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This paper follows a group of ten publications in this Journal reporting x-ray diffraction powder data for steroids. The data here reported is for a group of amino acid derivatives.

Powder analysis by x-ray diffraction can be an important aid in determining the chemical composition of small amounts of crystalline materials. To apply this technique requires that sets of the principal interplanar spacing data be available for comparison with data measured from photographic patterns of unknown powders. Barnes and Sheppard in 1954[1] and Sullivan and O'Brien in 1968[2] have published sets of x-ray diffraction powder data for various narcotics and their substitutes. Since 1958 a series of papers reporting similar data from the Edsel B. Ford Institute Physics laboratory for over 535 steroids and derivatives have been published in this Journal (Parsons et al[3-5]). The original DeBye-Scherrer powder diffraction technique used for

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Table I

Index to Amino Acid X-ray Diffraction Data

Pattern Number	Name	Molecular Formula	Melting Point (Uncorr. OC.)
1	N ACETYL L CYSTEINE	$C_5H_9NO_3S$	99-101
2	ACETYL L GLUTAMIC ACID	$C_7H_{11}NO_5$	193-194
3	CARBAMYL L GLUTAMIC ACID	$C_6H_{10}N_2O_5$	160
4	N-N DIMETHYL GLYCINE HCl	$C_4H_{10}ClNO_2$	189-190
5	L LEUCINE METHYL ESTER HCl	$C_7H_{16}ClNO_2$	152-153
6	DL LYSINE DIHYDROCHLORIDE	$C_6H_{16}Cl_2N_2O_2$	187-189
7	DL LYSINE HCl	$C_6H_{15}ClN_2O_2$	260-263
8	2 METHYL CREATININE SULFATE	$C_5H_{11}N_3O_5S$	118

