Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Understanding the solid state luminescence and piezochromic properties in polymorphs of an anthracene derivative

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Supporting Information

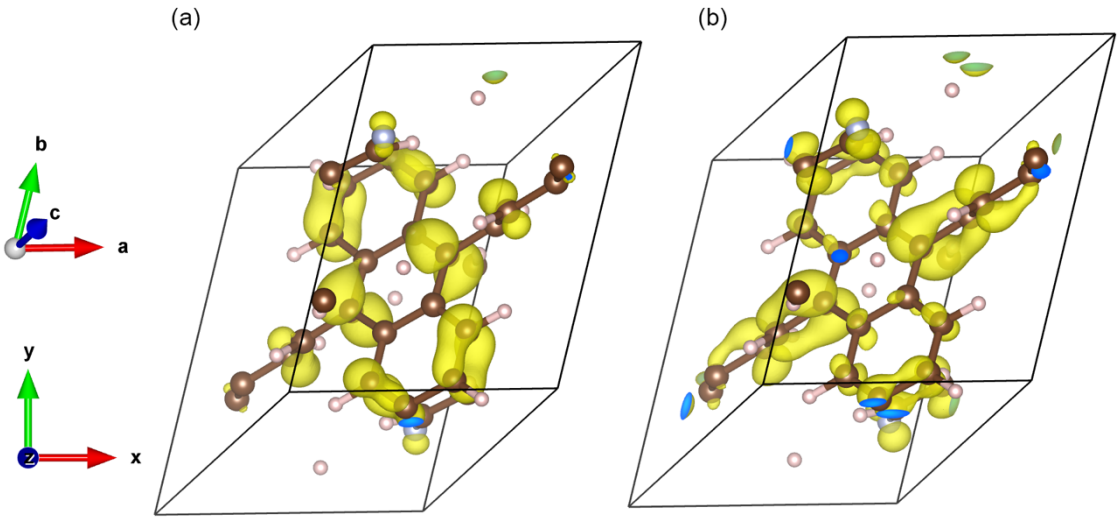

Figure S1. Electron density of (a) the HOMO and (b) the LOMO of the C1 crystal structure.

