ELECTRONIC SUPPORTING INFORMATION

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1. Procedure of energy calculations in CRYSTAL

1.1 Energy of interaction between single molecules

The calculation procedure of energy of intermolecular interactions between single molecules is rather complicated and has many steps. Additionally, the method differs depending on type of molecules involved in interaction. In the case when both interacting molecules are of the same type (two A molecules or two B molecules) procedure goes as follows. In the first step is calculated value of energy for single molecule (without any neighboring molecules) with empirical dispersion correction as well without it (Civalleri *et al.* 2008). Let's call them E_1 and E_{1+DC}.In the second step, similar calculation (with dispersion correction) is conducted, which gives us E_{2+DC},but this time for pair of interacting molecules (two interacting molecules only). Such a pair of interacting molecule we call a dimer. Because the common and general definition of a dimer is molecular complex consisting of two identical molecules linked together we think that use of such a nomenclature is justified. In the third step we calculate energy of such a dimer (energy without dispersion correction), which gives us E_3 , but atoms which belongs to second molecule are transformed into so called "ghosts" (by deleting the nuclear charge and the shell electron charges, but leaving the basis set centered at the atomic position). All described here energy calculations were conducted in CRYSTAL program package and "GHOSTS" option is implemented in this software. In a nutshell, this option is useful to evaluate the basis set superposition error (BSSE), in a periodic system. The periodic structure is maintained, and the energy of the isolated components computed, leaving the basis set of the other one(s) unaltered. For further information reader should look into proper manual devoted for CRYSTAL software. In the fourth step we act as in step 3rd but this time atoms which belong to first molecule are transformed into "ghosts" atoms and in this way we obtained energy E_4. In the fifth step we calculate BSSE for first molecule by subtracting from value of energy obtained in first step (without dispersion correction) energy calculated in third step ($E_1 - E_3 = E_{BSSE\_1}$). In the sixth step we calculate BSSE for second molecule by subtracting from value of energy obtained in first step (without dispersion correction) energy calculated in fourth step ($E_1 - E_4 = E_{BSSE\_2}$). Finally, our recipe for energy of interaction (E_{int}) between two molecules is as follows: ($E_{int} = E_{2+DC} -(2*E_{1+DC}) + E_{BSSE\_1} + E_{BSSE\_2}$). In the case when one of interacting molecules is type A and second one is type B procedure goes as follows. In the first step is calculated value of energy for single molecule type A and for single molecule type B (without any neighboring molecules) with empirical dispersion correction as well without it. In this way, as a result we obtain: E_{A1}, E_{A1+DC}, E_{B1} and E_{B1+DC}. Steps from 2 to 4 are in fact the same. We must just remember that this time our dimer consists of molecule type A and type B. That is why in fifth step we calculate BSSE in this way: $E_{A1} - E_3 = E_{BSSE\_1}$, and in the sixth step in this way: $E_{B1} - E_4 = E_{BSSE\_2}$ (we assume that type A molecule is molecule "first" in our dimer and type B molecule is molecule "second" in our dimer). Finally, our recipe for energy of interaction (E_{int}) between

two molecules (one A type and second B type) is as follows: (E_{int} = E_{2+DC} - E_{A1+DC} - E_{B1+DC} + E_{BSSE_1} + E_{BSSE_2}).

1.2 Energy of interactions between columns

The calculation procedure of energy of intermolecular interactions between columns of molecules is as follows. In the first step was calculated energy of separate column built of A type molecules and energy of separate column built of B type molecules. In the second step, were calculated energies of pairs of columns (column 1 with column 2, column 1 with column 3 and so on). Finally, from calculated energy of pairs of columns were subtracted energies of separate columns. Obviously, it was taken into account whether interacting columns are built of A type molecules, B type molecules or both and proper values calculated in step 1 were used.

1.3 Energy of interactions between double-columns

The calculation procedure of energy of intermolecular interactions between double-column is as follows. In the first step was calculated energy of separate central stake. Then, were calculated energies of pairs of double-column (central one with neighbouring double-column, six interactions in total). Finally, from calculated in this way energy of pair of interacting double-column was subtracted doubled energy of separate stake and, to obtain energy per column, this value was divided by two.

2. Data for charts on Figure 12

Table S1. Figure 12a. length of hydrogen bonds.

Green trendline in figure*			Blue trendline in figure**	
Pressure [GPa]	Distance [angstrom]		Pressure [GPa]	Distance [angstrom]
0	2.709		0	2.673
0.39	2.68		0.39	2.649
0.85	2.66		0.85	2.631
1.41	2.637		1.41	2.608
1.82	2.617		1.82	2.591
2.08	2.611		2.08	2.584
2.15	2.607		2.15	2.574
2.51	2.613		2.51	2.579
2.86	2.592		2.86	2.565
2.94	2.59		2.94	2.564
3.36	2.582		3.36	2.555
3.78	2.573		3.78	2.548
4.86	2.554		4.86	2.527
6.12	2.515		6.12	2.487
7.5	2.514		7.5	2.487

*green trendline correspond with OH...O bond between A type (donor) and B type (acceptor) molecule

**blue trendline correspond with OH...O bond between B type (donor) and A type (acceptor) molecule

Table S2. Figure 12b - Distances between parallel pyrene rings of neighbouring molecules lined up in columns.

Green trendline - A type molecules			Blue trendline - B type molecules	
Pressure [GPa]	Distance [angstrom]		Pressure [GPa]	Distance [angstrom]
0	3.405		0	3.413
0.39	3.379		0.39	3.382
0.85	3.347		0.85	3.347
1.41	3.313		1.41	3.313
1.82	3.297		1.82	3.296
2.08	3.282		2.08	3.281
2.51	-		2.51	3.248
2.86	-		2.86	3.231
2.94	3.236		2.94	3.234
3.36	3.216		3.36	3.215
3.78	3.198		3.78	3.193
4.86	3.152		4.86	3.152
6.12	3.126		6.12	3.123
7.5	3.065		7.5	3.065

Table S3. Figure 12c - Energy of intermolecular interaction between molecules connected by hydrogen bond.

Green trendline*			Blue trendline**	
Pressure [GPa]	Energy [kJ/mol]		Pressure [GPa]	Energy [kJ/mol]
0	-26.51		0	-27.098
0.39	-24.891		0.39	-26.111
0.85	-24.306		0.85	-25.079
1.41	-22.329		1.41	-23.199
2.86	-19.755		2.86	-18.033
4.86	-14.636		4.86	-15.04
7.5	-9.3614		7.5	-9.6765

*green trendline correspond with OH...O bond between A type (donor) and B type (acceptor) molecule

**blue trendline correspond with OH...O bond between B type (donor) and A type (acceptor) molecule

Table S4. Figure 12d - Energy of intermolecular interaction between neighbouring molecules with parallel pyrene rings.

Green trendline - A type molecules			Blue trendline - B type molecules	
Pressure [GPa]	Energy [kJ/mol]		Pressure [GPa]	Energy [kJ/mol]
0	-39.44		0	-39.685
0.39	-39.648		0.39	-40.056
0.85	-39.517		0.85	-39.875
1.41	-39.103		1.41	-39.634
2.86	-37.883		2.86	-37.206
4.86	-31.998		4.86	-33.119
7.5	-23.099		7.5	-24.441

Table S5. Angle between planes defined by pyrene rings, which belongs to different stacks of molecules.

Pressure [GPa]	Angle[deg.]
0	30.38
0.39	29.5
0.85	29.04
1.41	28.31
1.82	27.56
2.08	27.42
2.15	27.27
2.51	27.43
2.86	27.11
2.94	27.08
3.36	26.77
3.78	26.63
4.86	26.09
7.5	25.27

3. Multi-temperature X-ray measurements, tables of unit-cell parameters

Table S6. Table of unit-cell parameters in function of temperature.

Pressure/GPa	atm.	atm.	atm.	atm.
Temperature/K	310.02(10)	300.00(10)	279.99(10)	270.02(10)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
X-ray λ/Å	1.54184	1.54184	1.54184	1.54184
Space group	P 1 21 1	P 1 21 1	P 1 21 1	P 1 21 1
a/Å	13.8797(9)	13.8662(7)	13.8533(6)	13.8493(6)
b/Å	4.5834(2)	4.58166(18)	4.57353(17)	4.56956(16)
c/Å	16.6647(10)	16.6568(7)	16.6470(7)	16.6429(7)
β/°	89.990(6)	90.015(4)	90.006(4)	89.995(4)
Volume/Å^3	1060.14(11)	1058.21(8)	1054.73(7)	1053.25(7)
R_{int}	0.0434	0.0311	0.0299	0.034
Refl. collected	7035	7106	7084	7015
2Θ range for data collection	76.3577 2.6515	76.1116 2.6527	76.1454 2.6543	76.2169 2.655
Pressure/GPa	atm.	atm.	atm.	atm.
Temperature/K	259.98(10)	250.02(10)	239.98(10)	230.01(10)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
X-ray λ/Å	1.54184	1.54184	1.54184	1.54184
Space group	P 1 21 1	P 1 21 1	P 1 21 1	P 1 21 1
a/Å	13.8462(7)	13.8377(7)	13.8327(7)	13.8253(6)
b/Å	4.56671(18)	4.56471(18)	4.56126(18)	4.55989(15)
c/Å	16.6389(7)	16.6313(7)	16.6307(7)	16.6167(6)
β/°	90.008(4)	89.998(4)	90.013(4)	89.995(4)
Volume/Å^3	1052.11(8)	1050.52(8)	1049.30(8)	1047.55(6)
R_{int}	0.0293	0.0353	0.0318	0.0332
Refl. collected	7066	6992	7044	7037
2Θ range for data collection	76.2701 2.6556	76.416 2.6568	76.2677 2.6569	76.3619 2.6591
Pressure/GPa	atm.	atm.	atm.	atm.
Temperature/K	219.98(10)	210.02(10)	199.97(10)	190.03(10)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
X-ray λ/Å	1.54184	1.54184	1.54184	1.54184
Space group	P 1 21 1	P 1 21 1	P 1 21 1	P 1 21 1
a/Å	13.8211(6)	13.8115(5)	13.8039(5)	13.7983(5)
b/Å	4.55654(16)	4.55379(14)	4.55103(13)	4.54885(13)
c/Å	16.6176(6)	16.6052(5)	16.6046(5)	16.5972(5)
β/°	90.009(4)	90.010(3)	90.002(3)	90.021(3)
Volume/Å^3	1046.52(7)	1044.37(6)	1043.14(6)	1041.74(5)
R_{int}	0.0324	0.0329	0.0293	0.0323
Refl. collected	7038	7018	7013	7006
2Θ range for data collection	76.2976 2.659	76.3759 2.661	76.1689 2.6611	76.6037 2.6623

Pressure/GPa	atm.	atm.	atm.	atm.
Temperature/K	179.97(10)	170.03(10)	159.98(10)	150.03(10)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
X-ray λ/Å	1.54184	1.54184	1.54184	1.54184
Space group	P 1 21 1	P 1 21 1	P 1 21 1	P 1 21 1
a/Å	13.7934(4)	13.7896(5)	13.7827(5)	13.7768(4)
b/Å	4.54536(12)	4.54222(14)	4.54004(14)	4.53799(13)
c/Å	16.5872(5)	16.5883(5)	16.5843(5)	16.5780(5)
β/°	90.021(3)	90.024(3)	90.026(3)	90.020(3)
Volume/Å^3	1039.95(5)	1039.02(6)	1037.75(6)	1036.44(5)
R_{int}	0.0302	0.0313	0.0322	0.0328
Refl. collected	6989	6966	6961	6941
2Θ range for data collection	76.4337 2.6639	76.4391 2.6637	76.5164 2.6643	76.2451 2.6654
Pressure/GPa	atm.	atm.	atm.	atm.
Temperature/K	139.99(10)	130.02(10)	122(3)	110.02(12)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
X-ray λ/Å	1.54184	1.54184	1.54184	1.54184
Space group	P 1 21 1	P 1 21 1	P 1 21 1	P 1 21 1
a/Å	13.7702(4)	13.7678(4)	13.7629(4)	13.7570(5)
b/Å	4.53628(13)	4.53466(13)	4.53230(13)	4.53003(14)
c/Å	16.5687(5)	16.5652(5)	16.5628(5)	16.5589(5)
β/°	90.011(3)	90.025(3)	90.038(3)	90.035(3)
Volume/Å^3	1034.97(5)	1034.20(5)	1033.15(5)	1031.94(6)
R_{int}	0.029	0.0307	0.0293	0.0321
Refl. collected	6931	6916	6908	6901
2Θ range for data collection	76.3652 2.6669	76.2627 2.6674	76.2026 2.6678	76.5398 2.6684
Pressure/GPa	atm.	atm.		
Temperature/K	104(6)	90.1(4)		
Crystal system	monoclinic	monoclinic		
X-ray λ/Å	1.54184	1.54184		
Space group	P 1 21 1	P 1 21 1		
a/Å	13.7588(4)	13.7503(4)		
b/Å	4.52816(13)	4.52597(12)		
c/Å	16.5509(5)	16.5449(5)		
β/°	90.024(3)	90.024(3)		
Volume/Å^3	1031.16(5)	1029.65(5)		
R_{int}	0.0329	0.0311		
Refl. collected	6889	6874		
2Θ range for data collection	76.4045 2.6697	76.513 2.6707		

4. Multi-pressure X-ray measurements, tables of unit-cell parameters

Table S7. Table of unit-cell parameters in function of pressure.

