Electronic Supplementary Information For: Fundamentally Intertwined: Anharmonic Intermolecular Interactions Dictate Both Thermal Expansion and Terahertz Lattice Dynamics in Molecular Crystals

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1 Structure of TMA-Azo

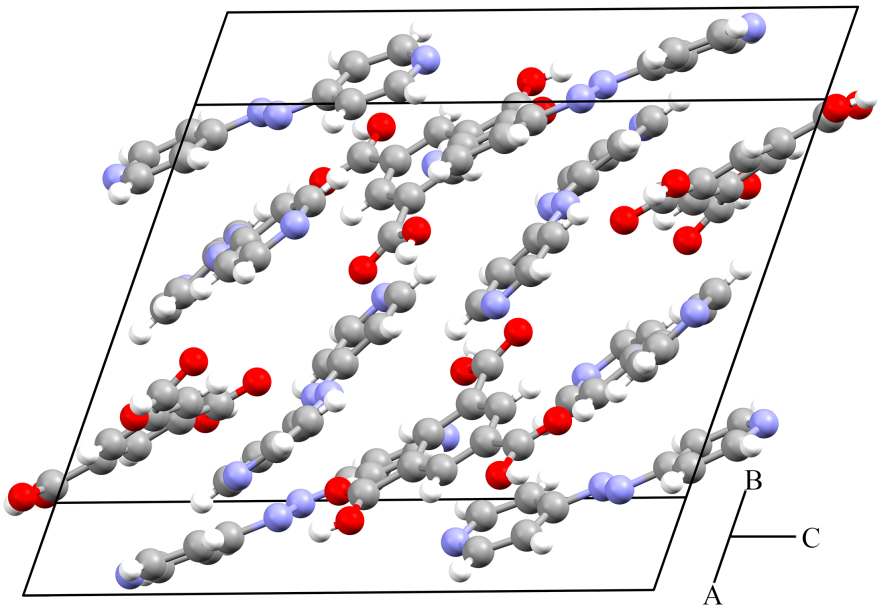

Figure 1: Structure of TMA-azo from the 100K single-crystal XRD structure.

2 Methods

2.1 Experimental

2.1.1 Synthesis of TMA-Azo

TMA-azo were obtained by dissolving a 2:3 molar equivalent of TMA (77 mg, 0.37 mmol) and azo (100 mg, 0.54 mmol) in 1mL of DMSO, as previously reported.[1] The clear orange homogeneous solution prepared was left on the benchtop overnight. Dark, orange-colored single crystals suitable for single crystal X-ray diffraction experiments were grown overnight. These crystals were dried on the filter paper overnight and were used for further spectroscopic data collection.

2.1.2 Single-Crystal X-ray Diffraction

Data collection, structure solution, and structure refinement were conducted at the X-ray Crystallographic Facility in the Department of Chemistry at the University of Rochester.

Data Collection: A crystal (0.4 mm $\times$ 0.354 mm $\times$ 0.126 mm) was placed onto a 100 μm MiTeGen cyoloop loop and mounted on a Rigaku XtaLAB Synergy-S Dualflex diffractometer equipped with a PhotonJet X-ray source operated at 50 W (50kV, 1 mA) to generate Cu Kα radiation (λ = 1.54184 Å). Crystals were transferred from the vial and placed on a glass slide in polyisobutylene. A Leica microscope with a Zeiss base was used to identify a suitable specimen for X-ray diffraction experiments from a representative sample of the material. A preliminary set of cell constants and an orientation matrix were calculated from a small sampling of reflections. A short pre-experiment was run at 100 K, from which an optimal data collection strategy was determined at this specific temperature and further used for data collection at subsequent temperatures. Data were collected with frame times of 0.07 and 0.29 seconds at a detector distance of 34.0 mm, and at temperatures of 100K, 110K, 130K, 150K, and 170K, with a transition rate of 2K/minute between the temperatures. The samples were optically centered with the aid of a video camera to ensure that no translations were observed as the crystal was rotated through all positions.

Structure solution and refinement: After data collection, the unit cell was re-determined using a subset of the full data collection. Intensity data were corrected for Lorentz, polarization, and background effects using CrysAlisPro. A numerical absorption correction was applied based over a multifaceted crystal and followed by a semi-empirical correction for absorption applied using the program SCALE3 ABSPACK. The structure was solved using SHELXT, and refined with SHELXL,[2] within the Olex2 software package.[3] All non-hydrogen atoms were refined with anisotropic displacement parameters. The azo and one of the pyridine rings in one of the crystallographically unique bipyridine molecules were modeled as positionally disordered over two sites

(A and B) at 170K. The two bipyridines showed no disorder before 170K and the crystal structure is fully ordered at temperatures 150K, 130K, 110K, and 100K. The site occupancy values for the A and B sites at 170K are located in the CIFs under the "_refine_special_details" section and are 0.94/0.06. To help model these disordered sites, SIMU and RIGU restraints were applied. Hydrogen atoms bound to carbon and oxygen atoms were located in the difference Fourier map and were geometrically constrained using the appropriate AFIX commands.

2.1.3 Terahertz Spectroscopy

All THz-TDS data were collected using a commercial Teraflash Pro spectrometer (Toptica Photonics AG). A pair of fiber-coupled photoconductive antennas served as emitter and a receiver, respectively, and two pairs of off-axis parabolic mirrors were utilized to collimate and focus the terahertz radiation. The entire was subjected to constant dry air purging to remove absorption features from atomspheric water vapor rotational transitions. Pellets were prepared for the THz-TDS experiments by mixing polytetrafluoroethylene (PTFE) with TMA-azo to a 3% w/w concentration. After mixing and grinding both in a mortar and pestle, the mixture was compressed to produce 3-mm thick sample tablets (compressed with ca. 225 MPa of pressure) in a 13-mm-diameter die (Specac). The temperature was controlled using liquid nitrogen in a vacuum-purged cryostat system. Frequency-domain terahertz power spectra were obtained by averaging 20,000 time-domain waveforms followed by performing a Fourier transformation. The presented absorption spectra were generating through division of the sample-containing spectra by that of a standard blank (PTFE reference). The peak positions were determined by fitting with Lorentzian functions.

2.1.4 Low-frequency Raman Spectroscopy

Raman data were obtained using a Coherent (Ondax) THz-Raman system, using a excitation laser centered at 785 nm (Coherent, Inc). The scattered light was analyzed using an Andor Shamrock SR-750 spectrograph with an iDus 416 CCD detector. Each Raman spectrum consisted of 300

acquisitions of 3 s exposure time windows, yielding a usable spectral range of 10 to 300 cm-1 and a spectral resolution of 0.6 cm-1. Low-frequency Raman spectra were obtained using polycrystalline powder samples of TMA-Azo. Microcrystalline samples were prepared by grinding in a mortar and pestle before experiments were performed at different temperatures between 80 K and 300 K in 10 K increments using a Lake Shore Cryotronics continuous flow liquid nitrogen cryostat.

2.2 Theory

The solid-state DFT simulations were performed using CRYSTAL23 software package,[4] with Perdew-Burke-Ernzerhof density functional[5] and 6-311G(2d,2p) basis set.[6] This computational approach was used to perform all the calculations. The experimental single-crystal XRD structure (at 100K) was used as the starting point for unconstrained geometry optimizations with an energy criterion of $\Delta E < 10^{-8}$ hartree. The low-frequency vibrational analysis was performed on the optimized structures to obtain the frequencies and normal modes. Frequencies were calculated via numerical differentiation within the harmonic approximation,[7,8] and IR and Raman intensities were determined analytically through the Coupled-Perturbed Kohn-Sham method.[9–11] The vibrational potentials were generated by extracting the mass-weighted eigenvector for the Raman active vibrational mode predicted 125.69 cm^{-1} that was described in the main text (see file "eigenvector_displacement.txt"). Subsequently, constrained volume optimizations were performed at a series of volumes (see Table 7). After complete optimization, the eigenvector from the frequency calculation was used to generate a series of structures in steps of $0.2Q$, where Q is the normalized vibrational eigenvector, which is normalized to the classical vibrational amplitude. Single-point energy calculations were performed to generate the potential energy curves shown in the main text.

