–Ci5–Ci9	109.5 (9)	103.3 (9)	105.4 (9)
Ci6–Ci5–Ci7	110.3 (8)	108.1 (9)	109.2 (10)
Ci6–Ci5–Ci9	107.6 (9)	111.7 (10)	110.7 (10)
Ci7–Ci5–Ci9	107.6 (10)	110.1 (10)	108.8 (10)
Ni1–Ci6–Ci5	114.9 (8)	114.8 (11)	121.5 (11)
Ni1–Ci6–Oi6	125.9 (11)	122.3 (15)	117.2 (15)
Ci5–Ci6–Oi6	118.1 (12)	117.4 (13)	119.9 (14)
Ci5–Ci7–Ci8	110.7 (11)	107.3 (11)	118.9 (11)
Ci5–Ci7–Hi7a	109.5	110.4	107.4
Ci5–Ci7–Hi7b	109.6	110.4	107.4
Ci8–Ci7–Hi7a	109.5	110.4	107.4
Ci8–Ci7–Hi7b	109.5	110.4	1.703
Hi7a–Ci7–Hi7b	108.0	107.9	108.0
Ci7–Ci8–Hi8a	108.0	108.0	108.0
Ci7–Ci8–Hi8b	108.0	107.9	107.9
Ci7–Ci8–Hi8c	107.9	108.0	107.9
Hi8a–Ci8–Hi8b	110.9	110.8	111.0
Hi8a–Ci8–Hi8c	111.0	111.0	111.0
Hi8b–Ci8–Hi8c	110.9	111.0	110.9
Ci5–Ci9–Ci10	124.6 (14)	126.4 (13)	123.5 (16)
Ci5–Ci9–Ci14	118.2 (15)	116.8 (14)	123.2 (15)
Ci10–Ci9–Ci14	117.2 (15)	116.6 (13)	112.2 (15)
Ci9–Ci10–Ci11	127.6 (15)	121.7 (15)	128.9 (18)
Ci9–Ci10–Hi10	116.1	119.2	115.5
Ci11–Ci10–Hi10	116.2	119.1	115.6

Ci10–Ci11–Ci12	112.3 (16)	119.9 (16)	114.0 (15)
Ci10–Ci11–Hi11	123.8	120.0	123.0
Ci12–Ci11–Hi11	123.9	120.1	123.0
Ci11–Ci12–Ci13	122.9 (15)	118.6 (12)	120.0 (12)
Ci11–Ci12–Hi12	118.6	120.8	120.0
Ci13–Ci12–Hi12	118.5	120.7	120.0
Ci12–Ci13–Ci14	122.8 (14)	119.5 (14)	120.1 (17)
Ci12–Ci13–Hi13	118.5	120.2	120.0
Ci14–Ci13–Hi13	118.7	120.2	119.9
Ci9–Ci14–Ci13	116.7 (16)	121.1 (16)	121.1 (16)
Ci9–Ci14–Hi14	121.6	119.5	119.5
Ci13–Ci14–Hi14	121.6	119.4	119.4

Torsion angles ($^{\circ}$) of form I of phenobarbital after Rietveld refinements.