Pressure / GPa	0.38(5)	0.62(5)	0.80(5)	0.88(5)
Temperature/K	296.54(13)	296.41(16)	296.00(15)	296.1(2)
X-ray wavelength/Å	0.56087	0.56087	0.56087	0.56087
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P 1 21 1	P 1 21 1	P 1 21 1	P 1 21 1
a/Å	13.784(4)	13.691(4)	13.44(8)	13.609(3)
b/Å	4.536(2)	4.4836(14)	4.4486(17)	4.4437(12)
c/Å	16.46(9)	16.45(9)	16.453(9)	16.29(5)
β/°	90.04(8)	90.05(9)	90.80(16)	90.37(5)
Volume/Å^3	1029(6)	1010(6)	983(6)	985(3)
R_{int}	0.1423	0.1268	0.1662	0.1489
Refl. collected	417	410	3225	2104
2Θ range for data collection	16.0459 2.3319	16.4042 2.3478	17.1422 1.9537	17.1094 2.362
Pressure / GPa	1.30(5)	1.55(5)	1.70(5)	2.12(5)
Temperature/K	296.1(5)	295.76(11)	296.0(2)	295.6(2)
X-ray λ/Å	0.56087	0.56087	0.56087	0.56087
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P 1 21 1	P 1 21 1	P 1 21 1	P 1 21 1
a/Å	13.447(8)	13.41(8)	13.357(7)	13.31(9)
b/Å	4.3913(14)	4.3464(19)	4.3764(11)	4.3077(17)
c/Å	16.27(17)	16.265(13)	16.18(15)	16.228(11)
β/°	90.33(16)	90.57(17)	90.23(16)	90.27(19)
Volume/Å^3	961(10)	948(6)	946(9)	931(6)
R_{int}	0.1873	0.1333	0.1356	0.0452
Refl. collected	321	1643	422	523
2Θ range for data collection	17.144 3.5871	17.1479 1.9763	17.1281 2.6073	17.1471 1.9807
Pressure / GPa	2.27(5)	2.83(5)	3.10(5)	3.20(5)
Temperature/K	296.04(13)	295.8(3)	296.0(5)	295.7(5)
X-ray λ/Å	0.56087	0.56087	0.56087	0.56087
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P 1 21 1	P 1 21 1	P 1 21 1	P 1 21 1
a/Å	13.354(4)	13.07(4)	12.757(13)	13.00(6)
b/Å	4.4408(10)	4.2836(8)	4.200(6)	4.2589(13)
c/Å	15.50(6)	16.240(5)	16.6(7)	16.306(5)
β/°	90.06(8)	90.57(8)	91.1(5)	90.90(10)
Volume/Å^3	919(3)	909(3)	890(30)	903(4)
R_{int}	0.2209	0.0825	0.6039	0.1142
Refl. collected	1948	1518	356	2503
2Θ range for data collection	17.1322 2.4072	17.1321 1.9793	17.0938 3.6333	17.0704 1.9715

5. Equation of state, atomic positions under pressure (0.01-7.5 GPa)

Lattice parameters (angstrom and degrees). Atoms in the asymmetric unit - 54, atoms in the unit cell - 108.

Table S8. Pressure = 0.01 GPa

VOLUME = 1016.540584 DENSITY = 1.425 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.70010264	4.48454192	16.54657524	90.000000	89.381489	90.000000

ATOM	X/A	Y/B	Z/C
1 T 8 O	-3.616916225637E-01	-2.719844625920E-01	4.291948428965E-01
2 T 1 H	-3.611723315599E-01	-7.339728181838E-02	4.033333500704E-01
3 T 6 C	-2.857628664907E-01	-3.154051414731E-01	4.819507038124E-01
4 T 6 C	-1.951372794762E-01	-1.803965774358E-01	4.697622842694E-01
5 T 6 C	-3.023538375878E-01	4.848568716700E-01	-4.537891177960E-01
6 T 1 H	-1.851128879155E-01	-2.627155016789E-02	4.198363510111E-01
7 T 6 C	-1.183946315366E-01	-2.436018765335E-01	-4.785029478563E-01
8 T 6 C	-2.234111121325E-01	4.206173668323E-01	-4.012478739112E-01
9 T 6 C	-3.953610183038E-01	3.458172793875E-01	-4.394628386166E-01
10 T 1 H	-4.834593953566E-02	-1.352117673096E-01	-4.875120042179E-01
11 T 6 C	-1.304275077420E-01	-4.438216262479E-01	-4.141569725075E-01
12 T 6 C	-2.376858445758E-01	2.204820180843E-01	-3.352202046555E-01
13 T 1 H	-4.555080053602E-01	3.966797618345E-01	-4.791155454723E-01
14 T 6 C	-4.081738568273E-01	1.523003218917E-01	-3.768158339688E-01
15 T 6 C	-5.253526275162E-02	4.849197909089E-01	-3.601973182153E-01
16 T 6 C	-3.304582264428E-01	8.402627304760E-02	-3.223728756923E-01
17 T 6 C	-1.592480129792E-01	1.566447125352E-01	-2.819255363043E-01
18 T 1 H	-4.779500785123E-01	4.401815728834E-02	-3.670524647171E-01
19 T 1 H	1.775197447157E-02	-4.088224462991E-01	-3.700166089787E-01
20 T 6 C	-6.619790600278E-02	2.943579777703E-01	-2.971395295718E-01
21 T 6 C	-3.429560701557E-01	-1.136753763793E-01	-2.573401144830E-01
22 T 6 C	-1.755334784131E-01	-3.894299056509E-02	-2.169475307382E-01
23 T 1 H	-6.580624792983E-03	2.466482554814E-01	-2.565858354633E-01
24 T 1 H	-4.130960531384E-01	-2.214982929251E-01	-2.484555999095E-01
25 T 6 C	-2.663043402445E-01	-1.736771519487E-01	-2.051944957009E-01
26 T 1 H	-1.160757087883E-01	-8.766418180876E-02	-1.760606803203E-01

27	T	1	H	-2.768823565561E-01	-3.288589992984E-01	-1.556329977782E-01
55	T	8	O	3.696749460152E-01	-2.671287411629E-01	-3.395861199988E-01
56	T	1	H	3.612014304309E-01	-7.242493346889E-02	-3.668290453510E-01
57	T	6	C	2.994350148212E-01	-3.193988715883E-01	-2.811798609904E-01
58	T	6	C	2.063841151930E-01	-1.943848561094E-01	-2.858960701240E-01
59	T	6	C	3.235929684304E-01	4.814955882177E-01	-2.187232433080E-01
60	T	1	H	1.898070323570E-01	-3.733257408273E-02	-3.337635098341E-01
61	T	6	C	1.347206709542E-01	-2.738464686178E-01	-2.296965176072E-01
62	T	6	C	2.496618142718E-01	4.009068322241E-01	-1.616138134157E-01
63	T	6	C	4.197325558725E-01	3.585134580673E-01	-2.106844014147E-01
64	T	1	H	6.233272424681E-02	-1.786944985329E-01	-2.343357148466E-01
65	T	6	C	1.537387452007E-01	-4.793416237500E-01	-1.681199954671E-01
66	T	6	C	2.715735202134E-01	1.970048454059E-01	-9.818721648910E-02
67	T	1	H	4.752124313471E-01	4.192064506124E-01	-2.548202668001E-01
68	T	6	C	4.408572717906E-01	1.690614683521E-01	-1.490041589253E-01
69	T	6	C	7.993912723989E-02	4.253727925092E-01	-1.115359484435E-01
70	T	6	C	3.678819084871E-01	8.004204404964E-02	-9.090008889906E-02
71	T	6	C	1.970313717298E-01	1.084667352633E-01	-4.225978584892E-02
72	T	1	H	-4.860441665227E-01	7.888219274837E-02	-1.435105745763E-01
73	T	1	H	6.675496758244E-03	-4.855951838173E-01	-1.179929757531E-01
74	T	6	C	1.003478101338E-01	2.274974965676E-01	-5.166723522817E-02
75	T	6	C	3.879772039338E-01	-1.209981162429E-01	-2.818807075644E-02
76	T	6	C	2.202745486764E-01	-9.468008135703E-02	1.909393977574E-02
77	T	1	H	4.324220134670E-02	1.565932390229E-01	-1.001239767737E-02
78	T	1	H	4.608661585282E-01	-2.137613886247E-01	-2.331079960945E-02
79	T	6	C	3.146935112750E-01	-2.072016963398E-01	2.593563962007E-02
80	T	1	H	1.637885089071E-01	-1.678896347475E-01	6.117325178814E-02
81	T	1	H	3.302869312833E-01	-3.661035385280E-01	7.346046807718E-02

Table S9. Pressure = 0.39GPa

VOLUME = 993.684257 DENSITY = 1.458 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.62084709	4.39350457	16.60567367	90.000000	89.406636	90.000000

	ATOM	X/A	Y/B	Z/C
1	T 8 O	-3.608566217541E-01	-2.680519822360E-01	4.289360647118E-01
2	T 1 H	-3.600420882043E-01	-6.620251717167E-02	4.024857692572E-01
3	T 6 C	-2.846478644109E-01	-3.132050192031E-01	4.815773871274E-01
4	T 6 C	-1.929581712130E-01	-1.795605244165E-01	4.690738430858E-01
5	T 6 C	-3.022615071253E-01	4.865211625173E-01	-4.538123470646E-01
6	T 1 H	-1.822671575735E-01	-2.441787933192E-02	4.189522963907E-01
7	T 6 C	-1.161571902599E-01	-2.445954569957E-01	-4.790400766146E-01
8	T 6 C	-2.232602726195E-01	4.203879984384E-01	-4.011486942225E-01
9	T 6 C	-3.963783219728E-01	3.489899189822E-01	-4.393178970682E-01
10	T 1 H	-4.528573117649E-02	-1.370675782819E-01	-4.881721428999E-01
11	T 6 C	-1.292448276866E-01	-4.453409083438E-01	-4.142924397715E-01
12	T 6 C	-2.385601940961E-01	2.197588703567E-01	-3.347686398089E-01
13	T 1 H	-4.565045374390E-01	4.012979704612E-01	-4.791539021144E-01
14	T 6 C	-4.101340995482E-01	1.546933867006E-01	-3.763489719979E-01
15	T 6 C	-5.143241844153E-02	4.822610557268E-01	-3.600387507791E-01
16	T 6 C	-3.323961354412E-01	8.462216287333E-02	-3.217645673691E-01
17	T 6 C	-1.601358134423E-01	1.544454800469E-01	-2.812467048320E-01
18	T 1 H	-4.806217021091E-01	4.663226444541E-02	-3.664788741192E-01
19	T 1 H	1.954392283639E-02	-4.114024173490E-01	-3.698285146964E-01
20	T 6 C	-6.612418680189E-02	2.916105162947E-01	-2.965598594835E-01
21	T 6 C	-3.458816132198E-01	-1.139487971272E-01	-2.564476271794E-01
22	T 6 C	-1.774004033676E-01	-4.179178217475E-02	-2.159597541144E-01
23	T 1 H	-6.611587552031E-03	2.440277905549E-01	-2.556624515519E-01
24	T 1 H	-4.168361539762E-01	-2.209446801383E-01	-2.474349393741E-01
25	T 6 C	-2.691851321998E-01	-1.758613324063E-01	-2.041629763929E-01
26	T 1 H	-1.179314331766E-01	-9.182468623119E-02	-1.748953948250E-01
27	T 1 H	-2.805359454196E-01	-3.322646157978E-01	-1.544686408507E-01
55	T 8 O	3.691458713099E-01	-2.637706477033E-01	-3.384494185835E-01
56	T 1 H	3.602969329712E-01	-6.609435334337E-02	-3.662839107680E-01
57	T 6 C	2.982828876609E-01	-3.173892899414E-01	-2.804892047320E-01
58	T 6 C	2.044299242021E-01	-1.923935903742E-01	-2.858820991385E-01
59	T 6 C	3.228390426104E-01	4.824658695587E-01	-2.176888198317E-01
60	T 1 H	1.875463898896E-01	-3.411102147984E-02	-3.339848327239E-01