Table II

d, A	I/I1	d, A	I/I1	d, A	I/I1	d, A	I/I1	d, A	I/I1	d, A	I/I1	d, A	I/I1
1		**2** cont.		**3** cont.		**4** cont.		**6** cont.		**7** cont.		**8** cont.	
6.27	.30	3.260	.25	2.435	.16	2.442	.11	5.85	.12	2.992	.08	3.270	.04
5.70	.25	3.237	.19	2.403	.12	2.387	.07	5.53	.05	2.951	.20	3.143	.19
4.809	.25	3.151	.16	2.376	.05	2.360	.07	5.08	.30	2.909	.16	3.002	.04
4.622	.06	3.049	.02	2.336	.08	2.332	.03	4.536	.11	2.862	.10	2.972	.09
4.437	.45	2.981	.07	2.271	.20	2.307	.13	4.488	.04	2.810	.05	2.938	.05
4.218	.70	2.927	.05	2.245	.15	2.231	.03	4.326	.08	2.759	.08	2.852	.06
3.887	.55	2.819	.25	2.225	.05	2.179	.04	4.211	.16	2.705	.70	2.796	.10
3.687	.20	2.693	.20	2.180	.04	2.130	.05	4.126	.13	2.684	.20	2.387	.07
3.385	.30	2.646	.09	2.149	.06	2.056	.04	4.037	.11	2.663	.08		
3.331	1.00	2.588	.12	2.127	.03	2.008	.06	3.932	.11	2.610	.05		
3.119	.12	2.545	.02	2.091	.02	1.981	.03	3.749	.30	2.565	.17		
3.015	.08	2.372	.07	2.066	.03	1.947	.03	3.682	.14	2.539	.40		
2.955	.40	2.306	.11	2.039	.05	1.811	.03	3.599	.30	2.375	.04		
2.835	.16	2.271	.09	2.015	.12	1.798	.03	3.554	.20	2.319	.50		
2.764	.30	2.259	.12	1.987	.03	1.779	.02	3.485	1.00	2.216	.10		
2.646	.04	2.251	.12	1.949	.08	1.760	.03	3.385	.07	2.172	.15		
2.549	.15	2.125	.07	1.914	.05	1.743	.01	3.293	.10	2.101	.05		
2.504	.06	2.102	.04	1.901	.03	1.723	.04	3.217	.25	2.060	.05		
2.466	.09	2.054	.05	1.890	.04	1.696	.04	3.145	.09	2.045	.06		
2.427	.09	2.033	.05	1.877	.03	1.668	.02	3.095	.11	2.036	.05		
2.375	.30	1.991	.12	1.846	.03	1.612	.03	2.990	.25	2.000	.12		
2.334	.13	1.950	.03	1.807	.03	1.536	.03	2.921	.15	1.981	.09		
2.282	.04	1.931	.03	1.785	.03	**5**		2.884	.06	1.963	.07		
2.208	.08	1.817	.05	1.737	.03			2.839	.09	1.894	.03		
2.124	.09	1.798	.04	1.712	.05	10.77	.55	2.786	.07	1.867	.05		
2.100	.05	1.765	.05	1.680	.02	8.55	.20	2.766	.06	1.827	.05		
2.075	.10	1.721	.03	1.665	.05	7.04	.90	2.745	.08	1.792	.05		
2.052	.13	1.698	.03	1.603	.03	5.35	.06	2.711	.11	1.747	.07		
2.033	.05	1.626	.03	1.539	.03	5.19	.45	2.665	.20	1.726	.04		
1.991	.08	1.527	.02	**4**		4.780	.08	2.637	.07	1.699	.05		
1.947	.05	1.495	.04			4.643	.16	2.525	.04	1.654	.03		
1.927	.05	**3**		7.15	.30	4.527	1.00	2.484	.06	1.576	.05		
1.900	.04			7.07	.10	4.253	.80	2.460	.05	1.548	.08		
1.872	.04	8.95	.01	6.96	.10	3.886	.50	2.425	.09	1.533	.08		
1.848	.03	6.15	.08	5.45	.15	3.773	.40	2.401	.10	1.473	.06		
1.830	.05	5.74	.25	5.37	.03	3.560	.70	2.371	.04	1.419	.05		
1.804	.04	5.57	.02	5.20	.03	3.498	.90	2.314	.06	1.390	.04		
1.783	.08	4.815	.17	4.999	.25	3.455	.06	2.255	.09				
1.758	.05	4.477	1.00	4.606	.85	3.324	.09	2.209	.04	**8**			
1.727	.05	4.455	.14	3.887	.13	3.135	.60	2.024	.04				
1.687	.06	4.077	.50	3.557	.20	3.058	.06	1.983	.04	10.72	.08		
1.658	.07	4.046	.20	3.528	1.00	2.965	.06	1.926	.09	7.89	.07		
1.648	.05	3.786	.60	3.507	.35	2.925	.08	1.834	.04	6.21	.04		
1.552	.04	3.532	.50	3.459	.02	2.698	.06			6.01	.10		
1.514	.05	3.452	.04	3.406	.19	2.662	.50	**7**		5.85	.09		
1.505	.05	3.373	.20	3.344	.35	2.647	.40			5.74	.20		
2		3.196	.09	3.224	.13	2.585	.09	8.95	.12	5.63	.25		
		3.154	.09	3.156	.11	2.539	.19	6.68	.18	5.35	1.00		
9.50	.07	3.127	.35	3.071	.05	2.495	.13	6.01	.05	4.908	.20		
6.97	.20	3.114	.25	3.055	.06	2.383	.11	5.65	.03	4.753	.30		
6.49	.20	3.062	.08	3.026	.17	2.305	.17	4.762	.12	4.409	.08		
6.13	.02	2.964	.03	3.006	.45	2.257	.09	4.660	.50	4.286	.07		
5.87	.02	2.910	.15	2.981	.12	2.191	.13	4.444	.08	4.198	.04		
4.643	.14	2.857	.09	2.969	.05	2.124	.08	4.140	.55	4.020	.05		
4.370	.25	2.767	.45	2.924	.10	2.108	.11	3.942	.30	3.948	.15		
4.114	.25	2.670	.12	2.882	.03	2.030	.11	3.887	.25	3.912	.45		
4.018	.20	2.631	.02	2.827	.04	2.008	.11	3.495	1.00	3.795	.08		
3.833	.30	2.567	.25	2.780	.12	**6**		3.459	.17	3.556	.10		
3.772	1.00	2.531	.12	2.716	.07			3.419	.85	3.437	.09		
3.466	.05	2.496	.09	2.601	.05	9.40	.02	3.368	.35	3.383	.08		
3.405	.14	2.475	.07	2.538	.14	8.48	.20	3.323	.25	3.344	.25		
								3.257	.15	3.320	.55		