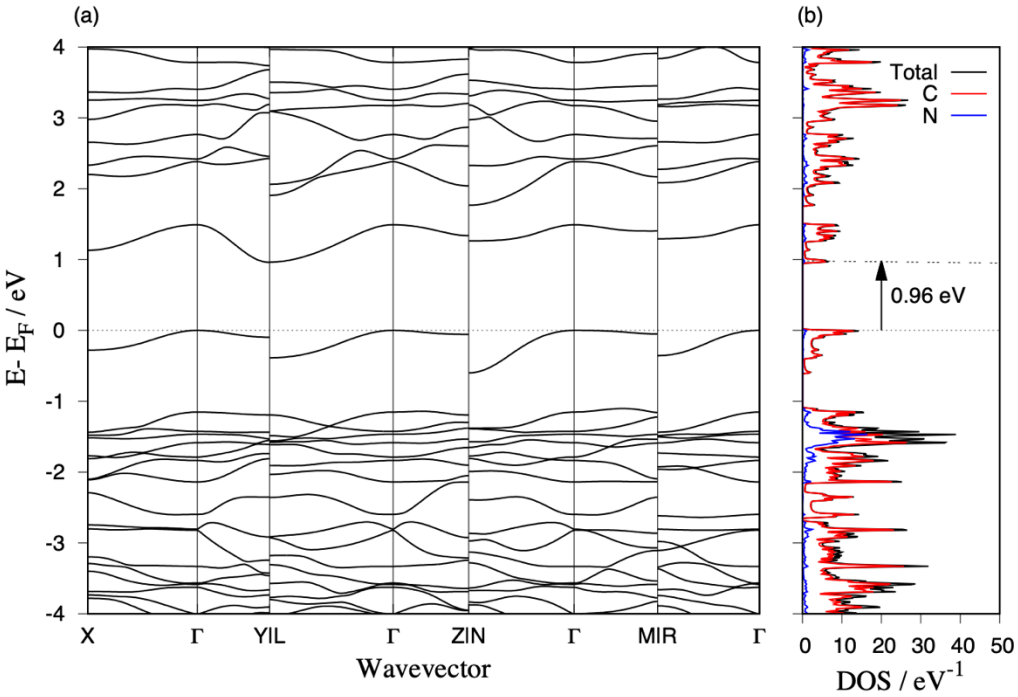

Figure S2. (a) Electronic band structure and (b) DOS of the C1 crystal structure at 6 GPa

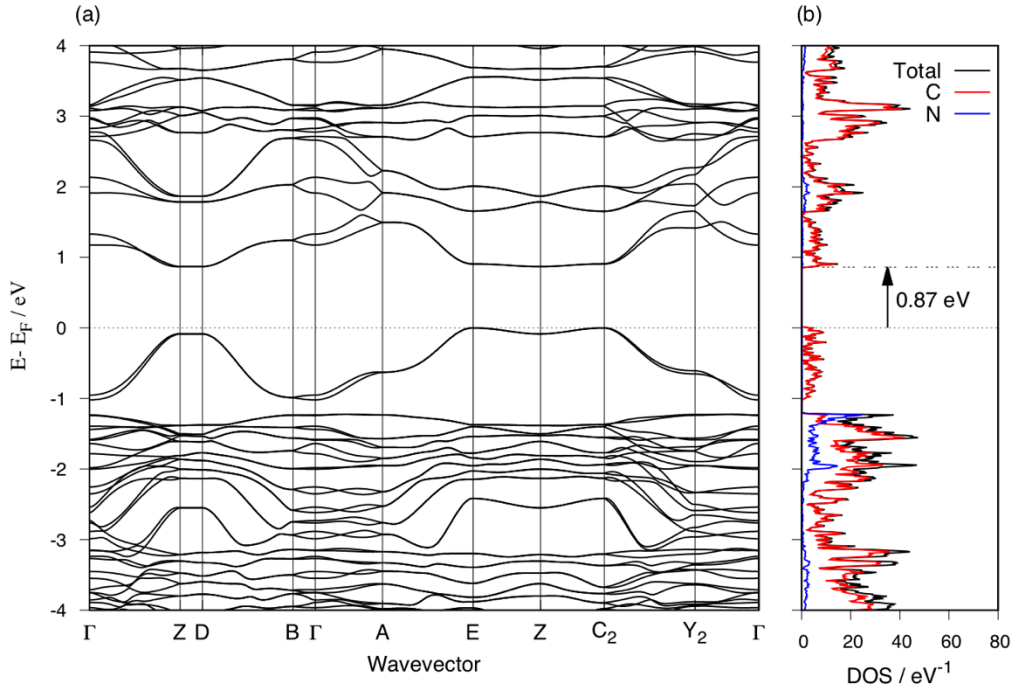

Figure S3. Electronic band structure and DOS of the C2 crystal structure at 6 GPa