3 Single-Crystal X-ray Diffraction Data

Table 1: Experimental single-crystal XRD data

Compound formula	$C_{29}H_{22}N_8O_6$	$C_{29}H_{22}N_8O_6$	$C_{29}H_{22}N_8O_6$	$C_{29}H_{22}N_8O_6$	$C_{29}H_{22}N_8O_6$
Formula weight	578.54	578.54	578.54	578.54	578.54
Temperature/K	100.00(10)	110.02(10)	130.01(10)	150.01(10)	170.00(10)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	13.9468 (2)	13.9549(2)	13.9761(10)	14.0001(10)	14.0295(10)
b (Å)	12.3892(10)	12.3882(10)	12.3862(10)	12.386(10)	12.3839(10)
c (Å)	16.6087(2)	16.6141(2)	16.6209(2)	16.6263(2)	16.6344(2)
α (degrees)	90	90	90	90	90
β (degrees)	110.401(10)	110.344(10)	110.219(10)	110.087(10)	109.943(10)
γ (degrees)	90	90	90	90	90
Volume (Å^3)	2689.80(6)	2693.02(6)	2699.95(5)	2707.72(5)	2716.75(5)
Z	4	4	4	4	4
ρ_{calc} (g/cm^3)	1.429	1.427	1.423	1.419	1.414
Absorption coefficient, μ/mm^1	0.867	0.866	0.864	0.861	0.858
F(000)	1200	1200	1200	1200	1200
Crystal size (mm)	0.4 × 0.35 × 0.13	0.4 × 0.35 × 0.13	0.4 × 0.35 × 0.13	0.4 × 0.35 × 0.13	0.4 × 0.35 × 0.13
Radiation Type	Cu K_α	Cu K_α	Cu K_α	Cu K_α	Cu K_α
Wavelength (Å)	1.54184	1.54184	1.54184	1.54184	1.54184
Reflections collected	34952	35109	35393	35564	35755
No. of independent reflections	5799	5808	5818	5836	5862
No. of reflections (I > 2σ (I))	5352	5381	5378	5402	5411
Data/restraints/parameter	5799/0/391	5808/0/391	5818/0/391	5836/0/391	5862/360/452
R_{int}	0.0526	0.0471	0.0488	0.0457	0.0460
R1 (I> 2σ (I))	0.0494	0.0490	0.0461	0.0442	0.0423
wR(F2) (I> 2σ (I))	0.1420	0.1376	0.1303	0.1247	0.1210
R1 (all data)	0.0521	0.0515	0.0488	0.0469	0.0450
wR(F2) (all data)	0.1447	0.1402	0.1328	0.1271	0.1235
Goodness-of-fit on F2	1.063	1.047	1.044	1.042	1.049
CCDC deposition number	2377598	2377599	2377600	2377601	2377602

Table 2: Experimental hydrogen bond distances from the single-crystal XRD data.

	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
100 K	O(6)-H(6)...N(8)#1	0.84	1.77	2.6064(16)	176.1
	O(1)-H(1)...N(1)	0.84	1.83	2.6660(17)	172.4
	O(3)-H(3)...N(5)	0.84	1.76	2.6007(16)	176
110 K	O(6)-H(6)...N(8)#1	0.84	1.77	2.6068(16)	173.7
	O(1)-H(1)...N(1)	0.84	1.83	2.6671(16)	174.3
	O(3)-H(3)...N(5)	0.84	1.76	2.6015(16)	175.6
130 K	O(6)-H(6)...N(8)#1	0.84	1.77	2.6082(15)	175.9
	O(1)-H(1)...N(1)	0.84	1.83	2.6688(16)	175.6
	O(3)-H(3)...N(5)	0.84	1.76	2.6021(15)	174.4
150 K	O(6)-H(6)...N(8)#1	0.84	1.77	2.6098(14)	175.5
	O(1)-H(1)...N(1)	0.84	1.83	2.6697(15)	174.6
	O(3)-H(3)...N(5)	0.84	1.76	2.6030(14)	175.9
170 K	O(6)-H(6)...N(8)#1	0.84	1.77	2.6107(14)	174.1
	O(1)-H(1)...N(1)	0.84	1.83	2.6728(14)	175.9
	O(3)-H(3)...N(5A)	0.84	1.77	2.6052(18)	175.5
	O(3)-H(3)...N(5B)	0.84	1.76	2.602(16)	176.6

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+3/2,-z+1/2

4 Peak Fitting Data

4.1 Low-Frequency Raman Data

Table 3: Center frequency of absorption features from the low-frequency Raman spectra.

Temp	Frequency (cm^{-1})									
90	87.5	97.5	105.7	122.7	136.7	154.8	186.0	198.0	215.5	225.5
100	87.5	97.2	105.7	122.6	137.0	155.0	185.0	198.0	215.1	225.5
110	87.5	96.9	105.7	122.5	135.5	155.0	185.0	198.0	215.0	225.5
120	87.1	96.6	105.7	122.2	136.0	154.0	185.0	198.0	216.1	225.3
130	87.2	96.3	105.4	121.9	135.0	154.3	185.0	198.0	215.1	225.5
140	86.6	95.9	105.3	121.4	135.0	154.0	184.8	198.0	214.8	224.9
150	86.6	95.6	105.3	120.8	135.0	154.0	184.0	198.0	214.8	224.9
160	86.6	95.0	104.7	120.4	134.5	154.0	184.0	198.0	214.8	224.9
170	86.2	94.3	104.0	120.1	135.0	154.0	184.0	198.0	214.1	224.2
180	86.1	94.1	103.0	119.7	135.0	154.0	184.0	198.0	214.1	223.5
190	85.3	93.5	103.5	119.4	135.0	154.0	184.0	198.0	213.6	223.0
200	85.2	93.3	103.5	119.0	134.5	152.6	183.2	197.8	213.3	223.0
210	85.0	93.0	103.5	118.8	134.5	152.6	183.2	197.8	213.3	223.0
220	84.5	92.7	103.0	118.7	134.2	152.7	183.2	197.8	213.3	223.0
230	84.5	92.7	103.0	118.5	134.2	152.7	183.2	197.8	212.7	223.0
240	84.4	92.6	103.0	118.3	134.0	152.9	183.2	197.8	212.7	222.4
250	84.0	92.3	103.0	118.0	134.0	152.9	183.2	197.8	212.7	222.4
260	83.7	92.0	103.0	117.8	134.0	152.9	183.2	197.8	212.7	222.4
270	83.7	92.0	102.0	117.1	134.0	155.0	183.2	197.8	212.5	222.2
280	83.6	92.0	102.0	116.6	134.0	153.1	183.2	197.8	212.3	222.0
290	83.2	91.7	102.0	116.2	134.0	154.5	183.2	197.8	212.1	221.7
300	83.2	91.7	102.0	115.3	134.0	154.3	183.2	197.8	211.8	221.3

Table 4: Full-width at half-maxima of the experimental absorption features from the low-frequency Raman spectra.