61	T	6	C	1.323932396606E-01	-2.730709018181E-01	-2.298760738959E-01
62	T	6	C	2.485081346988E-01	4.010462132071E-01	-1.607478437031E-01
63	T	6	C	4.197297480402E-01	3.592838151558E-01	-2.091516099838E-01
64	T	1	H	5.939359114806E-02	-1.782417746926E-01	-2.349843546735E-01
65	T	6	C	1.517995133776E-01	-4.795861989713E-01	-1.678874202523E-01
66	T	6	C	2.708086176014E-01	1.964988824969E-01	-9.687577582970E-02
67	T	1	H	4.754215471237E-01	4.198263048888E-01	-2.532945434938E-01
68	T	6	C	4.412383694190E-01	1.695574864824E-01	-1.469958895348E-01
69	T	6	C	7.756644665202E-02	4.237528050225E-01	-1.115206498297E-01
70	T	6	C	3.679019185773E-01	8.004531574372E-02	-8.899967707460E-02
71	T	6	C	1.958796144778E-01	1.069219667555E-01	-4.109455888097E-02
72	T	1	H	-4.851384901484E-01	7.900070107926E-02	-1.410911810800E-01
73	T	1	H	3.702266596824E-03	-4.875852841658E-01	-1.185300260164E-01
74	T	6	C	9.837351067135E-02	2.252235684139E-01	-5.117028862120E-02
75	T	6	C	3.884112195962E-01	-1.216097833302E-01	-2.583573738556E-02
76	T	6	C	2.195696349619E-01	-9.676965625258E-02	2.076872095959E-02
77	T	1	H	4.098721880653E-02	1.532347566282E-01	-9.649176522354E-03
78	T	1	H	4.618975138487E-01	-2.143635098948E-01	-2.059384310824E-02
79	T	6	C	3.147914391825E-01	-2.088216809919E-01	2.817327184231E-02
80	T	1	H	1.628386874639E-01	-1.708992452729E-01	6.279732926582E-02
81	T	1	H	3.307087454184E-01	-3.685191473938E-01	7.602854401874E-02

Table S10. Pressure = 0.85GPa

VOLUME = 971.149157 DENSITY = 1.492 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.52156963	4.34367158	16.53581495	90.000000	89.400723	90.000000

	ATOM		X/A	Y/B	Z/C
1	T	8 O	-3.614620089057E-01	-2.626233103698E-01	4.291633906152E-01
2	T	1 H	-3.607467669267E-01	-5.863721281902E-02	4.023567617721E-01
3	T	6 C	-2.844007079422E-01	-3.091794563464E-01	4.816017816601E-01
4	T	6 C	-1.920026657431E-01	-1.750724207206E-01	4.686419445468E-01
5	T	6 C	-3.020577612764E-01	4.886609579760E-01	-4.534725941204E-01
6	T	1 H	-1.814024247767E-01	-1.810996383088E-02	4.183241746981E-01
7	T	6 C	-1.145137014375E-01	-2.413393960850E-01	-4.794802222166E-01
8	T	6 C	-2.223697994620E-01	4.213528581513E-01	-4.008335990054E-01
9	T	6 C	-3.969012144180E-01	3.505420787336E-01	-4.386765092364E-01
10	T	1 H	-4.309223757257E-02	-1.332377752190E-01	-4.887793947555E-01
11	T	6 C	-1.276731891448E-01	-4.437463392694E-01	-4.143733243400E-01
12	T	6 C	-2.376913181276E-01	2.191974550919E-01	-3.340608750594E-01
13	T	1 H	-4.575075199053E-01	4.034125537710E-01	-4.786032603417E-01
14	T	6 C	-4.106345321140E-01	1.543863755641E-01	-3.753813183651E-01
15	T	6 C	-4.924168147835E-02	4.833244171192E-01	-3.600233147479E-01
16	T	6 C	-3.322387070787E-01	8.348906227196E-02	-3.207333671434E-01
17	T	6 C	-1.586091595856E-01	1.531243985193E-01	-2.804684931843E-01
18	T	1 H	-4.815114466923E-01	4.485849761215E-02	-3.653215218989E-01
19	T	1 H	2.215124942244E-02	-4.088855952595E-01	-3.699306689905E-01
20	T	6 C	-6.396438065327E-02	2.913122104622E-01	-2.961360158622E-01
21	T	6 C	-3.457296912147E-01	-1.168924984171E-01	-2.550879449740E-01
22	T	6 C	-1.759030912655E-01	-4.465282679645E-02	-2.147734373996E-01
23	T	1 H	-4.008620208253E-03	2.442176467942E-01	-2.550873601266E-01
24	T	1 H	-4.171953753689E-01	-2.246603945262E-01	-2.458541831052E-01
25	T	6 C	-2.683711650383E-01	-1.797683605607E-01	-2.027626090546E-01
26	T	1 H	-1.159446241128E-01	-9.511086626479E-02	-1.736008838175E-01
27	T	1 H	-2.797798272298E-01	-3.377893752188E-01	-1.528648176902E-01
55	T	8 O	3.701726431961E-01	-2.585486718648E-01	-3.382073909393E-01
56	T	1 H	3.611311567002E-01	-5.883648655883E-02	-3.664172241236E-01
57	T	6 C	2.985705951329E-01	-3.135667737380E-01	-2.802812615849E-01
58	T	6 C	2.039926175032E-01	-1.879537342824E-01	-2.859684552230E-01
59	T	6 C	3.232384971842E-01	4.842158606191E-01	-2.172193787450E-01
60	T	1 H	1.870004597715E-01	-2.772245050074E-02	-3.342269751320E-01

61	T	6	C	1.313578695241E-01	-2.704863662476E-01	-2.299439076795E-01
62	T	6	C	2.482723977737E-01	4.012609570861E-01	-1.602547864901E-01
63	T	6	C	4.208590402450E-01	3.603749726963E-01	-2.085084179660E-01
64	T	1	H	5.780057246287E-02	-1.754706835817E-01	-2.352417501026E-01
65	T	6	C	1.508216274125E-01	-4.792028955832E-01	-1.677143570447E-01
66	T	6	C	2.706736549125E-01	1.948185219378E-01	-9.607652076406E-02
67	T	1	H	4.769245921253E-01	4.213137951263E-01	-2.528539981857E-01
68	T	6	C	4.425009496459E-01	1.691088346489E-01	-1.459971596143E-01
69	T	6	C	7.585974101014E-02	4.219980134693E-01	-1.114612965236E-01
70	T	6	C	3.685336703951E-01	7.834569142588E-02	-8.791921283292E-02
71	T	6	C	1.950496090857E-01	1.032428310338E-01	-4.035410642085E-02
72	T	1	H	-4.833666608220E-01	7.775459873731E-02	-1.399519114932E-01
73	T	1	H	1.393997900325E-03	-4.894514950652E-01	-1.188251496363E-01
74	T	6	C	9.674912166805E-02	2.214449981377E-01	-5.082330910405E-02
75	T	6	C	3.891583204758E-01	-1.252880976879E-01	-2.447016303724E-02
76	T	6	C	2.188470051957E-01	-1.026791781124E-01	2.175448060817E-02
77	T	1	H	3.882248188680E-02	1.476557492557E-01	-9.416345562922E-03
78	T	1	H	4.632198647586E-01	-2.183894621362E-01	-1.909313507551E-02
79	T	6	C	3.148696991646E-01	-2.146511148130E-01	2.945346310060E-02
80	T	1	H	1.616185042004E-01	-1.787437242170E-01	6.371938410701E-02
81	T	1	H	3.308490913415E-01	-3.763164101489E-01	7.744867754232E-02

Table S11. Pressure = 1.41GPa

VOLUME = 948.763820 DENSITY = 1.527 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.43286461	4.26312161	16.56910209	90.000000	89.249912	90.000000

	ATOM		X/A	Y/B	Z/C
1	T	8 O	-3.621796490267E-01	-2.593887579325E-01	4.299325241821E-01
2	T	1 H	-3.611486103779E-01	-5.273468271710E-02	4.023923131076E-01
3	T	6 C	-2.843613078739E-01	-3.071834847134E-01	4.817620126680E-01
4	T	6 C	-1.912130003751E-01	-1.729430937078E-01	4.679173010964E-01
5	T	6 C	-3.022080556508E-01	4.895187951360E-01	-4.529349545044E-01
6	T	1 H	-1.806118847060E-01	-1.473354170815E-02	4.173454520510E-01
7	T	6 C	-1.131683799547E-01	-2.396309095625E-01	-4.805241110362E-01
8	T	6 C	-2.219674450681E-01	4.218808871769E-01	-4.006182627892E-01
9	T	6 C	-3.977769296708E-01	3.506624465936E-01	-4.374983351826E-01
10	T	1 H	-4.116580725307E-02	-1.311125561841E-01	-4.903473551699E-01
11	T	6 C	-1.265736534619E-01	-4.425901714456E-01	-4.149307682918E-01
12	T	6 C	-2.374372991726E-01	2.190914369242E-01	-3.334140785084E-01
13	T	1 H	-4.587094490968E-01	4.032625247842E-01	-4.773753975038E-01
14	T	6 C	-4.116338416006E-01	1.535536887045E-01	-3.738143288924E-01
15	T	6 C	-4.767566112490E-02	4.851005265875E-01	-3.607531360798E-01
16	T	6 C	-3.327120214747E-01	8.280623605493E-02	-3.193778052512E-01
17	T	6 C	-1.578212312226E-01	1.530826188834E-01	-2.800812598974E-01
18	T	1 H	-4.828751601975E-01	4.204084542453E-02	-3.633564075646E-01
19	T	1 H	2.408672276542E-02	-4.049812897472E-01	-3.710123325955E-01
20	T	6 C	-6.255083729570E-02	2.924251111596E-01	-2.964172011242E-01
21	T	6 C	-3.463025542521E-01	-1.186297897851E-01	-2.533647846422E-01
22	T	6 C	-1.752475537046E-01	-4.539950948099E-02	-2.139034853087E-01
23	T	1 H	-2.256792107108E-03	2.469436378592E-01	-2.554868154660E-01
24	T	1 H	-4.182942333804E-01	-2.272123741727E-01	-2.436087247636E-01
25	T	6 C	-2.684032767070E-01	-1.816197360071E-01	-2.013015308726E-01
26	T	1 H	-1.148186198693E-01	-9.548901842799E-02	-1.729664777659E-01
27	T	1 H	-2.799728507059E-01	-3.406794189018E-01	-1.511537699296E-01
55	T	8 O	3.703949059104E-01	-2.552004393876E-01	-3.381000654472E-01
56	T	1 H	3.611805703501E-01	-5.281132950587E-02	-3.669446397862E-01
57	T	6 C	2.980360941748E-01	-3.114586041541E-01	-2.804456676408E-01
58	T	6 C	2.026432716932E-01	-1.857844754911E-01	-2.865215886986E-01
59	T	6 C	3.230031942659E-01	4.852544177046E-01	-2.170916745113E-01
60	T	1 H	1.854125226848E-01	-2.392601242779E-02	-3.349063772543E-01

