Supporting Information

Modified Corrections for London Forces in Solid-State Density Functional Theory Calculations of Structure and Lattice Dynamics of Molecular Crystals

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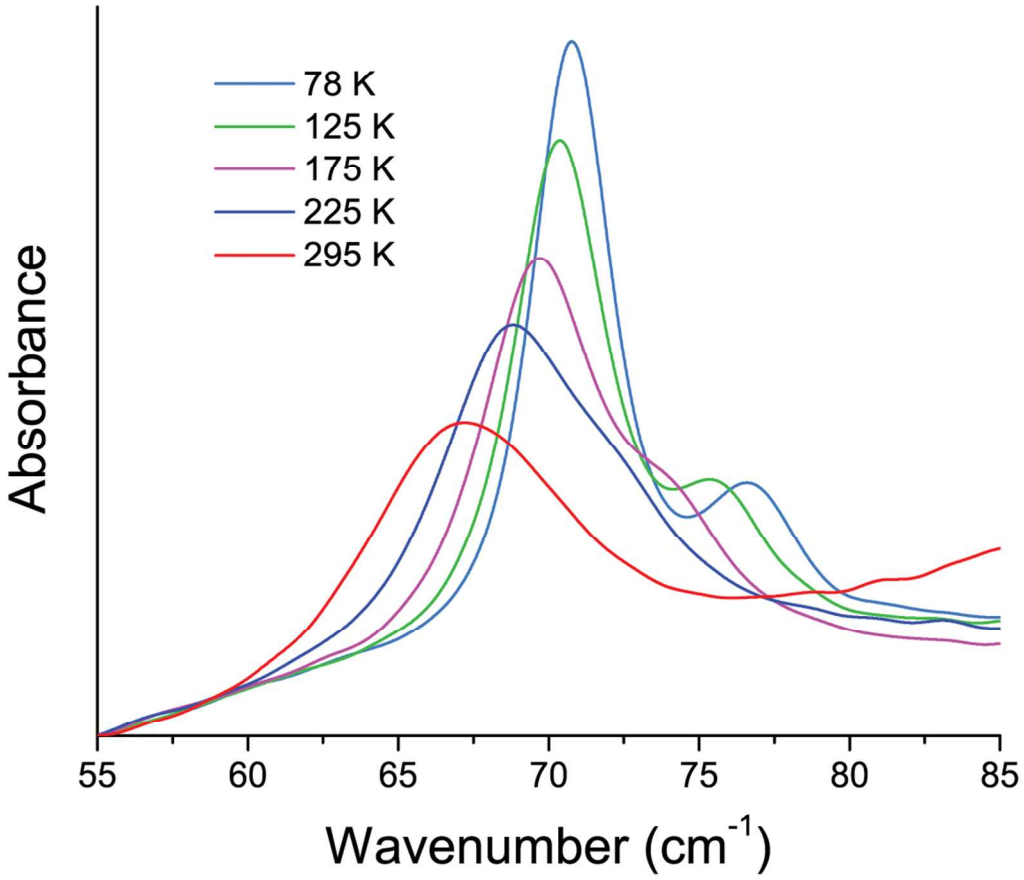

Figure S-1. Splitting of vibrational modes ν_1 and ν_2 of durene over the temperature range of 78 K to 295 K.

Table S-1. Calculated THz vibrational frequencies and IR intensities for durene using the dispersion parameter sets given in Table 1.

