

Elastic Anisotropy of Mechanically Responsive Molecular Solids

Dherya Bahl, Beth A. Young, and Lewis L. Stevens*

Material	$\nu_{L,max}$ (GHz)	$\nu_{L,peak}$ (GHz)	A^{BLS}	A^U	A^L
Acenaphthene	22.45	19.54	1.149	0.740	0.265
Adamantane	18.87	16.78	1.125	0.880	0.316
Anthracene	25.89	18.85	1.373	5.967	1.669

*Department of Pharmaceutical Sciences and Experimental Therapeutics, College of Pharmacy,
The University of Iowa, Iowa City, IA 52242*

Material	Density (g/mL)	Refractive index
Acenaphthene	1.15	1.69
Adamantane	1.07	1.57
Anthracene	1.25	1.89
Aspirin	1.40	1.55
Benzophenone	1.11	1.61
Biphenyl	1.00	1.57
Carbamazepine	1.25	1.75
Citric acid	1.67	1.58
Diphenyl sulfone	1.20	1.59
Hippuric acid	1.37	1.57
4- methylbenzophenone	1.07	1.58
Naphthalene	1.16	1.72
Resorcinol	1.28	1.58
Succinimide	1.41	1.48
1,2,4,5- tetramethylbenzene	0.89	1.48
1,3,5- trichlorobenzene	1.46	1.57
Thiourea	1.41	1.65
Trans-stilbene	0.97	1.63
Urotropine	1.34	1.59
Maleic acid	1.59	1.51
Urea	1.32	1.40
Melamine	1.57	1.87
2-methyl-1,3- cyclohexanedione	1.31	1.46
Succinic acid	1.57	1.45

SUPPORTING INFORMATION

Table S1. Density and refractive index data for our validation set of materials.

Aspirin	17.66	16.85	1.048	0.697	0.245
Benzophenone	20.39	17.20	1.185	0.760	0.285
Biphenyl	20.52	17.20	1.193	2.540	0.822
Carbamazepine	$V_{\max}^{23.86} (C_{ij})$	$V_{\max}^{19.12} (p-BLS)$	1.246	3.233	0.981
Citric acid	24.63	20.22	1.219	2.010	0.685
Diphenyl sulfone	20.52	16.92	1.213	4.330	1.238
Hippuric acid	23.00	19.12	1.203	3.480	1.040
4-methylbenzophenone	19.97	18.16	1.100	2.470	0.786
Naphthalene	24.79	17.21	1.440	12.550	2.565
Resorcinol	21.07	19.75	1.067	1.190	0.685
Succinimide	18.83	17.89	1.053	1.430	0.536
1,2,4,5-tetramethylbenzene	22.04	17.47	1.262	4.690	1.317
1,3,5-trichlorobenzene	17.35	14.58	1.190	0.330	0.123
Thiourea	27.30	18.98	1.438	8.250	1.966
Trans-stilbene	22.72	19.40	1.171	2.430	0.775
Urotropine	20.80	21.12	0.985	0.030	0.014
Maleic acid	31.94	16.23	1.968	37.220	4.499
Urea	33.59	21.74	1.545	11.900	3.052
Melamine	38.68	26.69	1.449	3.230	1.058
2-methyl-1,3-cyclohexanedione	36.04	18.85	1.912	8.190	2.008
Succinic acid	47.96	17.89	2.681	12.830	2.704

Table S2. Our characteristic frequencies – $v_{L,\max}$ and $v_{L,\text{peak}}$ – for determining elastic anisotropy using p-BLS (A^{BLS}). The calculated EAIs from Ranganathan et al. (A^{U}) and Kube (A^{L}).

Table S3. Maximum longitudinal sound velocities calculated

Acenaphthene	3454	3534
Adamantane	2834	3201
Anthracene	3789	3644
Aspirin	3200	3031
Benzophenone	3264	3373
Biphenyl	3948	3474
Carbamazepine	3029	3622
Citric acid	4159	4163
Diphenyl sulfone	3439	3426
Hippuric acid	4174	3902
4-methylbenzophenone	3495	3371
Naphthalene	3540	3834
Resorcinol	4747	3552
Succinimide	3314	3387
1,2,4,5-tetramethylbenzene	4243	3964
1,3,5-trichlorobenzene	2751	2947
Thiourea	4299	4390
Trans-stilbene	3844	3716
Urotropine	6511	3477
Maleic acid	5883	5627
Urea	6388	6382
Melamine	5789	5496
2-methyl-1,3-cyclohexanedione	6202	6083
Succinic acid	8938	8798

Figure S1. Powder BLS spectra for all materials. Characteristic frequencies are shown by the dashed gray lines.