Temp	Peak Full-width at Half-maxima (cm^{-1})									
90	4.8	5.7	6.2	6.5	4.0	5.5	8.0	6.0	5.0	4.3
100	4.8	5.8	6.0	6.9	3.0	4.5	6.0	6.0	4.5	4.3
110	4.8	6.0	6.0	6.9	3.0	4.5	6.0	6.2	4.5	4.3
120	4.8	6.0	6.0	6.9	3.0	4.5	6.0	6.2	4.5	4.3
130	4.8	6.0	6.0	7.1	3.0	4.5	6.0	6.2	4.5	4.3
140	4.9	6.3	6.3	7.4	3.0	4.7	6.2	6.2	4.7	4.4
150	4.9	6.3	6.6	7.2	4.2	7.0	9.0	6.2	4.7	4.4
160	5.0	6.4	6.5	7.4	4.5	7.0	9.0	6.2	4.7	4.4
170	5.0	6.6	6.3	8.1	4.0	7.0	9.0	6.2	4.7	4.4
180	5.0	6.6	6.5	8.5	4.0	7.0	9.0	6.2	5.3	4.4
190	5.4	7.3	6.5	8.6	4.5	7.0	9.0	6.2	5.2	5.6
200	5.8	7.5	6.7	9.0	4.0	7.2	9.0	6.2	5.3	5.6
210	5.8	7.5	6.8	9.2	4.0	7.2	9.0	6.2	5.3	5.6
220	5.8	7.7	7.2	9.6	5.0	7.3	9.0	6.2	5.8	6.1
230	6.1	7.8	7.2	10.3	5.0	7.3	9.0	6.2	6.0	6.7
240	7.0	8.7	8.2	10.8	6.0	10.0	9.0	6.2	6.8	7.2
250	7.5	8.7	8.2	11.2	6.0	10.0	9.0	6.2	6.8	7.2
260	7.5	8.7	8.2	12.0	6.0	10.0	9.0	6.8	6.8	7.2
270	7.5	8.7	8.2	12.5	8.0	9.0	11.0	6.9	7.0	7.2
280	7.5	8.7	8.2	13.0	8.0	9.3	11.0	6.9	7.0	7.2
290	7.5	8.7	8.2	14.2	8.0	9.2	15.0	8.0	7.0	7.2
300	8.0	8.7	8.2	15.1	8.0	9.2	15.0	10.0	7.0	9.0

4.2 Terahertz Time-domain Spectroscopy

Table 5: Center frequency of absorption features from the terahertz time-domain spectroscopy data.

Temperature		Center Frequency (cm^{-1})											
80	36.9	41.6	47.8	58.9	63.1	69.4	75.9	87.0	100.6	105.1	117.4	124.2	129.7
150	36.5	40.8	47.6	61.4	61.4	69.8	74.1	86.0	99.6	103.0	117.1	123.0	128.0
170	36.3	40.7	47.4	61.2	61.2	73.1	73.1	85.4	98.9	102.4	117.1	122.6	128.5
190	36.2	40.3	47.7	60.3	60.3	72.8	72.8	85.2	99.4	102.6	114.9	121.7	127.5
230	35.7	39.8	47.1	60.2	60.2	72.0	72.0	83.9	100.2	–	–	120.4	127.9
250	35.5	39.3	47.5	58.3	58.3	71.4	71.4	80.9	98.2	–	–	119.6	125.8
290	35.0	–	46.5	57.4	57.4	70.2	70.2	–	94.3	–	–	117.1	-

Table 6: Full-width at half-maxima of absorption features from the terahertz time-domain spectroscopy data.

Temperature		Full-width at Half-maxima (cm^{-1})											
80	1.2	1.4	1.7	2.2	1.6	1.4	1.8	1.9	3.1	1.6	2.6	3.0	1.6
150	1.6	1.6	1.5	3.0	1.6	1.7	3.2	2.4	2.1	22.6	2.6	2.8	1.2
170	1.7	1.6	1.7	2.4	2.4	3.9	3.9	1.7	2.9	2.6	3.1	2.7	1.7
190	1.6	1.6	2.3	2.7	2.7	3.6	3.6	1.9	2.7	2.2	3.0	2.8	2.4
230	1.8	1.9	2.8	2.2	2.2	3.5	3.5	1.6	2.8	-	-	3.5	2.2
250	1.9	1.7	3.4	3.8	3.8	3.4	3.4	7.4	2.6	-	-	3.2	3.9
290	2.1	-	3.6	3.6	3.6	3.0	3.0	-	3.5	-	-	4.7	-

5 Structure Information for Constrained Volume Optimizations

Table 7: Structures obtained from the constrained volume optimizations (CIF files available online).)

Volume (Å^3)	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ (dag)
2490.8974	13.7794	12.3943	15.9747	90.0000	114.0772	90.0000
2647.1565	14.0682	12.4256	16.2783	90.0000	111.5208	90.0000
2660.6181	14.1507	12.4149	16.2629	90.0000	111.3695	90.0000
2696.4546	14.3976	12.3948	16.4330	90.0000	109.9572	90.0000

6 Calculated Transition Frequencies and Intensities

6.1 Infrared

Table 8: DFT-predicted IR-active Vibrational Mode Frequency (cm^{-1}) and intensity (km mol^{-1})

Frequency	Intensity	Frequency	Intensity	Frequency	Intensity	Frequency	Intensity
20.7012	0.11	107.7903	1.86	231.8338	3.5	396.3117	152.62
36.9104	1.82	110.5966	23.52	235.9362	23.93	399.7179	41.59
38.664	10.13	112.5395	3.09	242.7563	3.57	414.5489	10.46
40.3511	0.4	113.1805	0.04	244.9248	17.33	458.7262	38.32
43.6786	0.32	117.4987	16.73	247.1793	189.97	459.2145	10.64
45.7745	0.81	121.0914	20.17	252.0508	10.46	469.5152	0.15
46.4804	2.38	121.2092	0.04	256.2609	82.8	470.2053	1.5
51.6877	2.44	122.0916	1.92	257.7572	35.2	498.9945	0.02
54.1604	0.21	127.5554	0.06	262.6187	14.9	501.1257	1.4
60.4999	0.49	128.3452	18.4	267.355	5.73	503.3336	1.87
61.047	9.03	132.9525	0.19	300.7239	69.3	506.0122	11.67
65.3856	0.58	133.324	0.66	302.3227	82.89	507.1559	131.23
66.0095	0.84	136.9742	7.11	307.5623	136.34	510.2054	18
67.774	0.4	137.3337	3.28	308.29	3.07	516.8027	153.58
68.5222	0.67	139.6573	1.14	311.2858	158.16	520.7357	25.53
72.5498	0.11	141.797	3.95	313.5481	70.5	524.7412	252.34
74.2011	3.72	143.8898	0.03	317.2277	73.83	524.944	18.06
77.3232	4.2	144.7754	6.83	319.0041	35.97	525.2094	38.54
81.8529	1.97	146.8807	0.62	319.8044	335.6	527.5671	233.41
85.4899	9.63	151.5662	17.98	339.3886	16.46	541.7823	0.8
85.6671	0.03	153.3559	6.73	362.1084	14.71	542.8103	532.58
88.0633	0.58	159.0889	0.34	362.1481	31.3	562.0341	903.73
90.181	8.62	164.5525	36.98	376.592	13.87	568.6249	285.98
92.0902	1.36	165.3313	5.38	376.856	4.7	569.6058	0.86
94.0985	3.03	170.3459	16.99	383.5483	38.2	569.8693	441.32
97.0243	5.48	199.3464	5.09	383.944	59.35	570.7562	5.98
97.5334	3.34	203.1089	5.92	386.9001	240.91	574.8187	24.96
99.9947	4.96	207.1176	61.76	388.7708	3.92	591.9929	81.02
102.4677	5.06	214.5934	198.42	392.8496	2.51	595.2835	701.88
104.4351	0.51	220.452	2.37	393.2191	59.5	649.5134	0.97
107.7583	0.59	224.6567	115.89	393.8188	0.16	651.2143	1.18

DFT-predicted IR-active Vibrational Mode Frequency (cm^{-1}) and intensity (km mol^{-1}) (continued).

