Supporting Information

for “Structure and piezochromism of 1-pyrenealdehyde at high pressure”

Daniel Tchoń & Anna Makal

Table of Contents

Section 1 – Crystal Structure

Table S1: Dependence of cell parameters on external pressure (see Figure 5 in main text).

EXPERIMENT				
Pressure [GPa]	**a [Å]**	**b [Å]**	**c [Å]**	**V [Å^3]**
0.000	6.92715(15)	8.3336(2)	10.4706(2)	542.32(2)
0.834	6.7049(9)	8.1989(12)	10.329(2)	509.65(16)
1.000	6.6950(8)	8.1846(11)	10.306(2)	506.95(16)
1.516	6.6139(17)	8.1151(16)	10.272(2)	495.3(2)
1.834	6.6007(14)	8.1331(19)	10.232(3)	492.5(2)
2.822	6.477(2)	8.041(2)	10.205(3)	477.5(3)
CALCULATIONS				
Pressure [GPa]	**a [Å]**	**b [Å]**	**c [Å]**	**V [Å^3]**
0	7.048	8.199	10.403	540.173
0.5	6.928	8.183	10.332	523.914
1	6.857	8.074	10.257	511.055
1.5	6.810	8.010	10.194	501.261
2	6.733	7.968	10.164	491.000
2.5	6.670	7.939	10.126	483.471
3	6.608	7.906	10.105	475.230
3.5	6.527	7.913	10.087	468.492
4	6.479	7.880	10.061	462.290
4.5	6.446	7.842	10.037	456.631
5	6.417	7.807	10.009	451.843
6	6.343	7.751	9.976	441.730
7	6.235	7.753	9.950	433.128
8	6.198	7.692	9.915	425.397
9	6.134	7.662	9.887	418.484
10	6.091	7.619	9.859	412.136

Table S2: Dependence of vertical separation and horizontal shift observed between "paired" and "offset" stacked PA molecules on external pressure (see Figure 6 in main text).

EXPERIMENT				
	dist. between "paired" molecules		**dist. between "offset" molecules**	
Pressure [GPa]	**vertical [Å]**	**horizontal [Å]**	**vertical [Å]**	**horizontal [Å]**
0.000	3.414	1.597	3.367	2.999
0.834	3.313	1.604	3.260	2.919
1.000	3.306	1.600	3.259	2.907
1.516	3.270	1.594	3.210	2.902
1.834	3.259	1.576	3.204	2.908
2.822	3.208	1.598	3.139	2.877
CALCULATIONS				
	dist. between "paired" molecules		**dist. between "offset" molecules**	
Pressure [GPa]	**vertical [Å]**	**horizontal [Å]**	**vertical [Å]**	**horizontal [Å]**
0	3.453	1.498	3.383	3.124
0.5	3.401	1.502	3.336	3.097
1	3.365	1.500	3.291	3.072
1.5	3.344	1.505	3.270	3.034
2	3.299	1.485	3.219	3.078
2.5	3.281	1.518	3.205	2.993
3	3.242	1.500	3.163	3.046
3.5	3.216	1.534	3.143	2.964
4	3.194	1.538	3.122	2.941
4.5	3.173	1.526	3.099	2.964
5	3.161	1.540	3.090	2.931
6	3.155	1.437	3.044	2.966
7	3.078	1.569	3.016	2.856
8	3.029	1.507	2.972	2.833
9	3.018	1.551	2.954	2.892
10	2.993	1.542	2.929	2.902

The centroids and mean planes used to obtain distances Table S2 were determined based solely on carbon atoms. Their precision was assumed to be on the same order of magnitude as C–C bond length precision, which is no larger then 0.02Å (experiment at 1.8 GPa) and only 0.0009Å in the reference structure). Assuming error propagation in calculation of the 'offset' distances, the uncertainties would not exceed 0.003Å for the structure at atmospheric pressure and 0.06Å at the remaining pressures.

Table S3: Dependence of C–H•••O hydrogen bonds' lengths and C–H•••O angles found between inversion-related moieties in PA structure on external pressure (see Figure 7 in main text).

EXPERIMENT						
Pressure [GPa]	**C4 – O1' distance [Å]**	**H4 – O1' distance [Å]**	**C4–H4–O1' angle [°]**	**C6 – O1' distance [Å]**	**H6 – O1' distance [Å]**	**C6–H6–O1' angle [°]**
0.000	3.4783(7)	2.69	142.8	3.7463(8)	3.03	135.5
0.834	3.408(7)	2.64	140.3	3.646(6)	2.94	133.9
1.000	3.401(6)	2.63	140.7	3.634(5)	2.92	134.2
1.516	3.348(5)	2.57	141.3	3.586(4)	2.88	133.9
1.834	3.382(16)	2.60	141.9	3.576(16)	2.89	131.5
2.822	3.295(9)	2.50	142.9	3.517(9)	2.79	135.7
THEORY						
Pressure [GPa]	**C4 – O1' distance [Å]**	**H4 – O1' distance [Å]**	**C4–H4–O1' angle [°]**	**C6 – O1' distance [Å]**	**H6 – O1' distance [Å]**	**C6–H6–O1' angle [°]**
0	3.481	2.460	146.53	3.750	2.845	137.67
0.5	3.433	2.420	144.50	3.744	2.780	136.58
1	3.361	2.388	145.56	3.646	2.761	136.89
1.5	3.311	2.363	145.41	3.590	2.718	137.12
2	3.292	2.347	144.97	3.563	2.693	136.91
2.5	3.265	2.325	144.33	3.518	2.647	136.93
3	3.249	2.314	143.89	3.497	2.628	136.65
3.5	3.223	2.301	142.34	3.447	2.581	136.29
4	3.211	2.289	142.28	3.425	2.557	136.49
4.5	3.199	2.277	142.38	3.410	2.541	136.49
5	3.184	2.263	142.30	3.387	2.517	136.64
6	3.164	2.242	142.47	3.364	2.495	136.52
7	3.132	2.225	140.72	3.309	2.444	135.96
8	3.114	2.292	139.45	3.296	2.448	136.57
9	3.094	2.183	141.25	3.268	2.404	135.88
10	3.077	2.164	141.52	3.250	2.386	135.86

Table S4: Dependence of selected covalent bond lengths in PA structure on external pressure.

EXPERIMENT					
Pressure [GPa]	**C17 – O1 distance [Å]**	**C1 – C17 distance [Å]**	**C1 – C2 distance [Å]**	**C2 – C15 distance [Å]**	**C15 – C16 distance [Å]**
0.000	1.212(1)	1.4728(8)	1.4182(8)	1.4238(7)	1.4268(7)
0.834	1.216(8)	1.478(7)	1.42(1)	1.417(6)	1.43(1)
1.000	1.226(7)	1.439(6)	1.427(9)	1.408(5)	1.427(7)
1.516	1.223(5)	1.471(4)	1.418(6)	1.434(4)	1.430(6)
1.834	1.24(2)	1.38(2)	1.49(3)	1.39(2)	1.41(3)
2.822	1.22(1)	1.468(9)	1.42(1)	1.437(8)	1.42(1)
THEORY					
Pressure [GPa]	**C17 – O1 distance [Å]**	**C1 – C17 distance [Å]**	**C1 – C2 distance [Å]**	**C2 – C15 distance [Å]**	**C15 – C16 distance [Å]**
0	1.228	1.469	1.423	1.428	1.427
0.5	1.228	1.467	1.422	1.427	1.426
1	1.228	1.466	1.421	1.426	1.425
1.5	1.229	1.465	1.420	1.425	1.424
2	1.229	1.464	1.420	1.424	1.424
2.5	1.229	1.462	1.419	1.424	1.423
3	1.229	1.462	1.418	1.423	1.422
3.5	1.229	1.461	1.417	1.422	1.422
4	1.229	1.460	1.416	1.421	1.421
4.5	1.229	1.459	1.416	1.421	1.420
5	1.229	1.458	1.415	1.420	1.419
6	1.230	1.457	1.414	1.418	1.418
7	1.230	1.454	1.412	1.417	1.417
8	1.230	1.450	1.412	1.414	1.415
9	1.230	1.451	1.410	1.414	1.415
10	1.230	1.450	1.409	1.413	1.414

Section 2 – Luminescence

Table S4: Observed positions of maxima of emitted wavelength and estimated positions of maxima of absorbed wavelength for given pressure values (see Figure 10 in main text).

