X-ray powder diffraction data for the second and third polymorphs of 1-methylhydantoin

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X-ray powder diffraction data for the two new polymorphs of 1-methylhydantoin, $C_4H_6N_2O_2$, are reported. The polymorph II (MH-**II**) crystallizes in the orthorhombic system with space group $Pna2_1$ [$a = 19.0323(7)$ Å, $b = 3.91269(8)$ Å, $c = 6.8311(7)$ Å, $Z' = 1$, $Z = 4$, unit cell volume $V = 508.70(3)$ Å^3. Polymorph III (MH-**III**) crystallizes in the orthorhombic system with space group $P2_12_12_1$ [$a = a = 7.82427(5)$, $b = 9.8230(5)$, $c = 20.2951(4)$, $Z' = 3$, $Z = 12$, unit cell volume $V = 1563.5(1)$ Å^3]. All measured lines, in each case, were indexed and are consistent with the space group. © *The Author(s), 2022. Published by Cambridge University Press on behalf of International Centre for Diffraction Data.* [doi:10.1017/S0885715622000136]

Key words: 1-methylhydantoin, polymorphism, X-ray powder diffraction

I. INTRODUCTION

Polymorphism is the result of the different crystalline forms in the solid-state produced by different packing of the molecules (Bernstein, 2002; Cruz-Cabeza and Bernstein, 2014). According to this definition, different polymorphs of the same compound can present different physical and chemical properties in the solid-state. Polymorphism is important in the pharmaceutical industry due to the need to control the physical and chemical properties of one specific product, such as its solubility, nonlinear optical activities, bioactivity, pharmacokinetics, and among others (Park *et al.*, 2003).

According to a recent report (Cruz-Cabeza *et al.*, 2015), one out of every two organic compounds reported in the Cambridge Structural Database version 5.43, March 2022 (Groom *et al.*, 2016) show polymorphism and are mainly due to crystallization conditions. A particular case occurs in the 1-methylhydantoin (1-methyl-imidazolidine-2,4-dione) compound for which three different conformational polymorphs have been reported to date (Nogueira *et al.*, 2020). Hydantoin compounds, and their analogs thiohydantoins, form a large group of derivatives widely applied in medicine and pharmacy because of their varied range of therapeutic properties (Avendaño López and González Trigo, 1985; Meusel and Gütschow, 2004).

Meanwhile, for 1-methylhydantoin molecule (Figure 1) have been found to have excellent anti-asthmatic and antitussive effects (Hahn *et al.*, 2014) and antidepressant properties (You *et al.*, 2013). This hydantoin is produced by bacterial creatinine deaminase in the intestinal tract of uremic patients (Yang *et al.*, 2007) and was found as a metabolite of the intelligence affecting substance dupracetam, a nootropic drug from the racetam family (Baune and Renger, 2014).

1-methylhydantoin is the active ingredient in the natural product *Ranae Oviductus*, which is obtained from the Northeast forest frog, a wild animal found in the mountainous area of northeast China. This product is used in the traditional Chinese medicine and has been used as an antitussive, anti-inflammatory, anti-fatigue, and antilipemic drug (Wang *et al.*, 2017; Liu *et al.*, 2019; Xu *et al.*, 2019).

The crystal structure of the three polymorphs of 1-methylhydantoin was studied from single-crystal X-ray diffraction. Polymorph MH-**I** crystallizes in the monoclinic space group $P2_1/c$ (Puszynska-Tuszkanow *et al.*, 2011; Nogueira *et al.*,

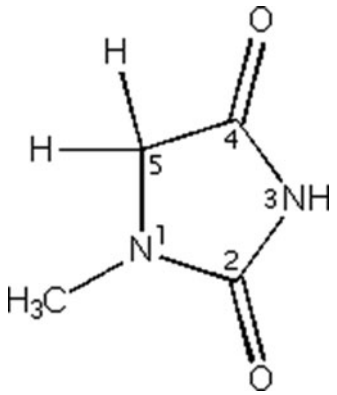

Figure 1. 1-Methylhydantoin structural molecule with ring atoms numbering.