Frequency	Intensity
652.2838	3.94
653.3424	3
654.9098	0.06
656.4304	8.91
658.2701	0.86
659.5354	17.93
668.6977	1.05
668.8001	12.26
678.7632	95.43
679.6126	0.4
686.3387	57.53
691.65	5.93
698.4608	50.72
700.1137	34.39
702.8602	38.36
709.8377	5.28
720.7382	0.02
722.3442	9.18
723.9821	1.01
725.4422	0.85
735.4717	426.9
738.0467	16.2
739.031	49.31
741.2891	36.33
743.3504	6.74
746.0011	58.28
765.987	2.54
766.2071	0.43
777.8262	2.42
777.9948	9.91
778.5676	14.74

Frequency	Intensity
779.381	14.5
822.5646	12.01
822.5969	10.19
831.641	0.52
835.2322	27.22
841.899	13.76
842.9966	760.44
845.5233	76.02
847.3282	3.87
847.6821	184.51
848.2502	0.14
851.3917	625.59
852.8341	137.79
854.6904	46.1
855.2575	8.85
857.4786	14.27
858.5728	2.31
864.7961	0.14
866.0024	47.94
872.6739	77.36
875.4949	14.21
912.5308	5.24
912.7544	35.02
913.143	51.29
913.3775	2.01
931.894	3.64
932.3108	5.84
932.3946	3.49
933.4274	0.52
934.3282	39.35
934.7065	6.02

Frequency	Intensity
949.0833	16.45
949.5148	5.75
954.7656	7.1
956.3102	1.12
958.5153	4.16
958.5359	0.48
960.8241	9.55
963.5723	5.14
969.5882	3.1
969.624	4.79
973.7815	7.54
975.5431	6.04
981.5855	7.7
981.7911	8.93
986.6253	12.87
987.2467	1
990.4572	0.17
990.8497	18.01
991.5868	0.83
992.9649	5.1
993.2946	20.95
994.4777	12.19
999.4884	1.35
1000.0096	2.01
1008.3848	60.19
1008.8809	12.09
1011.6377	60.57
1012.6898	0.02
1013.4275	1.46
1019.9043	3.31
1029.9419	1109.98

Frequency	Intensity
1032.8199	2.46
1033.4902	7.4
1034.5188	1118.04
1034.826	215.92
1043.2894	293.59
1043.8667	88.89
1046.4656	21.2
1048.7021	40.94
1049.6268	27.79
1056.7342	217.98
1058.5022	57.84
1061.2318	79.16
1062.4315	10.5
1063.164	28.01
1068.5768	808.74
1068.6646	19.14
1070.4885	19.98
1078.0688	373.93
1078.4097	0.46
1154.9161	68.54
1155.2861	521.95
1159.8241	41.24
1160.4728	36.13
1164.7482	8.09
1166.1894	512.91
1172.1463	574.16
1172.7353	208.47
1184.9641	48.27
1185.1962	4.6
1186.7914	17.14
1187.7585	90.27

DFT-predicted IR-active Vibrational Mode Frequency (cm^{-1}) and intensity (km mol^{-1}) (continued).

Frequency	Intensity
1189.0467	280.67
1189.8573	2.86
1190.6702	359.98
1190.8105	643.72
1195.6488	389.79
1196.4099	398.49
1197.0961	39.83
1197.8312	35.73
1211.067	2.4
1211.0994	12.19
1247.4801	76.65
1247.7041	0.15
1248.5526	89.14
1249.9652	24.11
1271.179	866.41
1271.2085	427.99
1277.7377	1699.66
1278.6542	1.37
1282.786	51.33
1283.2837	1205.82
1288.3685	41.36
1289.192	993.95
1291.4898	1348.07
1298.6372	101.13
1306.4812	10332.18
1307.376	627.8
1338.6886	4.18
1338.7509	37.64
1342.3944	4.85
1342.6144	1.07
1344.7491	118.4
1346.6763	33.5
1347.6345	205.26
1349.4645	7.74
1369.4413	58.84
1371.7885	206.58

Frequency	Intensity
1405.0907	13.48
1405.1213	151.56
1407.9375	28.75
1408.3325	514.04
1408.7728	430.01
1409.4217	124.64
1411.7243	3.09
1411.8765	333.78
1414.6216	392.57
1417.4033	28.2
1429.2596	132.96
1429.5199	470.03
1438.3113	66.72
1439.9834	355.15
1446.0375	20.73
1446.8477	0.04
1453.5471	47.43
1454.5202	0.83
1468.7429	10.81
1469.5019	201.03
1472.2735	6.93
1476.2278	1.9
1514.7923	0.19
1515.3249	236.86
1516.0595	3.07
1517.4997	1.86
1528.6767	17.88
1528.731	16.12
1533.1054	188.61
1534.8787	24.64
1539.1651	3.6
1539.9112	39.67
1577.5564	54.67
1578.0243	60.57
1585.5089	493.44
1586.6622	193.9

Frequency	Intensity
1590.9967	70.26
1591.5695	8.3
1592.9323	9.32
1593.7673	36.11
1601.8179	418.61
1602.1644	1.41
1604.4307	4.5
1604.5906	5.16
1612.5583	3274.8
1614.4626	229.88
1614.956	46.14
1616.1583	359.69
1617.8727	567.48
1619.5396	0.09
1623.309	59.88
1624.0135	13.27
1668.4832	4761.68
1671.9861	292.65
1685.2745	179.47
1685.6062	3798.37
1694.4436	909.38
1696.9875	356.54
1941.6069	50037.88
1954.7125	5638.73
1977.7559	22854.79
1991.0166	2188.73
2187.127	32537.32
2209.4022	5.2
3089.005	260.09
3089.0352	13.12
3095.1015	1.76
3095.2081	3.71
3100.8793	238.98
3101.1334	0.44
3114.6376	0.93
3114.8975	3.48

Frequency	Intensity
3129.8247	29.19
3129.8542	160.73
3130.1413	63.61
3130.3126	10.64
3139.0045	60.09
3139.0383	1.76
3148.5944	4.49
3148.638	0.11
3150.5555	175.4
3150.6253	14.65
3153.89	10.53
3153.9301	19.84
3159.7365	4.77
3159.7762	9.71
3163.4333	31.6
3163.5004	5.04
3166.9423	2.01
3167.0653	1.33
3170.1584	45.38
3170.2093	3.37
3173.2683	40.06
3173.2729	0.97
3179.4382	4.7
3179.5854	5.81
3181.8228	10.1
3181.9294	14.31
3185.7401	72.66
3185.8379	17.49
3189.6281	26.13
3189.7337	3.31

6.2 Raman

Table 9: DFT-Predicted Raman Active Vibrational Frequency (cm^{-1}) and response.

	Polycrystalline Response			Single-Crystalline Response					
Frequency	Total	$I_{\parallel}$	$I_{\perp}$	xx	xy	xz	yy	yz	zz
20.63	24.36	13.92	10.44	0	10.93	0	0	9.45	0
20.72	19.48	11.21	8.27	0.45	0	0.47	21.23	0	9.89
24.91	8.04	5	3.04	1.59	0	4.49	1.79	0	0.61
33.86	26.09	15.14	10.95	18.51	0	2.48	2.1	0	17.83
37.67	1.31	0.75	0.56	0	0.07	0	0	1.02	0
40.28	43.99	25.47	18.53	23.33	0	0.35	0.28	0	48.94
40.80	13.59	7.76	5.82	0	11.18	0	0	0.19	0
41.30	21.78	12.66	9.12	14.41	0	2.07	16.52	0	1.12
42.67	2.7	1.54	1.16	0	1.47	0	0	0.79	0
46.64	31.13	17.79	13.34	0	9.36	0	0	16.69	0
47.72	16.75	11.38	5.37	2.41	0	0.5	0.51	0	22.01
51.06	3.56	2.11	1.44	1.45	0	1.59	0.92	0	0.32
53.01	16.05	9.17	6.88	0	13.3	0	0	0.13	0
55.75	5.57	3.18	2.39	0	4.63	0	0	0.03	0
61.31	23.98	13.71	10.27	21.52	0	3.34	1.17	0	10.75
61.40	5.02	2.87	2.15	0	1.41	0	0	2.79	0
62.57	17.19	10.26	6.94	0.94	0	5.35	15.46	0	1.16
63.27	28.28	16.16	12.12	0	2.51	0	0	21.16	0
65.07	14.98	8.57	6.41	2.72	0	1.36	14.15	0	5.49
68.23	0.19	0.11	0.08	0	0.05	0	0	0.12	0
74.08	2.72	1.55	1.17	0	0.81	0	0	1.46	0
74.44	13.75	8.47	5.28	4.39	0	3.02	6.28	0	5.58
75.84	1.17	0.91	0.26	1.48	0	0.02	0.03	0	0.14
76.70	3.98	2.27	1.7	0	0.34	0	0	2.99	0
79.36	6.93	5.99	0.94	5.75	0	0.67	2.07	0	0.06
83.53	2.87	1.64	1.23	0	0.82	0	0	1.58	0
86.62	3.45	2.06	1.39	0.02	0	0.14	1.12	0	4.25
88.25	7.85	4.59	3.26	5.3	0	1.18	0.65	0	4.7
88.70	12.94	7.39	5.55	0	4.98	0	0	5.85	0
90.45	41.82	23.89	17.92	0	28.21	0	0	6.78	0