Luminescence measurements		**Theoretical calculations**	
Calculated pressure [GPa]	Observed peak of emitted wavelength [nm]	Set Pressure [GPa]	Estimated peak of absorbed wavelength [nm]
0.24	583	0	464
0.13	588	0.5	472
0.1	587	1	482
0.52	582	1.5	488
0.76	582	2	499
1.13	587	2.5	502
1.56	594	3	513
1.77	604	3.5	514
2.04	616	4	520
2.33	630	4.5	529
2.52	640	5	533
2.56	645	6	551
2.64	648	7	554
2.61	651	8	575
2.64	654	9	586
2.8	660	10	602
3.01	665		
3.1	674		
3.17	676		

Values presented in the second column are experimental and have been determined by a means of a following fitting process:
1) rough estimation – fit linear background + gauss signal to the experimental luminescence curve
2) background subtraction – subtract the linear background defined in the previous step
3) data cleaning – remove sharp Raman signals and points far (>25nm) from initial gauss maximum
4) final fitting – fit gauss signal to the modified luminescence curve and write down its position

Section 3 – Theoretical Calculations

All the theoretical calculations mentioned in the paper for investigated pyrene-1-carbaldehyde were performed in CRYSTAL09, using a B3LYP functional and 6-31G** basis set. The Coulomb and Exchange sums truncation criteria (7, 7, 7, 7, 29) and shrinking factors (8, 8) were increased relative to default values in all calculations.

Optimisation of the structures in high-pressure conditions was performed using FULLOPTG and EXTPRESS commands, with dispersion correction considered using GRIMME module with appropriate parameters. This allowed for both atomic positions and cell parameters to be optimised simultaneously.

Since CRYSTAL09 does not allow to include both dispersion and BSSE corrections during one computational process, whenever an interaction analysis was due, calculations were performed in two different variants in order to consider both errors in the final result. The first variant utilised a GRIMME procedure and was used to obtain both the energy without any corrections and the value of dispersion correction. The second variant used GHOSTS command and aimed to estimate Basis Set Superposition Error. A formula for corrected value of energy becomes then:

$$E_{corrected} = E_{without\ corrections} + \Delta E_{dispersion\ correction} + \Delta E_{BSSE}$$

In order to obtain PA cohesive energy, firstly the total bulk energy was obtained by fixing experimental cell parameters and refining only atomic positions. Then the energy of a single, isolated molecule was calculated based on its fixed geometry obtained in the previous step. The cohesive energy was then estimated as a difference between total crystal energy and twice the energy of a single molecule:

$$E_{cohesive} = E_{bulk} - 2\,E_{molecule}$$

In order to evaluate individual interactions within PA stacks stretched in the (100) direction, energy of investigated dimer formed by inversion-related moieties was calculated based on a fixed optimised bulk geometry and compared to twice the energy of a single monomer:

$$E_{interaction\ between\ dimers} = E_{dimer} - 2\,E_{molecule}$$

The interaction between neighbouring stacks was estimated slightly differently. The energy of infinite double rod, composed out of periodic one-dimensional lattice of (100)-translation related dimers, was compared to double the energy of a single infinite rod defined in the same way. In this approach the geometry of individual stacks, dimers and monomers was also not optimised and was exported out of optimised bulk structure mentioned in the previous paragraph instead.

$$E_{interaction\ between\ stacks} = E_{double\ rod} - 2\,E_{single\ rod}$$

Table S5: Coordinates of atoms in PA structures optimised by CRYSTAL09 (excerpt from output)

0 GPa

```
*******************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   540.173161 - DENSITY  1.415 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    7.04791353     8.19949134    10.40314393   109.279462  99.688798 100.729104
*******************************************************************************
        ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
          ATOM              X/A                 Y/B                 Z/C
*******************************************************************************
     1 T   6 C     2.111084139672E-01 -1.844577655017E-01 -1.928076350410E-01
     3 T   6 C     2.110166067421E-01 -1.498564370147E-01 -4.948592382986E-02
     5 T   6 C     1.661307046411E-01 -2.881490625219E-01  4.950857695730E-03
     7 T   1 H     1.338042802836E-01 -4.253483945400E-01 -6.643330020052E-02
     9 T   6 C     1.640184434340E-01 -2.487526977509E-01  1.426510081172E-01
    11 T   1 H     1.265459201102E-01 -3.551119511961E-01  1.813998083725E-01
    13 T   6 C     2.066967178206E-01 -6.804696580325E-02  2.393141369004E-01
    15 T   6 C     1.975127228582E-01 -2.641780862964E-02  3.801489934746E-01
    17 T   1 H     1.531550816959E-01 -1.354262004041E-01  4.152219989054E-01
    19 T   6 C     2.373982699245E-01  1.509434804698E-01  4.710527343629E-01
    21 T   1 H     2.232267208302E-01  1.831569889889E-01 -4.218303919009E-01
    23 T   6 C     2.901539502927E-01  2.895783511024E-01  4.237852634098E-01
    25 T   1 H     3.198527524032E-01  4.271778571173E-01  4.949662659550E-01
    27 T   6 C     3.010966062859E-01  2.538352976812E-01  2.841320065697E-01
    29 T   6 C     3.495194483567E-01  3.941330747108E-01  2.320820183023E-01
    31 T   1 H     3.820283578732E-01 -4.679785962713E-01  3.041618683114E-01
    33 T   6 C     3.528200755933E-01  3.559476953370E-01  9.506260124747E-02
    35 T   1 H     3.864241745573E-01  4.630126770826E-01  5.655853355375E-02
    37 T   6 C     3.077516117314E-01  1.749256395042E-01 -2.584597244216E-03
    39 T   6 C     3.111204396179E-01  1.353815857416E-01 -1.439211151593E-01
    41 T   1 H     3.489548252436E-01  2.441120776427E-01 -1.802498275750E-01
    43 T   6 C     2.644494840874E-01 -4.067593997727E-02 -2.359150356494E-01
    45 T   1 H     2.686646451899E-01 -6.991148823551E-02 -3.448153966062E-01
    47 T   6 C     2.588897298633E-01  3.192160932674E-02  4.550035114025E-02
    49 T   6 C     2.565754820411E-01  7.251485033425E-02  1.895000649785E-01
    51 T   6 C     1.530880207630E-01 -3.622685953113E-01 -3.057554319936E-01
    53 T   1 H     1.616380209474E-01 -3.558971555122E-01 -4.095778108085E-01
    55 T   8 O     9.564696722260E-02  4.911511029589E-01 -2.980931249100E-01
```