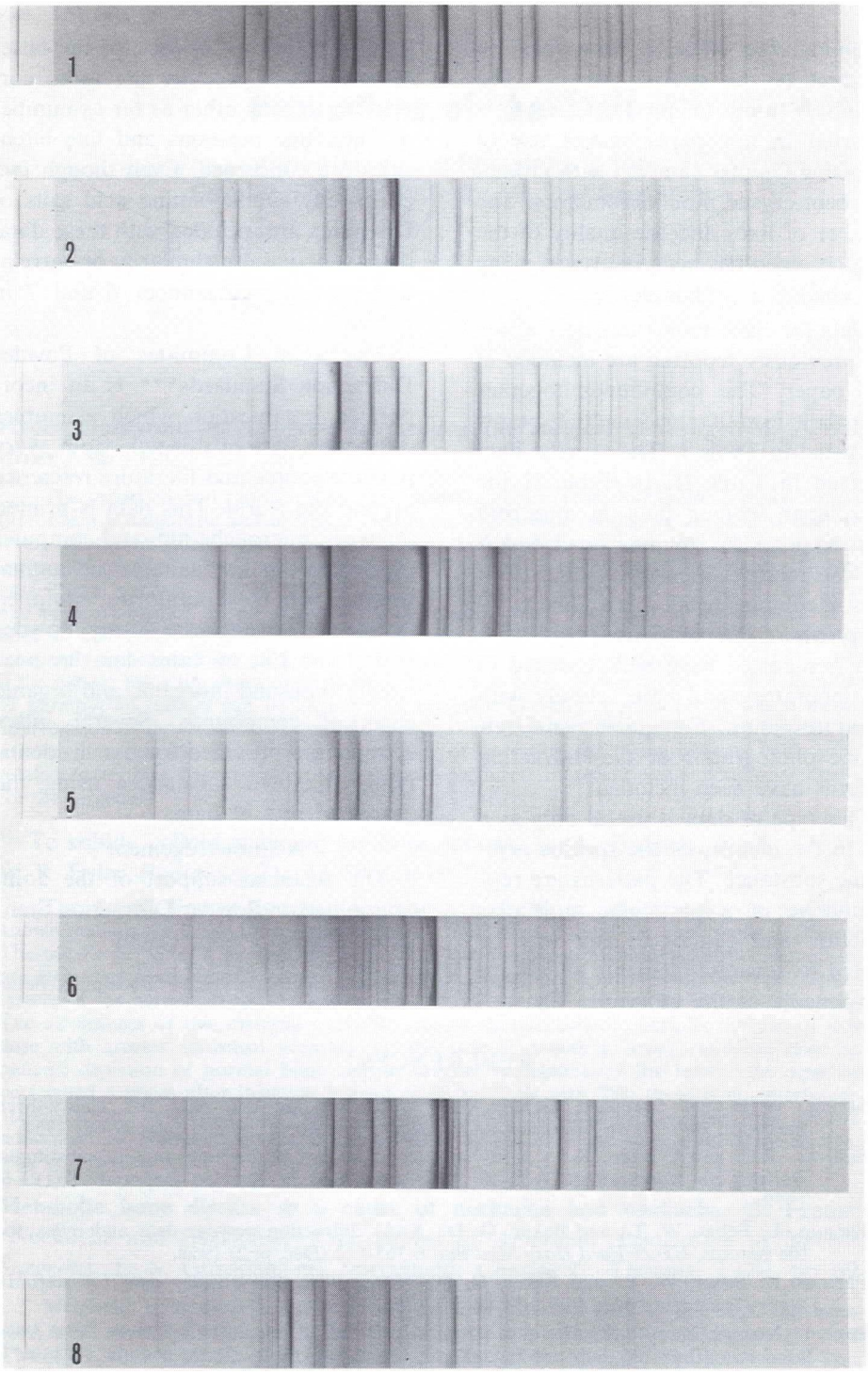

Figure 1

obtaining the data is described in the first of the steroid papers.[3] The technique used to produce the data reported in this paper makes use of focussing Guinier cameras with ground and bent crystal monochromators. The number of lines and the quality of the data obtained has been improved using this change in technique.

Data for eight amino acid derivatives not previously reported are included in this paper. The compounds together with their formulas and melting points are listed in Table I. The specific data is given in Table II. In Table II the interplanar spacing data in angstrom units appears in columns headed d,A and the relative intensity of diffraction lines in columns headed I/I_1. The melting points of the compounds for which data is reported have been checked in this laboratory and agree closely with literature values. For quick visual reference photographs of the diffraction patterns have been included.

This type of data is useful only as a key to the identity of the specific crystalline substance. The patterns are representative of a particular molecular structure and cannot in any way be related to separate elements which are components of the molecule. The degree of hydration or lack of the latter often produce patterns having no correlation to each other as far as number of lines, line positions and line intensities are concerned. Even though two chemically similar amino acid salts of DL-lysine are included with these data, there is no pattern similarity or correlation present (see number 6 and 7 in Figure 1).

The Joint Committee of Powder Diffraction Standards*** is an incorporated organization which assembles diffraction data of this type from every possible source and literature reference around the world. This data is printed on cards, microfiche film and computer tape, and made available in annual supplements to laboratories equipped to use it. To date the X-ray Powder Diffraction File contains data for over twenty thousand inorganic and organic chemical compounds. Several index systems are provided for use in identifying unknown substances using the described sets of data.

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