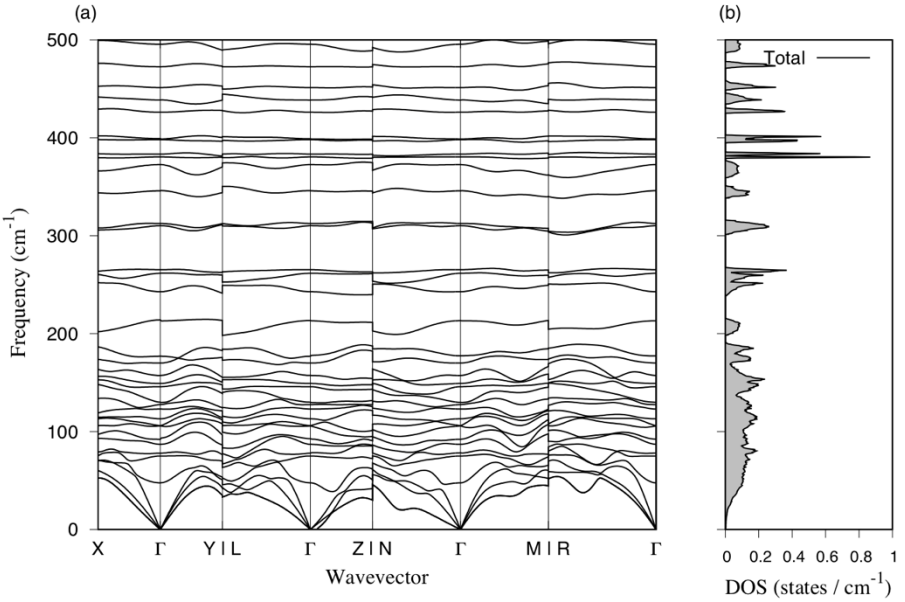

Figure S4. (a) Phonon dispersion and (b) phonon density of states for C1 at 0 GPa calculated with the DFPT method within Quantum Espresso.

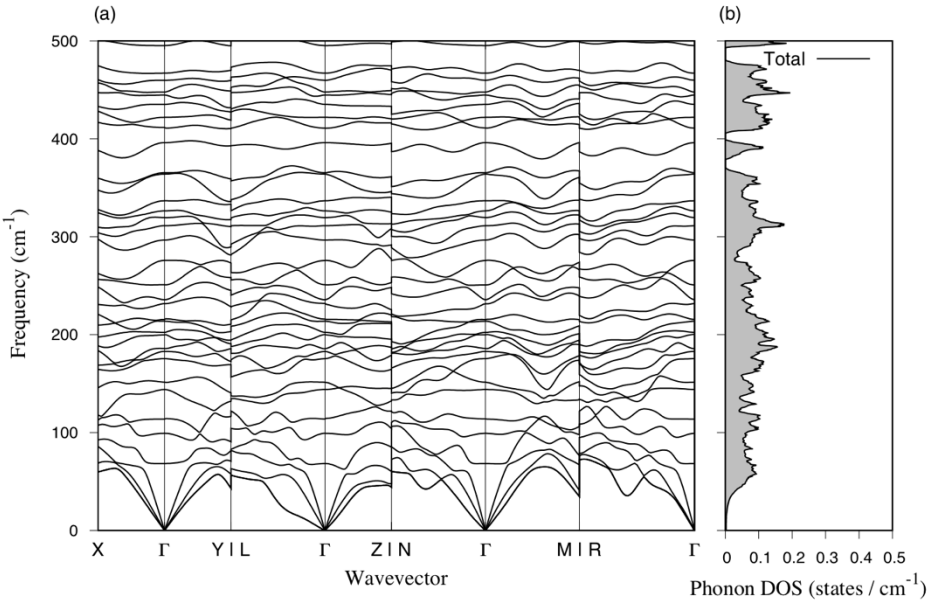

Figure S5. (a) Phonon dispersion and (b) phonon density of states for C1 at 6 GPa calculated with the DFPT method within Quantum Espresso.