0.5 GPa

```
*******************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   523.913802 - DENSITY  1.458 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.92816604     8.18327290    10.33210795   109.195852  99.442145 101.932026
*******************************************************************************
        ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
          ATOM              X/A                 Y/B                 Z/C
*******************************************************************************
     1 T   6 C     2.109519324267E-01 -1.842090846961E-01 -1.938346470960E-01
     3 T   6 C     2.118718288395E-01 -1.500372255764E-01 -4.957932006791E-02
     5 T   6 C     1.688370456357E-01 -2.894828586918E-01  5.377662309312E-03
     7 T   1 H     1.369110354957E-01 -4.272756489190E-01 -6.650418991320E-02
     9 T   6 C     1.681579847197E-01 -2.504034738024E-01  1.441092478505E-01
    11 T   1 H     1.315386582162E-01 -3.575818719237E-01  1.833274680033E-01
    13 T   6 C     2.106893729415E-01 -6.892705320059E-02  2.413609898704E-01
    15 T   6 C     2.027051972727E-01 -2.796730885488E-02  3.832185916894E-01
    17 T   1 H     1.594247975821E-01 -1.383451233183E-01  4.184725565954E-01
    19 T   6 C     2.408684896725E-01  1.501030317193E-01  4.743955750799E-01
    21 T   1 H     2.264907054391E-01  1.818165491077E-01 -4.178920119740E-01
    23 T   6 C     2.912276068540E-01  2.900771485897E-01  4.264960148531E-01
    25 T   1 H     3.188435832548E-01  4.280350211379E-01  4.977946926800E-01
    27 T   6 C     3.019118397058E-01  2.550399820342E-01  2.859990724337E-01
    29 T   6 C     3.483694943463E-01  3.966645966267E-01  2.334489242226E-01
    31 T   1 H     3.800884660712E-01 -4.648449261596E-01  3.058842710771E-01
    33 T   6 C     3.504666229414E-01  3.587848646941E-01  9.541175720196E-02
    35 T   1 H     3.824251417255E-01  4.666230020109E-01  5.639696723125E-02
    37 T   6 C     3.058480519113E-01  1.769185819011E-01 -2.728255835824E-03
    39 T   6 C     3.077183279232E-01  1.379004849772E-01 -1.451152669081E-01
    41 T   1 H     3.434081249723E-01  2.477627861023E-01 -1.818166789486E-01
    43 T   6 C     2.624395347324E-01 -3.903128974103E-02 -2.374599612709E-01
    45 T   1 H     2.662786289142E-01 -6.805116809154E-02 -3.470508572830E-01
    47 T   6 C     2.591580495761E-01  3.265395218810E-02  4.590667218932E-02
    49 T   6 C     2.584295748097E-01  7.291631924255E-02  1.909728314341E-01
    51 T   6 C     1.537622141871E-01 -3.629766710750E-01 -3.074501744346E-01
    53 T   1 H     1.636849983567E-01 -3.559713569180E-01 -4.116462697708E-01
    55 T   8 O     9.538635700797E-02  4.888411472617E-01 -3.000457942972E-01
```

1.0 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   511.055354 - DENSITY  1.495 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.85718038     8.07420117    10.25741040   108.866847 100.131464 100.592393
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.100683831276E-01 -1.846077143280E-01 -1.957550392552E-01
    3 T   6 C     2.108944049007E-01 -1.504633112224E-01 -5.074815194732E-02
    5 T   6 C     1.663766444077E-01 -2.908485741426E-01  4.638097203104E-03
    7 T   1 H     1.328073041316E-01 -4.294262263651E-01 -6.758688771545E-02
    9 T   6 C     1.662797315939E-01 -2.516365941044E-01  1.442153024885E-01
   11 T   1 H     1.284517173226E-01 -3.592965980611E-01  1.839039393948E-01
   13 T   6 C     2.109132639486E-01 -6.921512498951E-02  2.418548619593E-01
   15 T   6 C     2.034758438369E-01 -2.815675965298E-02  3.845443697083E-01
   17 T   1 H     1.591373269033E-01 -1.392662176181E-01  4.199135322228E-01
   19 T   6 C     2.429148529622E-01  1.510021429769E-01  4.760238443859E-01
   21 T   1 H     2.283135948428E-01  1.832913946706E-01 -4.157669189915E-01
   23 T   6 C     2.942290798825E-01  2.917263524068E-01  4.275615505979E-01
   25 T   1 H     3.223015361688E-01  4.305931425309E-01  4.988815210185E-01
   27 T   6 C     3.047189125567E-01  2.565444277624E-01  2.863316414566E-01
   29 T   6 C     3.520053380288E-01  3.990799101236E-01  2.332623919498E-01
   31 T   1 H     3.844641781169E-01 -4.615983307368E-01  3.058390850854E-01
   33 T   6 C     3.539437027916E-01  3.610259009670E-01  9.447755626147E-02
   35 T   1 H     3.864428622216E-01  4.696163842225E-01  5.507770704415E-02
   37 T   6 C     3.078906982564E-01  1.782505482633E-01 -4.056872003552E-03
   39 T   6 C     3.097649200433E-01  1.392287610453E-01 -1.471709935292E-01
   41 T   1 H     3.466556534153E-01  2.498538777547E-01 -1.841355793564E-01
   43 T   6 C     2.632995666354E-01 -3.868408376756E-02 -2.397816509710E-01
   45 T   1 H     2.679601532227E-01 -6.793030541928E-02 -3.498100289357E-01
   47 T   6 C     2.598816313365E-01  3.311143100176E-02  4.505731185403E-02
   49 T   6 C     2.597389850998E-01  7.345782016015E-02  1.909587740367E-01
   51 T   6 C     1.518424318479E-01 -3.639635512432E-01 -3.096049214151E-01
   53 T   1 H     1.619064552328E-01 -3.569668846439E-01 -4.144593170264E-01
   55 T   8 O     9.250869617235E-02  4.873229237981E-01 -3.017006566952E-01
```

1.5 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   501.260834 - DENSITY  1.524 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.81016022     8.00973154    10.19439316   108.778206 100.005462 100.504730
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.102487172093E-01 -1.842194763603E-01 -1.976806943291E-01
    3 T   6 C     2.107122797071E-01 -1.504233972766E-01 -5.203035503498E-02
    5 T   6 C     1.655916227177E-01 -2.920609478950E-01  3.461641652325E-03
    7 T   1 H     1.319684729755E-01 -4.313591871859E-01 -6.922660787217E-02
    9 T   6 C     1.653695557012E-01 -2.530651557135E-01  1.437414013471E-01
   11 T   1 H     1.272136278915E-01 -3.614933233970E-01  1.837165983653E-01
   13 T   6 C     2.107191054833E-01 -6.972499316033E-02  2.419811202295E-01
   15 T   6 C     2.034821564908E-01 -2.902717326011E-02  3.854411762040E-01
   17 T   1 H     1.584407963398E-01 -1.412475844147E-01  4.207072757446E-01
   19 T   6 C     2.434867552805E-01  1.511477295956E-01  4.775152348002E-01
   21 T   1 H     2.286277204974E-01  1.834477356335E-01 -4.137388664556E-01
   23 T   6 C     2.952342707008E-01  2.930774106504E-01  4.288692469432E-01
   25 T   1 H     3.234595014025E-01  4.326992926129E-01 -4.994426460023E-01
   27 T   6 C     3.057260856112E-01  2.582321790735E-01  2.869384087329E-01
   29 T   6 C     3.532641414439E-01  4.020716707556E-01  2.337380219434E-01
   31 T   1 H     3.857203112024E-01 -4.578237247262E-01  3.067185402193E-01
   33 T   6 C     3.551435323512E-01  3.641816398347E-01  9.422734907419E-02
   35 T   1 H     3.874636320514E-01  4.736711165035E-01  5.463375476829E-02
   37 T   6 C     3.087934325503E-01  1.804798012608E-01 -4.900712074992E-03
   39 T   6 C     3.109750408498E-01  1.418035856269E-01 -1.486924307949E-01
   41 T   1 H     3.482921982130E-01  2.534599312430E-01 -1.857015977227E-01
   43 T   6 C     2.644318720896E-01 -3.709940896273E-02 -2.418067389371E-01
   45 T   1 H     2.699022805452E-01 -6.626711417580E-02 -3.522642014141E-01
   47 T   6 C     2.602126841816E-01  3.409611362857E-02  4.433703486642E-02
   49 T   6 C     2.601179412105E-01  7.418881351518E-02  1.909574515038E-01
   51 T   6 C     1.514794183651E-01 -3.643143333747E-01 -3.120888082048E-01
   53 T   1 H     1.626888087059E-01 -3.569953473295E-01 -4.173165947063E-01
   55 T   8 O     9.051090871321E-02  4.859311901161E-01 -3.042474200436E-01
```