	Molecule 1	Molecule 2	Molecule 3
Ci6–Ni1–Ci2–Ni3	-6.6 (27)	3.6 (23)	-1.9 (27)
Ci6–Ni1–Ci2–Oi2	-175.8 (18)	169.2 (16)	169.6 (18)
Ci2–Ni1–Ci6–Ci5	3.4 (25)	19.2 (22)	13.6 (25)
Ci2–Ni1–Ci6–Oi6	-164.5 (19)	172.3 (16)	179.8 (18)
Ni1–Ci2–Ni3–Ci4	9.8 (25)	-13.6 (25)	-5.8 (30)
Oi2–Ci2–Ni3–Ci4	179.6 (17)	-177.4 (18)	-177.4 (18)
Ci2–Ni3–Ci4–Ci5	-9.7 (24)	-1.7 (25)	0.9 (26)
Ci2–Ni3–Ci4–Oi4	172.6 (17)	173.8 (17)	177.8 (19)
Ni3–Ci4–Ci5–Ci6	5.5 (19)	24.4 (17)	9.9 (19)
Ni3–Ci4–Ci5–Ci7	127.9 (14)	145.8 (13)	131.8 (14)
Ni3–Ci4–Ci5–Ci9	-116.7 (15)	-96.1 (15)	-111.9 (15)
Oi4–Ci4–Ci5–Ci6	-177.0 (17)	-150.9 (16)	-166.9 (17)
Oi4–Ci4–Ci5–Ci7	-54.6 (20)	-29.6 (21)	-45.0 (21)
Oi4–Ci4–Ci5–Ci9	60.9 (20)	88.5 (19)	71.3 (20)
Ci4–Ci5–Ci6–Ni1	-2.5 (18)	-32.2 (16)	-17.5 (20)
Ci4–Ci5–Ci6–Oi6	166.4 (15)	173.3 (14)	176.7 (16)
Ci7–Ci5–Ci6–Ni1	-122.2 (14)	-155.3 (12)	-138.9 (16)
Ci7–Ci5–Ci6–Oi6	46.6 (19)	50.2 (16)	55.3 (20)
Ci9–Ci5–Ci6–Ni1	120.6 (15)	83.4 (14)	101.3 (17)
Ci9–Ci5–Ci6–Oi6	-70.5 (18)	-71.1 (16)	-64.5 (20)
Ci4–Ci5–Ci7–Ci8	-63.2 (15)	-67.7 (14)	-63.3 (16)
Ci6–Ci5–Ci7–Ci8	63.0 (15)	56.1 (14)	61.7 (17)
Ci9–Ci5–Ci7–Ci8	-179.9 (13)	178.4 (12)	-177.4 (14)
Ci4–Ci5–Ci9–Ci10	-153.6 (16)	109.4 (18)	-64.6 (19)
Ci4–Ci5–Ci9–Ci14	30.1 (19)	-75.1 (17)	102.4 (18)
Ci6–Ci5–Ci9–Ci10	79.2 (19)	-11.7 (21)	171.3 (16)
Ci6–Ci5–Ci9–Ci14	-97.0 (16)	163.8 (14)	-21.7 (21)
Ci7–Ci5–Ci9–Ci10	-39.6 (20)	-131.9 (17)	51.3 (20)
Ci7–Ci5–Ci9–Ci14	144.2 (15)	43.7 (18)	-141.6 (16)
Ci5–Ci9–Ci10–Ci11	175.7 (16)	-177.5 (15)	175.3 (16)
Ci14–Ci9–Ci10–Ci11	-8.1 (28)	6.9 (25)	7.0 (28)
Ci5–Ci9–Ci14–Ci13	180.0 (14)	172.1 (14)	173.4 (15)
Ci10–Ci9–Ci14–Ci13	3.4 (25)	-11.9 (25)	-18.3 (25)
Ci9–Ci10–Ci11–Ci12	7.9 (27)	-7.3 (26)	-0.7 (28)
Ci10–Ci11–Ci12–Ci13	-3.7 (25)	12.2 (24)	5.2 (24)
Ci11–Ci12–Ci13–Ci14	0.2 (28)	-17.1 (24)	-16.8 (26)
Ci12–Ci13–Ci14–Ci9	0.0 (26)	17.4 (26)	24.2 (27)

Reduced atomic coordinates for form II of phenobarbital.