61	T	6	C	1.295214203376E-01	-2.699328639223E-01	-2.305210163712E-01
62	T	6	C	2.475188250798E-01	4.010000328668E-01	-1.601566858497E-01
63	T	6	C	4.214537358386E-01	3.616922425483E-01	-2.081098192380E-01
64	T	1	H	5.535029811544E-02	-1.751499864190E-01	-2.360622451984E-01
65	T	6	C	1.492356527149E-01	-4.800117922850E-01	-1.679979020133E-01
66	T	6	C	2.702444746787E-01	1.936713112695E-01	-9.564272124866E-02
67	T	1	H	4.777742258791E-01	4.227771779865E-01	-2.526221912626E-01
68	T	6	C	4.434528631327E-01	1.701086168062E-01	-1.452004394764E-01
69	T	6	C	7.367397029812E-02	4.191501268332E-01	-1.118666795567E-01
70	T	6	C	3.689703109524E-01	7.812447744372E-02	-8.712888044939E-02
71	T	6	C	1.940691441527E-01	1.002620035341E-01	-3.999634225409E-02
72	T	1	H	-4.818071831867E-01	7.879666074204E-02	-1.389291699459E-01
73	T	1	H	-1.451474542842E-03	-4.929143357355E-01	-1.195791621505E-01
74	T	6	C	9.489259976731E-02	2.174636528766E-01	-5.089995810276E-02
75	T	6	C	3.899237759275E-01	-1.265393122787E-01	-2.336860911198E-02
76	T	6	C	2.182153605178E-01	-1.068029139595E-01	2.243494073788E-02
77	T	1	H	3.658549651090E-02	1.418413071933E-01	-9.570897254134E-03
78	T	1	H	4.646296742414E-01	-2.194716699792E-01	-1.779264586508E-02
79	T	6	C	3.151136023309E-01	-2.178914230525E-01	3.046687224400E-02
80	T	1	H	1.606085562785E-01	-1.848364907234E-01	6.433878042853E-02
81	T	1	H	3.313370624402E-01	-3.810507992781E-01	7.859793638874E-02

Table S12. Pressure = 2.08GPa

VOLUME = 926.876312 DENSITY = 1.563 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.35820969	4.16516263	16.66056479	90.000000	89.146775	90.000000

	ATOM		X/A	Y/B	Z/C
1	T	8 O	-3.628602604310E-01	-2.576613710223E-01	4.305415289932E-01
2	T	1 H	-3.612653895252E-01	-4.803556857911E-02	4.020508989525E-01
3	T	6 C	-2.843927275220E-01	-3.067607131621E-01	4.816613441072E-01
4	T	6 C	-1.904519072096E-01	-1.733084151381E-01	4.668045299723E-01
5	T	6 C	-3.026272633059E-01	4.898379544073E-01	-4.525804723416E-01
6	T	1 H	-1.797027450933E-01	-1.464630034864E-02	4.158959190114E-01
7	T	6 C	-1.120141688993E-01	-2.400452662293E-01	-4.819534418115E-01
8	T	6 C	-2.219581921828E-01	4.220792226294E-01	-4.006264871062E-01
9	T	6 C	-3.989768313284E-01	3.511444628912E-01	-4.364140153951E-01
10	T	1 H	-3.940657996698E-02	-1.316212348304E-01	-4.924028186016E-01
11	T	6 C	-1.258433619738E-01	-4.424226011732E-01	-4.157699792980E-01
12	T	6 C	-2.377637095827E-01	2.195157330037E-01	-3.329294531080E-01
13	T	1 H	-4.601391669704E-01	4.033259308135E-01	-4.761888612488E-01
14	T	6 C	-4.131323687704E-01	1.538838857154E-01	-3.722517507692E-01
15	T	6 C	-4.662695567892E-02	4.863518334634E-01	-3.617802214327E-01
16	T	6 C	-3.338013455922E-01	8.338611379142E-02	-3.181171996376E-01
17	T	6 C	-1.577421317261E-01	1.538506719999E-01	-2.799085135859E-01
18	T	1 H	-4.847995638376E-01	4.110589927905E-02	-3.612122696590E-01
19	T	1 H	2.552782086966E-02	-4.019092540070E-01	-3.724508018050E-01
20	T	6 C	-6.183769046014E-02	2.938529158089E-01	-2.969773873576E-01
21	T	6 C	-3.476523283293E-01	-1.183360403451E-01	-2.516743183978E-01
22	T	6 C	-1.754323528676E-01	-4.457519197957E-02	-2.132481879198E-01
23	T	1 H	-1.321627687733E-03	2.498827975320E-01	-2.561747263797E-01
24	T	1 H	-4.201697380495E-01	-2.274390919183E-01	-2.412861968106E-01
25	T	6 C	-2.693126940601E-01	-1.813623692989E-01	-1.999701315704E-01
26	T	1 H	-1.146503115544E-01	-9.473819233024E-02	-1.725666084607E-01
27	T	1 H	-2.811123989974E-01	-3.413733106341E-01	-1.495968102779E-01
55	T	8 O	3.698511471269E-01	-2.535605354444E-01	-3.376382100962E-01
56	T	1 H	3.605950405991E-01	-4.794648675657E-02	-3.672178774877E-01
57	T	6 C	2.967835640775E-01	-3.110222547702E-01	-2.805231385019E-01
58	T	6 C	2.005887789162E-01	-1.856557391455E-01	-2.871712300170E-01
59	T	6 C	3.221701249696E-01	4.851526268676E-01	-2.168549190710E-01
60	T	1 H	1.830485954423E-01	-2.244067533851E-02	-3.357118039484E-01

61	T	6	C	1.271666506102E-01	-2.709932515152E-01	-2.312672833565E-01
62	T	6	C	2.463651454486E-01	4.001807645450E-01	-1.600060669229E-01
63	T	6	C	4.214055059689E-01	3.619765648352E-01	-2.075430010977E-01
64	T	1	H	5.236983844398E-02	-1.769385212191E-01	-2.371753864662E-01
65	T	6	C	1.472911573910E-01	-4.816124557742E-01	-1.683357576298E-01
66	T	6	C	2.695944700702E-01	1.928069367934E-01	-9.509883805007E-02
67	T	1	H	4.777992496733E-01	4.226888621835E-01	-2.521942630147E-01
68	T	6	C	4.439159503500E-01	1.708311955701E-01	-1.442120790680E-01
69	T	6	C	7.135787832648E-02	4.161948152936E-01	-1.123052897090E-01
70	T	6	C	3.691367913983E-01	7.844569686649E-02	-8.616512801981E-02
71	T	6	C	1.931052235620E-01	9.837854295773E-02	-3.949230710560E-02
72	T	1	H	-4.807799800180E-01	7.954530775570E-02	-1.376356619340E-01
73	T	1	H	-4.391848473812E-03	-4.965484158971E-01	-1.203807167916E-01
74	T	6	C	9.310870166210E-02	2.143336729277E-01	-5.089587037585E-02
75	T	6	C	3.906057252840E-01	-1.261943537743E-01	-2.198319524037E-02
76	T	6	C	2.177935647138E-01	-1.087111603463E-01	2.339435492889E-02
77	T	1	H	3.465026553036E-02	1.374711666234E-01	-9.559833002027E-03
78	T	1	H	4.659045378463E-01	-2.189961899777E-01	-1.616294610748E-02
79	T	6	C	3.155358736632E-01	-2.185736339932E-01	3.183819849299E-02
80	T	1	H	1.600158468795E-01	-1.880411595673E-01	6.531940794541E-02
81	T	1	H	3.321872800505E-01	-3.823538200389E-01	8.023356182651E-02

Table S13. Pressure = 2.86GPa

VOLUME = 905.331174 DENSITY = 1.600 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.26510546	4.13097734	16.52376024	90.000000	89.009268	90.000000

	ATOM		X/A	Y/B	Z/C
1	T	8 O	-3.643702051980E-01	-2.488276808502E-01	4.316195464856E-01
2	T	1 H	-3.628145359330E-01	-3.730108396736E-02	4.028175787513E-01
3	T	6 C	-2.848259274116E-01	-2.999114023775E-01	4.822787242309E-01
4	T	6 C	-1.904722795805E-01	-1.648255393237E-01	4.667228964470E-01
5	T	6 C	-3.025738733070E-01	4.933804210674E-01	-4.516974695954E-01
6	T	1 H	-1.802564881377E-01	-3.335611831801E-03	4.156459640710E-01
7	T	6 C	-1.111126887722E-01	-2.328489603655E-01	-4.822855508275E-01
8	T	6 C	-2.209901064638E-01	4.245918341398E-01	-3.999899536346E-01
9	T	6 C	-3.993251036884E-01	3.524763930100E-01	-4.350978217106E-01
10	T	1 H	-3.816516123046E-02	-1.229494768837E-01	-4.930350833549E-01
11	T	6 C	-1.245041644491E-01	-4.379054969951E-01	-4.157460299695E-01
12	T	6 C	-2.362804274100E-01	2.193793698638E-01	-3.318904868282E-01
13	T	1 H	-4.611129604953E-01	4.047292562881E-01	-4.748731590656E-01
14	T	6 C	-4.129402294999E-01	1.520717665388E-01	-3.706337577555E-01
15	T	6 C	-4.438544232112E-02	4.905112027399E-01	-3.619200647142E-01
16	T	6 C	-3.327221990606E-01	8.118538707176E-02	-3.165742466249E-01
17	T	6 C	-1.553346153065E-01	1.531596207642E-01	-2.790379246701E-01
18	T	1 H	-4.846918289038E-01	3.620552273183E-02	-3.593052523258E-01
19	T	1 H	2.794324025578E-02	-3.951266046801E-01	-3.728772081514E-01
20	T	6 C	-5.909068078472E-02	2.953505471051E-01	-2.967441490143E-01
21	T	6 C	-3.459780487366E-01	-1.237007646840E-01	-2.498316781706E-01
22	T	6 C	-1.724875314728E-01	-4.796873869030E-02	-2.119397832690E-01
23	T	1 H	2.075345797711E-03	2.517962192675E-01	-2.560026880684E-01
24	T	1 H	-4.186692009152E-01	-2.353262503282E-01	-2.390909810987E-01
25	T	6 C	-2.667233149209E-01	-1.874491537671E-01	-1.982999058884E-01
26	T	1 H	-1.110156125684E-01	-9.850243279453E-02	-1.713183345698E-01
27	T	1 H	-2.781333431775E-01	-3.503596303956E-01	-1.477996331258E-01
55	T	8 O	3.709508841128E-01	-2.446520644847E-01	-3.383620882009E-01
56	T	1 H	3.617006201185E-01	-3.687822136655E-02	-3.681611042332E-01
57	T	6 C	2.972119054293E-01	-3.048251819802E-01	-2.810213486446E-01
58	T	6 C	2.003012604864E-01	-1.792583533090E-01	-2.875101462992E-01
59	T	6 C	3.228304000425E-01	4.881847519377E-01	-2.172800161571E-01
60	T	1 H	1.825690576367E-01	-1.300598801475E-02	-3.360274475153E-01

61 T 6 C 1.264237502984E-01 -2.683675600220E-01 -2.313363841729E-01
62 T 6 C 2.465530894488E-01 3.999402670452E-01 -1.601396318529E-01
63 T 6 C 4.228314050288E-01 3.651881185936E-01 -2.082419941833E-01
64 T 1 H 5.101871638546E-02 -1.749743588230E-01 -2.370720644107E-01
65 T 6 C 1.467487145920E-01 -4.821942085167E-01 -1.683455274759E-01
66 T 6 C 2.700510672096E-01 1.895252810206E-01 -9.513220207530E-02
67 T 1 H 4.794359596347E-01 4.277514639217E-01 -2.533428896966E-01
68 T 6 C 4.456759535700E-01 1.715394707757E-01 -1.447079315351E-01
69 T 6 C 7.020508423444E-02 4.117250608018E-01 -1.122261638586E-01
70 T 6 C 3.703820781782E-01 7.576544863956E-02 -8.638101351863E-02
71 T 6 C 1.929888065809E-01 9.129747594989E-02 -3.936721089705E-02
72 T 1 H -4.784264570038E-01 8.052072509402E-02 -1.382934503190E-01
73 T 1 H -6.174276560847E-03 4.983185208022E-01 -1.203446737038E-01
74 T 6 C 9.219414793337E-02 2.067020864201E-01 -5.073554984368E-02
75 T 6 C 3.920884843045E-01 -1.323386965767E-01 -2.216571079950E-02
76 T 6 C 2.178937687509E-01 -1.195379438731E-01 2.348501003186E-02
77 T 1 H 3.329961008619E-02 1.265336644510E-01 -9.374683621453E-03
78 T 1 H 4.679606914514E-01 -2.253046310075E-01 -1.658443900665E-02
79 T 6 C 3.164469136622E-01 -2.289133688175E-01 3.173560238438E-02
80 T 1 H 1.597143714978E-01 -2.025715990121E-01 6.545252168743E-02
81 T 1 H 3.332182397061E-01 -3.962688723030E-01 7.996476642944E-02

Table S14. Pressure = 3.78GPa

VOLUME = 884.103620 DENSITY = 1.638 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.18745752	4.09422939	16.37683270	90.000000	89.047705	90.000000