2.0 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   490.999701 - DENSITY  1.556 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.73255856     7.96799353    10.16376397   108.482922 101.168177  99.944268
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.085450671376E-01 -1.851461402537E-01 -1.974852161411E-01
    3 T   6 C     2.102960272610E-01 -1.514271172582E-01 -5.143062461303E-02
    5 T   6 C     1.660907982479E-01 -2.934206332493E-01  4.320462567529E-03
    7 T   1 H     1.315767410029E-01 -4.329530731971E-01 -6.862532813002E-02
    9 T   6 C     1.676082546506E-01 -2.544838555663E-01  1.450819650080E-01
   11 T   1 H     1.296396513309E-01 -3.631023820182E-01  1.852319263003E-01
   13 T   6 C     2.138726031419E-01 -7.089157262579E-02  2.435621964446E-01
   15 T   6 C     2.076127193783E-01 -3.038517499836E-02  3.873119201291E-01
   17 T   1 H     1.630095450373E-01 -1.431299838119E-01  4.224429571697E-01
   19 T   6 C     2.468659280249E-01  1.500871412866E-01  4.792810514377E-01
   21 T   1 H     2.318419200366E-01  1.824173329503E-01 -4.120195501295E-01
   23 T   6 C     2.976111891913E-01  2.924067713770E-01  4.303816840596E-01
   25 T   1 H     3.246413948104E-01  4.322372422082E-01 -4.982025448900E-01
   27 T   6 C     3.079260388883E-01  2.576985490627E-01  2.883247807655E-01
   29 T   6 C     3.549990574838E-01  4.019281312033E-01  2.349439764720E-01
   31 T   1 H     3.878957162129E-01 -4.577419895134E-01  3.080231723361E-01
   33 T   6 C     3.561924695054E-01  3.641169628622E-01  9.515668300205E-02
   35 T   1 H     3.888180734421E-01  4.739449675441E-01  5.550810646194E-02
   37 T   6 C     3.083948743747E-01  1.801310035218E-01 -4.280170975988E-03
   39 T   6 C     3.086603834326E-01  1.416380816632E-01 -1.485221235392E-01
   41 T   1 H     3.450244080609E-01  2.537398237146E-01 -1.856219850267E-01
   43 T   6 C     2.617998973249E-01 -3.761228289295E-02 -2.417820592514E-01
   45 T   1 H     2.663683670598E-01 -6.683165007248E-02 -3.524791942763E-01
   47 T   6 C     2.605196427477E-01  3.336615081531E-02  4.515729440259E-02
   49 T   6 C     2.622085801684E-01  7.337906926650E-02  1.922565981871E-01
   51 T   6 C     1.499354421126E-01 -3.655021980599E-01 -3.121952784944E-01
   53 T   1 H     1.614515868850E-01 -3.579064445344E-01 -4.174736757297E-01
   55 T   8 O     8.879665297464E-02  4.842212238616E-01 -3.046131291642E-01
```

2.5 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   483.470674 - DENSITY  1.580 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.66989780     7.93902198    10.12617725   108.694006 100.178775 100.403639
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.087355313265E-01 -1.849682048873E-01 -1.994921318862E-01
    3 T   6 C     2.102229115501E-01 -1.517024524302E-01 -5.300992209210E-02
    5 T   6 C     1.661004890806E-01 -2.948092141518E-01  2.604577426777E-03
    7 T   1 H     1.323405164590E-01 -4.348816896998E-01 -7.079405013297E-02
    9 T   6 C     1.673247826485E-01 -2.561558930871E-01  1.438512605288E-01
   11 T   1 H     1.295926872769E-01 -3.654534672014E-01  1.841580515401E-01
   13 T   6 C     2.136600963179E-01 -7.185490905908E-02  2.429640975965E-01
   15 T   6 C     2.079114007223E-01 -3.184116555809E-02  3.874146594617E-01
   17 T   1 H     1.630520990048E-01 -1.456024145353E-01  4.224017470837E-01
   19 T   6 C     2.476755611092E-01  1.494143306064E-01  4.801589351056E-01
   21 T   1 H     2.328370055979E-01  1.815799477995E-01 -4.104935834469E-01
   23 T   6 C     2.983912766951E-01  2.928378888475E-01  4.312908561632E-01
   25 T   1 H     3.256413121490E-01  4.331725181237E-01 -4.966506344777E-01
   27 T   6 C     3.082794996169E-01  2.586146746492E-01  2.885526179148E-01
   29 T   6 C     3.552322457628E-01  4.040445196505E-01  2.353173527104E-01
   31 T   1 H     3.878442848148E-01 -4.550202894262E-01  3.089141023545E-01
   33 T   6 C     3.560182752436E-01  3.664600906276E-01  9.490591602831E-02
   35 T   1 H     3.880508708360E-01  4.770195433503E-01  5.522270031456E-02
   37 T   6 C     3.082926418155E-01  1.817362943826E-01 -5.159359837485E-03
   39 T   6 C     3.088715304692E-01  1.436673163371E-01 -1.499090740059E-01
   41 T   1 H     3.452009414300E-01  2.567259156642E-01 -1.868617939415E-01
   43 T   6 C     2.624754535304E-01 -3.633791990707E-02 -2.437203591883E-01
   45 T   1 H     2.678936022221E-01 -6.541757577043E-02 -3.547560655972E-01
   47 T   6 C     2.603871192066E-01  3.385186997111E-02  4.416414882637E-02
   49 T   6 C     2.621231309422E-01  7.354847214202E-02  1.917843967476E-01
   51 T   6 C     1.497082805344E-01 -3.658910566061E-01 -3.147254114349E-01
   53 T   1 H     1.623055706382E-01 -3.579142933156E-01 -4.202097625861E-01
   55 T   8 O     8.703148848629E-02  4.828552822005E-01 -3.073155193186E-01
```

