Supplementary Materials for

Phase transformation in two-dimensional covalent organic frameworks under compressive loading

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1. Supplementary figures

Fig. S1 The electron density of DTPA/Ag(111) interface.
Fig. S2 Relationship between the binding energy of DTPA/Ag(111) interface and the interfacial distance, which was obtained from DFT and MD calculations.
Fig. S3 Stress-strain curves of a 20 nm×20 nm graphene sheet compressed in x and y directions. The inset shows the molecular structure of the graphene sheet considered.
**Fig. S4** Relative energy $E_R$ as a function of strain $\varepsilon$ of DTPA sheets when they are compressed in (a) $x$ direction and (b) $y$ direction. Here the dashed lines are results fitted by $E_R \propto \varepsilon^2$. 
**Fig. S5** Stress-strain curves of a freestanding DTPA monolayer subjected to the compression in $x$ and $y$ directions. Here, the insets show the side view of the molecular structure of the DTPA monolayer before and after the buckling instability.
Fig. S6 Crystal structures of the transformed phases of seven-layered DTPA sheets when they are compressed along (a) y direction and (b) x direction.
2. Atomic coordinates of phases I, II and III unit cells of the DTPA sheet

|    |   |   |   |
|----|---|---|---|
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| C  | 72.8993912000 | 85.4179688000 | 0.0000000000 |
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| C  | 75.2296219000 | 85.4158173000 | 0.0000000000 |
| C  | 75.2913895000 | 86.8197022000 | 0.0000000000 |
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| C  | 72.8166580000 | 91.0936356000 | 0.0000000000 |
| N  | 74.0665131000 | 88.9660568000 | 0.0000000000 |
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| C  | 75.3143005000 | 91.0936356000 | 0.0000000000 |
| C  | 76.5339966000 | 88.9806366000 | 0.0000000000 |
| C  | 77.7243042000 | 89.7269287000 | 0.0000000000 |
| C  | 77.8251648000 | 91.1287766000 | 0.0000000000 |
| C  | 80.2888947000 | 91.1976395000 | 0.0000000000 |
| C  | 82.7853852000 | 91.2215424000 | 0.0000000000 |
| C  | 85.2779846000 | 91.1897507000 | 0.0000000000 |
| C  | 71.5735245000 | 91.7453690000 | 0.0000000000 |
| C  | 74.0645676000 | 91.7148896000 | 0.0000000000 |
| C  | 76.5610510000 | 91.7432175000 | 0.0000000000 |
| C  | 79.0245285000 | 91.8151779000 | 0.0000000000 |
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| N  | 82.7835694000 | 93.9750444000 | 0.0000000000 |
| C  | 82.7873230000 | 95.4010391000 | 0.0000000000 |
| C  | 84.0194473000 | 93.2604294000 | 0.0000000000 |
| C  | 85.2535172000 | 93.9562760000 | 0.0000000000 |
| C  | 85.1722031000 | 95.3498764000 | 0.0000000000 |
| C  | 86.5422135000 | 91.8059769000 | 0.0000000000 |
| C  | 86.4417420000 | 93.2071152000 | 0.0000000000 |
| C  | 81.5698319000 | 96.1203156000 | 0.0000000000 |
| C  | 81.6271897000 | 97.5237198000 | 0.0000000000 |
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| C | 83.9565202000 | 97.5207291000 | 0.0000000000 |
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| H | 82.7859630068 | 90.1295496188 | 0.0000000000 |
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| H | 80.6878538628 | 98.0766766041 | 0.0000000000 |
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| H | 71.9570742406 | 84.8695610941 | 0.0000000000 |
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| H | 71.5657561754 | 92.8352832318 | 0.0000000000 |