	x	y	z
Na1	0.1502 (12)	0.4812 (4)	0.673 (3)
Ca2	0.2452 (13)	0.4559 (4)	0.768 (4)
Na3	0.3407 (14)	0.4890 (4)	0.844 (3)
Ca4	0.3568 (12)	0.5456 (4)	0.822 (4)
Ca5	0.2544 (8)	0.5838 (4)	0.725 (1)
Ca6	0.1570 (13)	0.5437 (4)	0.634 (3)
Oa2	0.2463 (15)	0.4045 (4)	0.786 (3)
Oa4	0.4540 (11)	0.5642 (7)	0.895 (2)
Oa6	0.0664 (11)	0.5673 (7)	0.542 (2)
Ca7	0.3200 (18)	0.6127 (5)	0.558 (2)
Ca8	0.3648 (17)	0.5715 (8)	0.404 (2)
Ca9	0.2162 (17)	0.6255 (7)	0.888 (3)
Ca10	0.2773 (14)	0.6748 (6)	0.949 (3)
Ca11	0.2216 (12)	0.7084 (8)	1.090 (3)
Ca12	0.1031 (12)	0.6992 (6)	1.151 (3)
Ca13	0.0582 (17)	0.6450 (5)	1.109 (3)
Ca14	0.1099 (15)	0.6087 (7)	0.972 (3)
Ha1	0.0677 (13)	0.4676 (4)	0.631 (3)
Ha3	0.4097 (14)	0.4674 (4)	0.929 (3)
Ha7a	0.3921 (18)	0.6350 (5)	0.621 (2)
Ha7b	0.2546 (18)	0.6406 (5)	0.491 (2)
Ha8a	0.3219 (17)	0.5341 (8)	0.412 (2)
Ha8b	0.4582 (17)	0.5663 (8)	0.433 (2)
Ha8c	0.3447 (17)	0.5893 (8)	0.270 (2)
Ha10	0.3584 (14)	0.6867 (6)	0.898 (3)
Ha11	0.2683 (12)	0.7411 (8)	1.156 (3)
Ha12	0.0498 (12)	0.7294 (6)	1.215 (3)
Ha13	-0.0101 (17)	0.6295 (5)	1.185 (3)
Ha14	0.0707 (15)	0.5717 (7)	0.928 (3)
Nb1	0.3322 (10)	0.0098 (6)	0.387 (3)
Cb2	0.2112 (11)	0.0309 (7)	0.372 (3)
Nb3	0.1369 (14)	0.0125 (6)	0.209 (2)
Cb4	0.1682 (15)	-0.0369 (6)	0.112 (3)
Cb5	0.2764 (8)	-0.0753 (4)	0.198 (1)
Cb6	0.3770 (9)	-0.0398 (7)	0.309 (4)
Ob2	0.1765 (14)	0.0766 (5)	0.440 (2)
Ob4	0.0942 (13)	-0.0589 (8)	-0.010 (2)
Ob6	0.4860 (9)	-0.0579 (8)	0.331 (3)
Cb7	0.3336 (19)	-0.1063 (5)	0.023 (2)

Cb8	0.3802 (20)	-0.0698 (8)	-0.140 (2)
Cb9	0.2247 (12)	-0.1184 (7)	0.339 (3)
Cb10	0.1113 (12)	-0.1197 (7)	0.426 (3)
Cb11	0.0808 (11)	-0.1635 (7)	0.548 (3)
Cb12	0.1779 (10)	-0.2002 (8)	0.620 (3)
Cb13	0.2923 (12)	-0.1994 (9)	0.536 (3)
Cb14	0.3131 (14)	-0.1620 (7)	0.387 (3)
Hb1	0.3965 (10)	0.0340 (6)	0.468 (3)
Hb3	0.0577 (14)	0.0357 (6)	0.160 (2)
Hb7a	0.2671 (19)	-0.1313 (5)	-0.043 (2)
Hb7b	0.4042 (19)	-0.1319 (5)	0.080 (2)
Hb8a	0.3078 (20)	-0.0577 (8)	-0.236 (2)
Hb8b	0.4420 (20)	-0.0951 (8)	-0.208 (2)
Hb8c	0.4214 (20)	-0.0357 (8)	-0.076 (2)
Hb10	0.0476 (12)	-0.0877 (7)	0.398 (3)
Hb11	-0.0067 (11)	-0.1686 (7)	0.589 (3)
Hb12	0.1678 (10)	-0.2273 (8)	0.731 (3)
Hb13	0.3616 (12)	-0.2272 (9)	0.583 (3)
Hb14	0.3917 (14)	-0.1646 (7)	0.314 (3)
Nc1	0.1507 (14)	0.3514 (4)	0.372 (3)
Cc2	0.2420 (15)	0.3817 (6)	0.289 (5)
Nc3	0.3500 (14)	0.3539 (5)	0.238 (3)
Cc4	0.3842 (12)	0.2979 (5)	0.274 (4)
Cc5	0.2830 (8)	0.2635 (4)	0.361 (1)
Cc6	0.1599 (16)	0.2940 (5)	0.413 (4)
Oc2	0.2118 (16)	0.4300 (5)	0.239 (3)
Oc4	0.4840 (12)	0.2738 (8)	0.248 (3)
Oc6	0.0820 (14)	0.2719 (8)	0.506 (2)
Cc7	0.3285 (23)	0.2325 (5)	0.555 (2)
Cc8	0.3864 (20)	0.2698 (9)	0.723 (3)
Cc9	0.2487 (13)	0.2152 (8)	0.210 (3)
Cc10	0.3283 (16)	0.1715 (8)	0.150 (3)
Cc11	0.2952 (12)	0.1362 (9)	-0.009 (3)
Cc12	0.1763 (11)	0.1380 (9)	-0.113 (3)
Cc13	0.0992 (14)	0.1810 (9)	-0.040 (3)
Cc14	0.1331 (14)	0.2218 (9)	0.105 (3)