set 1

	mode ν_1^D		mode ν_2^D		mode ν_3^D	
s_6	freq[a]	int[b]	freq	int	freq	int
0.35	26.29	0.39	49.98	0.27	57.33	0.26
0.45	26.21	0.43	55.10	0.38	64.92	0.31
0.55	39.86	0.47	63.16	0.44	75.05	0.19
0.65	43.89	0.48	71.98	0.56	85.86	0.14
0.75	41.66	0.59	79.64	0.53	93.77	0.14
0.85	51.77	0.30	89.37	0.54	105.52	0.28

set 2

	mode ν_1^D		mode ν_2^D		mode ν_3^D	
S_6	freq	int	freq	int	freq	int
0.35	36.00	0.25	56.93	0.31	57.65	0.26
0.45	35.72	0.39	61.58	0.40	63.40	0.15
0.55	38.88	0.39	66.39	0.51	73.14	0.20
0.65	42.42	0.29	75.63	0.36	72.96	0.57
0.75	45.77	0.33	75.27	0.70	86.42	0.21
0.85	45.56	0.29	79.34	0.90	89.94	0.22

set 3

	mode ν_1^D		mode ν_2^D		mode ν_3^D	
s_6	freq	int	freq	int	freq	int
0.35	33.65	0.19	56.28	0.17	60.92	0.42
0.45	35.70	0.23	61.31	0.26	65.82	0.39
0.55	35.89	0.42	65.30	0.33	70.40	0.44
0.65	40.59	0.39	71.74	0.41	76.56	0.38
0.75	43.59	0.43	77.06	0.52	82.96	0.39
0.85	48.67	0.40	84.27	0.69	87.42	0.47

[a]Frequency (cm^{-1}); [b]Intensity (km mol^{-1})

Table S-2. Calculated THz vibrational frequencies and IR intensities for durene using the 6-31G(d,p) and 6-311G(d,p) basis sets with dispersion parameter *set 2*.

cc-pVDZ

	mode ν_1^D		mode ν_2^D		mode ν_3^D	
s_6	freq[a]	int[b]	freq	int	freq	int
0.35	36.00	0.25	56.93	0.31	57.65	0.26
0.45	35.72	0.39	61.58	0.40	63.40	0.15
0.55	38.88	0.39	66.39	0.51	73.14	0.20
0.65	42.42	0.29	75.63	0.36	72.96	0.57
0.75	45.77	0.33	75.27	0.70	86.42	0.21
0.85	45.56	0.29	79.34	0.90	89.94	0.22

6-31G(d,p)

	mode ν_1^D		mode ν_2^D		mode ν_3^D	
s_6	freq	int	freq	int	freq	int
0.35	26.75	0.38	51.26	0.54	63.56	0.54
0.45	30.20	0.39	58.91	0.67	67.40	0.33
0.55	35.92	0.36	64.74	0.65	73.69	0.18
0.65	41.25	0.48	70.26	0.94	81.67	0.24
0.75	45.12	0.39	74.99	1.13	87.53	0.34
0.85	47.64	0.59	79.79	1.30	90.90	0.23

6-311G(d,p)

	mode ν_1^D		mode ν_2^D		mode ν_3^D	
s_6	freq	int	freq	int	freq	int
0.35	22.30	0.31	46.10	0.27	55.03	0.35
0.45	26.59	0.31	54.29	0.42	61.14	0.28
0.55	33.82	0.28	62.93	0.59	67.63	0.13
0.65	38.43	0.34	67.69	0.71	78.48	0.27
0.75	42.61	0.32	73.00	0.73	85.58	0.22
0.85	44.70	0.33	77.84	0.93	89.50	0.18

[a]Frequency (cm^{-1}); [b]Intensity (km mol^{-1})

Table S-3. Naphthalene unit cell dimensions obtained for the dispersion parameters sets provided in Table 1.

