

## Supplementary Material

### Alanine at 13.6 GPa and its Pressure-Induced Amorphisation at 15 GPa

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Tables containing complete details of PIXEL energies for each hydrogen bond at pressure points between ambient pressure and 13.60 GPa.

The pressure points between ambient conditions and 9.85 GPa are from our previous investigation into the effects of pressure on L-alanine. Data for 11.74 and 13.60 GPa are from the current experiment. All energies are given in units of  $\text{kJmol}^{-1}$ .

N1-H3...O2

Pressure/GPa	Coulombic	Polarisation	Dispersive	Repulsive	Total
<b>Ambient</b>	-127.9	-34.1	-24.3	37.8	-148.4
<b>1.03</b>	-139.3	-42	-27.4	56.1	-152.6
<b>2.29</b>	-136.6	-40	-26.5	50.5	-152.6
<b>4.30</b>	-136.7	-44.5	-29.6	63.3	-147.5
<b>8.04</b>	-141.7	-49.4	-32.5	75.8	-147.8
<b>9.85</b>	-157.3	-60.6	-34.5	108.6	-143.8
<b>11.74</b>	-159.2	-63.2	-36.5	124.7	-134.2
<b>13.60</b>	-160.9	-67.1	-38.8	143.7	-123.1

N1-H2...O2

Pressure/GPa	Coulombic	Polarisation	Dispersive	Repulsive	Total
<b>Ambient</b>	-114.6	-33.7	-17.3	42.9	-122.7
<b>1.03</b>	-119.9	-38.3	-17.3	58.3	-117.2
<b>2.29</b>	-126.5	-41.6	-19.5	59	-128.7
<b>4.30</b>	-126.7	-42.9	-21.2	64	-126.8
<b>8.04</b>	-130.5	-43.3	-22.2	64.4	-131.6
<b>9.85</b>	-148.1	-56.1	-24.6	107.3	-121.5
<b>11.74</b>	-150.3	-64.3	-24.4	124.3	-114.7
<b>13.60</b>	-141	-64.3	-24.9	120.4	-109.8

N1-H1...O1

<b>Pressure/GPa</b>	<b>Coulombic</b>	<b>Polarisation</b>	<b>Dispersive</b>	<b>Repulsive</b>	<b>Total</b>
<b>Ambient</b>	-20.4	-23.7	-12.1	26.3	-29.8
<b>1.03</b>	-27.2	-26.1	-12.5	34.9	-30.9
<b>2.29</b>	-24.8	-27.4	-13	33.7	-31.5
<b>4.30</b>	-29.6	-31.2	-14.9	43.6	-32.2
<b>8.04</b>	-34.3	-38.3	-16.9	57.6	-31.8
<b>9.85</b>	-52.7	-54.1	-19	95	-30.7
<b>11.74</b>	-57.9	-57.2	-19.5	105.4	-29.2
<b>13.60</b>	-49.2	-48.6	-19.1	85	-31.9