Hc1	0.0684 (14)	0.3728 (4)	0.399 (3)
Hc3	0.4105 (14)	0.3768 (5)	0.162 (3)
Hc7a	0.3925 (23)	0.2019 (5)	0.523 (2)
Hc7b	0.2535 (23)	0.2131 (5)	0.602 (2)
Hc8a	0.4661 (20)	0.2500 (9)	0.779 (3)
Hc8b	0.3237 (20)	0.2737 (9)	0.827 (3)
Hc8c	0.4041 (20)	0.3082 (9)	0.669 (3)
Hc10	0.4174 (16)	0.1692 (8)	0.211 (3)
Hc11	0.3549 (12)	0.1039 (9)	-0.040 (3)
Hc12	0.1528 (11)	0.1149 (9)	-0.236 (3)
Hc13	0.0064 (14)	0.1782 (9)	-0.075 (3)
Hc14	0.0830 (14)	0.2588 (9)	0.113 (3)

Bond lengths (\AA) of form II of phenobarbital.

	Molecule 1	Molecule 2	Molecule 3
Ni1–Ci2	1.362 (20)	1.372 (17)	1.390 (26)
Ni1–Ci6	1.364 (14)	1.360 (23)	1.381 (17)
Ni1–Hi1	1.030	1.030	1.030
Ci2–Ni3	1.370 (19)	1.384 (22)	1.377 (23)
Ci2–Oi2	1.217 (13)	1.219 (21)	1.217 (19)
Ni3–Ci4	1.357 (14)	1.372 (21)	1.375 (17)
Ni3–Hi3	1.030	1.030	1.030
Ci4–Ci5	1.516 (16)	1.533 (17)	1.534 (20)
Ci4–Oi4	1.211 (19)	1.223 (22)	1.221 (20)
Ci5–Ci6	1.519 (15)	1.529 (18)	1.544 (20)
Ci5–Ci7	1.554 (18)	1.542 (17)	1.554 (15)
Ci5–Ci9	1.536 (21)	1.548 (21)	1.548 (22)
Ci6–Oi6	1.234 (19)	1.230 (15)	1.220 (28)
Ci7–Ci8	1.510 (22)	1.536 (23)	1.532 (23)
Ci7–Hi7a	1.011	1.010	1.010
Ci7–Hi7b	1.010	1.010	1.010
Ci8–Hi8a	1.009	1.010	1.010
Ci8–Hi8b	1.010	1.010	1.010
Ci8–Hi8c	1.010	1.009	1.010
Ci9–Ci10	1.392 (23)	1.394 (22)	1.391 (26)
Ci9–Ci14	1.388 (26)	1.398 (22)	1.388 (23)
Ci10–Ci11	1.389 (24)	1.397 (26)	1.384 (26)
Ci10–Hi10	1.010	1.009	1.010
Ci11–Ci12	1.393 (20)	1.394 (21)	1.408 (20)
Ci11–Hi11	1.010	1.010	1.009
Ci12–Ci13	1.393 (19)	1.394 (20)	1.395 (26)
Ci12–Hi12	1.010	1.010	1.009
Ci13–Ci14	1.386 (24)	1.390 (26)	1.398 (29)
Ci13–Hi13	1.009	1.010	1.009
Ci14–Hi14	1.010	1.009	1.010

Bond angles ($^{\circ}$) of form II of phenobarbital.