	ATOM	X/A	Y/B	Z/C
1	T 8 O	-3.656079675609E-01	-2.376056670491E-01	4.319619254641E-01
2	T 1 H	-3.640712147966E-01	-2.385526336403E-02	4.028840618596E-01
3	T 6 C	-2.851668735386E-01	-2.913175260655E-01	4.823957365688E-01
4	T 6 C	-1.903644087835E-01	-1.554953823756E-01	4.664016617969E-01
5	T 6 C	-3.026694762355E-01	4.986507476144E-01	-4.513417549201E-01
6	T 1 H	-1.805187308305E-01	9.127346657540E-03	4.152148760700E-01
7	T 6 C	-1.102634961498E-01	-2.260715880761E-01	-4.826530674589E-01
8	T 6 C	-2.203645555064E-01	4.275618185112E-01	-3.996680242487E-01
9	T 6 C	-3.999083848002E-01	3.568688014203E-01	-4.345475372559E-01
10	T 1 H	-3.693291971748E-02	-1.154249087035E-01	-4.934769942210E-01
11	T 6 C	-1.234567477121E-01	-4.340574518276E-01	-4.158008485964E-01
12	T 6 C	-2.353909897526E-01	2.195147837484E-01	-3.312074697148E-01
13	T 1 H	-4.621788159146E-01	4.103907376821E-01	-4.744699935412E-01
14	T 6 C	-4.132379906406E-01	1.533133224780E-01	-3.697899933338E-01
15	T 6 C	-4.264510702984E-02	4.928351461392E-01	-3.619067505423E-01
16	T 6 C	-3.323118968585E-01	8.053302246615E-02	-3.156317693587E-01
17	T 6 C	-1.537145962670E-01	1.514057953434E-01	-2.783117297781E-01
18	T 1 H	-4.851638342580E-01	3.553809831653E-02	-3.583210124528E-01
19	T 1 H	2.992370531572E-02	-3.910768532970E-01	-3.729486225873E-01
20	T 6 C	-5.710754121756E-02	2.950440640856E-01	-2.963578609796E-01
21	T 6 C	-3.452429487465E-01	-1.278464498656E-01	-2.486626848877E-01
22	T 6 C	-1.705478466942E-01	-5.300762554408E-02	-2.108961417249E-01
23	T 1 H	4.534606623623E-03	2.513788459138E-01	-2.554469276317E-01
24	T 1 H	-4.182239876379E-01	-2.407056572031E-01	-2.377404929949E-01
25	T 6 C	-2.652010766525E-01	-1.941857453720E-01	-1.971953401918E-01
26	T 1 H	-1.085239706284E-01	-1.052024971172E-01	-1.701952105418E-01
27	T 1 H	-2.763837133517E-01	-3.606602415855E-01	-1.467077476507E-01
55	T 8 O	3.716293011453E-01	-2.338134829719E-01	-3.382893228508E-01
56	T 1 H	3.623376415119E-01	-2.349069279350E-02	-3.682310040567E-01
57	T 6 C	2.972482089790E-01	-2.980281787541E-01	-2.810197529572E-01
58	T 6 C	1.996690463601E-01	-1.727760625236E-01	-2.876123601064E-01
59	T 6 C	3.231243498063E-01	4.910383628830E-01	-2.172550002280E-01
60	T 1 H	1.817154374522E-01	-3.148931176063E-03	-3.361189799408E-01

61	T	6	C	1.254508964012E-01	-2.665162136791E-01	-2.313893034104E-01
62	T	6	C	2.465206546201E-01	3.991521949985E-01	-1.599639433562E-01
63	T	6	C	4.237585468611E-01	3.677528973398E-01	-2.084108268953E-01
64	T	1	H	4.944328588822E-02	-1.745568463653E-01	-2.371725755236E-01
65	T	6	C	1.460830664814E-01	-4.834549789829E-01	-1.682370893791E-01
66	T	6	C	2.703364945215E-01	1.855576454515E-01	-9.478550538465E-02
67	T	1	H	4.804453797161E-01	4.320867844917E-01	-2.539156936152E-01
68	T	6	C	4.469385644164E-01	1.709010812953E-01	-1.446938469093E-01
69	T	6	C	6.910781344292E-02	4.066651725207E-01	-1.121014688724E-01
70	T	6	C	3.713158328316E-01	7.202258486567E-02	-8.611842162260E-02
71	T	6	C	1.928906470650E-01	8.374557523111E-02	-3.890702229190E-02
72	T	1	H	-4.767160340432E-01	7.936297568574E-02	-1.384303666543E-01
73	T	1	H	-7.818432676805E-03	4.926346191310E-01	-1.204023299508E-01
74	T	6	C	9.141138500664E-02	1.986927172279E-01	-5.039594764824E-02
75	T	6	C	3.932966411798E-01	-1.397354740882E-01	-2.181182944747E-02
76	T	6	C	2.180656154588E-01	-1.307907003901E-01	2.401507612649E-02
77	T	1	H	3.222429537190E-02	1.153411569291E-01	-9.051984233538E-03
78	T	1	H	4.696136424389E-01	-2.333323006086E-01	-1.642699611008E-02
79	T	6	C	3.172859317669E-01	-2.401690602771E-01	3.214886217138E-02
80	T	1	H	1.596342461491E-01	-2.170783833929E-01	6.603615606421E-02
81	T	1	H	3.342270258214E-01	-4.113121349788E-01	8.023433079316E-02

Table S15. Pressure = 4.86GPa

VOLUME = 863.027908 DENSITY = 1.678 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.11073730	4.05724783	16.22879389	90.000000	88.652841	90.000000

	ATOM		X/A	Y/B	Z/C
1	T	8 O	-3.673080500698E-01	-2.285579637982E-01	4.343891689878E-01
2	T	1 H	-3.655726436136E-01	-1.285287285436E-02	4.048362755635E-01
3	T	6 C	-2.857496336464E-01	-2.847766269917E-01	4.839132905777E-01
4	T	6 C	-1.907179449046E-01	-1.469018444753E-01	4.667557179799E-01
5	T	6 C	-3.025475141239E-01	-4.987366422429E-01	-4.495189727111E-01
6	T	1 H	-1.815466763399E-01	2.084315859120E-02	4.153676582501E-01
7	T	6 C	-1.097039540590E-01	-2.185583601860E-01	-4.829008077257E-01
8	T	6 C	-2.193393606133E-01	4.295087888499E-01	-3.984371111794E-01
9	T	6 C	-3.999493871015E-01	3.562699804259E-01	-4.319499062498E-01
10	T	1 H	-3.617506235285E-02	-1.060187670176E-01	-4.942818929797E-01
11	T	6 C	-1.222838237800E-01	-4.293726707037E-01	-4.155988892114E-01
12	T	6 C	-2.336577087742E-01	2.186314780246E-01	-3.294641638681E-01
13	T	1 H	-4.627342901428E-01	4.092386789794E-01	-4.717660683673E-01
14	T	6 C	-4.125667117016E-01	1.491485473380E-01	-3.668201163659E-01
15	T	6 C	-4.053499055795E-02	4.976682162263E-01	-3.622319489080E-01
16	T	6 C	-3.307808137229E-01	7.687227480764E-02	-3.129513030551E-01
17	T	6 C	-1.510237400948E-01	1.505273431049E-01	-2.770955070632E-01
18	T	1 H	-4.843841641799E-01	2.730173274781E-02	-3.548327092089E-01
19	T	1 H	3.201804815184E-02	-3.828864245168E-01	-3.738746724482E-01
20	T	6 C	-5.427761910410E-02	2.967561307419E-01	-2.962595808494E-01
21	T	6 C	-3.428334616875E-01	-1.346125862034E-01	-2.455162769007E-01
22	T	6 C	-1.670767370795E-01	-5.642338721224E-02	-2.090553863262E-01
23	T	1 H	8.005008369435E-03	2.535367147208E-01	-2.556798938157E-01
24	T	1 H	-4.157458962791E-01	-2.508033807183E-01	-2.337946401307E-01
25	T	6 C	-2.618715188847E-01	-2.007924048622E-01	-1.945259653495E-01
26	T	1 H	-1.043741749316E-01	-1.084851858096E-01	-1.686356577804E-01
27	T	1 H	-2.725265546038E-01	-3.699623484152E-01	-1.437732856834E-01
55	T	8 O	3.722708512789E-01	-2.243909058720E-01	-3.403552035940E-01
56	T	1 H	3.634421906033E-01	-1.145732101434E-02	-3.705625894422E-01
57	T	6 C	2.973669372299E-01	-2.908848785502E-01	-2.824886730067E-01
58	T	6 C	1.990717270091E-01	-1.663039631972E-01	-2.885586669681E-01
59	T	6 C	3.236981410999E-01	4.957454625736E-01	-2.186069204059E-01
60	T	1 H	1.807431362588E-01	6.196363118085E-03	-3.370190295650E-01

61	T	6	C	1.246456416194E-01	-2.647084145611E-01	-2.317148435549E-01
62	T	6	C	2.468726240074E-01	3.993840487248E-01	-1.607330105438E-01
63	T	6	C	4.252147651205E-01	3.751854562130E-01	-2.102460212889E-01
64	T	1	H	4.799757490458E-02	-1.744455218549E-01	-2.370437114156E-01
65	T	6	C	1.456947807409E-01	-4.848412182547E-01	-1.685454899273E-01
66	T	6	C	2.712573015071E-01	1.828374761167E-01	-9.553779592919E-02
67	T	1	H	4.819156533114E-01	4.433826637754E-01	-2.563470366187E-01
68	T	6	C	4.491025305998E-01	1.766777177786E-01	-1.462739947513E-01
69	T	6	C	6.834786729220E-02	4.000194511272E-01	-1.120572437480E-01
70	T	6	C	3.731086149347E-01	7.184405953150E-02	-8.734043183301E-02
71	T	6	C	1.934413397279E-01	7.545937993219E-02	-3.930615579513E-02
72	T	1	H	-4.737191153336E-01	8.872827349587E-02	-1.401378566294E-01
73	T	1	H	-9.246579454792E-03	4.841198075640E-01	-1.201433853967E-01
74	T	6	C	9.114029862566E-02	1.886103017304E-01	-5.039928120849E-02
75	T	6	C	3.955578082560E-01	-1.439341662853E-01	-2.318007546133E-02
76	T	6	C	2.190640921023E-01	-1.433297058812E-01	2.336951895014E-02
77	T	1	H	3.165835318281E-02	1.005604782022E-01	-8.917659344391E-03
78	T	1	H	4.725052877679E-01	-2.366136564960E-01	-1.831704696722E-02
79	T	6	C	3.191445832295E-01	-2.508785927209E-01	3.095381444164E-02
80	T	1	H	1.603697402413E-01	-2.346419048528E-01	6.554333821149E-02
81	T	1	H	3.364160309434E-01	-4.264822688939E-01	7.861660530379E-02

Table S16. Pressure = 6.12GPa

VOLUME = 842.222427 DENSITY = 1.720 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.01496154	3.82416827	16.92273185	90.000000	89.403277	90.000000