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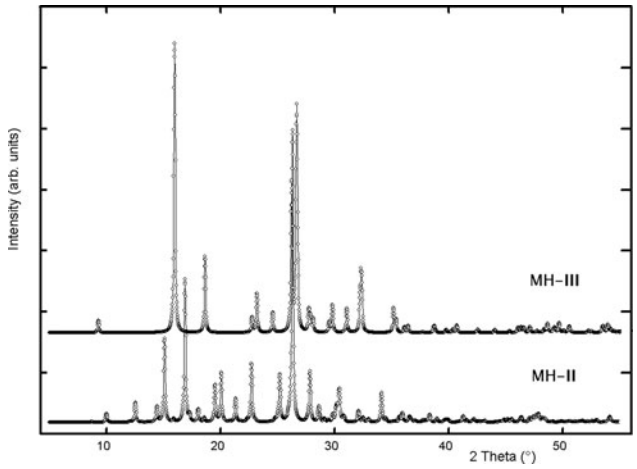

Figure 2. X-ray powder diffraction patterns of 1-methylhydantoin polymorphs MH-**II** and MH-**III**.

2014) with CSD-database refcode EWUVEY (CSD, version 5.43, March 2022), polymorph MH-**II** crystallizes in the orthorhombic space group $Pna2_1$, EWUEY01 (Nogueira *et al.*, 2017) and the polymorph MH-**III** (Nogueira *et al.*, 2020) crystallize in the orthorhombic space group $P2_12_12_1$, EWUEY02. In MH-**I**, the molecules form dimers which then associate in chains, while in MH-**II** and MH-**III**, the molecules form chains directly (Nogueira *et al.*, 2020).

Following our investigation on hydantoin and thiohydantoin derivative compounds (Seijas *et al.*, 2010; Delgado *et al.*, 2020, 2021, 2022; Hernández *et al.*, 2021) in previous work, we reported the X-ray powder diffraction data for the polymorph I of 1-methylhydantoin MH-**I** (Delgado *et al.*, 2015) in the Powder Diffraction File database with code PDF-00-066-1563 (Gates-Rector and Blanton, 2019) and report now the X-ray powder data for the two new polymorphs MH-**II** and MH-**III**.

II. EXPERIMENTAL

1-methylhydantoin 99% was a commercial material, purchased from Aldrich. Polymorphs II and III were synthesized using previous procedures. MH-**II** was obtained by recrystallization from methanol (Nogueira *et al.*, 2017), and MH-**III** was obtained by recrystallization from an aqueous solution of $MgCl_2$ (Nogueira *et al.*, 2020). MH-**II** crystals are colorless plates (m.p. 160–161 °C), and MH-**III** crystals are colorless thinner plates almost needles (m.p. 166–168 °C), both stable in air.

A. X-ray powder diffraction data

For the X-ray Powder Diffraction analyses, a small quantify of each of the two samples was ground mechanically using an agate mortar and pestle. The resulting fine powders were sieved to pass 46 (micron) and mounted on flat zero-background holders coated with a thin layer of petroleum jelly. The X-ray powder diffraction data were collected at room temperature 293(1) K, in θ/θ reflection mode using a Bruker D8 Advance diffractometer and monocromatized Cu$K\alpha$ radiation (λ = 1.54056 Å) with Bragg-Brentano geometry with fixed slits using an LYNX-eye position sensitive detector (PSD). The specimen was scanned from 5° to 55° 2θ, with a step size of 0.02° and a counting time of 5 s per step. Silicon (SRM 640) was used as an external standard to establish 2-theta-zero. The analytical software package WinPLOTR (Roisnel and Rodríguez-Carvajal, 2001) was used to establish the positions of the peaks, background reduction, and to determine the peak intensities of the diffraction peaks.

III. RESULTS AND DISCUSSION

The X-ray powder patterns of 1-methylhydantoin polymorphs are shown in Figure 2. The first peak positions, in each case, were indexed using the program DICVOL06 (Boultif and Louër, 2004), which gave a unique solution in orthorhombic cells with unit cell similar to those reported by single-crystal data (see Table I) for MH-**II** (Nogueira *et al.*, 2017) and MH-**III** (Nogueira *et al.*, 2020), and figures of merit M_{20} = 35.2 (de Wolff, 1968), F_{20} (36.8 (0.0077, 71) (Smith and Snyder, 1979), and M_{17} = 31.4, F_{17} (40.8 (0.0059, 71), respectively.