3.0 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   475.230336 - DENSITY  1.608 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.60787821     7.90591167    10.10503429   108.421080 101.339514  99.918697
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.069959491728E-01 -1.858194854776E-01 -1.989507290237E-01
    3 T   6 C     2.099658108537E-01 -1.525375027601E-01 -5.213154417424E-02
    5 T   6 C     1.667826906730E-01 -2.958572569026E-01  3.714032660185E-03
    7 T   1 H     1.321515282591E-01 -4.361274003505E-01 -6.987740129568E-02
    9 T   6 C     1.697031707640E-01 -2.571991269428E-01  1.453354166531E-01
   11 T   1 H     1.321181901572E-01 -3.666186731182E-01  1.857492961415E-01
   13 T   6 C     2.168269303800E-01 -7.271430457622E-02  2.446169891517E-01
   15 T   6 C     2.118998507513E-01 -3.284334094516E-02  3.892266471573E-01
   17 T   1 H     1.676627822381E-01 -1.470499440307E-01  4.240753742903E-01
   19 T   6 C     2.507375016866E-01  1.486249644083E-01  4.817731616094E-01
   21 T   1 H     2.357337632212E-01  1.808114511789E-01 -4.090174233818E-01
   23 T   6 C     3.003539900180E-01  2.923282916410E-01  4.326861412184E-01
   25 T   1 H     3.262384085120E-01  4.327922583711E-01 -4.956071315615E-01
   27 T   6 C     3.102075682641E-01  2.582016424432E-01  2.899510778996E-01
   29 T   6 C     3.566520661366E-01  4.038620563295E-01  2.365390007700E-01
   31 T   1 H     3.895780780518E-01 -4.550387868478E-01  3.101450284958E-01
   33 T   6 C     3.569222604178E-01  3.663101834945E-01  9.597262478662E-02
   35 T   1 H     3.893064049036E-01  4.771153188755E-01  5.626623962316E-02
   37 T   6 C     3.078859602478E-01  1.813602293774E-01 -4.310621515432E-03
   39 T   6 C     3.063427997815E-01  1.433992087067E-01 -1.494460588461E-01
   41 T   1 H     3.414670118226E-01  2.567895491342E-01 -1.865092367820E-01
   43 T   6 C     2.595431361955E-01 -3.689235022947E-02 -2.433502285937E-01
   45 T   1 H     2.635842707007E-01 -6.607010932609E-02 -3.546232409618E-01
   47 T   6 C     2.607749162318E-01  3.323257662673E-02  4.520111504245E-02
   49 T   6 C     2.642266339463E-01  7.292415301989E-02  1.931961334612E-01
   51 T   6 C     1.480954528546E-01 -3.669736479575E-01 -3.144467314604E-01
   53 T   1 H     1.603319685017E-01 -3.587003196282E-01 -4.199814416694E-01
   55 T   8 O     8.579054813436E-02  4.812903043699E-01 -3.072788739535E-01
```

3.5 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   468.491946 - DENSITY  1.631 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.52672334     7.91330861    10.08673577   108.712804 100.320807 100.752777
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.064957403351E-01 -1.865296621324E-01 -2.005314017250E-01
    3 T   6 C     2.100239954863E-01 -1.536655397563E-01 -5.341135717815E-02
    5 T   6 C     1.684147275419E-01 -2.976293531992E-01  2.316797717809E-03
    7 T   1 H     1.350965907987E-01 -4.381038982584E-01 -7.164039204951E-02
    9 T   6 C     1.718195640789E-01 -2.592326782474E-01  1.443084339779E-01
   11 T   1 H     1.357116945351E-01 -3.690634584752E-01  1.848610695869E-01
   13 T   6 C     2.181951861906E-01 -7.442322528889E-02  2.440901957888E-01
   15 T   6 C     2.144810271435E-01 -3.504888997367E-02  3.892777570197E-01
   17 T   1 H     1.710204502706E-01 -1.500112543657E-01  4.240054042141E-01
   19 T   6 C     2.531081587269E-01  1.467409883037E-01  4.824764140643E-01
   21 T   1 H     2.387642643006E-01  1.785727399592E-01 -4.077308960446E-01
   23 T   6 C     3.015169451285E-01  2.911551170023E-01  4.334615165414E-01
   25 T   1 H     3.269513667613E-01  4.316743610229E-01 -4.942478643622E-01
   27 T   6 C     3.104329804484E-01  2.575449000000E-01  2.901500014267E-01
   29 T   6 C     3.559644162588E-01  4.039619983838E-01  2.369532365328E-01
   31 T   1 H     3.886246476507E-01 -4.546881421531E-01  3.110700558513E-01
   33 T   6 C     3.551516430864E-01  3.666436065837E-01  9.587554268035E-02
   35 T   1 H     3.867295541697E-01  4.778193225412E-01  5.620238618206E-02
   37 T   6 C     3.061599327597E-01  1.813134956605E-01 -4.942124350998E-03
   39 T   6 C     3.039154692358E-01  1.437526401177E-01 -1.504925106163E-01
   41 T   1 H     3.379030215694E-01  2.578121646672E-01 -1.873476554758E-01
   43 T   6 C     2.581406658338E-01 -3.685272003801E-02 -2.448512135928E-01
   45 T   1 H     2.621336003235E-01 -6.588248721308E-02 -3.564394413611E-01
   47 T   6 C     2.602076284604E-01  3.249195890685E-02  4.441339441471E-02
   49 T   6 C     2.644889705612E-01  7.192549794815E-02  1.928150817335E-01
   51 T   6 C     1.477616777236E-01 -3.679846494665E-01 -3.165105096378E-01
   53 T   1 H     1.611841268915E-01 -3.592942195802E-01 -4.220410915890E-01
   55 T   8 O     8.416131789806E-02  4.794792140170E-01 -3.097123848090E-01
```