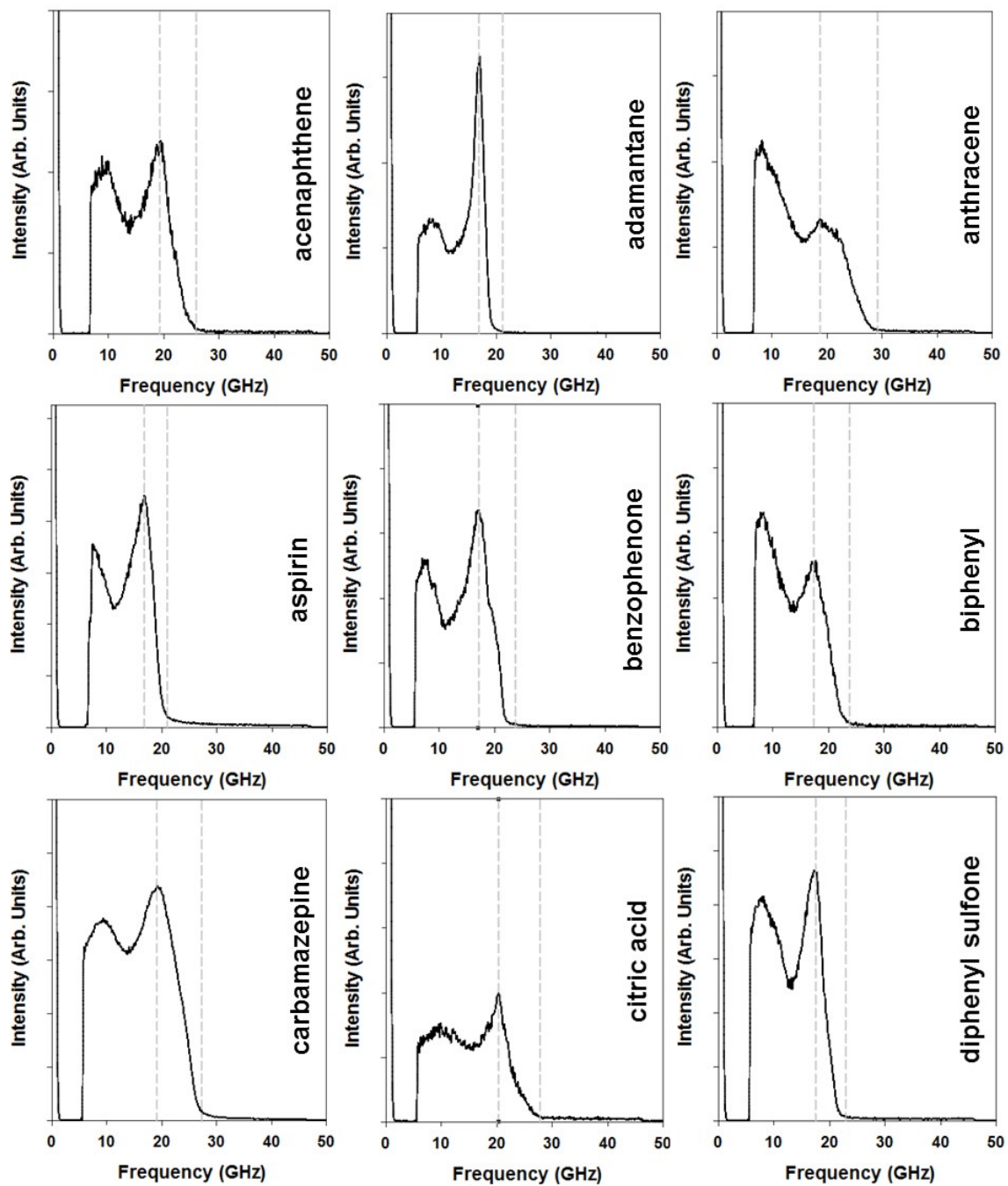


Figure S1 continued.