To confirm the unit cell parameters, Rietveld (Rietveld, 1969) refinements were carried out using the FULLPROF program (Rodríguez-Carvajal, 2021). The starting structure model used was that of the single-crystal structures reported for the polymorph MH-**II** (Nogueira *et al.*, 2017) and polymorph MH-**III** (Nogueira *et al.*, 2020). In each case, the peak profiles were described using a parametrized pseudo-Voight function (Thompson *et al.*, 1987), the background was described by the automatic interpolation of 20 points throughout the whole patterns, and the thermal motion of the atoms was described by one overall isotropic temperature factor B. The figures of merit of refinements were R_{exp} = 4.4, R_{wp} = 6.2 for MH-**II** and R_{exp} = 4.2, R_{wp} = 5.8 for MH-**III**. Figure 3 shows the very good fit between the observed and calculated patterns. These refinement results confirmed that the polymorphs MH-**II** and MH-**III** crystallize in the

TABLE I. Crystal data for the polymorphs **II** and **III** of 1-methylhydantoin

	MH-II	MH-II	MH-III	MH-III
Space group	$Pna2_1$ (No. 33)	$Pna2_1$ (No. 33)	$P2_12_12_1$ (No. 19)	$P2_12_12_1$ (No. 19)
Z (Z')	4(1)	4(1)	12(3)	12(3)
T (K)	293(2)	295(2)	293(2)	295(2)
Unit cell parameters (Å, °)	a = 19.0258(4)	a = 19.0323(7)	a = 7.8466(2)	a = 7.82427(5)
	b = 3.9121(1)	b = 3.91269(8)	b = 9.8257(3)	b = 9.8230(5)
	c = 6.8288(1)	c = 6.8311(3)	c = 20.3107(7)	c = 20.2951(4)
Vol (Å^3)	508.27(2)	508.70(3)	1565.92(8)	1563.5(1)
	Single crystal		Single crystal	
Reference	Nogueira *et al.* (2017)	This work	Nogueira *et al.* (2020)	This work

Z' = molecules in asymmetric unit.

