Supporting Information for:

The Structural Behavior of $Li_2B_{10}H_{10}$

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How to view phonon animations using the V_Sim software*

The **Li2B10H10_phonons.xyz** and **Li2B10D10_phonons.xyz** files contain the information needed to view the animated (gamma-point) phonon normal modes from the DFT-optimized 0 K $^{7}Li_2{}^{11}B_{10}H_{10}$ and $^{7}Li_2{}^{11}B_{10}D_{10}$ structures, respectively, following the steps below:

- Get the V_Sim software (It is free, and there is no need to install).
- Go to the following webpage and download the Win32 binaries:
  http://www-drfmc.cea.fr/L_Sim/V_Sim/download.html
- Unzip the zip file to wherever you want to put the software.

- Click "~V_Sim\bin\V_sim.exe" to start the V_Sim program, then open the **Li2B10H10_phonons.xyz** or **Li2B10D10_phonons.xyz** file to view the phonon animations.
- To build bonds in the structure, check the box on the left side of the "Pairs" button, and click the "Pairs" button.
- Highlight a pair and click the "Auto set" button to allow bonding.
- Adjust the "Link parameters," if desired.
- Adjust the element color, radius, etc. on the "Elements" tab, if desired.
- Go to the "Phonons" tab, highlight a phonon mode, and click the "Play" button to view a phonon animation.

* N.B., the use of this software does not imply its recommendation or endorsement by NIST.

Table S1. List of phonon symmetries and the corresponding phonon energies at the gamma point from the DFT-optimized $^{7}Li_2{}^{11}B_{10}H_{10}$ structure at 0 K. The number before the symmetry symbol denotes the degeneracy. (N.B.: Infrared-active modes = A2, E1 and Raman-active modes = A1, E1, E2.) Modes below 300 cm^{-1} possess translational and/or librational character.

Phonon Symm.	Energy (meV)	Energy (cm^{-1})
B1	4.4	35.81
2E1	8.9	71.43
B2	9.9	79.99
2E1	12.9	103.74
2E2	14.9	120.25
B2	15.3	123.38
2E1	15.9	128.48
A2	15.9	128.66
B1	17.2	138.42
2E2	17.9	144.75
B1	22.9	184.37
2E1	25.5	205.66
2E2	28.0	226.29
A2	28.4	229.08
2E1	28.7	231.84
A1	28.9	232.99
B2	29.7	239.85
B1	33.2	267.78
2E1	34.0	274.57
2E1	36.4	293.91
2E2	37.0	298.71
B2	37.1	299.58
2E2	57.3	462.30
A1	57.7	465.65
2E1	59.0	476.18
B1	59.1	477.01
A2	59.6	481.00
2E2	59.7	481.44
A2	66.5	536.35
2E2	66.7	538.13
B1	66.8	538.72
2E1	66.9	539.36
A2	71.2	574.57
2E2	71.8	579.58
B1	72.0	581.21
2E1	72.3	583.59
2E2	76.0	613.32
A1	76.4	616.47
2E1	76.7	619.09
B2	76.8	619.30
2E2	77.0	621.09
A1	77.3	623.45
2E2	81.3	656.05
A2	81.4	656.85
2E1	82.8	667.98
B2	83.3	671.91
2E2	84.0	677.96
A1	84.3	680.09
B1	84.5	681.35
2E1	84.8	683.83
2E1	87.2	703.11
A1	87.7	707.42
2E2	87.8	708.12
B2	88.0	710.28
B1	89.8	724.49
2E1	90.9	733.70
B2	91.1	735.01
2E1	91.7	739.63
A2	92.9	749.58
2E2	93.7	756.14
2E2	95.2	768.14
A1	95.8	773.01
A2	100.1	807.71
2E2	100.5	810.63
2E1	100.6	811.21
B2	101.4	818.06
B1	102.4	825.98
2E1	102.4	826.26
2E1	102.9	829.88
B2	103.3	833.04
2E2	103.9	838.50
A1	104.8	845.41
B1	105.4	850.20
2E1	105.5	851.24
2E2	106.9	862.07
A1	107.0	863.60
A2	108.0	871.05
2E2	108.4	874.28
A2	109.3	881.97
2E2	109.5	883.05
B1	109.9	886.90
2E1	110.0	887.26
2E1	110.3	889.45
B2	110.5	891.51
A2	113.2	913.23
2E2	113.3	913.77
2E2	113.4	915.14
A1	113.6	916.46
B1	114.1	920.78
2E1	114.4	922.89
2E2	115.3	930.12
A1	115.4	931.08
B1	116.0	935.73
2E1	116.4	938.81
A2	116.5	940.23
2E2	116.6	940.62
2E1	121.3	978.22
B1	121.5	980.44
B2	121.7	982.09
2E1	122.1	985.11
A2	123.1	993.36
2E2	123.5	996.59
A2	126.1	1017.05
2E2	126.3	1019.06
2E2	129.1	1041.28
A1	129.1	1041.43
B1	130.5	1052.57
2E1	130.7	1054.55
2E1	134.9	1088.41
B2	135.1	1090.17
2E1	310.7	2506.74
A1	311.0	2508.89
2E2	311.1	2509.69
A2	311.1	2509.96
B1	311.3	2511.27
B2	311.3	2511.42
2E2	311.3	2511.63
2E1	311.3	2511.77
B1	313.1	2526.01
2E1	313.4	2528.07
B2	313.4	2528.41
A1	313.5	2529.21
A2	313.7	2530.56
2E1	313.8	2531.42
2E2	314.1	2533.72
2E1	314.4	2536.74
B2	314.6	2538.42
2E2	315.1	2542.37
2E2	316.2	2551.11
A1	316.4	2552.77

