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Pancake-bonding of semiquinone radicals under variable temperature and pressure conditions

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Table S1. The angles between the principal axes of the strain ellipsoid and the crystallographic axes

Linear strain in phase 1 – from 100 to 210 K				
Temperature, K	strain direction	angle to axis ***a***, °	angle to axis ***b***, °	angle to axis ***c***, °
120	1	90.0	0.0	90.0
	2	75.2(0.4)	90.0	170.0(0.4)
	3	165.2(0.4)	90.0	100.0(0.4)
150	1	90.0	0.0	90.0
	2	80.0(0.4)	90.0	174.8(0.4)
	3	170.0(0.4)	90.0	95.2(0.4)
180	1	90.0	0.0	90.0
	2	79.8(0.3)	90.0	174.5(0.3)
	3	169.8(0.3)	90.0	95.5(0.3)
210	1	90.0	0.0	90.0
	2	82.1(0.4)	90.0	176.9(0.4)
	3	172.1(0.4)	90.0	93.1(0.4)
Linear strain in phase 2 – from 240 K to 370 K				
270	1	90.0	0.0	90.0
	2	83.4(0.4)	90.0	178.1(0.4)
	3	173.4(0.4)	90.0	91.9(0.4)
293	1	Circular section of strain ellipsoid - no eigenvector defined		
	2			
	3	6.1(0.2)	90.0	88.6(0.2)
310	1	Circular section of strain ellipsoid - no eigenvector defined		
	2			
	3	4.7(0.4)	90.0	90.0(0.4)
340	1	Circular section of strain ellipsoid - no eigenvector defined		
	2			
	3	5.1(0.4)	90.0	89.6(0.4)
370	1	Circular section of strain ellipsoid - no eigenvector defined		
	2			
	3	4.4(0.4)	90.0	90.3(0.4)

Table S2. Linear strain in the directions of the principal axes of the strain ellipsoid

Temperature, K	Axis 1	Axis 2	Axis 3
The linear strain in phase 1 – from 100 to 210 K			
100	0	0	0
120	0.00088(3)	0.00092(3)	0.00182(3)
150	0.00120(3)	0.00145(3)	0.00428(3)
180	0.00141(3)	0.00182(3)	0.00682(3)
210	0.00166(3)	0.00217(3)	0.00896(3)
The linear strain in phase 2 – from 240 K to 370 K			
240	0	0	0
270	0.00039(3)	0.00052(3)	0.00280(3)
293	0.00080(2)	0.00080(2)	0.00495(3)
310	0.00123(2)	0.00123(2)	0.00663(3)

340	0.00192(2)	0.00192(2)	0.01000(4)
370	0.00280(2)	0.00280(2)	0.01353(4)

Table S3. Linear strain in the directions of the principal axes of strain ellipsoid

Pressure, GPa	1	2	3
0	0	0	0
0.25	-0.00549(10)	-0.00208(28)	-0.00087(12)
0.49	-0.018248(93)	-0.0056(26)	-0.00419(11)
0.86	-0.035703(98)	-0.00982(15)	-0.00982(15)
1.42	-0.052786(92)	-0.01565(14)	-0.01565(14)
1.85	-0.064656(90)	-0.01957(13)	-0.01957(13)
2.55	-0.07826(11)	-0.02608(13)	-0.02095(30)
3.26	-0.094611(92)	-0.03338(11)	-0.02535(26)
3.95	-0.103475(95)	-0.03739(11)	-0.02758(27)
4.80	-0.11765(14)	-0.04573(18)	-0.03006(44)
5.48	-0.12534(18)	-0.04783(24)	-0.03239(63)
6.00	-0.13333(21)	-0.05227(25)	-0.03375(63)

Table S4. The angles between the principal axes of the strain ellipsoid and the crystallographic axes

Linear strain in phase 1 – from 0 to 1.85 GPa				
Pressure, GPa	strain direction	angle to axis ***a***, °	angle to axis ***b***, °	angle to axis ***c***, °
0.25	1	2.7(1.1)	90.0	97.4(1.1)
	2	90.0	180.0	90.0
	3	92.7(1.1)	90.0	172.6(1.1)
0.49	1	1.0(0.4)	90.0	95.6(0.4)
	2	90.0	180.0	90.0
	3	174.4(0.4)	90.0	174.4(0.3)
0.86	1	0.9(0.2)	90.0	93.8(0.2)
	2	Circular section of strain ellipsoid - no eigenvector defined		
	3			
1.42	1	2.0(0.2)	90.0	92.6(0.2)
	2	Circular section of strain ellipsoid - no eigenvector defined		
	3			
1.85	1	2.9(0.1)	90.0	91.9(0.1)
	2	Circular section of strain ellipsoid - no eigenvector defined		
	3			
Linear strain in phase 2 – from 2.55 GPa to 6 GPa				
3.26	1	19.9(0.4)	90.0	75.7(0.4)

	2	70.1(0.4)	90.0	165.7(0.4)
	3	90.0	0.0	90.0
3.95	1	19.8(0.3)	90.0	76.0(0.3)
	2	70.2(0.3)	90.0	166.0(0.3)
	3	90.0	0.0	90.0
4.80	1	20.9(0.4)	90.0	75.1(0.4)
	2	69.1(0.4)	90.0	165.1(0.4)
	3	90.0	0.0	90.0
5.48	1	21.4(0.4)	90.0	74.8(0.4)
	2	68.6(0.4)	90.0	164.8(0.4)
	3	90.0	0.0	90.0
6.00	1	21.3(0.4)	90.0	75.1(0.4)
	2	68.7(0.4)	90.0	165.1(0.4)
	3	90.0	0.0	90.0

Table S5. The changes in the geometrical parameters characterising the pancake interactions

Temperature, K	Cg…plane(Cg2), Å		Cg…Cg2, Å	
	A	B	A	B
100	2.872(1)	3.430(1)	3.519(1)	3.977(1)
120	2.875(1)	3.437(1)	3.523(1)	3.986(1)
150	2.880(1)	3.445(1)	3.529(1)	3.994(1)
180	2.890(1)	3.451(1)	3.535(1)	4.005(1)
210	2.895(1)	3.457(1)	3.541(1)	4.012(1)
240	2.907(1)	3.467(1)	3.550(1)	4.029(1)
270	2.912(1)	3.476(1)	3.556(1)	4.041(1)
293	2.918(1)	3.483(1)	3.559(1)	4.052(1)
310	2.925(1)	3.484(1)	3.565(1)	4.055(1)
340	2.939(1)	3.494(1)	3.572(1)	4.067(1)
370	2.953(1)	3.496(1)	3.583(1)	4.074(1)