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| H | 76.4874728446 | 92.8259260827 | 0.0000000000 |
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| H       | 63.4185808023          | 66.9869619000          | 0.0000000000        |
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| H       | 59.9056753417          | 61.5095533395          | 0.0000000000        |
| H       | 67.2760079012          | 64.3854018938          | 0.0000000000        |
| H       | 68.0677971606          | 62.2147357673          | 0.0000000000        |
| H       | 68.956862891           | 60.0338391091          | 0.0000000000        |
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| H       | 63.8624373415          | 57.0761405781          | 0.0000000000        |
| H       | 61.5759190533          | 57.5211364592          | 0.0000000000        |
| H       | 57.6326294347          | 60.3124857101          | 0.0000000000        |
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| H       | 60.1347818084          | 56.8124860465          | 0.0000000000        |
| H       | 59.4537932223          | 54.7925807648          | 0.0000000000        |
| H       | 58.7109953202          | 52.513577234           | 0.0000000000        |
| H       | 54.5890496122          | 51.6687532603          | 0.0000000000        |
| H       | 52.9446506287          | 53.5149046103          | 0.0000000000        |
| H       | 51.2581009770          | 55.2942620148          | 0.0000000000        |
Phase III

| Element | X (Å)          | Y (Å)          | Z (Å)          | E (eV)         |
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| C       | 77.1980362000  | 40.2147102000  | 0.0000000000   |                |
| C       | 78.2020569000  | 39.2204361000  | 0.0000000000   |                |
| C       | 79.4850769000  | 39.8125687000  | 0.0000000000   |                |
| C       | 59.8797500000  | 43.5814133000  | 0.0000000000   |                |
| C       | 61.1722641000  | 43.0332184000  | 0.0000000000   |                |
| C       | 61.5242996000  | 41.6870728000  | 0.0000000000   |                |
| C       | 62.1872560000  | 41.1682091000  | 0.0000000000   |                |
| C       | 62.2572560000  | 43.9392472000  | 0.0000000000   |                |
| C       | 63.8375100000  | 42.0956612000  | 0.0000000000   |                |
| C       | 63.5963211000  | 43.4830666000  | 0.0000000000   |                |
| C       | 65.2301331000  | 41.6288948000  | 0.0000000000   |                |
| C       | 64.6319657000  | 44.4416809000  | 0.0000000000   |                |
| C       | 66.1990662000  | 42.6444664000  | 0.0000000000   |                |
| C       | 65.9849168000  | 44.0276108000  | 0.0000000000   |                |
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| C       | 76.4349442000  | 42.6315613000  | 0.0000000000   |                |
| C       | 77.4073486000  | 41.6189118000  | 0.0000000000   |                |
| C       | 77.9912568000  | 44.1659203000  | 0.0000000000   |                |
| C       | 78.7512512000  | 42.0905495000  | 0.0000000000   |                |
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| C       | 80.3711701000  | 43.9390030000  | 0.0000000000   |                |
| C       | 81.1157230000  | 41.6876831000  | 0.0000000000   |                |
| C       | 81.4587708000  | 43.0362587000  | 0.0000000000   |                |
| C       | 82.7500992000  | 43.5895653000  | 0.0000000000   |                |