	ATOM	X/A	Y/B	Z/C
1	T 8 O	-3.627929205029E-01	-2.560802628346E-01	4.282561050332E-01
2	T 1 H	-3.609877038068E-01	-3.341843449305E-02	3.973094791929E-01
3	T 6 C	-2.823926745365E-01	-3.077093742755E-01	4.788343716991E-01
4	T 6 C	-1.853575055536E-01	-1.742983831934E-01	4.628400793236E-01
5	T 6 C	-3.035239869306E-01	4.902674342957E-01	-4.540798257920E-01
6	T 1 H	-1.738802218689E-01	-1.072089163855E-02	4.114422983929E-01
7	T 6 C	-1.065346283125E-01	-2.374616914549E-01	-4.839653680642E-01
8	T 6 C	-2.221365271485E-01	4.217607946212E-01	-4.017076217886E-01
9	T 6 C	-4.035610057721E-01	3.537252738023E-01	-4.378365321211E-01
10	T 1 H	-3.202140894196E-02	-1.166039905864E-01	-4.922216338870E-01
11	T 6 C	-1.229603311033E-01	-4.413719438996E-01	-4.171837958578E-01
12	T 6 C	-2.405882140286E-01	2.189687607514E-01	-3.330254705721E-01
13	T 1 H	-4.651443971489E-01	4.087832524230E-01	-4.781657056710E-01
14	T 6 C	-4.199420495497E-01	1.539353655061E-01	-3.727593284652E-01
15	T 6 C	-4.371036321166E-02	4.961295277042E-01	-3.615323441916E-01
16	T 6 C	-3.398658172706E-01	8.193702617930E-02	-3.182710207161E-01
17	T 6 C	-1.602723406575E-01	1.567368363035E-01	-2.788891026620E-01
18	T 1 H	-4.935382672792E-01	3.716824579614E-02	-3.610989195732E-01
19	T 1 H	2.996170352257E-02	-3.802197337742E-01	-3.710791790024E-01
20	T 6 C	-6.192323770724E-02	3.051790735544E-01	-2.955289003047E-01
21	T 6 C	-3.561697852205E-01	-1.245517736219E-01	-2.513910509305E-01
22	T 6 C	-1.802534040738E-01	-4.526108216209E-02	-2.116099958821E-01
23	T 1 H	-1.943886882234E-03	2.739061833734E-01	-2.530144973256E-01
24	T 1 H	-4.310996656484E-01	-2.362955709477E-01	-2.410319110559E-01
25	T 6 C	-2.771525547415E-01	-1.885977484903E-01	-1.990851552962E-01
26	T 1 H	-1.189980699537E-01	-9.480248535341E-02	-1.701419835229E-01
27	T 1 H	-2.908818766346E-01	-3.560330478901E-01	-1.488408074959E-01
55	T 8 O	3.703397561618E-01	-2.512158437937E-01	-3.332298786246E-01
56	T 1 H	3.595049618344E-01	-3.512739394722E-02	-3.660470104488E-01
57	T 6 C	2.941177823648E-01	-3.126570012632E-01	-2.788346888879E-01
58	T 6 C	1.954258767540E-01	-1.814554838680E-01	-2.879049612950E-01
59	T 6 C	3.203181216963E-01	4.783071057641E-01	-2.143155513879E-01
60	T 1 H	1.775390339691E-01	-1.043794961338E-02	-3.368823628856E-01

61	T	6	C	1.206225817994E-01	-2.648300820632E-01	-2.322931030035E-01
62	T	6	C	2.429963470530E-01	3.976362373587E-01	-1.578725410349E-01
63	T	6	C	4.218625944279E-01	3.462943527298E-01	-2.042708815696E-01
64	T	1	H	4.397220001106E-02	-1.660171822669E-01	-2.390039084110E-01
65	T	6	C	1.414517012161E-01	-4.791013464078E-01	-1.680455824739E-01
66	T	6	C	2.673394448575E-01	1.893764424302E-01	-9.158085015934E-02
67	T	1	H	4.783546483871E-01	3.967408745270E-01	-2.498690631213E-01
68	T	6	C	4.456355912949E-01	1.542591353877E-01	-1.396657408156E-01
69	T	6	C	6.359703701078E-02	4.201429703905E-01	-1.125239317524E-01
70	T	6	C	3.694757702053E-01	7.071100046853E-02	-8.136202461093E-02
71	T	6	C	1.892295211464E-01	9.899933079987E-02	-3.605560862686E-02
72	T	1	H	-4.777923674582E-01	5.083892570338E-02	-1.326347386287E-01
73	T	1	H	-1.415903834921E-02	-4.886428905385E-01	-1.219269547870E-01
74	T	6	C	8.658847499718E-02	2.164792817067E-01	-4.956671448131E-02
75	T	6	C	3.918408994381E-01	-1.346394664720E-01	-1.566245898249E-02
76	T	6	C	2.150508211359E-01	-1.080814510359E-01	2.867466249155E-02
77	T	1	H	2.723862225036E-02	1.401824659991E-01	-8.225504378424E-03
78	T	1	H	4.687367323356E-01	-2.351482484964E-01	-9.072279165767E-03
79	T	6	C	3.155212323267E-01	-2.213888436595E-01	3.837532776710E-02
80	T	1	H	1.562887971327E-01	-1.859625293675E-01	7.084754591895E-02
81	T	1	H	3.333907765369E-01	-3.879337701677E-01	8.759038536259E-02

Table S17. Pressure = 7.50GPa

VOLUME = 822.867102 DENSITY = 1.760 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
12.96819476	3.98391261	15.93457044	90.000000	88.261343	90.000000

ATOM		X/A	Y/B	Z/C
1 T	8 O	-3.699987722713E-01	-2.092237446785E-01	4.375008705676E-01
2 T	1 H	-3.681435219507E-01	1.097304804737E-02	4.071837031137E-01
3 T	6 C	-2.864972318650E-01	-2.705210828028E-01	4.857318205056E-01
4 T	6 C	-1.909481589447E-01	-1.293840613905E-01	4.669420701335E-01
5 T	6 C	-3.022969973711E-01	-4.920646499519E-01	-4.472361919739E-01
6 T	1 H	-1.828358302522E-01	4.478991898334E-02	4.153026498867E-01
7 T	6 C	-1.084317864552E-01	-2.042413887774E-01	-4.833462848314E-01
8 T	6 C	-2.176245433374E-01	4.335845901735E-01	-3.967823271328E-01
9 T	6 C	-4.002287026635E-01	3.586116855262E-01	-4.287565240530E-01
10 T	1 H	-3.444415021355E-02	-8.842158687240E-02	-4.951937200084E-01
11 T	6 C	-1.201851581492E-01	-4.209791005156E-01	-4.153162474656E-01
12 T	6 C	-2.309713404836E-01	2.169418774697E-01	-3.269550684606E-01
13 T	1 H	-4.637865059215E-01	4.122156076384E-01	-4.687505338422E-01
14 T	6 C	-4.118960761561E-01	1.447858569279E-01	-3.629494221730E-01
15 T	6 C	-3.689699887708E-02	-4.948084159330E-01	-3.624500178842E-01
16 T	6 C	-3.286786156209E-01	7.136454290676E-02	-3.092422499734E-01
17 T	6 C	-1.467484098474E-01	1.474788730089E-01	-2.750943670878E-01
18 T	1 H	-4.838018851172E-01	1.750374192560E-02	-3.503043101933E-01
19 T	1 H	3.572666460189E-02	-3.696007586483E-01	-3.747341297045E-01
20 T	6 C	-4.965852597003E-02	2.982945666659E-01	-2.957261646842E-01
21 T	6 C	-3.394961779052E-01	-1.467070774586E-01	-2.410966636447E-01
22 T	6 C	-1.616857930059E-01	-6.533645536982E-02	-2.061200622750E-01
23 T	1 H	1.363355279353E-02	2.558804481153E-01	-2.552985338180E-01
24 T	1 H	-4.125030972741E-01	-2.677367777335E-01	-2.282654814019E-01
25 T	6 C	-2.569178895761E-01	-2.148260187237E-01	-1.907042968987E-01
26 T	1 H	-9.793597436124E-02	-1.186318251098E-01	-1.658151529686E-01
27 T	1 H	-2.668247227162E-01	-3.899544033453E-01	-1.396667202044E-01
55 T	8 O	3.734214855935E-01	-2.050011183759E-01	-3.427527686766E-01
56 T	1 H	3.653318480697E-01	1.348086756296E-02	-3.734030442286E-01
57 T	6 C	2.975127283446E-01	-2.771127979490E-01	-2.842342161163E-01
58 T	6 C	1.979795247848E-01	-1.530807782335E-01	-2.897182363497E-01
59 T	6 C	3.246216551620E-01	-4.966457688562E-01	-2.202278704125E-01
60 T	1 H	1.790196119772E-01	2.527396242958E-02	-3.381886862502E-01

61	T	6	C	1.232532624172E-01	-2.602463047081E-01	-2.319963766905E-01
62	T	6	C	2.474725799835E-01	3.990976397384E-01	-1.614862621958E-01
63	T	6	C	4.275511075202E-01	3.856382166573E-01	-2.126625770779E-01
64	T	1	H	4.546286910991E-02	-1.728457700948E-01	-2.366950861781E-01
65	T	6	C	1.450856251651E-01	-4.867259430719E-01	-1.686908705573E-01
66	T	6	C	2.728377549295E-01	1.763607355930E-01	-9.618266654819E-02
67	T	1	H	4.842124199773E-01	4.602757324814E-01	-2.597550270151E-01
68	T	6	C	4.526314540836E-01	1.824420861127E-01	-1.482678309723E-01
69	T	6	C	6.711028982225E-02	3.894316813102E-01	-1.117011926103E-01
70	T	6	C	3.760938872164E-01	6.809921224629E-02	-8.869527629712E-02
71	T	6	C	1.944524323823E-01	6.019404653581E-02	-3.936150429789E-02
72	T	1	H	-4.689215357390E-01	9.851891053155E-02	-1.423866065336E-01
73	T	1	H	-1.159736319034E-02	4.713413003134E-01	-1.195898437320E-01
74	T	6	C	9.078624496337E-02	1.715250905170E-01	-4.994526483208E-02
75	T	6	C	3.993304581444E-01	-1.553336119816E-01	-2.462015200802E-02
76	T	6	C	2.208305451838E-01	-1.665046115056E-01	2.306432892340E-02
77	T	1	H	3.087322889666E-02	7.600131537865E-02	-8.219724542496E-03
78	T	1	H	4.772549922394E-01	-2.480367264498E-01	-2.058505711217E-02
79	T	6	C	3.223292692732E-01	-2.723576382253E-01	2.986081030955E-02
80	T	1	H	1.617004260451E-01	-2.653602763591E-01	6.554233804707E-02
81	T	1	H	3.401807834565E-01	-4.560168616754E-01	7.692625838574E-02

6. Equation of state, atomic positions under pressure (1.82-3.36 GPa)

Lattice parameters (angstrom and degrees). Atoms in the asymmetric unit - 54, atoms in the unit cell - 108.

Table S18. Pressure = 1.82GPa

VOLUME = 934.869799 DENSITY = 1.549 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.39210890	4.17778038	16.71090041	90.000000	89.190941	90.000000

ATOM	X/A	Y/B	Z/C
1 T 8 O	-3.624420387443E-01	-2.614056608885E-01	4.301813391055E-01
2 T 1 H	-3.609033295070E-01	-5.251886429218E-02	4.017672955252E-01
3 T 6 C	-2.843331200309E-01	-3.093721335262E-01	4.814447656137E-01
4 T 6 C	-1.905898577589E-01	-1.763016087018E-01	4.667925040756E-01
5 T 6 C	-3.026725485911E-01	4.886706436277E-01	-4.528472488625E-01
6 T 1 H	-1.796986787127E-01	-1.887807764262E-02	4.159034591880E-01
7 T 6 C	-1.124457522756E-01	-2.421725884834E-01	-4.818896089999E-01
8 T 6 C	-2.222756852339E-01	4.215448743999E-01	-4.008486489819E-01
9 T 6 C	-3.988505122285E-01	3.507674117590E-01	-4.367672988747E-01
10 T 1 H	-3.999509045134E-02	-1.341191110521E-01	-4.922894313177E-01
11 T 6 C	-1.263375441796E-01	-4.434831974297E-01	-4.158122721878E-01
12 T 6 C	-2.381814631370E-01	2.199105123563E-01	-3.332644384359E-01
13 T 1 H	-4.598340722336E-01	4.028539818628E-01	-4.764808065550E-01
14 T 6 C	-4.131054769935E-01	1.544815963511E-01	-3.727022368219E-01
15 T 6 C	-4.737474033823E-02	4.856352205568E-01	-3.618202087015E-01
16 T 6 C	-3.340316522078E-01	8.428077811501E-02	-3.185996338311E-01
17 T 6 C	-1.584223574859E-01	1.547076143164E-01	-2.802370751464E-01
18 T 1 H	-4.846930310603E-01	4.268250182422E-02	-3.616773435278E-01
19 T 1 H	2.469168579609E-02	-4.034771985684E-01	-3.724367824087E-01
20 T 6 C	-6.267369354564E-02	2.940481364594E-01	-2.971728498483E-01
21 T 6 C	-3.479879830488E-01	-1.164732880157E-01	-2.522685267907E-01
22 T 6 C	-1.761972972155E-01	-4.283939456332E-02	-2.137618825951E-01
23 T 1 H	-2.344845003262E-03	2.495915994037E-01	-2.563682172532E-01
24 T 1 H	-4.203489200616E-01	-2.252297413159E-01	-2.419467500298E-01
25 T 6 C	-2.698955211560E-01	-1.790599611204E-01	-2.005863574194E-01
26 T 1 H	-1.156645788414E-01	-9.305880943892E-02	-1.730347317915E-01
27 T 1 H	-2.816889073035E-01	-3.384808515660E-01	-1.503052055568E-01