Table S2. List of phonon symmetries and the corresponding phonon energies at the gamma point from the DFT-optimized $^{7}Li_2{}^{11}B_{10}D_{10}$ structure at 0 K. The number before the symmetry symbol denotes the degeneracy. (N.B.: Infrared-active modes = A2, E1 and Raman-active modes = A1, E1, E2.) Modes below 300 cm^{-1} possess translational and/or librational character.

Phonon Symm.	Energy (meV)	Energy (cm^{-1})
B1	4.3	34.37
2E1	8.5	68.75
B2	9.4	76.23
2E1	11.7	94.65
B2	14.1	113.60
2E2	14.3	115.61
A2	14.7	118.27
2E1	14.7	118.43
B1	15.8	127.56
2E2	16.6	133.61
B1	22.6	182.57
2E1	25.2	203.27
2E2	28.0	225.73
A2	28.2	227.39
2E1	28.4	229.40
A1	28.8	232.68
B2	29.5	238.18
B1	33.0	266.07
2E1	33.8	272.92
2E1	36.3	292.55
2E2	36.9	297.38
B2	37.0	298.26
2E2	52.0	419.63
A1	52.5	423.56
2E1	53.2	429.27
B1	53.3	430.06
A2	54.2	436.92
2E2	54.2	437.43
A2	57.7	465.73
2E2	58.5	471.58
B1	59.0	475.97
2E1	59.4	479.46
2E1	60.2	485.82
B1	60.4	487.33
A2	61.2	493.44
2E2	61.4	495.22
2E1	64.1	517.52
2E2	64.3	518.77
A1	65.0	524.62
B2	65.1	524.88
2E2	65.4	527.81
A2	65.5	528.16
B1	67.3	542.79
2E1	67.4	543.77
A2	70.1	565.34
2E2	70.6	569.21
2E1	70.8	571.48
B2	71.0	572.80
2E2	71.3	575.04
A1	71.5	577.18
B1	72.1	581.74
2E1	73.3	591.23
2E2	75.2	606.58
A1	75.3	607.48
B1	77.0	621.49
2E2	77.1	622.05
2E1	77.2	623.20
A1	77.4	624.49
2E1	77.6	626.17
B2	78.0	629.19
A2	79.7	643.17
2E2	79.9	644.81
2E1	82.3	664.11
B2	82.4	664.94
2E2	82.8	667.65
A1	83.0	669.20
A2	83.9	676.62
2E2	84.2	678.97
A1	85.9	692.93
2E2	85.9	693.10
2E1	86.4	696.72
B2	86.6	698.64
B2	87.2	703.41
B1	87.3	704.68
2E1	87.4	705.06
2E1	87.5	705.85
2E2	89.4	721.40
A2	89.4	721.45
2E2	89.9	725.49
B1	90.0	726.11
A1	90.0	726.17
2E1	90.5	729.92
2E1	91.2	735.92
B2	91.4	737.44
2E1	92.9	749.10
B1	93.2	751.66
2E2	94.2	760.19
A2	94.3	760.63
2E2	94.3	760.99
A1	94.6	763.50
A1	95.7	771.77
2E2	95.7	771.96
B2	97.9	789.73
2E1	98.0	790.45
B1	106.7	860.45
2E1	106.8	861.25
A2	107.4	866.27
2E2	107.6	868.21
2E2	110.6	892.48
A2	110.6	892.49
2E1	111.0	895.88
B1	111.1	896.26
A2	114.1	920.20
2E2	114.1	920.32
B1	114.3	922.21
2E1	114.4	922.90
A1	120.5	971.90
2E2	120.5	972.19
2E1	121.8	982.82
B2	121.9	983.27
2E1	229.8	1853.51
A1	229.9	1854.75
2E2	230.1	1856.10
A2	230.2	1857.22
2E2	230.3	1858.16
B2	230.4	1858.40
B1	230.4	1858.65
2E1	230.4	1858.75
B2	231.6	1868.82
B1	231.7	1868.96
2E1	231.8	1869.68
2E1	232.1	1872.70
A2	232.2	1873.09
A1	232.3	1873.74
2E2	232.6	1876.47
2E2	233.1	1880.79
2E1	233.9	1886.91
B2	234.0	1887.60
2E2	235.3	1898.16
A1	235.4	1898.70