| C       | 51.1106033000  | 45.3222695000  | 0.0000000000   |                |
| C       | 51.1031647000  | 46.7295189000  | 0.0000000000   |                |
| C       | 52.3781204000  | 44.7656784000  | 0.0000000000   |                |
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| C       | 55.9517746000  | 45.6317864000  | 0.0000000000   |                |
| C       | 57.1117859000  | 47.7573815000  | 0.0000000000   |                |
| C       | 58.3714230000  | 45.5900421000  | 0.0000000000   |                |
| C       | 58.2801132000  | 46.9903488000  | 0.0000000000   |                |
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| C       | 60.6866837000  | 45.7655487000  | 0.0000000000   |                |
| C       | 61.9842148000  | 45.3113175000  | 0.0000000000   |                |
| C   | 63.0277863000 | 46.2039566000 | 0.0000000000 |
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| C   | 66.9229736000 | 45.0727615000 | 0.0000000000 |
| C   | 66.6749726000 | 46.4624787000 | 0.0000000000 |
| C   | 65.3344193000 | 46.7929268000 | 0.0000000000 |
| C   | 68.9518510000 | 46.8380852000 | 0.0000000000 |
| C   | 67.6784973000 | 47.3838463000 | 0.0000000000 |
| C   | 70.1096268000 | 45.0743080000 | 0.0000000000 |
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| C   | 73.6689966000 | 46.8312683000 | 0.0000000000 |
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| C   | 75.9439164000 | 46.4511605000 | 0.0000000000 |
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| C   | 74.9248810000 | 48.7843972000 | 0.0000000000 |
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| C   | 52.2553558000 | 56.4745827000 | 0.0000000000 |
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| C   | 53.3928070000 | 55.6603241000 | 0.0000000000 |
| C   | 54.6433411000 | 56.3324242000 | 0.0000000000 |
| C   | 55.7475510000 | 54.1924667000 | 0.0000000000 |
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
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| C       | 70.1450882000 | 56.1752892000 | 0.0000000000 |
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| C       | 51.0927429000 | 58.7363739000 | 0.0000000000 |
| C       | 52.2172928000 | 56.1752892000 | 0.0000000000 |
| N       | 54.6841355000 | 57.7478218000 | 0.0000000000 |
| C       | 53.5313111000 | 59.9022636000 | 0.0000000000 |
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| C       | 55.9216462000 | 58.4375725000 | 0.0000000000 |
| C       | 55.9383850000 | 59.8353640000 | 0.0000000000 |
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| C       | 58.3249970000 | 58.5602532000 | 0.0000000000 |
| C       | 58.3191220000 | 59.9689598000 | 0.0000000000 |
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| C       | 68.9364700000 | 58.3669777000 | 0.0000000000 |
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| C       | 68.8753434000 | 59.7618065000 | 0.0000000000 |
| C       | 70.0912704000 | 57.5816841000 | 0.0000000000 |
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| N       | 71.3197327000 | 59.7175026000 | 0.0000000000 |
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| C       | 72.5370407000 | 60.4352417000 | 0.0000000000 |
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| C       | 59.1075516000 | 62.2766380000 | 0.0000000000 |
| C       | 60.0229187000 | 63.3486862000 | 0.0000000000 |
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| N       | 62.3984909000 | 63.9582214000 | 0.0000000000 |