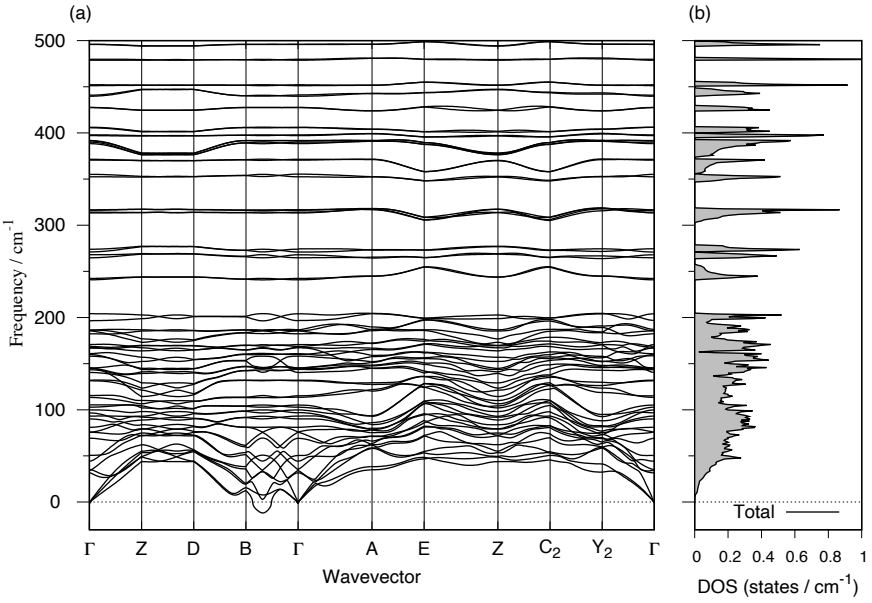

Figure S6. (a) Phonon dispersion and (b) phonon density of states for C2 at 0 GPa calculated with the DFPT method within Quantum Espresso.

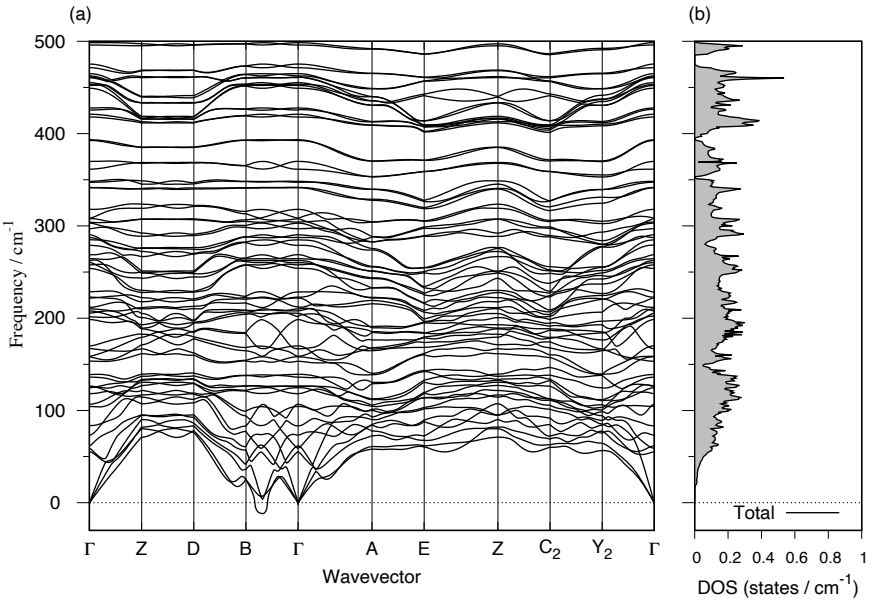

Figure S7. (a) Phonon dispersion and (b) phonon density of states for C2 at 6 GPa calculated with the DFPT method within Quantum Espresso.