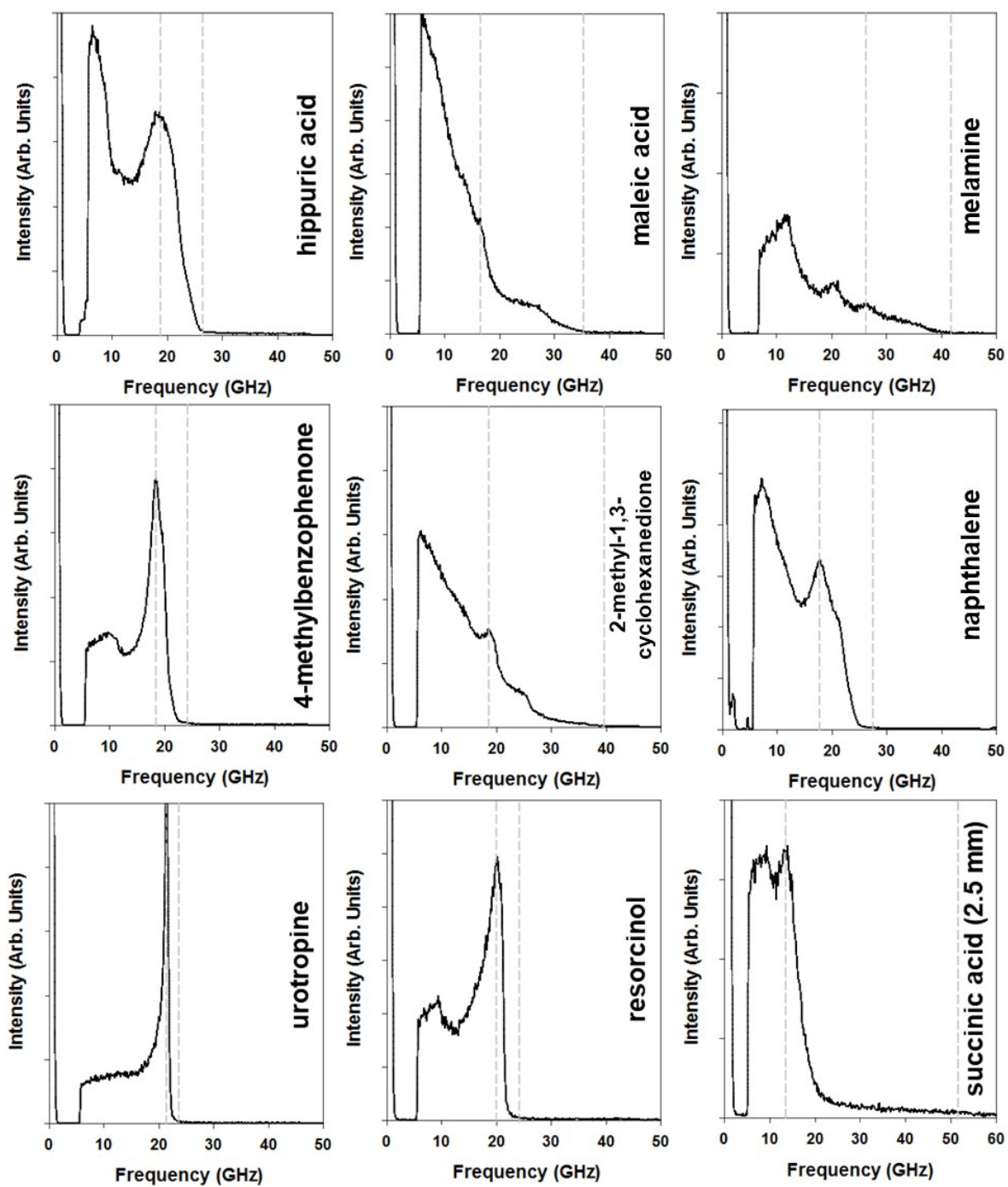


Figure S1 continued.