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| C       | 63.7510758000 | 63.5358811000 | 0.0000000000 |
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| C       | 74.9712602000 | 61.9495964000 | 0.0000000000 |
| C       | 76.1791382000 | 62.5775109000 | 0.0000000000 |
| C       | 77.2819824000 | 61.7370873000 | 0.0000000000 |
| C       | 76.5253449000 | 63.9366978000 | 0.0000000000 |
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| C       | 81.2655792000 | 62.9498330000 | 0.0000000000 |
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| C       | 83.2638245000 | 60.8709756000 | 0.0000000000 |
| C       | 83.5372467000 | 62.2619095000 | 0.0000000000 |
| C       | 82.8645554000 | 64.7139435000 | 0.0000000000 |
| C       | 80.4762573000 | 67.1721802000 | 0.0000000000 |
| C       | 60.7231369000 | 65.7711334000 | 0.0000000000 |
| C       | 62.0764694000 | 65.3397827000 | 0.0000000000 |
| C       | 61.4533692000 | 68.1996765000 | 0.0000000000 |
| C       | 62.7507706000 | 67.6304245000 | 0.0000000000 |
| C       | 63.1168213000 | 66.2898789000 | 0.0000000000 |
| C       | 64.4240189000 | 65.8061905000 | 0.0000000000 |
| C       | 78.2197952000 | 65.7862244000 | 0.0000000000 |
| C       | 79.5250920000 | 66.2714996000 | 0.0000000000 |
| C       | 79.8924104000 | 67.6126557000 | 0.0000000000 |
| C       | 80.5661011000 | 65.3221359000 | 0.0000000000 |
| C       | 81.1890793000 | 68.1861649000 | 0.0000000000 |
| C       | 81.9217834000 | 65.7557984000 | 0.0000000000 |
| C       | 82.1659393000 | 67.1585465000 | 0.0000000000 |
| C       | 60.4742737000 | 70.6184769000 | 0.0000000000 |
| C       | 60.7175598000 | 72.0212173000 | 0.0000000000 |
| C       | 61.4521332000 | 69.5917053000 | 0.0000000000 |
| C       | 62.0715027000 | 72.4539032000 | 0.0000000000 |
| C       | 62.7484207000 | 70.1641235000 | 0.0000000000 |
| C       | 63.1143417000 | 71.5058823000 | 0.0000000000 |
| C       | 64.4199219000 | 71.9873810000 | 0.0000000000 |
|   |   |   |   |
|---|---|---|---|
| C | 78.2194138000 | 71.9752046000 | 0.0000000000 |
| C | 79.5273590000 | 71.4906693000 | 0.0000000000 |
| C | 79.8910522000 | 70.1470871000 | 0.0000000000 |
| C | 81.1886978000 | 69.5777130000 | 0.0000000000 |
| C | 80.5667191000 | 72.4414902000 | 0.0000000000 |
| C | 81.9209214000 | 72.0067368000 | 0.0000000000 |
| C | 82.1659393000 | 70.6021729000 | 0.0000000000 |
| C | 59.7762833000 | 73.0650330000 | 0.0000000000 |
| C | 59.1099091000 | 75.5199738000 | 0.0000000000 |
| C | 59.3868027000 | 76.9081116000 | 0.0000000000 |
| N | 62.3947678000 | 73.8355942000 | 0.0000000000 |
| C | 61.9839480000 | 76.1959763000 | 0.0000000000 |
| C | 63.0292740000 | 76.5390854000 | 0.0000000000 |
| C | 63.7487183000 | 74.2591553000 | 0.0000000000 |
| C | 64.0567322000 | 75.6229477000 | 0.0000000000 |
| C | 64.8080450000 | 73.3220825000 | 0.0000000000 |
| C | 66.1192093000 | 73.8263397000 | 0.0000000000 |
| C | 65.3724899000 | 76.0298309000 | 0.0000000000 |
| C | 66.4716187000 | 75.1836853000 | 0.0000000000 |
| C | 68.9209748000 | 75.1941528000 | 0.0000000000 |
| C | 67.6809769000 | 75.8052750000 | 0.0000000000 |
| C | 71.3256912000 | 75.2728958000 | 0.0000000000 |
| C | 70.1082611000 | 75.9161530000 | 0.0000000000 |
| C | 72.5436096000 | 75.9179840000 | 0.0000000000 |
| C | 73.7304001000 | 75.1971970000 | 0.0000000000 |
| C | 74.9700166000 | 75.8077011000 | 0.0000000000 |
| C | 76.5244675000 | 73.8212281000 | 0.0000000000 |
| C | 76.1775284000 | 75.1797943000 | 0.0000000000 |
| C | 77.2793808000 | 76.0250855000 | 0.0000000000 |