	Polycrystalline Response			Single-Crystalline Response					
Frequency	Total	$I_{\parallel}$	$I_{\perp}$	xx	xy	xz	yy	yz	zz
91.97	4.62	2.86	1.76	5.1	0	0.98	0.21	0	0.21
92.85	6.72	3.84	2.88	0	0.69	0	0	4.94	0
93.65	56.69	32.39	24.3	0	15.51	0	0	31.93	0
94.39	9.78	5.61	4.18	0.54	0	0.65	6.23	0	8.28
95.28	9.72	5.55	4.17	0	1.36	0	0	6.77	0
98.25	8.9	5.09	3.81	2.26	0	5.46	1.52	0	0.18
100.19	7.05	4.03	3.02	0	3.2	0	0	2.7	0
101.23	14.35	8.6	5.75	0.67	0	3.1	1.57	0	15.1
102.31	7.98	4.9	3.09	2.6	0	4.94	0.26	0	0.22
104.20	9.91	5.66	4.25	0	1.48	0	0	6.82	0
109.18	3.58	2.05	1.54	0	1.8	0	0	1.2	0
109.93	11.69	6.72	4.97	14.34	0	0	2.94	0	2.23
111.07	24.1	15.1	9	12.25	0	1.48	15.11	0	8.47
111.37	6.69	3.82	2.87	0	3.01	0	0	2.59	0
114.25	3.94	2.25	1.69	0	0.02	0	0	3.28	0
115.49	72.41	41.38	31.03	0	34.21	0	0	26.38	0
119.14	13.64	8.08	5.56	13.03	0	2.68	0	0	4.1
120.81	3.73	2.13	1.6	0	0.01	0	0	3.11	0
122.89	45.52	26.14	19.38	41.22	0	3.93	0.05	0	26.9
123.69	8.71	5.41	3.31	0.15	0	5.57	2.75	0	0.03
125.70	86.14	49.22	36.92	0	28.88	0	0	43.2	0
125.93	44.32	25.32	18.99	0	4.31	0	0	32.78	0
127.02	32.89	19.02	13.87	26.87	0	2.72	0.72	0	21.74
131.99	129.21	73.83	55.37	0	15.38	0	0	92.74	0
132.21	28.99	17.27	11.73	21.43	0	0.51	5.09	0	20.16
137.20	11.36	7.46	3.91	0.87	0	7.43	1.91	0	0.24
142.71	18.6	13.09	5.52	4.58	0	0.35	6.8	0	16.17
147.14	19.82	11.32	8.49	0	10.38	0	0	6.2	0
150.51	8.97	5.13	3.85	0	4.25	0	0	3.25	0
151.55	7.17	4.98	2.19	0	0	1.32	0.05	0	8.26
178.78	0.28	0.16	0.12	0.04	0	0.07	0.1	0	0.18
182.63	0.2	0.11	0.09	0	0.16	0	0	0	0

	Polycrystalline Response			Single-Crystalline Response					
Frequency	Total	$I_{\parallel}$	$I_{\perp}$	xx	xy	xz	yy	yz	zz
185.71	0.12	0.07	0.05	0	0.1	0	0	0	0
194.31	2.45	1.4	1.04	1.95	0	0	2.07	0	0.06
200.38	2.99	1.71	1.28	0	0.39	0	0	2.12	0
202.55	5.07	2.97	2.11	1.27	0	2.52	1.86	0	0.25
209.26	13.45	8.45	5	7.04	0	0.1	6.79	0	7.58
214.63	2.88	1.65	1.24	0	1.55	0	0	0.86	0
218.81	8.29	4.74	3.55	0	2.86	0	0	4.08	0
219.82	6.57	3.92	2.65	7.59	0	0.31	2.59	0	0
225.61	3.18	2.04	1.14	0.25	0	0.08	0.08	0	4.57
226.41	0.95	0.54	0.41	0	0.35	0	0	0.45	0
227.66	2.14	1.51	0.63	0.44	0	0.44	1.72	0	0.19
232.95	3.46	1.98	1.48	0	1.34	0	0	1.55	0
235.88	4.21	3.12	1.09	0.06	0	0.7	0.33	0	4.4
236.95	0.33	0.19	0.14	0	0.13	0	0	0.15	0
270.24	0.75	0.43	0.32	0	0.18	0	0	0.45	0
273.17	1.47	1	0.47	1.11	0	0.38	0.15	0	0.24
276.10	3.68	3.15	0.53	0.65	0	0.01	4.25	0	0
276.26	0.44	0.25	0.19	0	0.02	0	0	0.35	0
279.96	1.35	0.77	0.58	1	0	0.15	0.96	0	0
282.02	0.31	0.18	0.13	0	0.15	0	0	0.12	0
284.01	2.55	1.73	0.82	0.4	0	0.21	2.97	0	0.16
286.09	0.97	0.56	0.42	0	0.48	0	0	0.34	0
287.91	0.19	0.16	0.03	0.02	0	0.01	0	0	0.22
305.17	1.22	0.7	0.52	0	1	0	0	0.01	0
325.51	10.59	9.3	1.29	4.7	0	2.04	0.84	0	4.3
325.88	0.6	0.34	0.26	0	0.25	0	0	0.25	0
338.68	5.29	4.76	0.53	4.06	0	0.13	2.46	0	0.04
341.10	0.47	0.27	0.2	0	0.15	0	0	0.25	0
343.32	2.82	2.79	0.03	1.36	0	0.04	1.03	0	0.87
345.78	3.9	3.75	0.15	1.89	0	0.26	1.32	0	1.02
347.01	1.14	0.65	0.49	0	0.39	0	0	0.56	0
349.05	1.09	0.62	0.47	0	0.32	0	0	0.6	0
353.94	1.91	1.13	0.78	1.74	0	0.55	0.08	0	0.22
354.31	0.31	0.17	0.13	0	0.01	0	0	0.24	0
355.54	1.16	0.66	0.5	0	0.55	0	0	0.43	0
357.21	0.15	0.08	0.06	0	0.08	0	0	0.05	0
359.99	0.42	0.26	0.17	0.13	0	0.01	0.26	0	0.28
371.85	5.55	4.08	1.47	0.28	0	0.37	6.81	0	0.41