	Molecule 1	Molecule 2	Molecule 3
Ci2–Ni1–Ci6	123.8 (10)	127.7 (12)	124.7 (12)
Ci2–Ni1–Hi1	118.7	116.1	117.7
Ci6–Ni1–Hi1	117.5	116.1	117.5
Ni1–Ci2–Ni3	112.3 (14)	115.8 (13)	119.6 (15)
Ni1–Ci2–Oi2	124.7 (10)	125.1 (14)	115.9 (13)
Ni3–Ci2–Oi2	123.0 (10)	113.6 (16)	123.5 (14)
Ci2–Ni3–Ci4	129.4 (10)	120.0 (14)	126.5 (12)
Ci2–Ni3–Hi3	114.3	120.3	117.0
Ci4–Ni3–Hi3	116.2	119.7	116.5
Ni3–Ci4–Ci5	121.5 (9)	119.9 (12)	114.3 (10)
Ni3–Ci4–Oi4	116.6 (12)	121.0 (15)	127.6 (13)
Ci5–Ci4–Oi4	121.9 (13)	116.4 (14)	118.1 (12)
Ci4–Ci5–Ci6	105.1 (9)	110.6 (9)	119.2 (10)
Ci4–Ci5–Ci7	103.4 (9)	107.2 (10)	113.8 (10)
Ci4–Ci5–Ci9	105.5 (9)	109.0 (10)	107.0 (9)
Ci6–Ci5–Ci7	109.6 (9)	108.8 (10)	103.4 (11)
Ci6–Ci5–Ci9	118.1 (10)	110.4 (9)	107.6 (10)
Ci7–Ci5–Ci9	113.5 (10)	110.9 (10)	104.9 (10)
Ni1–Ci6–Ci5	126.1 (9)	113.8 (13)	115.3 (10)
Ni1–Ci6–Oi6	118.1 (12)	125.5 (12)	120.6 (14)
Ci5–Ci6–Oi6	114.7 (13)	120.6 (10)	123.5 (16)
Ci5–Ci7–Ci8	113.9 (11)	110.9 (14)	116.2 (10)
Ci5–Ci7–Hi7a	108.5	107.2	108.4
Ci5–Ci7–Hi7b	107.5	107.0	106.9
Ci8–Ci7–Hi7a	110.4	106.7	108.1
Ci8–Ci7–Hi7b	108.4	109.8	109.0
Hi7a–Ci7–Hi7b	107.9	107.9	107.9
Ci7–Ci8–Hi8a	109.9	110.0	107.8
Ci7–Ci8–Hi8b	106.5	105.4	107.2
Ci7–Ci8–Hi8c	107.6	108.5	109.0
Hi8a–Ci8–Hi8b	111.0	110.9	110.9
Hi8a–Ci8–Hi8c	110.9	111.0	110.9
Hi8b–Ci8–Hi8c	110.9	110.9	110.9
Ci5–Ci9–Ci10	126.1 (15)	131.7 (13)	126.4 (16)
Ci5–Ci9–Ci14	112.0 (15)	110.9 (14)	115.5 (15)
Ci10–Ci9–Ci14	121.9 (16)	117.4 (13)	117.3 (15)
Ci9–Ci10–Ci11	116.4 (15)	123.1 (14)	121.8 (18)
Ci9–Ci10–Hi10	123.8	118.7	119.1
Ci11–Ci10–Hi10	119.8	118.1	118.4

Ci10–Ci11–Ci12	123.6 (14)	117.2 (16)	123.6 (15)
Ci10–Ci11–Hi11	119.9	123.0	118.0
Ci12–Ci11–Hi11	116.6	119.7	117.8
Ci11–Ci12–Ci13	115.0 (13)	119.1 (11)	111.6 (13)
Ci11–Ci12–Hi12	123.9	122.0	124.6
Ci13–Ci12–Hi12	121.0	119.0	123.3
Ci12–Ci13–Ci14	122.2 (13)	121.7 (14)	126.7 (19)
Ci12–Ci13–Hi13	120.7	119.4	116.9
Ci14–Ci13–Hi13	116.9	118.9	115.3
Ci9–Ci14–Ci13	118.1 (16)	119.3 (16)	118.2 (17)
Ci9–Ci14–Hi14	119.4	118.8	120.5
Ci13–Ci14–Hi14	122.4	121.9	120.1

Torsion angles ($^{\circ}$) of form II of phenobarbital after Rietveld refinements.