| C | 77.8340320000 | 73.3142929000 | 0.0000000000 |
| C | 78.8964540000 | 74.2501450000 | 0.0000000000 |
| C | 78.5921631000 | 75.6167374000 | 0.0000000000 |
| N | 80.2490387000 | 73.8265915000 | 0.0000000000 |
| C | 81.2621155000 | 74.8147736000 | 0.0000000000 |
| C | 79.6163864000 | 76.5345764000 | 0.0000000000 |
| C | 80.9488832000 | 76.1865997000 | 0.0000000000 |
| C | 82.8613206000 | 73.0509033000 | 0.0000000000 |
| C | 82.6237412000 | 74.4335709000 | 0.0000000000 |
| C | 83.5352555000 | 75.5039063000 | 0.0000000000 |
| C | 83.2629624000 | 76.8936310000 | 0.0000000000 |
| C | 52.3899002000 | 77.0824051000 | 0.0000000000 |
| C | 51.1032867000 | 77.5955506000 | 0.0000000000 |
| C | 51.0708008000 | 79.0043716000 | 0.0000000000 |
| C | 52.1845551000 | 79.8740082000 | 0.0000000000 |
|   | X           | Y           | Z           |
|---|-------------|-------------|-------------|
| C | 68.9349824000 | 86.7450791000 | 0.0000000000 |
| C | 68.8625718000 | 88.1409988000 | 0.0000000000 |
| C | 67.7220230000 | 88.9747314000 | 0.0000000000 |
| C | 70.0959854000 | 85.9568558000 | 0.0000000000 |
| C | 70.1174393000 | 88.7954700000 | 0.0000000000 |
| C | 71.3270493000 | 86.6609726000 | 0.0000000000 |
| C | 72.5592393000 | 85.9519882000 | 0.0000000000 |
| N | 71.3348618000 | 88.0757599000 | 0.0000000000 |
| C | 72.5545197000 | 88.7914353000 | 0.0000000000 |
| C | 73.7261811000 | 86.7342377000 | 0.0000000000 |
| C | 73.8059380000 | 88.1307755000 | 0.0000000000 |
| C | 74.9537736000 | 88.9589082000 | 0.0000000000 |
| C | 51.0951004000 | 91.0882797000 | 0.0000000000 |
| C | 51.1187970000 | 92.4979553000 | 0.0000000000 |
| C | 52.1915040000 | 90.2151083000 | 0.0000000000 |
| C | 52.3910141000 | 93.0349579000 | 0.0000000000 |
| C | 53.4607544000 | 90.8353577000 | 0.0000000000 |
| C | 53.5273438000 | 92.2433960000 | 0.0000000000 |
| N | 54.6387482000 | 90.0542069000 | 0.0000000000 |
| C | 54.7717972000 | 92.8309632000 | 0.0000000000 |
| C | 55.8875428000 | 90.7203369000 | 0.0000000000 |
| C | 55.9536264000 | 92.1270981000 | 0.0000000000 |
| C | 57.0895920000 | 89.9843370000 | 0.0000000000 |
| C | 57.1665955000 | 92.7955475000 | 0.0000000000 |
| C | 58.2686997000 | 90.7329941000 | 0.0000000000 |
| C | 58.3795548000 | 92.1318436000 | 0.0000000000 |
| C | 59.5780106000 | 92.7702255000 | 0.0000000000 |
| C | 60.7018128000 | 91.9554826000 | 0.0000000000 |
| C | 63.0487422000 | 91.5350876000 | 0.0000000000 |
| C | 61.9969864000 | 92.4143448000 | 0.0000000000 |
| C | 64.3668518000 | 91.9281060000 | 0.0000000000 |
| C | 65.3613281000 | 90.9635240000 | 0.0000000000 |
| C | 66.7006455000 | 91.3017655000 | 0.0000000000 |
| C | 66.9416962000 | 92.6924515000 | 0.0000000000 |
| C | 67.7045441000 | 90.3811264000 | 0.0000000000 |
| C | 68.9768982000 | 90.9288330000 | 0.0000000000 |
| C | 70.1352921000 | 90.1949081000 | 0.0000000000 |
| C | 71.3399429000 | 90.8441238000 | 0.0000000000 |
| C | 72.5406342000 | 90.1897888000 | 0.0000000000 |
| C | 74.9749756000 | 90.3648148000 | 0.0000000000 |
| C | 73.7031174000 | 90.9128876000 | 0.0000000000 |
| C | 77.3183136000 | 90.9519578000 | 0.0000000000 |
| C | 75.9776382000 | 91.2882538000 | 0.0000000000 |
| C | 75.7348480000 | 92.6789398000 | 0.0000000000 |
| C | 78.3127823000 | 91.9189682000 | 0.0000000000 |
| C | 79.6315232000 | 91.5317930000 | 0.0000000000 |
|    |    |    |    |    |    |
|----|----|----|----|----|----|
| C  | 80.6789398000 | 92.4201813000 | 0.0000000000 |
| C  | 81.9753494000 | 91.9661942000 | 0.0000000000 |