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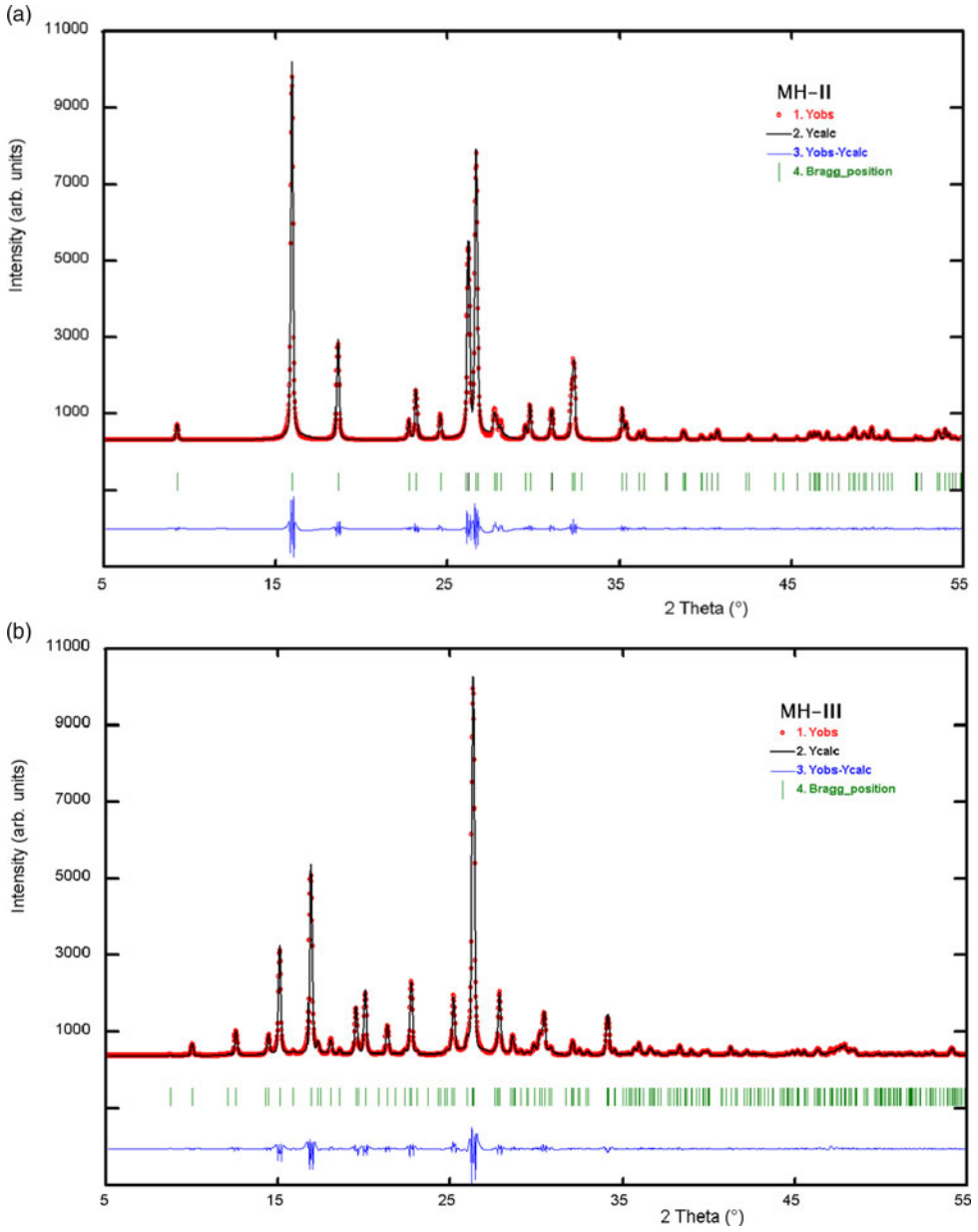

Figure 3. Rietveld refinement plots of 1-methylhydantoin polymorphs (a) MH-**II** and (b) MH-**III**.

orthorhombic space groups $Pna2_1$ and $P2_12_12_1$, respectively. All measured lines were indexed and were consistent with the mentioned space groups. The resulting X-ray powder diffraction data for both polymorphs of 1-methylhydantoin, together with the observed 2θ angles, the d-spacing's as well as the relative intensities of the reflections, are given in Tables II and III, respectively. Table I shows the crystal data for the polymorphs II and III of 1-methylhydantoin compared with those reported (Nogueira *et al.*, 2017, 2020) in the CSD database.

TABLE II. X-ray powder diffraction data of 1-methylhydantoin polymorph 2 (MH-**II**)

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	H	K	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$
9.290	9.5154	42.0	2	0	0	9.286	9.5114	−0.004
15.960	5.5489	1000.0	2	0	1	15.958	5.5483	−0.002
18.630	4.7577	267.0	4	0	0	18.634	4.7587	0.004
22.760	3.9040	53.2	4	0	1	22.758	3.9037	−0.002
23.200	3.8323	135.2	1	1	0	23.190	3.8306	−0.010
24.580	3.6185	62.0	2	1	0	24.581	3.6186	0.001
26.230	3.3950	7.6	0	1	1	26.227	3.3946	−0.003
26.650	3.3422	508.0	1	1	1	26.649	3.3420	−0.001
26.750	3.3300	674.4	3	1	0	26.748	3.3298	−0.002