4.0 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   462.289863 - DENSITY  1.653 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.47855527     7.88013391    10.06144379   108.711414 100.345273 100.576512
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.058164709849E-01 -1.867073178128E-01 -2.015166303925E-01
    3 T   6 C     2.096691988460E-01 -1.539821786653E-01 -5.409794045638E-02
    5 T   6 C     1.680594078667E-01 -2.985253787546E-01  1.602591890813E-03
    7 T   1 H     1.346066028269E-01 -4.393639060015E-01 -7.263253240840E-02
    9 T   6 C     1.718199727927E-01 -2.601862538637E-01  1.439324064268E-01
   11 T   1 H     1.356726666712E-01 -3.703347248897E-01  1.845913053942E-01
   13 T   6 C     2.187603071297E-01 -7.494010518019E-02  2.440702214955E-01
   15 T   6 C     2.154584015847E-01 -3.575483966096E-02  3.896138623839E-01
   17 T   1 H     1.717767152230E-01 -1.513119072973E-01  4.241695712945E-01
   19 T   6 C     2.544307739916E-01  1.465632157834E-01  4.831466054987E-01
   21 T   1 H     2.401150402764E-01  1.784999260208E-01 -4.068072130939E-01
   23 T   6 C     3.028995773675E-01  2.915288982832E-01  4.341042628064E-01
   25 T   1 H     3.282664144866E-01  4.324169081388E-01 -4.934089144969E-01
   27 T   6 C     3.115708441018E-01  2.580756274310E-01  2.904831913105E-01
   29 T   6 C     3.571834632939E-01  4.051191715624E-01  2.373425134763E-01
   31 T   1 H     3.899856763278E-01 -4.531420030197E-01  3.117060584765E-01
   33 T   6 C     3.560262585465E-01  3.678258028489E-01  9.593734313368E-02
   35 T   1 H     3.875498232154E-01  4.794132851285E-01  5.625199162765E-02
   37 T   6 C     3.063946251036E-01  1.820437048466E-01 -5.257087577909E-03
   39 T   6 C     3.036278705307E-01  1.446393575018E-01 -1.511440853426E-01
   41 T   1 H     3.374976175757E-01  2.592157518167E-01 -1.879553716551E-01
   43 T   6 C     2.576243474952E-01 -3.646770973720E-02 -2.458153440501E-01
   45 T   1 H     2.615401782320E-01 -6.555996344880E-02 -3.576445531805E-01
   47 T   6 C     2.603403655903E-01  3.263584042664E-02  4.406072982338E-02
   49 T   6 C     2.651604523650E-01  7.198277221324E-02  1.928076208716E-01
   51 T   6 C     1.466482910679E-01 -3.685049044754E-01 -3.178391506725E-01
   53 T   1 H     1.603285764324E-01 -3.596557663634E-01 -4.235378324617E-01
   55 T   8 O     8.227804794008E-02  4.784331445965E-01 -3.111431138488E-01
```

4.5 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   456.631341 - DENSITY  1.673 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.44624189     7.84175411    10.03716119   108.550206 100.940384 100.206790
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.051821405422E-01 -1.868028645373E-01 -2.015806372407E-01
    3 T   6 C     2.094877899926E-01 -1.540615645115E-01 -5.387549179790E-02
    5 T   6 C     1.677186422194E-01 -2.990258237094E-01  1.943591275688E-03
    7 T   1 H     1.336581941075E-01 -4.402303641556E-01 -7.246555621519E-02
    9 T   6 C     1.720214783927E-01 -2.606264012148E-01  1.445802645411E-01
   11 T   1 H     1.354501058693E-01 -3.709968743125E-01  1.853604165952E-01
   13 T   6 C     2.197068857379E-01 -7.497337400544E-02  2.448873193595E-01
   15 T   6 C     2.165818678304E-01 -3.585458515477E-02  3.906293314084E-01
   17 T   1 H     1.728739307337E-01 -1.519072626483E-01  4.250764310389E-01
   19 T   6 C     2.552895916703E-01  1.469180384382E-01  4.841576107727E-01
   21 T   1 H     2.406464773565E-01  1.790042008694E-01 -4.057921473310E-01
   23 T   6 C     3.036703078381E-01  2.923106668905E-01  4.349661336951E-01
   25 T   1 H     3.285381705193E-01  4.335697786099E-01 -4.926983398761E-01
   27 T   6 C     3.126831113690E-01  2.588816620785E-01  2.912603167367E-01
   29 T   6 C     3.584597862165E-01  4.063636275652E-01  2.380118942876E-01
   31 T   1 H     3.913932811558E-01 -4.515311074129E-01  3.124102715841E-01
   33 T   6 C     3.573127843074E-01  3.690370675513E-01  9.641057757265E-02
   35 T   1 H     3.891608181195E-01  4.809906442753E-01  5.668274664897E-02
   37 T   6 C     3.069082730306E-01  1.828255808547E-01 -4.992825679947E-03
   39 T   6 C     3.033228491700E-01  1.454676209108E-01 -1.511955731040E-01
   41 T   1 H     3.367997006232E-01  2.604611880565E-01 -1.880975118232E-01
   43 T   6 C     2.569298050566E-01 -3.613997129781E-02 -2.459958125066E-01
   45 T   1 H     2.604269025372E-01 -6.539027615941E-02 -3.580258296970E-01
   47 T   6 C     2.607650368620E-01  3.298844985733E-02  4.445225642000E-02
   49 T   6 C     2.661426619720E-01  7.235802869014E-02  1.934928330980E-01
   51 T   6 C     1.457707855929E-01 -3.689744896359E-01 -3.181215250600E-01
   53 T   1 H     1.593231762723E-01 -3.599885373552E-01 -4.239723892716E-01
   55 T   8 O     8.127811911831E-02  4.774748427133E-01 -3.115018654362E-01
```

5.0 GPa

LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME= 451.843460 - DENSITY 1.691 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
6.41719719	7.80721097	10.00934505	108.619894	100.614419	100.209305

ATOMS IN THE ASYMMETRIC UNIT 28 - ATOMS IN THE UNIT CELL: 56

ATOM	X/A	Y/B	Z/C
1 T 6 C	2.053016545866E-01	-1.865131531451E-01	-2.026214257159E-01
3 T 6 C	2.093146551943E-01	-1.539253635944E-01	-5.465128317703E-02
5 T 6 C	1.671096256333E-01	-2.996437320520E-01	1.049019751569E-03
7 T 1 H	1.332785573819E-01	-4.413210912507E-01	-7.364880014647E-02
9 T 6 C	1.711060341781E-01	-2.612941652103E-01	1.439907703494E-01
11 T 1 H	1.344269444960E-01	-3.720839121873E-01	1.848923216828E-01
13 T 6 C	2.191090597005E-01	-7.503266347774E-02	2.446712973681E-01
15 T 6 C	2.160938425215E-01	-3.612720931305E-02	3.907965522708E-01
17 T 1 H	1.719717556949E-01	-1.528926578742E-01	4.250684365743E-01
19 T 6 C	2.551985205764E-01	1.473308827721E-01	4.847683079169E-01
21 T 1 H	2.403729607038E-01	1.795367279524E-01	-4.048690103733E-01
23 T 6 C	3.039932540396E-01	2.934598844430E-01	4.356264789051E-01
25 T 1 H	3.290885686181E-01	4.352209141637E-01	-4.916959530643E-01
27 T 6 C	3.130196984472E-01	2.602150209449E-01	2.915703644844E-01
29 T 6 C	3.591686173078E-01	4.084963261180E-01	2.384301981158E-01
31 T 1 H	3.921574248835E-01	-4.488567990250E-01	3.131329408955E-01
33 T 6 C	3.580661721917E-01	3.711705405728E-01	9.647502464611E-02
35 T 1 H	3.898285476818E-01	4.836580339425E-01	5.675724500856E-02
37 T 6 C	3.074404584080E-01	1.843413952755E-01	-5.336226892383E-03
39 T 6 C	3.041281908363E-01	1.471234815312E-01	-1.518526766252E-01
41 T 1 H	3.379069965604E-01	2.627376712814E-01	-1.886723292600E-01
43 T 6 C	2.576941858726E-01	-3.516061002542E-02	-2.470021572710E-01
45 T 1 H	2.617995126375E-01	-6.449553063260E-02	-3.592361022269E-01
47 T 6 C	2.608406555376E-01	3.375884904915E-02	4.403435974076E-02
49 T 6 C	2.660517727163E-01	7.305543888398E-02	1.933754716265E-01
51 T 6 C	1.453078723096E-01	-3.691902219255E-01	-3.194677266783E-01
53 T 1 H	1.589353234944E-01	-3.601370603054E-01	-4.256047727289E-01
55 T 8 O	8.015055224499E-02	4.766474818954E-01	-3.127829966909E-01

6.0 GPa

LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME= 441.729749 - DENSITY 1.730 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
6.34308196	7.75058340	9.97607251	108.332566	101.729969	99.524922