| C  | 83.0943222000 | 92.7843476000 | 0.0000000000 |
| C  | 59.8836670000 | 94.1381607000 | 0.0000000000 |
| C  | 61.1740036000 | 94.6934128000 | 0.0000000000 |
| C  | 61.5219422000 | 96.0424805000 | 0.0000000000 |
| C  | 62.2663117000 | 93.7912750000 | 0.0000000000 |
| C  | 62.8112870000 | 96.5669480000 | 0.0000000000 |
| N  | 63.6041810000 | 94.2558530000 | 0.0000000000 |
| C  | 63.8781738000 | 95.6438530000 | 0.0000000000 |
| C  | 64.6448593000 | 95.4364385000 | 0.0000000000 |
| C  | 65.2197189000 | 96.1191565000 | 0.0000000000 |
| C  | 66.1943512000 | 96.1122840000 | 0.0000000000 |
| C  | 65.9943466000 | 95.7272568000 | 0.0000000000 |
| C  | 76.6800919000 | 93.7160450000 | 0.0000000000 |
| C  | 76.4732590000 | 95.1001740000 | 0.0000000000 |
| C  | 78.0299530000 | 93.2991943000 | 0.0000000000 |
| C  | 77.4464035000 | 96.1125180000 | 0.0000000000 |
| N  | 79.0725327000 | 94.2558530000 | 0.0000000000 |
| C  | 78.7873420000 | 95.6447200000 | 0.0000000000 |
| C  | 80.4075089000 | 93.7952957000 | 0.0000000000 |
| C  | 79.8547212000 | 96.5701065000 | 0.0000000000 |
| C  | 81.1458054000 | 96.0474701000 | 0.0000000000 |
| C  | 81.4948404000 | 94.6997360000 | 0.0000000000 |
| C  | 82.7858124000 | 94.1545170000 | 0.0000000000 |
| C  | 83.1362839000 | 97.9189302000 | 0.0000000000 |
| C  | 84.4160843000 | 98.5133744000 | 0.0000000000 |
| C  | 85.4240732000 | 97.5220185000 | 0.0000000000 |
| C  | 77.2347412000 | 97.5144300000 | 0.0000000000 |
| C  | 78.2407456000 | 98.5104520000 | 0.0000000000 |
| C  | 79.5236435000 | 97.9205094000 | 0.0000000000 |
| H  | 80.3467600999 | 98.6378397453 | 0.0000000000 |
| H  | 81.9669111762 | 96.7687541985 | 0.0000000000 |
| H  | 83.6311758679 | 94.8372913092 | 0.0000000000 |
| H  | 82.1763692243 | 90.8955258476 | 0.0000000000 |
| H  | 79.8670021740 | 90.4664065293 | 0.0000000000 |
| H  | 77.6135280781 | 89.9070220018 | 0.0000000000 |
| H  | 74.7599662717 | 93.1421549297 | 0.0000000000 |
| H  | 75.4392136191 | 95.4494702668 | 0.0000000000 |
| H  | 76.2087736421 | 97.8799386633 | 0.0000000000 |
| H  | 75.9102355563 | 88.4413871308 | 0.0000000000 |
| H  | 74.6823677561 | 86.1964633074 | 0.0000000000 |
| H  | 73.4654128153 | 84.0701893538 | 0.0000000000 |
| H  | 73.4834262346 | 91.9661103729 | 0.0000000000 |
| H  | 71.3427776385 | 91.9360372510 | 0.0000000000 |
| H  | 69.1940192967 | 91.9838477977 | 0.0000000000 |
| H | x   | y       | z       |
|---|-----|---------|---------|
| H | 66.7652004628 | 88.4597816847 | 0.0000000000 |
| H | 67.9775574535 | 86.2112340634 | 0.0000000000 |
| H | 69.1826404845 | 84.0781697077 | 0.0000000000 |
| H | 65.0730651413 | 89.1733507360 | 0.0000000000 |
| H | 62.8332395649 | 90.4663207011 | 0.0000000000 |
| H | 60.6681596391 | 90.8784146454 | 0.0000000000 |
| H | 59.0672924700 | 94.8571899399 | 0.0000000000 |
| H | 60.7031756795 | 96.7630669083 | 0.0000000000 |
| H | 62.3124418714 | 98.6353591135 | 0.0000000000 |
| H | 66.4491408191 | 97.8919599241 | 0.0000000000 |
| H | 67.2278397028 | 95.4653919070 | 0.0000000000 |
| H | 67.9163867623 | 93.1576561145 | 0.0000000000 |
| H | 59.1080307071 | 90.0547191473 | 0.0000000000 |
| H | 57.8835940057 | 88.0146504620 | 0.0000000000 |
| H | 56.6186890746 | 85.9802792188 | 0.0000000000 |
| H | 52.3442447539 | 86.0986727892 | 0.0000000000 |
| H | 51.2141207711 | 88.3375342290 | 0.0000000000 |
| H | 50.0986329300 | 90.6440881376 | 0.0000000000 |
| H | 52.4676436059 | 94.1212903695 | 0.0000000000 |
| H | 54.8151707141 | 93.9225084211 | 0.0000000000 |