Set 1

s_6	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)	d (g cm^{-3})
0.35	8.37978	5.96697	8.85961	126.0711	358.069	1.188
0.45	8.33298	5.88504	8.81984	126.2255	348.916	1.219
0.55	8.24368	5.80068	8.78596	126.4707	337.856	1.259
0.65	8.11050	5.75034	8.76265	126.6906	327.705	1.298
0.75	8.14644	5.68385	8.74450	127.4587	321.406	1.323
0.85	8.03070	5.61544	8.67998	127.0297	312.489	1.361

Set 2

s_6	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)	d (g cm^{-3})
0.35	8.47469	6.04393	8.89454	125.8999	369.041	1.152
0.45	8.32841	5.96820	8.85454	126.0942	355.639	1.196
0.55	8.31669	5.93859	8.83990	126.1222	352.666	1.206
0.65	8.24045	5.88248	8.82923	126.3428	344.740	1.234
0.75	8.14394	5.86594	8.82107	126.5401	338.569	1.256
0.85	8.18826	5.77624	8.78345	126.4612	334.117	1.273

Set 3

s_6	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)	d (g cm^{-3})
0.35	8.55527	6.00398	8.89075	125.6747	370.980	1.146
0.45	8.58898	5.95411	8.87440	125.6421	368.819	1.153
0.55	8.49318	5.90051	8.84317	125.8721	359.110	1.184
0.65	8.41003	5.85924	8.83422	126.1236	351.627	1.210
0.75	8.43548	5.82773	8.76370	125.6861	349.923	1.215
0.85	8.39165	5.79205	8.73167	125.5512	345.292	1.232

Table S-4. Naphthalene unit cell dimensions for the cc-pVDZ, 6-31G(d,p), and 6-311G(d,p) basis sets using dispersion parameter *set 2*.

cc-pVDZ

s_6	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	V (Å^3)	d (g cm^{-3})
0.35	8.47469	6.04393	8.89454	125.900	369.041	1.152
0.45	8.32841	5.96820	8.85454	126.094	355.639	1.196
0.55	8.31669	5.93859	8.83990	126.122	352.666	1.206
0.65	8.24045	5.88248	8.82923	126.343	344.740	1.234
0.75	8.14394	5.86594	8.82107	126.540	338.569	1.256
0.85	8.18826	5.77624	8.78345	126.461	334.117	1.273

6-31G(d,p)

s_6	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	V (Å^3)	d (g cm^{-3})
0.35	8.37292	5.98008	8.83713	125.769	359.022	1.185
0.45	8.31873	5.92608	8.82586	126.128	351.426	1.210
0.55	8.20609	5.90327	8.81741	126.419	343.717	1.237
0.65	8.13391	5.87704	8.80304	126.569	337.972	1.258
0.75	8.10748	5.82791	8.77321	126.604	332.778	1.278
0.85	8.08227	5.78387	8.74586	126.689	327.845	1.297

6-311G(d,p)

s_6	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	V (Å^3)	d (g cm^{-3})
0.35	8.49445	6.03640	8.87539	125.751	369.336	1.152
0.45	8.40512	5.96443	8.83451	125.913	358.700	1.186
0.55	8.35702	5.91045	8.81920	125.966	352.568	1.206
0.65	8.28339	5.86643	8.79764	126.100	345.427	1.231
0.75	8.16387	5.84480	8.79635	126.457	337.590	1.260
0.85	8.11418	5.81072	8.77315	126.482	332.593	1.279

Table S-5. Experimental temperature dependence of the naphthalene unit cell dimensions obtained from the Cambridge Structural Database (CSD) [Allen, F. *Acta Crystallogr. Sect. B* **2002**, *58*, 380-388].

Temperature (K)	CSD refcode	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	V (Å^3)
10	NAPHTA23	8.085(<1)	5.938(<1)	8.633(<1)	124.67(<1)	340.831
30	NAPHTA24	8.085(<1)	5.938(<1)	8.634(<1)	124.65(<1)	341.029
60	NAPHTA25	8.093(<1)	5.940(<1)	8.635(<1)	124.52(<1)	342.031
90	NAPHTA26	8.113(<1)	5.940(<1)	8.649(<1)	124.47(<1)	343.583
120	NAPHTA27	8.127(<1)	5.945(<1)	8.659(<1)	124.35(<1)	345.456
150	NAPHTA28	8.145(<1)	5.950(<1)	8.665(<1)	124.19(<1)	347.355
180	NAPHTA29	8.165(<1)	5.955(<1)	8.670(<1)	124.00(<1)	349.462
220	NAPHTA30	8.194(<1)	5.960(<1)	8.675(<1)	123.69(<1)	352.533

Table S-6. Durene unit cell dimensions obtained for dispersion parameters sets provided in Table 1.