55	T	8	O	3.696049263438E-01	-2.574343712930E-01	-3.374075191349E-01
56	T	1	H	3.603497123932E-01	-5.271442973136E-02	-3.669591195982E-01
57	T	6	C	2.967553687569E-01	-3.136818057578E-01	-2.803843055139E-01
58	T	6	C	2.008726072013E-01	-1.880119092479E-01	-2.870925856073E-01
59	T	6	C	3.219731407316E-01	4.836767500786E-01	-2.167181054607E-01
60	T	1	H	1.834696814502E-01	-2.584538918191E-02	-3.356415181578E-01
61	T	6	C	1.275698012564E-01	-2.717638825213E-01	-2.313032717893E-01
62	T	6	C	2.462985554399E-01	4.001887891848E-01	-1.599846081423E-01
63	T	6	C	4.208991079399E-01	3.602354326522E-01	-2.072745436001E-01
64	T	1	H	5.303095249650E-02	-1.772045834067E-01	-2.372936118854E-01
65	T	6	C	1.475244993602E-01	-4.812582477039E-01	-1.683888366121E-01
66	T	6	C	2.693582067711E-01	1.938856704163E-01	-9.510256315400E-02
67	T	1	H	4.772376223484E-01	4.200804946338E-01	-2.517627511818E-01
68	T	6	C	4.432335225187E-01	1.700130524071E-01	-1.440041501260E-01
69	T	6	C	7.174756099792E-02	4.180644512685E-01	-1.124334232718E-01
70	T	6	C	3.685906816580E-01	7.909087763667E-02	-8.606732556163E-02
71	T	6	C	1.930137622746E-01	1.009816918356E-01	-3.959122796804E-02
72	T	1	H	-4.817019800410E-01	7.845345555324E-02	-1.373614032358E-01
73	T	1	H	-3.751050484604E-03	-4.943265860635E-01	-1.205304634040E-01
74	T	6	C	9.332852146061E-02	2.172157137269E-01	-5.106975676767E-02
75	T	6	C	3.898664443563E-01	-1.243158362678E-01	-2.188296857981E-02
76	T	6	C	2.175322135076E-01	-1.047088255177E-01	2.332852242640E-02
77	T	1	H	3.498190064543E-02	1.415791460497E-01	-9.781000452743E-03
78	T	1	H	4.649245246567E-01	-2.172303983262E-01	-1.591076748170E-02
79	T	6	C	3.149508037582E-01	-2.149320763129E-01	3.188485994221E-02
80	T	1	H	1.598516405800E-01	-1.825407254535E-01	6.520931714686E-02
81	T	1	H	3.314930968030E-01	-3.774008430857E-01	8.035080113982E-02

Table S19. Pressure = 2.15 GPa

VOLUME = 924.752495 DENSITY = 1.566 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.35197061	4.16135617	16.64532594	90.000000	89.156646	90.000000

	ATOM	X/A	Y/B	Z/C
1	T 8 O	-3.630758612154E-01	-2.566457074164E-01	4.305455685146E-01
2	T 1 H	-3.615168465596E-01	-4.682340013989E-02	4.020102811645E-01
3	T 6 C	-2.845029284482E-01	-3.058108055568E-01	4.816422317868E-01
4	T 6 C	-1.905305956570E-01	-1.723965206678E-01	4.666891878834E-01
5	T 6 C	-3.026874847604E-01	4.907539311563E-01	-4.525177650162E-01
6	T 1 H	-1.798290320840E-01	-1.375487197873E-02	4.157029707974E-01
7	T 6 C	-1.119953864974E-01	-2.391793357236E-01	-4.820754492627E-01
8	T 6 C	-2.218999458588E-01	4.227764530850E-01	-4.006053937039E-01
9	T 6 C	-3.990866613152E-01	3.522314408170E-01	-4.362566913568E-01
10	T 1 H	-3.936184732347E-02	-1.307494347426E-01	-4.926059088019E-01
11	T 6 C	-1.257523310680E-01	-4.416843791359E-01	-4.158228800077E-01
12	T 6 C	-2.376250463238E-01	2.198901530702E-01	-3.328409383155E-01
13	T 1 H	-4.603423566893E-01	4.046833896371E-01	-4.759774330879E-01
14	T 6 C	-4.131510379927E-01	1.544975161626E-01	-3.720511593533E-01
15	T 6 C	-4.641320979679E-02	4.869400897257E-01	-3.618615120177E-01
16	T 6 C	-3.336932642579E-01	8.368680804435E-02	-3.179715206530E-01
17	T 6 C	-1.574711438878E-01	1.540225705650E-01	-2.798614506472E-01
18	T 1 H	-4.848138067377E-01	4.162724783238E-02	-3.609012400715E-01
19	T 1 H	2.575775348253E-02	-4.012147442448E-01	-3.725801112639E-01
20	T 6 C	-6.154348115912E-02	2.941229954667E-01	-2.970410581585E-01
21	T 6 C	-3.474469975869E-01	-1.185580170629E-01	-2.515058090639E-01
22	T 6 C	-1.750559917614E-01	-4.488941822105E-02	-2.132050681529E-01
23	T 1 H	-9.356303141797E-04	2.496481341623E-01	-2.562360266940E-01
24	T 1 H	-4.199333361397E-01	-2.280645856027E-01	-2.410381908599E-01
25	T 6 C	-2.689580447615E-01	-1.819523166190E-01	-1.998877472729E-01
26	T 1 H	-1.142194576774E-01	-9.569056259248E-02	-1.725021132724E-01
27	T 1 H	-2.806216372774E-01	-3.427398976752E-01	-1.495520274465E-01
55	T 8 O	3.700187960998E-01	-2.526741017770E-01	-3.375632400799E-01
56	T 1 H	3.607436315555E-01	-4.687134296319E-02	-3.671787556076E-01
57	T 6 C	2.968486474934E-01	-3.105671092234E-01	-2.804990409666E-01
58	T 6 C	2.006241332192E-01	-1.850705418897E-01	-2.871957336868E-01
59	T 6 C	3.221820893598E-01	4.851790116338E-01	-2.168067607761E-01
60	T 1 H	1.831158653381E-01	-2.147022704197E-02	-3.357402757767E-01

61	T	6	C	1.271199781482E-01	-2.708449380731E-01	-2.313328230744E-01
62	T	6	C	2.463072411240E-01	3.999749713245E-01	-1.599737587459E-01
63	T	6	C	4.214503382177E-01	3.618481807848E-01	-2.074636905738E-01
64	T	1	H	5.229125844744E-02	-1.768004846267E-01	-2.372912159971E-01
65	T	6	C	1.471942204625E-01	-4.818116966893E-01	-1.683704265207E-01
66	T	6	C	2.695087121399E-01	1.922359129047E-01	-9.503255039900E-02
67	T	1	H	4.778720195642E-01	4.226078109149E-01	-2.521397128491E-01
68	T	6	C	4.439425332835E-01	1.703324747931E-01	-1.441042150528E-01
69	T	6	C	7.116374109427E-02	4.156049696722E-01	-1.123907232447E-01
70	T	6	C	3.690957138584E-01	7.779129718573E-02	-8.604977783734E-02
71	T	6	C	1.929323511479E-01	9.748535700396E-02	-3.946206148983E-02
72	T	1	H	-4.807399753734E-01	7.879052064606E-02	-1.375334169191E-01
73	T	1	H	-4.621650728528E-03	-4.971811686494E-01	-1.205388481438E-01
74	T	6	C	9.288178748793E-02	2.133498367985E-01	-5.096018658798E-02
75	T	6	C	3.905066670182E-01	-1.272031315195E-01	-2.183022054549E-02
76	T	6	C	2.175764971205E-01	-1.099012121218E-01	2.346913424771E-02
77	T	1	H	3.436424951118E-02	1.361279586215E-01	-9.662446269414E-03
78	T	1	H	4.658225138981E-01	-2.201259853707E-01	-1.594571472110E-02
79	T	6	C	3.153624224328E-01	-2.197969972340E-01	3.197081117706E-02
80	T	1	H	1.597344872689E-01	-1.894916426852E-01	6.536408910412E-02
81	T	1	H	3.319848911271E-01	-3.838444547638E-01	8.039075706129E-02

Table S20. Pressure = 2.51GPa

VOLUME = 914.454717 DENSITY = 1.584 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.28954878	4.22007183	16.30891641	90.000000	88.814431	90.000000

ATOM		X/A	Y/B	Z/C
1 T	8 O	-3.653530600969E-01	-2.450807167227E-01	4.328744203312E-01
2 T	1 H	-3.642096740656E-01	-3.609518132681E-02	4.048097638866E-01
3 T	6 C	-2.855693099351E-01	-2.960973748416E-01	4.835950756122E-01
4 T	6 C	-1.919816512102E-01	-1.587108313176E-01	4.680854968037E-01
5 T	6 C	-3.020920168555E-01	4.950938980660E-01	-4.505750406308E-01
6 T	1 H	-1.826433046503E-01	3.748064193953E-03	4.171202940410E-01
7 T	6 C	-1.121305783586E-01	-2.269185450591E-01	-4.812201709123E-01
8 T	6 C	-2.200145811097E-01	4.263223698046E-01	-3.991375735718E-01
9 T	6 C	-3.980167728805E-01	3.518291679303E-01	-4.338539669105E-01
10 T	1 H	-3.976858909796E-02	-1.155894493439E-01	-4.919468205519E-01
11 T	6 C	-1.242791326091E-01	-4.342317170595E-01	-4.149707290076E-01
12 T	6 C	-2.340257190982E-01	2.190480948232E-01	-3.311394969045E-01
13 T	1 H	-4.602131627429E-01	4.037707645913E-01	-4.734022081715E-01
14 T	6 C	-4.103914690250E-01	1.492787287322E-01	-3.695956133355E-01
15 T	6 C	-4.351326112007E-02	4.931846126513E-01	-3.616085216214E-01
16 T	6 C	-3.296831063574E-01	7.866471262800E-02	-3.156815972182E-01
17 T	6 C	-1.524906475492E-01	1.525666196615E-01	-2.786069975408E-01
18 T	1 H	-4.815344912195E-01	3.209654062080E-02	-3.582575773648E-01
19 T	1 H	2.831538322336E-02	-3.922119998341E-01	-3.727810709066E-01
20 T	6 C	-5.688532870535E-02	2.955318096366E-01	-2.966953890297E-01
21 T	6 C	-3.416227153646E-01	-1.279103712768E-01	-2.490243955808E-01
22 T	6 C	-1.684132362761E-01	-5.005821040072E-02	-2.115280268970E-01
23 T	1 H	4.876321795316E-03	2.498408526082E-01	-2.563944562030E-01
24 T	1 H	-4.135637271476E-01	-2.417087978142E-01	-2.381859936135E-01
25 T	6 C	-2.618774834716E-01	-1.910923672844E-01	-1.976794281771E-01
26 T	1 H	-1.065771130510E-01	-1.005867054262E-01	-1.710256176821E-01
27 T	1 H	-2.722979138915E-01	-3.546538760676E-01	-1.471707208729E-01
55 T	8 O	3.722850722707E-01	-2.400948029728E-01	-3.404055121855E-01
56 T	1 H	3.633950934240E-01	-3.459055350909E-02	-3.694903298522E-01
57 T	6 C	2.988920506767E-01	-3.004052361732E-01	-2.819881073564E-01
58 T	6 C	2.022828171872E-01	-1.754614836129E-01	-2.874653484938E-01
59 T	6 C	3.243076485729E-01	4.918720195945E-01	-2.184854922845E-01
60 T	1 H	1.846341280743E-01	-8.991018872288E-03	-3.357526425153E-01