| H | 57.1396435828 | 93.8819508153 | 0.0000000000 |
| H | 56.6482757048 | 84.0855881732 | 0.0000000000 |
| H | 57.9273066106 | 82.0082923365 | 0.0000000000 |
| H | 59.2514408268 | 79.7807920852 | 0.0000000000 |
| H | 61.0474157690 | 78.2430248006 | 0.0000000000 |
| H | 63.2777342793 | 77.6013386676 | 0.0000000000 |
| H | 65.3978130814 | 77.1044377817 | 0.0000000000 |
| H | 66.9891850107 | 77.8903032324 | 0.0000000000 |
| H | 67.9907559902 | 79.9490523728 | 0.0000000000 |
| H | 69.1850263702 | 82.0780361048 | 0.0000000000 |
| H | 52.3726959729 | 83.9749520489 | 0.0000000000 |
| H | 51.2439940446 | 81.7756991177 | 0.0000000000 |
| H | 50.0804636088 | 79.4587418133 | 0.0000000000 |
| H | 52.4607315828 | 75.9967842231 | 0.0000000000 |
| H | 54.7691504677 | 76.1594040065 | 0.0000000000 |
| H | 56.8965859070 | 76.2059620949 | 0.0000000000 |
| H | 58.1339468191 | 75.0606797812 | 0.0000000000 |
| H | 58.7261724629 | 72.7629966697 | 0.0000000000 |
| H | 59.4312406469 | 70.2999301066 | 0.0000000000 |
| H | 59.4363506107 | 67.4959913498 | 0.0000000000 |
| H | 58.7304635613 | 65.0340991280 | 0.0000000000 |
| H | 58.1315653789 | 62.7357701396 | 0.0000000000 |
| H | 56.8932961222 | 61.5863769897 | 0.0000000000 |
| H | 54.7615012687 | 61.6126970592 | 0.0000000000 |
| H | 52.4540189221 | 61.7524128463 | 0.0000000000 |
| H | 59.2718588500 | 58.0258094993 | 0.0000000000 |
|      | X1   | Y1   | Z1   | X2   | Y2   | Z2   | X3   | Y3   | Z3   | X4   | Y4   | Z4   | X5   | Y5   | Z5   | X6   | Y6   | Z6   | X7   | Y7   | Z7   | X8   | Y8   | Z8   | X9   | Y9   | Z9   | X10 | Y10  | Z10  | X11 | Y11  | Z11  | X12 | Y12  | Z12  | X13 | Y13  | Z13  | X14 | Y14  | Z14  | X15 | Y15  | Z15  | X16 | Y16  | Z16  | X17 | Y17  | Z17  | X18 | Y18  | Z18  | X19 | Y19  | Z19  | X20 | Y20  | Z20  |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
H 73.6799780140  74.1121831179  0.0000000000
H 84.5987109541  62.5173688815  0.0000000000
H 83.9175078910  65.0084595101  0.0000000000
H 83.2068962442  67.4806796327  0.0000000000
H 81.6343523584  59.5215709196  0.0000000000
H 79.3777425386  50.1664264808  0.0000000000
H 77.2689735860  50.1664264808  0.0000000000
H 75.7557904414  59.8709651769  0.0000000000
H 74.6438252777  57.8110738347  0.0000000000
H 73.4481740545  55.6822163106  0.0000000000
H 73.453386103  53.6829918140  0.0000000000
H 74.662331990  51.5454183103  0.0000000000
H 75.8847942470  49.2966719245  0.0000000000
H 77.5815632737  47.8291272611  0.0000000000
H 79.8286186725  47.2658226965  0.0000000000
H 82.1342488433  46.8429806463  0.0000000000
H 83.5963344876  42.9037565619  0.0000000000
H 81.9327498572  40.9666237528  0.0000000000
H 80.308462339  39.0954478831  0.0000000000
H 76.1717373972  39.8541198373  0.0000000000
H 75.3966908888  42.2952956447  0.0000000000
H 74.7208785838  44.6112060501  0.0000000000
H 73.4518036824  45.7773244671  0.0000000000
H 71.3121697075  45.8202970515  0.0000000000
H 69.1825510976  45.787497055  0.0000000000
H 67.9069065008  44.6267719671  0.0000000000
H 67.2387000321  42.3105389774  0.0000000000
H 66.4653072121  39.8643764731  0.0000000000
H 62.3312246387  39.0962964375  0.0000000000
H 60.7095388270  40.9587947830  0.0000000000
H 59.0636177304  42.8615108102  0.0000000000
H 57.1128757811  43.8551511569  0.0000000000
H 54.7897050826  43.8492953570  0.0000000000
H 52.4396932438  43.6784766645  0.0000000000
H 50.1159310223  47.1904862465  0.0000000000
H 51.2629253997  49.4787143819  0.0000000000
H 52.4092572987  51.6888157165  0.0000000000