ATOMS IN THE ASYMMETRIC UNIT 28 - ATOMS IN THE UNIT CELL: 56

ATOM	X/A	Y/B	Z/C
1 T 6 C	2.036071099673E-01	-1.870917529155E-01	-2.026563042685E-01
3 T 6 C	2.088542074685E-01	-1.544142847295E-01	-5.424126879396E-02
5 T 6 C	1.667877994325E-01	-3.005796690891E-01	1.751766499183E-03
7 T 1 H	1.317105764019E-01	-4.427168837696E-01	-7.318152102728E-02
9 T 6 C	1.722430219813E-01	-2.621053622867E-01	1.451898300979E-01
11 T 1 H	1.348588553681E-01	-3.730793542904E-01	1.863061374681E-01
13 T 6 C	2.216966455892E-01	-7.535704998115E-02	2.460760736012E-01
15 T 6 C	2.192880065112E-01	-3.651502278657E-02	3.924948839267E-01
17 T 1 H	1.754520082704E-01	-1.539605213181E-01	4.266550907636E-01
19 T 6 C	2.578365331666E-01	1.475273419720E-01	4.862864994259E-01
21 T 1 H	2.427501868667E-01	1.800256286542E-01	-4.033782338400E-01
23 T 6 C	3.060494065698E-01	2.941218450564E-01	4.367689912582E-01
25 T 1 H	3.299599760935E-01	4.363412078477E-01	-4.909978091129E-01
27 T 6 C	3.153825877817E-01	2.608639786614E-01	2.926435995159E-01
29 T 6 C	3.614811051927E-01	4.096049925559E-01	2.392239529123E-01
31 T 1 H	3.949062605147E-01	-4.472858122185E-01	3.138812187017E-01
33 T 6 C	3.599791566923E-01	3.721792193949E-01	9.699743929730E-02
35 T 1 H	3.923891793943E-01	4.851085755440E-01	5.720886790807E-02
37 T 6 C	3.077156802190E-01	1.848467675155E-01	-5.072931709165E-03
39 T 6 C	3.023136809486E-01	1.476969714811E-01	-1.521023242463E-01
41 T 1 H	3.347513864178E-01	2.638541134779E-01	-1.891809286267E-01
43 T 6 C	2.553194954297E-01	-3.524577017879E-02	-2.473314859289E-01
45 T 1 H	2.581888215478E-01	-6.488687510827E-02	-3.599060320617E-01
47 T 6 C	2.614641415670E-01	3.378938875967E-02	4.460801371161E-02
49 T 6 C	2.682125790205E-01	7.318009236186E-02	1.944391166304E-01
51 T 6 C	1.436067943992E-01	-3.702345479093E-01	-3.197453579680E-01
53 T 1 H	1.572200771364E-01	-3.608945843524E-01	-4.260028205763E-01
55 T 8 O	7.834084485727E-02	4.749006594707E-01	-3.132472913854E-01

7.0 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   433.127704 - DENSITY  1.764 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.23525070     7.75275633     9.95036490   108.721511 100.414320 100.391594
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.022654605581E-01 -1.883005361941E-01 -2.047693505033E-01
    3 T   6 C     2.086481333398E-01 -1.559480861949E-01 -5.593459826940E-02
    5 T   6 C     1.683841523869E-01 -3.027558182054E-01 -2.550775762565E-05
    7 T   1 H     1.346687251914E-01 -4.452093615942E-01 -7.540599596902E-02
    9 T   6 C     1.746199105627E-01 -2.643228380385E-01  1.439068953299E-01
   11 T   1 H     1.391618452950E-01 -3.756371028877E-01  1.853209057945E-01
   13 T   6 C     2.234120894608E-01 -7.706595042981E-02  2.453258158332E-01
   15 T   6 C     2.226901241229E-01 -3.860339887217E-02  3.924659249722E-01
   17 T   1 H     1.798173138086E-01 -1.568631285739E-01  4.265253472749E-01
   19 T   6 C     2.613691692967E-01  1.459491506767E-01  4.870600196070E-01
   21 T   1 H     2.474911282688E-01  1.783619817055E-01 -4.017497884455E-01
   23 T   6 C     3.083556860780E-01  2.932226712683E-01  4.375740407707E-01
   25 T   1 H     3.321390486242E-01  4.355753493454E-01 -4.894041134692E-01
   27 T   6 C     3.163948171573E-01  2.603917029597E-01  2.926753902805E-01
   29 T   6 C     3.617340133981E-01  4.099219989041E-01  2.394797220060E-01
   31 T   1 H     3.953471992366E-01 -4.465460299379E-01  3.147401965356E-01
   33 T   6 C     3.584998430893E-01  3.724795656467E-01  9.655243480042E-02
   35 T   1 H     3.899122491983E-01  4.857477437073E-01  5.672261070944E-02
   37 T   6 C     3.057981929469E-01  1.845708500194E-01 -6.106208402937E-03
   39 T   6 C     2.989779787425E-01  1.476767540933E-01 -1.536968373767E-01
   41 T   1 H     3.300447627258E-01  2.645610600678E-01 -1.905116279145E-01
   43 T   6 C     2.526277851951E-01 -3.572555669620E-02 -2.495096879682E-01
   45 T   1 H     2.544147557038E-01 -6.551796901762E-02 -3.626648264825E-01
   47 T   6 C     2.608734461211E-01  3.281888030456E-02  4.345830111627E-02
   49 T   6 C     2.688369941776E-01  7.218107650945E-02  1.938027574909E-01
   51 T   6 C     1.422530658900E-01 -3.718563504898E-01 -3.223347330836E-01
   53 T   1 H     1.560170093343E-01 -3.622274742382E-01 -4.288968797967E-01
   55 T   8 O     7.647491649227E-02  4.723747320019E-01 -3.158357356953E-01
```

8.0 GPa