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TABLE II. Continued

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	H	K	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$
27.730	3.2145	220.4	2	0	2	27.728	3.2143	−0.002
27.880	3.1975	53.8	2	1	1	27.878	3.1973	−0.002
28.108	3.1718	38.8	6	0	0	28.109	3.1719	0.001
29.530	3.0219	25.2	4	1	0	29.534	3.0223	0.004
29.820	2.9933	43.4	3	1	1	29.823	2.9936	0.003
31.060	2.8768	92.1	6	0	1	31.061	2.8768	0.001
32.240	2.7745	41.8	4	0	2	32.237	2.7742	−0.003
32.370	2.7635	127.5	4	1	1	32.368	2.7633	−0.002
32.800	2.7282	100.1	5	1	0	32.799	2.7281	−0.001
35.170	2.5497	83.3	1	1	2	35.167	2.5495	−0.003
35.400	2.5335	40.9	5	1	1	35.398	2.5334	−0.002
36.130	2.4837	17.9	2	1	2	36.133	2.4839	0.003
36.430	2.4638	20.0	6	1	0	36.435	2.4641	0.005
38.710	2.3241	20.6	6	0	2	38.709	2.3241	−0.001
38.820	2.3177	8.6	6	1	1	38.821	2.3178	0.001
39.800	2.2632	8.7	4	1	2	39.795	2.2629	−0.005
40.360	2.2326	9.6	7	1	0	40.364	2.2328	0.004
40.710	2.2144	23.5	2	0	3	40.711	2.2144	0.001
42.560	2.1221	10.8	7	1	1	42.565	2.1223	0.005
44.050	2.0538	10.6	4	0	3	44.053	2.0539	0.003
45.350	1.9982	5.1	6	1	2	45.347	1.9980	−0.003
46.080	1.9679	15.6	0	1	3	46.085	1.9681	0.005
46.340	1.9574	14.0	1	1	3	M 46.345	1.9576	0.005
46.580	1.9482	11.8	8	1	1	46.578	1.9481	−0.002
47.120	1.9271	16.0	2	1	3	47.118	1.9270	−0.002
47.750	1.9031	4.2	10	0	0	47.750	1.9031	0.000
48.390	1.8795	10.3	3	1	3	48.386	1.8794	−0.004
48.610	1.8715	3.1	1	2	1	48.607	1.8714	−0.003
48.670	1.8693	2.9	3	2	0	M 48.667	1.8692	−0.003
48.680	1.8687	23.3	7	1	2	M 48.684	1.8689	0.004
49.220	1.8496	10.4	6	0	3	49.219	1.8496	−0.001
49.350	1.8449	8.0	2	2	1	49.354	1.8450	0.004
49.690	1.8333	26.5	10	0	1	49.689	1.8332	−0.001
50.120	1.8185	3.6	4	1	3	50.120	1.8185	0.000
50.580	1.8030	17.7	3	2	1	50.579	1.8030	−0.001
52.260	1.7489	4.8	4	2	1	M 52.260	1.7489	0.000
52.330	1.7467	1.8	8	1	2	M 52.333	1.7468	0.003
52.550	1.7399	4.3	5	2	0	52.554	1.7400	0.004
53.500	1.7114	17.2	10	1	0	53.498	1.7113	−0.002
53.620	1.7077	12.8	0	0	4	53.623	1.7077	0.003
53.970	1.6975	25.6	0	2	2	53.971	1.6975	0.001
54.200	1.6908	12.3	1	2	2	54.202	1.6908	0.002
54.550	1.6808	3.8	2	0	4	54.550	1.6808	0.000

TABLE III. X-ray powder diffraction data of 1-methylhydantoin polymorph 3 (MH-**III**)

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	H	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$
8.700	10.1551	2.6	0	0	2	8.707	10.1467	0.007
9.990	8.8465	43.2	0	1	1	9.996	8.8412	0.006
12.090	7.3142	3.6	1	0	1	12.089	7.3145	−0.001
12.530	7.0583	88.4	0	1	2	12.532	7.0574	0.002
14.260	6.2056	3.6	1	0	2	14.262	6.2046	0.002
14.440	6.1287	70.0	1	1	0	14.441	6.1282	0.001
15.090	5.8661	388.4	1	1	1	15.089	5.8666	−0.001
15.900	5.5691	6.1	0	1	3	15.894	5.5711	−0.006
16.890	5.2448	672.0	1	1	2	16.887	5.2457	−0.003
17.300	5.1214	39.3	1	0	3	17.298	5.1220	−0.002
18.050	4.9103	48.7	0	2	0	18.046	4.9112	−0.004
18.570	4.7739	14.9	0	2	1	18.572	4.7734	0.002
19.530	4.5414	166.8	1	1	3	19.529	4.5416	−0.001
19.680	4.5071	12.8	0	1	4	19.678	4.5076	−0.002
20.070	4.4204	227.7	0	2	2	20.069	4.4206	−0.001
21.330	4.1620	102.0	1	2	0	21.329	4.1623	−0.001