	Polycrystalline Response			Single-Crystalline Response					
Frequency	Total	$I_{\parallel}$	$I_{\perp}$	xx	xy	xz	yy	yz	zz
411.98	0.32	0.19	0.13	0.15	0	0	0.15	0	0.22
412.06	0.31	0.18	0.13	0	0.22	0	0	0.05	0
422.95	0.1	0.06	0.04	0	0.01	0	0	0.07	0
423.12	0.76	0.68	0.08	0.28	0	0.04	0.62	0	0.01
448.77	1.92	1.1	0.82	0	0.34	0	0	1.27	0
450.67	1.99	1.27	0.72	0.48	0	0	0.01	0	2.69
451.44	2.96	1.72	1.25	2.98	0	0	0.01	0	1.94
454.37	0.16	0.09	0.07	0	0.13	0	0	0	0
454.66	0.77	0.66	0.11	0.61	0	0	0.01	0	0.41
458.85	0.61	0.35	0.26	0	0.04	0	0	0.47	0
464.12	0.3	0.17	0.13	0	0	0	0	0.25	0
467.99	2.25	1.96	0.3	1.5	0	0.35	0.71	0	0.07
471.49	0.22	0.2	0.02	0.23	0	0	0.04	0	0.01
471.90	0.1	0.06	0.04	0	0.05	0	0	0.04	0
472.56	0.1	0.08	0.02	0	0	0.01	0.07	0	0.04
474.97	0.51	0.29	0.22	0	0	0	0	0.43	0
487.64	2.35	2	0.35	0.6	0	0.54	0.14	0	1.35
488.37	0.11	0.06	0.05	0	0.09	0	0	0	0
506.00	0.2	0.14	0.07	0.04	0	0.03	0.19	0	0.02
511.88	0.07	0.04	0.03	0	0.01	0	0	0.05	0
512.91	0.72	0.41	0.31	0	0	0.44	0.23	0	0.09
514.08	0.02	0.01	0.01	0	0	0	0	0.02	0
515.93	2.43	1.88	0.55	0	0	0	3.45	0	0.03
517.31	1.07	0.61	0.46	0	0.63	0	0	0.26	0
532.72	0.06	0.03	0.03	0	0.02	0	0	0.03	0
535.21	1.51	1.43	0.08	0.2	0	0.05	1.13	0	0.42
585.87	0.24	0.14	0.1	0	0.1	0	0	0.1	0
586.99	24.66	15.44	9.22	4.2	0	1.76	31.89	0	0.07
587.37	3.04	2.25	0.79	1.28	0	0.86	0.08	0	1.42
587.88	20.34	11.62	8.72	0	8.08	0	0	8.94	0
588.67	8.22	5.02	3.2	2.4	0	0.41	10.15	0	0
590.38	0.12	0.07	0.05	0	0.08	0	0	0.02	0
592.64	3.77	2.16	1.62	0	1.59	0	0	1.57	0
593.44	0.61	0.35	0.26	0.03	0	0.33	0.26	0	0.07
601.18	0.09	0.05	0.04	0	0.06	0	0	0.01	0
602.01	0.31	0.18	0.13	0.31	0	0.07	0.01	0	0.05
610.56	9.29	5.56	3.73	2.43	0	1.31	10.17	0	0.04
610.81	3.59	2.05	1.54	0	1.49	0	0	1.52	0
618.82	0.69	0.4	0.3	0	0.26	0	0	0.32	0

	Polycrystalline Response			Single-Crystalline Response					
Frequency	Total	$I_{\parallel}$	$I_{\perp}$	xx	xy	xz	yy	yz	zz
622.95	6.32	4.07	2.25	5.66	0	1.95	0.43	0	0.05
630.18	0.02	0.01	0.01	0	0.01	0	0	0	0
630.95	4.31	2.51	1.8	2.69	0	0.98	2.27	0	0.25
631.98	3.87	2.29	1.58	2.24	0	0.21	3.57	0	0.16
638.47	0.43	0.25	0.18	0	0.05	0	0	0.31	0
650.79	0.21	0.13	0.08	0	0	0	0.28	0	0.04
652.40	0.64	0.37	0.27	0	0.47	0	0	0.06	0
653.42	4.3	3.71	0.59	1.14	0	0.22	0.01	0	4.13
653.70	0.21	0.12	0.09	0	0.14	0	0	0.03	0
663.03	1.15	0.84	0.32	1.4	0	0.12	0.04	0	0.05
663.36	2.28	1.3	0.98	0	0.89	0	0	1.02	0
665.36	0.55	0.31	0.24	0	0.01	0	0	0.45	0
666.69	0.64	0.36	0.27	0.11	0	0.17	0.52	0	0.1
667.78	9.8	8.1	1.7	0.27	0	0.27	12.41	0	0.24
670.37	0.71	0.4	0.3	0	0.45	0	0	0.15	0
689.82	9.61	9.22	0.39	4.82	0	0.66	2.59	0	2.99
689.92	0.36	0.21	0.15	0	0.01	0	0	0.29	0
699.65	2	1.14	0.86	0	0.41	0	0	1.27	0
699.94	0.49	0.29	0.21	0	0	0.27	0.19	0	0.08
700.77	0.2	0.11	0.09	0	0.01	0	0	0.15	0
700.86	2.6	1.49	1.11	0.92	0	0.22	0.29	0	2.68
740.18	2.45	1.4	1.05	0	0.81	0	0	1.23	0
740.22	2.61	1.62	0.98	0	0	0.62	0.32	0	2.65
742.54	7.2	4.48	2.73	3.31	0	0.33	0.88	0	6.78
744.79	7.97	4.55	3.42	0	1.11	0	0	5.56	0
756.65	0.99	0.87	0.12	1.04	0	0.05	0.08	0	0.08
759.98	1.79	1.02	0.77	0	0.38	0	0	1.11	0
762.00	0.16	0.09	0.07	0	0.04	0	0	0.1	0
763.83	0.21	0.16	0.06	0	0	0.01	0	0	0.28
764.48	0.42	0.24	0.18	0	0.35	0	0	0	0
765.13	2.05	1.81	0.24	0.01	0	0.07	1.81	0	0.72
766.48	0.3	0.17	0.13	0	0.22	0	0	0.03	0
768.12	2.22	1.31	0.91	0.44	0	0.15	1.39	0	1.55
768.73	2.76	1.58	1.18	0	2.25	0	0	0.06	0
772.44	0.63	0.37	0.27	0.22	0	0.18	0.35	0	0.12
775.83	1.89	1.66	0.23	0.41	0	0.44	0.52	0	0.67
775.85	1.22	0.7	0.52	0	0.03	0	0	0.99	0
780.78	0.77	0.44	0.33	0	0.21	0	0	0.43	0
782.47	2.26	1.78	0.48	2.2	0	0.06	0.76	0	0.12

	Polycrystalline Response			Single-Crystalline Response					
Frequency	Total	$I_{\parallel}$	$I_{\perp}$	xx	xy	xz	yy	yz	zz
784.88	0.58	0.33	0.25	0.21	0	0.34	0.05	0	0.02
784.92	1.47	0.84	0.63	0	0.27	0	0	0.96	0
821.25	2.54	1.45	1.09	0	1.48	0	0	0.64	0
821.33	0.22	0.14	0.08	0.08	0	0	0.04	0	0.21
821.76	3.17	1.82	1.35	0.59	0	1.15	2.2	0	0.21
821.80	0.5	0.28	0.21	0	0.41	0	0	0	0
838.85	2.06	1.18	0.88	0	0.15	0	0	1.57	0
839.06	2.85	1.66	1.19	0.23	0	1.14	1.15	0	1.06
839.15	2.36	1.35	1.01	0	1.98	0	0	0	0
840.06	7.05	5.6	1.45	4.14	0	1.65	0	0	2.5
840.72	1.59	0.98	0.6	0.63	0	0.16	1.47	0	0.14
840.75	0.37	0.21	0.16	0	0.25	0	0	0.06	0
854.21	1.6	1.13	0.47	0.31	0	0.14	1.24	0	0.6
854.77	0.06	0.03	0.02	0	0.04	0	0	0	0
860.89	0.81	0.67	0.15	0.06	0	0	1.06	0	0
861.25	0.12	0.07	0.05	0	0	0	0	0.1	0
861.83	0.41	0.23	0.18	0	0.23	0	0	0.11	0
862.82	0.35	0.21	0.15	0.18	0	0.06	0.01	0	0.28
866.51	2.78	2.15	0.63	3.34	0	0.05	0.44	0	0.12
867.78	2.13	1.22	0.91	0	1.71	0	0	0.07	0
873.61	1.03	0.61	0.42	0.53	0	0	0.35	0	0.81
873.63	0.47	0.27	0.2	0	0.03	0	0	0.36	0
875.64	0.05	0.03	0.02	0	0	0	0	0.04	0
877.21	4.4	3.25	1.15	0	0	0.65	5.19	0	0.01
884.66	7.58	6.66	0.92	1.27	0	1.57	1.56	0	3.98
884.78	0.54	0.31	0.23	0	0.22	0	0	0.23	0
886.70	0.71	0.4	0.3	0	0.59	0	0	0	0
888.49	2.93	2.7	0.23	0.7	0	0.01	2.84	0	0.14
891.68	30.77	26.71	4.06	15.3	0	6.97	3.82	0	7.76
892.22	1.77	1.01	0.76	0	1.22	0	0	0.27	0
892.32	48.9	44.18	4.72	17.37	0	8.96	10.7	0	16.82
893.68	0.28	0.16	0.12	0	0.18	0	0	0.05	0
894.64	12.87	12.66	0.21	3.17	0	0.27	5.38	0	6.22
895.50	1.22	0.7	0.52	0	1.02	0	0	0	0
899.58	3.09	2.69	0.4	2.68	0	0.17	0.01	0	1.07
900.06	1.66	0.95	0.71	0	1.09	0	0	0.29	0
905.67	15.06	8.61	6.45	0	8.56	0	0	4.04	0
906.83	116.98	104.43	12.55	13.48	0	2.84	125.36	0	7.22
910.39	6.27	3.59	2.69	0	1.83	0	0	3.42	0
910.66	52.46	45.33	7.13	6.21	0	0.95	60.82	0	0.87
910.93	1.33	0.76	0.57	0	0.93	0	0	0.18	0
917.61	98.86	91.28	7.58	37.58	0	14.05	21.49	0	37.51