```
********************************************************************************
   LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=   425.396735 - DENSITY  1.796 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    6.19754468     7.69194356     9.91479377   108.345463 101.707400  99.675637
********************************************************************************
       ATOMS IN THE ASYMMETRIC UNIT   28 - ATOMS IN THE UNIT CELL:   56
         ATOM              X/A                 Y/B                  Z/C
********************************************************************************
    1 T   6 C     2.018817426063E-01 -1.879454162881E-01 -2.041187798543E-01
    3 T   6 C     2.084832341526E-01 -1.554450491413E-01 -5.493048862703E-02
    5 T   6 C     1.672219289391E-01 -3.027371760991E-01  1.254346449752E-03
    7 T   1 H     1.320996868803E-01 -4.457038294213E-01 -7.425697571053E-02
    9 T   6 C     1.740861413302E-01 -2.641600816840E-01  1.455894559717E-01
   11 T   1 H     1.370553216619E-01 -3.756705496938E-01  1.872006725797E-01
   13 T   6 C     2.243715208726E-01 -7.637740298473E-02  2.470930346193E-01
   15 T   6 C     2.233132261713E-01 -3.792245280821E-02  3.943843320173E-01
   17 T   1 H     1.802294526143E-01 -1.568371281348E-01  4.283602766334E-01
   19 T   6 C     2.613309878390E-01  1.472469245074E-01  4.886290721157E-01
   21 T   1 H     2.464848065145E-01  1.799847487126E-01 -4.003979964793E-01
   23 T   6 C     3.085117435684E-01  2.950089441043E-01  4.387590903936E-01
   25 T   1 H     3.311330565514E-01  4.379132204696E-01 -4.888669668079E-01
   27 T   6 C     3.177288608547E-01  2.620961716606E-01  2.939662997941E-01
   29 T   6 C     3.634909685053E-01  4.121044295900E-01  2.404417682686E-01
   31 T   1 H     3.971517824449E-01 -4.438801956003E-01  3.155217434677E-01
   33 T   6 C     3.609452676480E-01  3.745677095245E-01  9.738236764815E-02
   35 T   1 H     3.932203702935E-01  4.883320107140E-01  5.745848445520E-02
   37 T   6 C     3.071997320592E-01  1.861231571367E-01 -5.392653149942E-03
   39 T   6 C     2.994081846805E-01  1.492531644351E-01 -1.533780920883E-01
   41 T   1 H     3.298012152067E-01  2.666281946353E-01 -1.905416365917E-01
   43 T   6 C     2.525389385541E-01 -3.487850330470E-02 -2.491427980932E-01
   45 T   1 H     2.539801664122E-01 -6.496242376868E-02 -3.624971470143E-01
   47 T   6 C     2.617212856601E-01  3.387552872395E-02  4.450173818599E-02
   49 T   6 C     2.701925848208E-01  7.333241901067E-02  1.952135880302E-01
   51 T   6 C     1.416499967674E-01 -3.720029659158E-01 -3.218682758995E-01
   53 T   1 H     1.555573109787E-01 -3.621225800294E-01 -4.285482308431E-01
   55 T   8 O     7.540389546618E-02  4.715525684658E-01 -3.155758268772E-01
```

9.0 GPa

LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME= 418.483940 - DENSITY 1.826 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
6.13374652	7.66180956	9.88728458	108.388712	101.562259	99.635557

ATOMS IN THE ASYMMETRIC UNIT 28 - ATOMS IN THE UNIT CELL: 56

	ATOM	X/A	Y/B	Z/C
1	T 6 C	2.010456416484E-01	-1.884224541917E-01	-2.050786316133E-01
3	T 6 C	2.083047280786E-01	-1.560085204365E-01	-5.554325500592E-02
5	T 6 C	1.671728025567E-01	-3.038188888098E-01	6.875502235758E-04
7	T 1 H	1.320003276688E-01	-4.471759872558E-01	-7.508075214367E-02
9	T 6 C	1.744711843510E-01	-2.651665528312E-01	1.453980036362E-01
11	T 1 H	1.373973292332E-01	-3.768896753367E-01	1.872325827720E-01
13	T 6 C	2.253190087642E-01	-7.690512534447E-02	2.471938068515E-01
15	T 6 C	2.247516082284E-01	-3.861273776983E-02	3.948738643710E-01
17	T 1 H	1.816035355272E-01	-1.581723106876E-01	4.287066560617E-01
19	T 6 C	2.628560206416E-01	1.471181274505E-01	4.894121781329E-01
21	T 1 H	2.481515800078E-01	1.800807067843E-01	-3.992760200063E-01
23	T 6 C	3.098862130205E-01	2.953941473769E-01	4.394148411596E-01
25	T 1 H	3.322608339959E-01	4.386809211739E-01	-4.880622524446E-01
27	T 6 C	3.190024667595E-01	2.626098248203E-01	2.942882617568E-01
29	T 6 C	3.646964961939E-01	4.132023250073E-01	2.407457630803E-01
31	T 1 H	3.984293498376E-01	-4.423325153041E-01	3.159947546062E-01
33	T 6 C	3.616389581759E-01	3.755598125368E-01	9.729852874359E-02
35	T 1 H	3.937365640768E-01	4.896918675438E-01	5.730575110229E-02
37	T 6 C	3.072380144519E-01	1.866224269414E-01	-5.799569750310E-03
39	T 6 C	2.983792698427E-01	1.498791671437E-01	-1.542113044219E-01
41	T 1 H	3.280357953733E-01	2.678083599459E-01	-1.913856243026E-01
43	T 6 C	2.513410246134E-01	-3.481868085126E-02	-2.502550576585E-01
45	T 1 H	2.521210363622E-01	-6.514760905397E-02	-3.639768175455E-01
47	T 6 C	2.619636386076E-01	3.383052819050E-02	4.416101914105E-02
49	T 6 C	2.711351026751E-01	7.333697425001E-02	1.952495911512E-01
51	T 6 C	1.406365198174E-01	-3.728873385773E-01	-3.230531576902E-01
53	T 1 H	1.543556196610E-01	-3.628474309888E-01	-4.300065503741E-01
55	T 8 O	7.434869663662E-02	4.700227628222E-01	-3.166579015090E-01

10.0 GPa

LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME= 412.136113 - DENSITY 1.854 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
6.09063855	7.61857664	9.85907445	108.240387	102.052177	99.249027

ATOMS IN THE ASYMMETRIC UNIT 28 - ATOMS IN THE UNIT CELL: 56

	ATOM	X/A	Y/B	Z/C
1	T 6 C	2.003532008816E-01	-1.885158682413E-01	-2.053515750829E-01
3	T 6 C	2.080408485158E-01	-1.560554572935E-01	-5.549441247981E-02
5	T 6 C	1.664590151213E-01	-3.043232343845E-01	8.857044381804E-04
7	T 1 H	1.306319396748E-01	-4.480936515190E-01	-7.504378438033E-02
9	T 6 C	1.742506817891E-01	-2.655530889039E-01	1.459479186593E-01
11	T 1 H	1.363952895282E-01	-3.774262765631E-01	1.879930503050E-01
13	T 6 C	2.261513324390E-01	-7.684658570098E-02	2.479126599176E-01
15	T 6 C	2.256008105206E-01	-3.864017735539E-02	3.958316873254E-01
17	T 1 H	1.822362103007E-01	-1.588069262428E-01	4.295537156553E-01
19	T 6 C	2.635022072186E-01	1.476601883846E-01	4.903269490150E-01
21	T 1 H	2.483896040099E-01	1.809357837739E-01	-3.983182658446E-01
23	T 6 C	3.106650596348E-01	2.963934111389E-01	4.400891899218E-01
25	T 1 H	3.324070414183E-01	4.401414343842E-01	-4.876473168217E-01
27	T 6 C	3.203072319501E-01	2.636035364360E-01	2.948769582651E-01
29	T 6 C	3.662121319012E-01	4.146657541464E-01	2.411651656655E-01
31	T 1 H	4.001229691420E-01	-4.404175439912E-01	3.163961120894E-01
33	T 6 C	3.632400651695E-01	3.769210475309E-01	9.750061280803E-02
35	T 1 H	3.956994598990E-01	4.914836842911E-01	5.747986006165E-02
37	T 6 C	3.079486677281E-01	1.875321532533E-01	-5.811729913595E-03
39	T 6 C	2.981262861591E-01	1.508738259747E-01	-1.545949697194E-01
41	T 1 H	3.270952374285E-01	2.692926232078E-01	-1.919586714930E-01
43	T 6 C	2.505952978924E-01	-3.444309827923E-02	-2.507498243117E-01
45	T 1 H	2.508478701402E-01	-6.502070305205E-02	-3.647387702673E-01
47	T 6 C	2.624874167169E-01	3.427042045555E-02	4.434592274804E-02
49	T 6 C	2.722118478832E-01	7.384230711349E-02	1.957672914626E-01
51	T 6 C	1.396615255511E-01	-3.734121238998E-01	-3.234659686054E-01
53	T 1 H	1.529603801974E-01	-3.632048627638E-01	-4.306687639177E-01
55	T 8 O	7.349090812396E-02	4.689065797870E-01	-3.169888923342E-01

Table S6: Dependence of calculated HOCO energy, LUCO energy and band gap of PA on external pressure (see Figure 8 in main text).

Pressure [GPa]	LUCO energy [eV]	HOCO energy [eV]	Band gap [eV]
0	-5.169152	-2.499394	2.669758
0.5	-5.114240	-2.484861	2.629379
1	-5.079669	-2.505557	2.574112
1.5	-5.051219	-2.511135	2.540084
2	-4.988306	-2.504066	2.484240
2.5	-4.972082	-2.500043	2.472040
3	-4.906713	-2.487562	2.419151
3.5	-4.877432	-2.465859	2.411572
4	-4.843791	-2.460964	2.382826
4.5	-4.798022	-2.454185	2.343837
5	-4.779292	-2.452504	2.326788
6	-4.684199	-2.435033	2.249166
7	-4.633967	-2.397317	2.236650
8	-4.540569	-2.385291	2.155279
9	-4.480218	-2.364562	2.115656
10	-4.407889	-2.347536	2.060353