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TABLE III. Continued

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	H	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$
22.350	3.9743	15.3	0	2	3	22.351	3.9742	0.001
22.660	3.9207	35.0	2	0	0	22.659	3.9208	−0.001
22.730	3.9087	245.3	1	1	4	22.735	3.9079	0.005
23.080	3.8502	12.2	1	2	2	M 23.076	3.8509	−0.004
24.420	3.6419	4.3	2	1	0	24.424	3.6414	0.004
24.820	3.5841	9.4	2	1	1	24.820	3.5842	0.000
25.100	3.5448	28.9	1	2	3	25.099	3.5449	−0.001
25.220	3.5282	210.0	0	2	4	25.216	3.5287	−0.004
25.970	3.4280	43.1	2	1	2	25.975	3.4274	0.005
26.250	3.3920	213.3	2	0	3	26.249	3.3922	−0.001
26.320	3.3832	218.2	1	1	5	M 26.315	3.3838	−0.005
26.330	3.3819	1000.0	0	0	6	M 26.327	3.3822	−0.003
27.570	3.2326	5.9	0	3	1	27.572	3.2323	0.002
27.700	3.2177	9.4	1	2	4	27.698	3.2179	−0.002
27.800	3.2063	47.5	2	1	3	27.800	3.2063	0.000
27.870	3.1984	181.9	0	1	6	27.874	3.1980	0.004
28.620	3.1163	55.1	0	3	2	M 28.623	3.1159	0.003
28.720	3.1057	12.4	1	0	6	M 28.720	3.1057	0.000
29.120	3.0639	7.3	2	2	0	29.118	3.0641	−0.002
29.540	3.0213	2.4	1	3	0	29.540	3.0214	0.000
29.870	2.9887	30.8	1	3	1	29.873	2.9884	0.003
30.150	2.9616	47.7	1	1	6	M 30.154	2.9612	0.004
30.190	2.9577	12.5	2	1	4	M 30.184	2.9583	−0.006
30.300	2.9472	44.4	0	3	3	30.302	2.9471	0.002
30.450	2.9331	136.1	2	2	2	30.448	2.9333	−0.002
30.740	2.9060	12.0	1	2	5	30.742	2.9058	0.002
30.850	2.8959	12.2	1	3	2	30.852	2.8957	0.002
32.040	2.7910	7.1	2	2	3	32.039	2.7911	−0.001
32.100	2.7860	30.1	0	2	6	32.105	2.7856	0.005
32.170	2.7801	14.8	0	1	7	32.165	2.7805	−0.005
32.430	2.7584	3.6	1	3	3	32.426	2.7587	−0.004
32.520	2.7509	14.7	0	3	4	32.519	2.7510	−0.001
32.910	2.7192	3.4	1	0	7	32.910	2.7192	0.000
33.020	2.7104	8.9	2	1	5	33.020	2.7104	0.000
34.130	2.6248	106.2	1	2	6	M 34.128	2.6249	−0.002
34.160	2.6225	3.3	2	2	4	M 34.155	2.6229	−0.005
34.190	2.6203	37.3	1	1	7	M 34.186	2.6206	−0.004
34.520	2.5960	17.7	1	3	4	M 34.521	2.5959	0.001
35.690	2.5135	18.9	2	3	0	M 35.696	2.5131	0.006
35.790	2.5067	3.1	3	1	1	35.792	2.5066	0.002
35.940	2.4966	8.6	0	2	7	M 35.941	2.4965	0.001
35.980	2.4939	29.9	2	3	1	M 35.978	2.4941	−0.002
36.220	2.4779	8.1	2	1	6	36.217	2.4782	−0.003
36.560	2.4557	2.8	0	4	0	M 36.561	2.4556	0.001
36.630	2.4511	12.2	3	1	2	36.630	2.4511	0.000
36.720	2.4453	5.2	2	2	5	36.718	2.4455	−0.002
36.810	2.4396	1.3	2	3	2	M 36.813	2.4394	0.003
37.060	2.4237	6.5	1	3	5	37.062	2.4236	0.002
37.780	2.3791	8.5	1	2	7	37.784	2.3789	0.004
37.990	2.3665	7.6	3	1	3	37.992	2.3663	0.002
38.370	2.3439	7.9	1	1	8	M 38.371	2.3438	0.001
38.380	2.3433	21.2	1	4	0	M 38.379	2.3434	−0.001
38.990	2.3080	6.7	0	4	3	M 38.987	2.3082	−0.003
39.000	2.3075	11.1	3	2	0	M 39.001	2.3074	0.001
39.660	2.2706	4.5	2	2	6	M 39.656	2.2708	−0.004
39.830	2.2613	8.1	3	1	4	39.832	2.2612	0.002
39.970	2.2537	8.9	0	2	8	M 39.968	2.2538	−0.002
41.040	2.1974	1.7	3	0	5	M 41.036	2.1976	−0.004
41.570	2.1706	27.9	0	3	7	M 41.571	2.1705	0.001
42.100	2.1445	3.5	3	1	5	42.098	2.1445	−0.002
42.260	2.1367	12.2	2	3	5	M 42.261	2.1367	0.001
43.210	2.0919	4.7	1	3	7	M 43.211	2.0918	0.001
44.540	2.0325	3.2	3	3	1	44.540	2.0325	0.000
44.740	2.0239	3.3	3	1	6	44.740	2.0238	0.000
44.900	2.0170	11.6	2	3	6	44.895	2.0172	−0.005
45.160	2.0060	6.9	3	2	5	M 45.162	2.0059	0.002