	Polycrystalline Response			Single-Crystalline Response					
Frequency	Total	$I_{\parallel}$	$I_{\perp}$	xx	xy	xz	yy	yz	zz
927.61	0.26	0.15	0.11	0	0.1	0	0	0.12	0
928.41	4.05	2.71	1.34	0.26	0	2.1	0	0	1.84
929.38	1.67	0.95	0.71	0	1.19	0	0	0.21	0
931.00	9.51	9.02	0.49	4.76	0	0.8	3.44	0	1.92
931.72	0.29	0.16	0.12	0	0.03	0	0	0.21	0
937.33	17.67	17.33	0.35	7.39	0	0.53	8.12	0	4.54
937.80	0.15	0.08	0.06	0	0.06	0	0	0.06	0
941.54	5.15	3.7	1.45	1.11	0	2.59	0.08	0	1.36
945.40	0.94	0.54	0.4	0	0.7	0	0	0.09	0
945.48	7.69	6.15	1.53	0.32	0	0	10.48	0	0
948.86	8.42	7.3	1.12	0.14	0	0	10.07	0	0.95
949.86	0.11	0.06	0.05	0	0.09	0	0	0	0
955.00	0.58	0.33	0.25	0	0.3	0	0	0.18	0
955.96	2.93	2.63	0.29	0.06	0	0.05	2.8	0	0.81
956.51	2.37	1.71	0.66	0.81	0	0.92	0.02	0	0.89
961.16	0.21	0.13	0.08	0.13	0	0.1	0	0	0
961.71	1.49	0.85	0.64	0	0.65	0	0	0.6	0
963.08	0.02	0.01	0.01	0	0.01	0	0	0	0
970.39	3.84	2.48	1.36	1.06	0	1.46	0.55	0	1.55
970.44	0.58	0.33	0.25	0	0.36	0	0	0.12	0
1042.18	106.96	61.12	45.84	0	67.59	0	0	21.92	0
1042.61	947.82	859.74	88.08	154.5	0	48.94	880.73	0	80.45
1043.76	74.24	42.42	31.82	0	43.07	0	0	19.05	0
1044.07	195.38	112.14	83.25	23.46	0	40.78	178.79	0	42.61
1047.21	958.75	818.4	140.35	376.03	0	244	88.42	0	335.16
1050.25	44.09	25.2	18.9	0	19.99	0	0	16.9	0
1056.31	7.76	4.43	3.33	0	3.33	0	0	3.16	0
1056.58	8.53	5.82	2.71	0.22	0	0.9	10.35	0	0.8
1066.47	8.05	6.94	1.1	1.88	0	2.14	2.52	0	2.04
1066.89	8.69	4.97	3.73	0	5.45	0	0	1.83	0
1067.99	0.18	0.1	0.08	0	0.15	0	0	0.01	0
1068.23	148.35	132.65	15.7	42.55	0	30.54	48.61	0	39.94
1069.91	236.34	189.32	47.02	4	0	0.2	326.49	0	1.06
1070.77	42.46	24.26	18.2	0	27.16	0	0	8.37	0
1071.99	116.58	66.62	49.96	0	75.77	0	0	21.79	0
1073.00	129.58	112.62	16.96	12.27	0	0.99	153.9	0	3.52
1076.94	26.97	22.43	4.54	10.08	0	8.55	4.85	0	4.88
1077.51	0.33	0.19	0.14	0	0.01	0	0	0.26	0
1088.07	10.45	5.97	4.48	0	5.47	0	0	3.27	0
1088.44	111.26	90.39	20.86	48.3	0	31.21	1.93	0	42.14
1090.59	47.25	33.22	14.02	17.74	0	16.82	1.88	0	18.53

	Polycrystalline Response			Single-Crystalline Response					
Frequency	Total	$I_{\parallel}$	$I_{\perp}$	xx	xy	xz	yy	yz	zz
1091.19	1.24	0.71	0.53	0	0.45	0	0	0.58	0
1123.04	5.27	3.01	2.26	0	0.72	0	0	3.69	0
1123.11	1.24	0.86	0.38	0.07	0	0.39	0.19	0	0.87
1124.91	0.39	0.22	0.17	0	0.03	0	0	0.29	0
1125.71	5.34	4.53	0.81	2.23	0	1.1	0.13	0	2.65
1144.12	2.66	2.28	0.38	2.11	0	0.26	0.94	0	0
1144.78	2.82	1.61	1.21	0	1.31	0	0	1.06	0
1149.64	96.14	85.17	10.97	11.72	0	0.74	108.68	0	3.59
1151.57	51.96	29.69	22.27	0	31.87	0	0	11.6	0
1155.22	33.81	30.81	3	10.04	0	2.33	26.47	0	1.95
1155.73	0.91	0.52	0.39	0	0.15	0	0	0.61	0
1160.04	0.13	0.07	0.06	0	0.11	0	0	0	0
1161.81	98.44	78.14	20.3	47.74	0	29.84	0.88	0	30.8
1162.01	5.75	5.54	0.21	2.03	0	0.35	2.79	0	1.46
1169.22	0.94	0.53	0.4	0	0.1	0	0	0.68	0
1178.30	13.21	8.13	5.08	3.72	0	3.92	4.37	0	5.49
1178.34	3.43	1.96	1.47	0	2.26	0	0	0.61	0
1204.43	2	1.53	0.47	0.92	0	0.73	0.5	0	0.01
1204.65	7.86	4.49	3.37	0	2.26	0	0	4.32	0
1208.00	39.41	22.52	16.89	0	18.22	0	0	14.76	0
1208.55	8.23	4.71	3.52	0.01	0	2.37	5.22	0	3.79
1210.88	6.56	3.75	2.81	0	1.36	0	0	4.14	0
1211.85	62.49	47.77	14.72	0.22	0	0.02	89.26	0	0.93
1213.63	42.81	34.94	7.86	0.18	0	0.68	55.94	0	1.86
1215.02	1.7	0.97	0.73	0	1.02	0	0	0.41	0
1232.32	53.24	46.73	6.51	22.78	0	12.08	11.84	0	11.21
1233.39	4.04	2.31	1.73	0	0.01	0	0	3.37	0
1263.67	0.25	0.14	0.1	0.1	0	0.03	0.06	0	0.18
1263.98	3.4	1.94	1.46	0	1.73	0	0	1.11	0
1267.28	1.14	0.65	0.49	0	0.95	0	0	0	0
1267.69	0.64	0.5	0.14	0.11	0	0	0.78	0	0.03
1267.78	16.3	9.32	6.99	0	9.3	0	0	4.35	0
1268.46	11.67	9.44	2.22	8.07	0	2.92	0.22	0	2.15
1270.37	0.79	0.45	0.34	0	0.01	0	0	0.65	0
1270.40	47.46	37.22	10.24	21.42	0	14.68	0.15	0	16.67
1273.56	50.13	40.61	9.53	30.18	0	12.27	0.31	0	14.87
1275.43	0.59	0.34	0.25	0	0.09	0	0	0.41	0
1285.64	6.35	3.63	2.72	0	2.83	0	0	2.49	0
1285.77	12.34	11.2	1.14	5.15	0	1.95	4.96	0	1.78
1294.01	134.14	107.06	27.08	1.91	0	0.05	186.28	0	0.58
1295.48	1.19	0.68	0.51	0	0.88	0	0	0.11	0