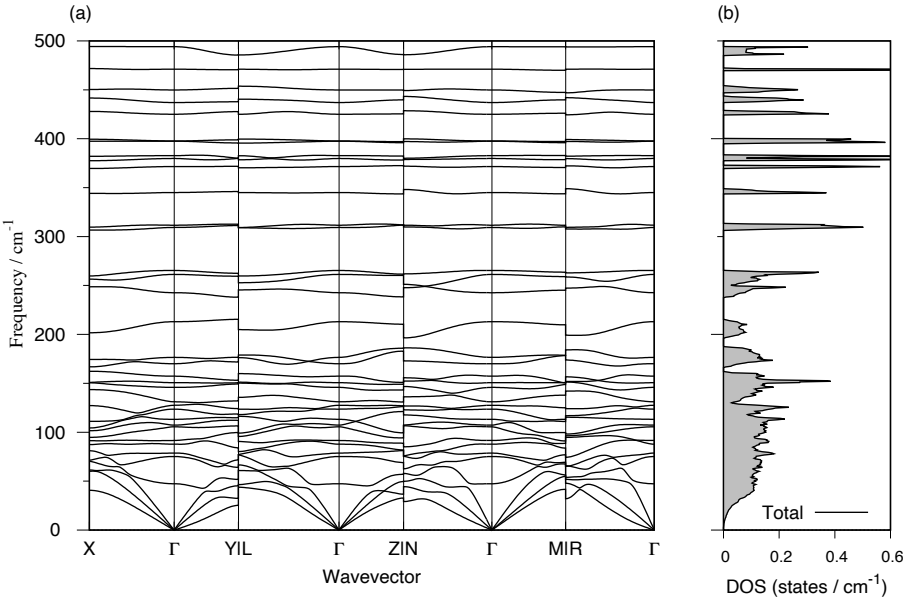

Figure S8. (a) Phonon dispersion and (b) phonon density of states for C1 at 0 GPa calculated with the finite-displacement method with VASP and the Phonopy package.

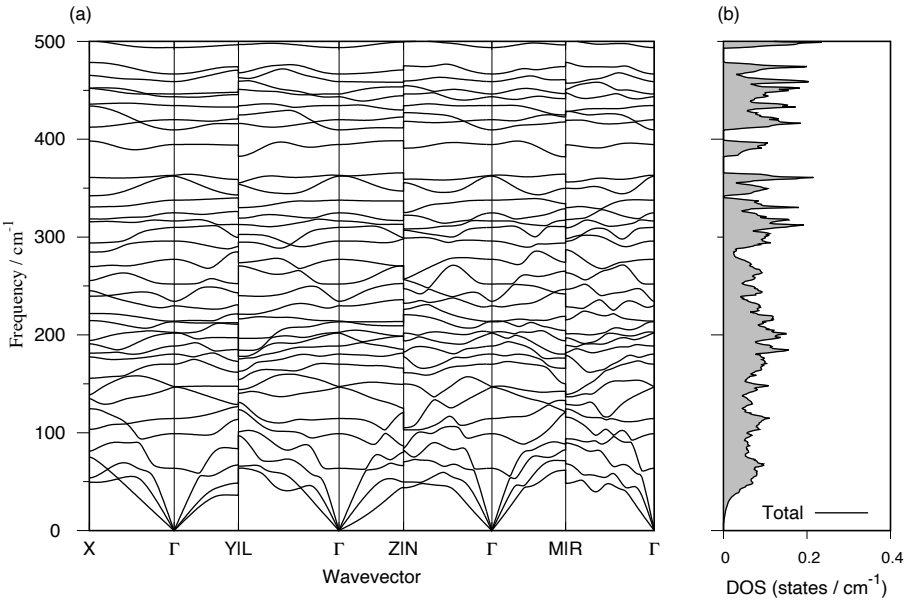

Figure S9. (a) Phonon dispersion and (b) phonon density of states for C1 at 6 GPa calculated with the finite-displacement method with VASP and the Phonopy package.