61	T	6	C	1.284360770643E-01	-2.669139520667E-01	-2.308383569707E-01
62	T	6	C	2.480868480415E-01	4.007496855181E-01	-1.609265674120E-01
63	T	6	C	4.241583884456E-01	3.709377315178E-01	-2.100709423679E-01
64	T	1	H	5.321515665731E-02	-1.741172444153E-01	-2.358628888334E-01
65	T	6	C	1.485252003856E-01	-4.823712117442E-01	-1.683471398129E-01
66	T	6	C	2.713968524922E-01	1.884130762475E-01	-9.637467544833E-02
67	T	1	H	4.808216639614E-01	4.370776470947E-01	-2.553386536178E-01
68	T	6	C	4.468751091734E-01	1.754980228620E-01	-1.469046147318E-01
69	T	6	C	7.199441072799E-02	4.086166588959E-01	-1.120064221538E-01
70	T	6	C	3.715451344473E-01	7.568111820330E-02	-8.834397907770E-02
71	T	6	C	1.942851260790E-01	8.677544044372E-02	-4.044124203696E-02
72	T	1	H	-4.772347439110E-01	8.686237565426E-02	-1.409768770192E-01
73	T	1	H	-4.264918092613E-03	4.938695815198E-01	-1.196539516477E-01
74	T	6	C	9.369443757368E-02	2.014479595343E-01	-5.110248824525E-02
75	T	6	C	3.929799282633E-01	-1.349922323606E-01	-2.472653775933E-02
76	T	6	C	2.188770139293E-01	-1.267705745775E-01	2.169139080918E-02
77	T	1	H	3.463076896666E-02	1.186372395980E-01	-9.817003967215E-03
78	T	1	H	4.687140065717E-01	-2.268112675405E-01	-1.968082804636E-02
79	T	6	C	3.171985020521E-01	-2.353601918534E-01	2.920605507330E-02
80	T	1	H	1.605976171896E-01	-2.124923811800E-01	6.359801798293E-02
81	T	1	H	3.336933654832E-01	-4.046964979782E-01	7.685167976964E-02

Table S21. Pressure = 2.94GPa

VOLUME = 903.390798 DENSITY = 1.603 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.26054720	4.12747720	16.50777559	90.000000	89.055405	90.000000

	ATOM	X/A	Y/B	Z/C
1	T 8 O	-3.644873103652E-01	-2.477131633322E-01	4.314675852408E-01
2	T 1 H	-3.630140643500E-01	-3.588161435013E-02	4.026468590174E-01
3	T 6 C	-2.848952300116E-01	-2.988154092894E-01	4.821813025650E-01
4	T 6 C	-1.905059693423E-01	-1.637174550486E-01	4.666362907263E-01
5	T 6 C	-3.026533198997E-01	4.944865733400E-01	-4.517265717726E-01
6	T 1 H	-1.803029835510E-01	-2.223647715621E-03	4.154951137869E-01
7	T 6 C	-1.110912987541E-01	-2.319232863110E-01	-4.823104330897E-01
8	T 6 C	-2.209983412706E-01	4.254344351003E-01	-3.999793701137E-01
9	T 6 C	-3.994576157994E-01	3.538258855976E-01	-4.351271471655E-01
10	T 1 H	-3.810736470481E-02	-1.220277293709E-01	-4.930605282847E-01
11	T 6 C	-1.244714704860E-01	-4.372037681177E-01	-4.157242182334E-01
12	T 6 C	-2.362645902279E-01	2.198945468210E-01	-3.318278364442E-01
13	T 1 H	-4.612904540472E-01	4.061794170415E-01	-4.749237641967E-01
14	T 6 C	-4.130357973903E-01	1.529406176533E-01	-3.706371605163E-01
15	T 6 C	-4.427161179050E-02	4.908715410619E-01	-3.618738542726E-01
16	T 6 C	-3.327540119447E-01	8.175310708920E-02	-3.165421968510E-01
17	T 6 C	-1.552369694775E-01	1.532673984401E-01	-2.789511358342E-01
18	T 1 H	-4.847703893420E-01	3.687112780878E-02	-3.592893147258E-01
19	T 1 H	2.811802287792E-02	-3.949970038277E-01	-3.728500730812E-01
20	T 6 C	-5.895372439453E-02	2.953922142454E-01	-2.966927720542E-01
21	T 6 C	-3.459806051443E-01	-1.237077955863E-01	-2.497978187723E-01
22	T 6 C	-1.723299853390E-01	-4.852969892587E-02	-2.118959286938E-01
23	T 1 H	2.297458678440E-03	2.510089567532E-01	-2.559444874841E-01
24	T 1 H	-4.186649860990E-01	-2.355131542694E-01	-2.390109274002E-01
25	T 6 C	-2.665975955872E-01	-1.881502641882E-01	-1.983064970104E-01
26	T 1 H	-1.108102167583E-01	-1.000472931930E-01	-1.712272103132E-01
27	T 1 H	-2.779283522298E-01	-3.519440229907E-01	-1.478743945157E-01
55	T 8 O	3.710634431674E-01	-2.438903104670E-01	-3.382203375832E-01
56	T 1 H	3.617519365674E-01	-3.580896260239E-02	-3.680143984810E-01
57	T 6 C	2.972610892523E-01	-3.046076638774E-01	-2.809460562906E-01
58	T 6 C	2.003421404449E-01	-1.787530768647E-01	-2.874975476414E-01
59	T 6 C	3.228266794008E-01	4.879121104646E-01	-2.171881817713E-01
60	T 1 H	1.826447353471E-01	-1.214969869663E-02	-3.360263547019E-01

61	T	6	C	1.264246706610E-01	-2.681056875071E-01	-2.313617808111E-01
62	T	6	C	2.465217338683E-01	3.997003749823E-01	-1.600412524487E-01
63	T	6	C	4.228137075660E-01	3.643900897074E-01	-2.081291189473E-01
64	T	1	H	5.100665759943E-02	-1.745668969022E-01	-2.371110599752E-01
65	T	6	C	1.467207467907E-01	-4.822011955660E-01	-1.683178443098E-01
66	T	6	C	2.699971499048E-01	1.889942834399E-01	-9.498266931657E-02
67	T	1	H	4.793752696723E-01	4.264280932924E-01	-2.533206881846E-01
68	T	6	C	4.456384812757E-01	1.703788321868E-01	-1.445540829744E-01
69	T	6	C	7.011512989990E-02	4.117407635839E-01	-1.122141152942E-01
70	T	6	C	3.703363074695E-01	7.484433455736E-02	-8.617713060977E-02
71	T	6	C	1.928905373125E-01	9.076867477038E-02	-3.923520966139E-02
72	T	1	H	-4.785063546488E-01	7.863467380394E-02	-1.381777400980E-01
73	T	1	H	-6.267031074923E-03	4.986123680284E-01	-1.203737995828E-01
74	T	6	C	9.207658725278E-02	2.063937195146E-01	-5.067665770795E-02
75	T	6	C	3.919695432957E-01	-1.335771478652E-01	-2.190304552933E-02
76	T	6	C	2.177307162711E-01	-1.203757873350E-01	2.367869225194E-02
77	T	1	H	3.318424087724E-02	1.262122605353E-01	-9.290442163954E-03
78	T	1	H	4.678151355861E-01	-2.270105792998E-01	-1.624795003948E-02
79	T	6	C	3.162808659566E-01	-2.300931420670E-01	3.199501014792E-02
80	T	1	H	1.594985160759E-01	-2.033215268380E-01	6.563122982945E-02
81	T	1	H	3.330170596459E-01	-3.976794174144E-01	8.026704259824E-02

Table S22 Pressure = 3.36GPa

VOLUME = 893.163215 DENSITY = 1.622 g/cm^3

A	B	C	ALPHA	BETA	GAMMA
13.22040383	4.11011167	16.44032328	90.000000	88.915047	90.000000

	ATOM	X/A	Y/B	Z/C
1	T 8 O	-3.654213061881E-01	-2.437315635674E-01	4.323715913161E-01
2	T 1 H	-3.638689513409E-01	-3.114141808332E-02	4.033093478056E-01
3	T 6 C	-2.852389813673E-01	-2.959268901101E-01	4.826896018452E-01
4	T 6 C	-1.907062368809E-01	-1.601173097385E-01	4.665797196999E-01
5	T 6 C	-3.026343294145E-01	4.957060825994E-01	-4.510465211321E-01
6	T 1 H	-1.808346691998E-01	2.671930478217E-03	4.153155229195E-01
7	T 6 C	-1.108014125790E-01	-2.287815523944E-01	-4.826362741048E-01
8	T 6 C	-2.204875446385E-01	4.262755812899E-01	-3.995775951668E-01
9	T 6 C	-3.995576735982E-01	3.537699599704E-01	-4.340483703241E-01
10	T 1 H	-3.770333745269E-02	-1.181874268840E-01	-4.936905101965E-01
11	T 6 C	-1.238523112248E-01	-4.351649090429E-01	-4.158150606463E-01
12	T 6 C	-2.353816348886E-01	2.195356277717E-01	-3.311735224885E-01
13	T 1 H	-4.617169070013E-01	4.061231612560E-01	-4.737494831975E-01
14	T 6 C	-4.127602395292E-01	1.513912624762E-01	-3.693622931342E-01
15	T 6 C	-4.316568221190E-02	4.930900750619E-01	-3.621725820806E-01
16	T 6 C	-3.319900982165E-01	8.024569430261E-02	-3.154366849271E-01
17	T 6 C	-1.538472780380E-01	1.530030212048E-01	-2.785206583958E-01
18	T 1 H	-4.844841711902E-01	3.376346786989E-02	-3.577143993895E-01
19	T 1 H	2.921286167585E-02	-3.911115633160E-01	-3.734044718816E-01
20	T 6 C	-5.748052149460E-02	2.963453436168E-01	-2.967669501913E-01
21	T 6 C	-3.447884766387E-01	-1.265081027934E-01	-2.484622530047E-01
22	T 6 C	-1.705665893274E-01	-4.972459402368E-02	-2.111509786657E-01
23	T 1 H	4.117693728148E-03	2.525090970507E-01	-2.561393586273E-01
24	T 1 H	-4.174890451073E-01	-2.396853735873E-01	-2.373395406954E-01
25	T 6 C	-2.649335803562E-01	-1.907744008648E-01	-1.971757568901E-01
26	T 1 H	-1.086928468936E-01	-1.009092122686E-01	-1.705986512778E-01
27	T 1 H	-2.759765614773E-01	-3.556669074183E-01	-1.465990476978E-01
55	T 8 O	3.715999213823E-01	-2.396268518613E-01	-3.388740827610E-01
56	T 1 H	3.624331608697E-01	-3.054872506546E-02	-3.688344173746E-01
57	T 6 C	2.974642176712E-01	-3.014052934237E-01	-2.814281148415E-01
58	T 6 C	2.001980190350E-01	-1.758463632912E-01	-2.878728569752E-01
59	T 6 C	3.231708733922E-01	4.899126664141E-01	-2.175892066454E-01
60	T 1 H	1.823772735191E-01	-7.932017582288E-03	-3.364146293243E-01

61	T	6	C	1.260656932183E-01	-2.673253140693E-01	-2.315640687528E-01
62	T	6	C	2.466454764066E-01	3.997174410490E-01	-1.602812350983E-01
63	T	6	C	4.235733758044E-01	3.673299368634E-01	-2.086533757759E-01
64	T	1	H	5.033770669464E-02	-1.745909304692E-01	-2.372669963031E-01
65	T	6	C	1.464702122484E-01	-4.828750894817E-01	-1.684783476246E-01
66	T	6	C	2.702825345722E-01	1.876191634139E-01	-9.517410287952E-02
67	T	1	H	4.802618767103E-01	4.310251227261E-01	-2.540303779946E-01
68	T	6	C	4.466047970539E-01	1.723694743146E-01	-1.449520337453E-01
69	T	6	C	6.959061804966E-02	4.086462359982E-01	-1.123198442114E-01
70	T	6	C	3.710295154457E-01	7.447515682501E-02	-8.647060826437E-02
71	T	6	C	1.929020965297E-01	8.697789650748E-02	-3.934550352855E-02
72	T	1	H	-4.771817001995E-01	8.173859534918E-02	-1.385960675130E-01
73	T	1	H	-7.110825677056E-03	4.946685488411E-01	-1.205104919064E-01
74	T	6	C	9.169261853453E-02	2.017709644460E-01	-5.076075524597E-02
75	T	6	C	3.928160684585E-01	-1.356016267944E-01	-2.219565204029E-02
76	T	6	C	2.178892018916E-01	-1.259519092714E-01	2.352578381856E-02
77	T	1	H	3.256867586954E-02	1.194650443546E-01	-9.403589780063E-03
78	T	1	H	4.689748853571E-01	-2.284792040413E-01	-1.666780655009E-02
79	T	6	C	3.168608710991E-01	-2.347945318120E-01	3.172273473006E-02
80	T	1	H	1.594818162120E-01	-2.111907065149E-01	6.549612858434E-02
81	T	1	H	3.336947359056E-01	-4.041467642803E-01	7.988731610818E-02