	Polycrystalline			Single-Crystalline					
Frequency	Total	I_par	I_perp	xx	xy	xz	yy	yz	zz
1301.62	182.21	104.12	78.09	0	113.39	0	0	39.08	0
1302.23	538.93	483.51	55.43	77.24	0	33.72	507.8	0	43.8
1308.17	47.54	27.16	20.37	0	20.45	0	0	19.33	0
1309.71	373.72	258.87	114.85	145.84	0	127.07	24.58	0	147.81
1322.08	3.02	1.72	1.29	0	0.97	0	0	1.55	0
1322.30	3.09	2.57	0.51	1.09	0	0.02	3.05	0	0.04
1324.91	0.2	0.11	0.08	0	0.09	0	0	0.07	0
1328.78	35.52	30.81	4.7	16.4	0	8.36	5.06	0	8.94
1364.17	1000	823	177	435.47	0	289.99	45.01	0	318.39
1364.19	5.42	3.1	2.32	0	0.1	0	0	4.43	0
1364.58	356.68	203.81	152.86	0	204.15	0	0	94.31	0
1366.12	686.36	515.68	170.68	0.19	0	1.89	1000	0	0.05
1376.03	139.28	112.33	26.95	58.15	0	43.7	4.22	0	44.98
1376.86	20.64	11.79	8.85	0	7.31	0	0	9.96	0
1380.07	15.07	13.03	2.04	1.37	0	0.62	16.89	0	0.55
1381.55	8.4	4.8	3.6	0	5.33	0	0	1.7	0
1386.13	25.7	14.69	11.02	0	15.79	0	0	5.72	0
1386.91	67.95	54.3	13.65	0.18	0	0	94.09	0	1.31
1419.77	5.03	2.88	2.16	0	1.27	0	0	2.94	0
1420.26	4.07	2.99	1.08	1.77	0	1.8	0.04	0	0.63
1427.32	1.83	1.22	0.61	0.53	0	0.4	1.15	0	0.37
1428.06	0.44	0.25	0.19	0	0.1	0	0	0.27	0
1431.05	7.87	5.7	2.17	2.02	0	3.49	0	0	2.76
1431.54	3.25	1.86	1.39	0	1.56	0	0	1.16	0
1433.85	5.59	3.19	2.4	0	2.47	0	0	2.21	0
1434.31	2.93	2.07	0.86	1.4	0	1.42	0.14	0	0.06
1441.42	0.03	0.02	0.01	0	0.03	0	0	0	0
1441.45	17.42	10.58	6.83	6.36	0	7.01	4.5	0	3.52
1444.05	1.47	0.84	0.63	0	0.01	0	0	1.23	0
1444.41	8.6	5.13	3.47	5.27	0	2.43	3.27	0	0.72
1451.23	4.23	3.77	0.46	2.84	0	0.08	2.49	0	0
1453.02	2.19	1.25	0.94	0	0.57	0	0	1.27	0
1453.83	6.89	3.93	2.95	0	4.99	0	0	0.77	0
1454.59	13.55	7.94	5.61	0.88	0	6.13	3.95	0	5.37
1456.84	108.25	75.78	32.47	48.22	0	41.6	3.11	0	30.32
1457.72	1.84	1.05	0.79	0	1.28	0	0	0.26	0
1460.20	87.13	68.94	18.19	2.41	0	0.48	120.01	0	0
1461.38	81.1	46.34	34.76	0	52.79	0	0	15.07	0
1489.45	58.72	54.42	4.3	12.97	0	1.75	52.29	0	5.05
1492.26	10.67	6.1	4.57	0	5.98	0	0	2.95	0
1515.79	16.34	14.08	2.26	0.45	0	0.7	18.25	0	1.69
1519.33	5.1	2.92	2.19	0	0.83	0	0	3.44	0
1528.60	0.01	0.01	0	0	0	0	0	0.01	0

	Polycrystalline Response			Single-Crystalline Response					
Frequency	Total	$I_{\parallel}$	$I_{\perp}$	xx	xy	xz	yy	yz	zz
1528.72	42.55	40.14	2.41	16.77	0	4.62	14.31	0	12.36
1721.50	28.55	22.12	6.42	0.23	0	0	40.72	0	0
1722.74	5.43	3.1	2.33	0	4.07	0	0	0.47	0
1779.07	43.82	35.36	8.46	0.22	0	0.01	60.04	0	0.97
1788.28	7.54	4.31	3.23	0	1.73	0	0	4.58	0
1954.26	78	65.74	12.26	39.11	0	15.41	1.06	0	34.75
1963.84	0.52	0.3	0.22	0	0.31	0	0	0.12	0
2780.07	22.5	17.06	5.44	12.5	0	7.26	0	0	5.72
2780.14	0.62	0.36	0.27	0	0.11	0	0	0.41	0
2785.63	6.1	3.49	2.61	0	2.74	0	0	2.37	0
2785.64	11.84	10.65	1.19	2.23	0	1.63	8.04	0	1.73
2790.77	6.08	5.01	1.07	2.58	0	1.85	0.41	0	1.68
2790.86	1.24	0.71	0.53	0	0.63	0	0	0.41	0
2803.17	3.7	2.11	1.58	0	1.03	0	0	2.07	0
2803.25	14.68	13.3	1.38	1.81	0	0.92	13.37	0	1.81
2816.61	0.52	0.3	0.22	0	0.24	0	0	0.19	0
2816.71	19.78	17.61	2.17	13.78	0	2.44	5.99	0	1.06
2817.49	15.57	10.32	5.25	16.7	0	2.32	2.32	0	0.73
2817.56	1.03	0.59	0.44	0	0.86	0	0	0.01	0
2825.05	9.56	8.69	0.87	2.56	0	0.72	7.58	0	0.63
2825.17	5.43	3.1	2.33	0	3.02	0	0	1.53	0
2833.70	9.25	7.84	1.41	0.49	0	0.02	11.77	0	0.2
2833.72	0.92	0.53	0.39	0	0.54	0	0	0.23	0
2835.38	0.28	0.16	0.12	0	0.06	0	0	0.18	0
2835.39	12.21	9.79	2.43	0.3	0	0.02	16.8	0	0.02
2838.44	0.59	0.34	0.25	0	0.18	0	0	0.31	0
2838.53	2.41	2.15	0.26	0.16	0	0.08	2.56	0	0.26
2844.11	8.47	7.81	0.65	4.11	0	0.88	3.98	0	0.84
2844.30	1.58	0.9	0.68	0	0.74	0	0	0.57	0
2847.19	0.03	0.02	0.01	0	0	0	0	0.03	0
2847.61	3.45	2.74	0.71	0.1	0	0.02	4.73	0	0
2850.26	11.8	9.76	2.04	0.31	0	0	15.68	0	0.21
2850.46	0.64	0.36	0.27	0	0.53	0	0	0	0
2853.07	16.05	13.17	2.88	12.99	0	3.35	0.51	0	1.98
2853.12	2.06	1.18	0.88	0	1.44	0	0	0.28	0
2855.93	13.02	10.72	2.3	7.68	0	3.32	0.37	0	3.28
2855.95	0.48	0.28	0.21	0	0.24	0	0	0.17	0
2861.59	0.13	0.07	0.06	0	0.03	0	0	0.08	0
2861.68	4.84	4.18	0.65	0.35	0	0.01	5.9	0	0.15
2863.67	2.08	1.19	0.89	0	1.72	0	0	0.02	0
2863.76	5.59	4.69	0.89	0.36	0	0	7.18	0	0.05
2867.22	6.95	6.08	0.86	4.4	0	1.27	0.71	0	1.5
2867.25	1.53	0.88	0.66	0	0.65	0	0	0.63	0
2870.74	5.86	5.4	0.46	3.29	0	0.44	2.87	0	0.35
2870.79	1.98	1.13	0.85	0	1.46	0	0	0.2	0

7 References

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