Set 1

s_6	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	V (Å^3)	d (g cm^{-3})
0.35	11.88380	5.54079	6.87050	111.7306	420.243	1.060
0.45	11.73395	5.46083	6.76054	111.3432	403.486	1.104
0.55	11.55836	5.38714	6.68793	111.1718	388.326	1.147
0.65	11.49738	5.30799	6.62264	111.7908	375.287	1.187
0.75	11.45363	5.23590	6.52208	111.5104	363.888	1.224
0.85	11.41692	5.17611	6.42881	111.2145	354.167	1.258

Set 2

s_6	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	V (Å^3)	d (g cm^{-3})
0.35	12.04503	5.59591	6.96725	112.2882	434.527	1.025
0.45	11.89204	5.56299	6.91267	112.1515	423.556	1.052
0.55	11.74693	5.53640	6.86144	111.9214	413.974	1.076
0.65	11.78097	5.47480	6.75885	111.3365	406.056	1.097
0.75	11.58708	5.46763	6.75265	111.3978	398.318	1.118
0.85	11.53496	5.42516	6.70068	110.9755	391.535	1.138

Set 3

s_6	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	V (Å^3)	d (g cm^{-3})
0.35	12.13430	5.59481	6.89991	112.1337	433.909	1.026
0.45	12.03697	5.55137	6.84083	112.1009	423.528	1.052
0.55	11.92680	5.52357	6.79016	111.9912	414.779	1.074
0.65	11.83383	5.49375	6.75998	112.0186	407.426	1.093
0.75	11.78312	5.45838	6.72031	111.9119	401.004	1.111
0.85	11.88164	5.36731	6.69821	112.1902	395.524	1.126

Table S-7. Durene unit cell dimensions for the cc-pVDZ, 6-31G(d,p), and 6-311G(d,p) basis sets using dispersion parameter *set 2*.

cc-pVDZ

s_6	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)	d (g cm^{-3})
0.35	12.04503	5.59591	6.96725	112.2882	434.5271	1.025
0.45	11.89204	5.56299	6.91267	112.1515	423.5561	1.052
0.55	11.74693	5.53640	6.86144	111.9214	413.9739	1.076
0.65	11.78097	5.47480	6.75885	111.3365	406.0560	1.097
0.75	11.58708	5.46763	6.75265	111.3978	398.3175	1.118
0.85	11.53496	5.42516	6.70068	110.9755	391.5347	1.138

6-31G(d,p)

s_6	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)	d (g cm^{-3})
0.35	11.85907	5.62989	6.89118	111.8749	426.9650	1.043
0.45	11.74973	5.58562	6.84160	111.7318	417.0984	1.068
0.55	11.65698	5.54551	6.80295	111.7690	408.4082	1.091
0.65	11.58834	5.50507	6.76662	111.7229	401.0184	1.111
0.75	11.55548	5.45861	6.73041	111.7273	394.3727	1.129
0.85	11.56321	5.39398	6.69010	111.5879	388.0034	1.148

6-311G(d,p)

s_6	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)	d (g cm^{-3})
0.35	11.90454	5.63551	6.98043	111.4983	435.7227	1.022
0.45	11.78965	5.58556	6.90427	111.4308	423.2233	1.052
0.55	11.61296	5.56611	6.85239	111.3299	412.5913	1.079
0.65	11.53423	5.52546	6.80517	111.3731	403.8796	1.103
0.75	11.47899	5.48452	6.75678	111.3046	396.3147	1.124
0.85	11.45621	5.43248	6.70494	111.0601	389.4133	1.144