	Molecule 1	Molecule 2	Molecule 3
Ci6–Ni1–Ci2–Ni3	8.4 (23)	-25.4 (25)	1.2 (30)
Ci6–Ni1–Ci2–Oi2	-172.1 (17)	-177.7 (18)	170.4 (19)
Ci2–Ni1–Ci6–Ci5	-14.3 (24)	-1.7 (25)	0.6 (27)
Ci2–Ni1–Ci6–Oi6	178.2 (16)	-177.9 (18)	171.8 (20)
Ni1–Ci2–Ni3–Ci4	-6.1 (25)	21.5 (22)	-5.3 (31)
Oi2–Ci2–Ni3–Ci4	174.5 (17)	177.0 (15)	-173.7 (20)
Ci2–Ni3–Ci4–Ci5	8.4 (26)	7.2 (22)	6.6 (27)
Ci2–Ni3–Ci4–Oi4	-175.5 (17)	167.6 (16)	-172.5 (21)
Ni3–Ci4–Ci5–Ci6	-10.4 (18)	-32.1 (18)	-4.2 (21)
Ni3–Ci4–Ci5–Ci7	115.2 (16)	89.4 (16)	118.0 (16)
Ni3–Ci4–Ci5–Ci9	-125.4 (15)	-150.5 (14)	-126.6 (15)
Oi4–Ci4–Ci5–Ci6	173.7 (16)	166.6 (15)	175.0 (17)
Oi4–Ci4–Ci5–Ci7	-60.7 (19)	-71.9 (17)	-62.8 (20)
Oi4–Ci4–Ci5–Ci9	58.8 (18)	48.2 (17)	52.6 (21)
Ci4–Ci5–Ci6–Ni1	13.8 (18)	28.4 (18)	1.0 (22)
Ci4–Ci5–Ci6–Oi6	-178.3 (14)	-155.2 (16)	-169.9 (18)
Ci7–Ci5–Ci6–Ni1	-103.5 (17)	-92.3 (16)	-121.0 (17)
Ci7–Ci5–Ci6–Oi6	64.3 (17)	84.1 (19)	68.2 (23)
Ci9–Ci5–Ci6–Ni1	-124.4 (15)	145.8 (14)	128.4 (16)
Ci9–Ci5–Ci6–Oi6	-67.8 (16)	-37.8 (20)	-42.5 (23)
Ci4–Ci5–Ci7–Ci8	62.7 (14)	56.5 (16)	55.1 (18)
Ci6–Ci5–Ci7–Ci8	-49.0 (15)	-63.1 (16)	-75.7 (16)
Ci9–Ci5–Ci7–Ci8	176.5 (13)	175.3 (13)	171.7 (14)
Ci4–Ci5–Ci9–Ci10	81.9 (19)	-15.1 (22)	62.4 (21)
Ci4–Ci5–Ci9–Ci14	-98.0 (15)	166.7 (13)	-107.2 (17)
Ci6–Ci5–Ci9–Ci10	-161.0 (16)	106.5 (20)	-168.4 (18)
Ci6–Ci5–Ci9–Ci14	19.1 (19)	-71.6 (16)	22.0 (20)
Ci7–Ci5–Ci9–Ci10	-30.6 (21)	-132.9 (18)	-58.8 (21)
Ci7–Ci5–Ci9–Ci14	149.4 (13)	49.0 (16)	131.6 (16)
Ci5–Ci9–Ci10–Ci11	175.8 (15)	178.8 (16)	-168.8 (16)
Ci14–Ci9–Ci10–Ci11	-4.2 (25)	-3.1 (26)	0.6 (28)
Ci5–Ci9–Ci14–Ci13	-174.2 (14)	169.4 (14)	177.0 (15)
Ci10–Ci9–Ci14–Ci13	5.8 (26)	-9.0 (25)	6.5 (27)
Ci9–Ci10–Ci11–Ci12	-8.6 (25)	14.4 (26)	-5.5 (29)
Ci10–Ci11–Ci12–Ci13	18.6 (24)	-13.3 (24)	2.5 (26)
Ci11–Ci12–Ci13–Ci14	-16.7 (24)	1.7 (26)	5.4 (28)
Ci12–Ci13–Ci14–Ci9	5.2 (25)	9.9 (26)	-10.2 (31)