Electronic Supplementary Data

Growth, Structural Characterization, and Nonlinear Optical Properties of L-Lysinium hydrogen Adipate Single Crystals: An Integrated Experimental and DFT Study

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Table S1. Bond Lengths (Å)

Bond	Length (Å)		Bond		Length (Å)
	XRD	DFT		XRD	DFT
C1-C2	1.536(4)	1.557	C13-C14	1.499(4)	1.501
C1-O1	1.221(6)	1.266	C13-O11	1.195(4)	1.228
C1-O2	1.217(5)	1.264	C13-O12	1.263(5)	1.346
N1-C2	1.495(5)	1.509	C14-C15	1.498(5)	1.523
C2-C3	1.527(5)	1.54	C15-C16	1.508(4)	1.528
C3-C4	1.523(4)	1.541	C16-C17	1.510(5)	1.523
C4-C5	1.516(5)	1.544	C17-C18	1.493(4)	1.532
C5-C6	1.504(5)	1.531	C18-O19	1.203(4)	1.264
C6-N7	1.482(6)	1.471	C18-O20	1.300(5)	1.262

Table S2. Bond Angles (°)

Angle	Degrees (°)		Angle	Degrees (°)	
	XRD	DFT		XRD	DFT
C2-C1-O1	117.6(4)	113.89	C14-C13-O11	120.4(4)	125.01
C2-C1-O2	118.8(4)	116.85	C14-C13-O12	116.2(3)	113.0
O1-C1-O2	123.6(4)	129.19	O11-C13-O12	123.4(4)	121.92
C1-C2-N1	107.8(3)	112.41	C13-C14-C15	115.7(3)	111.84
C1-C2-C3	112.2(3)	110.85	C14-C15-C16	113.6(3)	110.51
N1-C2-C3	108.7(3)	107.55	C15-C16-C17	113.0(3)	111.71
C2-C3-C4	114.5(3)	114.78	C16-C17-C18	114.1(3)	114.34
C3-C4-C5	111.3(3)	113.47	C17-C18-O19	123.2(3)	113.98
C4-C5-C6	114.6(3)	113.39	C17-C18-O20	113.6(3)	116.41
C5-C6-N7	111.4(3)	110.47	O19-C18-O20	123.2(4)	129.61

Table S3. Dihedral (Torsion) Angles (º)

Dihedral	**Degrees (º)**		**Dihedral**	**Degrees (º)**	
	XRD	**DFT**		**XRD**	**DFT**
O1-C1-C2-N1	-16.1(5)	-14.68	C4-C5-C6-N7	-174.8(3)	-85.93
O1-C1-C2-C3	103.6(4)	105.72	O11-C13-C14-C15	-6.3(6)	118.29
O2-C1-C2-N1	165.4(4)	168.28	O12-C13-C14-C15	173.3(3)	-64.79
O2-C1-C2-C3	-74.9(5)	-71.31	C13-C14-C15-C16	173.6(3)	-173.94
C1-C2-C3-C4	169.5(3)	55.03	C14-C15-C16-C17	174.8(3)	-179.11
N1-C2-C3-C4	-71.4(4)	178.29	C15-C16-C17-C18	-178.0(3)	-178.6
C2-C3-C4-C5	172.4(3)	-97.12	C16-C17-C18-O19	-4.1(5)	-178.28
C3-C4-C5-C6	175.7(3)	146.35	C6-C17-C18-O20	174.4(3)	1.95