Continued

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TABLE III. Continued

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	H	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$
45.180	2.0052	4.6	0	3	8	M 45.178	2.0053	−0.002
45.240	2.0026	6.1	3	3	2	45.242	2.0026	0.002
45.570	1.9889	14.5	2	4	3	45.565	1.9891	−0.005
45.610	1.9872	0.1	0	1	10	45.607	1.9874	−0.003
45.720	1.9827	0.1	1	2	9	45.723	1.9826	0.003
46.170	1.9644	0.1	1	0	10	46.166	1.9646	−0.004
46.270	1.9604	0.2	4	0	0	46.271	1.9604	0.001
46.400	1.9552	10.1	0	5	1	M 46.397	1.9553	−0.003
46.420	1.9544	10.2	2	0	9	M 46.415	1.9546	−0.005
46.430	1.9540	11.2	2	2	8	46.432	1.9540	0.002
46.500	1.9513	0.3	4	0	1	46.499	1.9513	−0.001
46.720	1.9426	0.6	1	3	8	M 46.716	1.9427	−0.004
46.760	1.9410	8.7	3	0	7	M 46.753	1.9413	−0.007
47.080	1.9286	9.5	0	5	2	47.077	1.9287	−0.003
47.140	1.9263	4.1	1	4	6	M 47.141	1.9262	0.001
47.160	1.9255	37.0	2	4	4	M 47.161	1.9254	0.001
47.180	1.9247	8.0	4	0	2	M 47.178	1.9248	−0.002
47.240	1.9224	19.2	4	1	0	47.238	1.9225	−0.002
47.380	1.9171	23.5	2	1	9	47.380	1.9170	0.000
47.470	1.9136	3.1	4	1	1	47.463	1.9139	−0.007
47.670	1.9061	3.3	3	2	6	M 47.669	1.9061	−0.001
47.680	1.9057	0.6	1	5	0	M 47.683	1.9056	0.003
47.710	1.9046	18.7	3	1	7	M 47.713	1.9045	0.003
47.860	1.8989	10.1	2	3	7	M 47.860	1.8989	0.000
47.910	1.8971	14.1	1	5	1	M 47.905	1.8973	−0.005
47.970	1.8948	10.1	3	3	4	47.968	1.8949	−0.002
48.130	1.8889	2.1	4	1	2	48.131	1.8889	0.001
48.190	1.8867	5.6	0	5	3	48.195	1.8865	0.005
48.300	1.8827	14.8	4	0	3	48.293	1.8829	−0.007
48.500	1.8754	15.7	0	2	10	M 48.496	1.8755	−0.004
48.550	1.8736	0.1	0	4	7	M 48.544	1.8738	−0.006
48.570	1.8728	0.1	1	5	2	M 48.569	1.8729	−0.001
49.010	1.8570	0.5	0	3	9	49.010	1.8570	0.000
49.160	1.8517	2.8	2	4	5	49.156	1.8519	−0.004
49.230	1.8493	0.6	4	1	3	49.230	1.8492	0.000
49.660	1.8342	1.5	1	5	3	49.661	1.8342	0.001
49.730	1.8318	0.2	0	5	4	49.727	1.8319	−0.003
49.820	1.8287	1.5	4	0	4	49.823	1.8286	0.003
49.940	1.8246	3.3	3	3	5	M 49.939	1.8247	−0.001
49.960	1.8239	0.6	1	2	10	M 49.956	1.8241	−0.004
50.000	1.8226	0.6	1	4	7	M 50.003	1.8225	0.003
50.060	1.8205	0.4	3	0	8	M 50.064	1.8204	0.004
50.190	1.8161	0.7	2	2	9	50.191	1.8161	0.001
50.270	1.8134	0.8	4	2	1	M 50.270	1.8134	0.000
50.280	1.8131	2.4	0	1	11	M 50.278	1.8132	−0.002
50.460	1.8070	1.7	1	3	9	M 50.459	1.8071	−0.001
50.510	1.8054	0.2	3	2	7	M 50.509	1.8054	−0.001
50.600	1.8024	0.1	2	0	10	50.603	1.8022	0.003
50.740	1.7977	0.6	4	1	4	50.739	1.7977	−0.001
50.800	1.7957	0.6	1	0	11	50.797	1.7958	−0.003
50.910	1.7921	0.8	4	2	2	50.911	1.7921	0.001
50.980	1.7898	0.8	3	1	8	M 50.977	1.7899	−0.003
51.120	1.7852	2.2	2	3	8	M 51.118	1.7853	−0.002
51.160	1.7839	0.4	1	5	4	M 51.161	1.7839	0.001
51.200	1.7826	0.2	3	4	1	M 51.195	1.7828	−0.005
51.510	1.7726	2.9	2	1	10	51.509	1.7726	−0.001
51.520	1.7723	0.5	2	4	6	M 51.515	1.7725	−0.005
51.650	1.7682	0.5	0	5	5	M 51.647	1.7682	−0.003
51.700	1.7666	1.3	1	1	11	M 51.701	1.7665	0.001
51.740	1.7653	1.9	4	0	5	M 51.741	1.7653	0.001
51.770	1.7643	1.6	0	4	8	M 51.770	1.7643	0.000
51.830	1.7624	1.7	3	4	2	51.828	1.7625	−0.002
51.970	1.7580	0.2	4	2	3	M 51.966	1.7581	−0.004
52.020	1.7564	3.3	2	5	0	M 52.023	1.7564	0.003
52.230	1.7499	6.3	2	5	1	M 52.232	1.7498	0.002
52.270	1.7486	2.8	3	3	6	M 52.272	1.7486	0.002

Continued

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TABLE III. Continued

$2\theta_{obs}$ (°)	d_{obs} (Å)	$(I/I_o)_{obs}$	H	k	l	$2\theta_{cal}$ (°)	d_{cal} (Å)	$\Delta 2\theta$
52.630	1.7375	0.3	4	1	5	52.633	1.7374	0.003
52.860	1.7305	2.4	2	5	2	M 52.856	1.7306	−0.004
52.870	1.7302	5.6	3	4	3	M 52.871	1.7302	0.001

IV. DEPOSITED DATA

Cif files MH-II.cif and MH-III.cif contain the raw powder diffraction data for second and third polymorphs of 1-methylhydantoin. You may request this data from the ICDD at info@icdd.com.

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