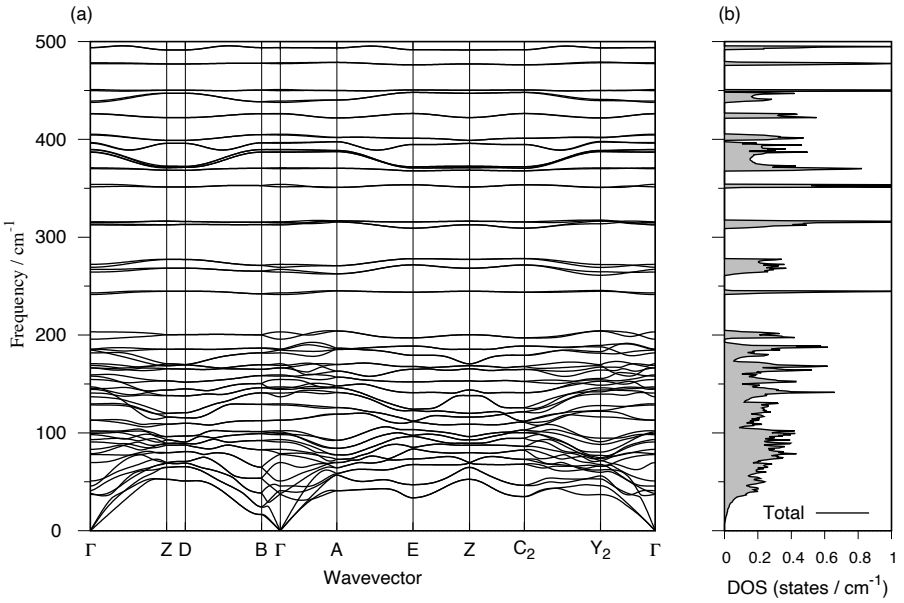

Figure S10. (a) Phonon dispersion and (b) phonon density of states for C2 at 0 GPa calculated with the finite-displacement method with VASP and the Phonopy package.

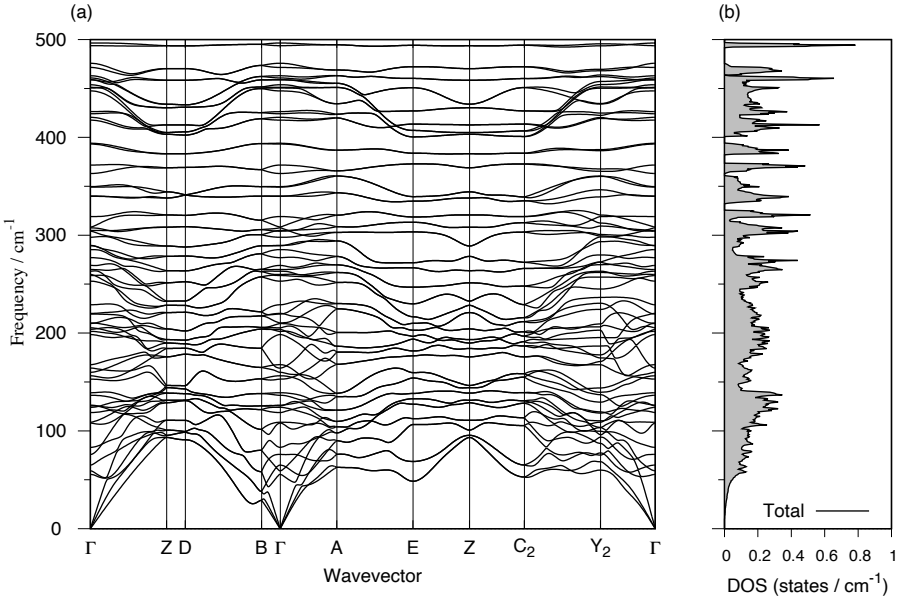

Figure S11. (a) Phonon dispersion and (b) phonon density of states for C2 at 6 GPa calculated with the finite-displacement method with VASP and the Phonopy package.

Table S1. comparison of theoretical and experimentally determined parameters of the BP4VA crystal structures at 0 and 6PGa calculated with PBE-D3

		C1			C2	
	Exp	0 GPa	6 GPa	Exp	0 GPa	6 GPa
a (Å)	6.85	6.62	4.70	7.60	7.72	7.16
b (Å)	9.23	9.20	10.23	5.71	5.58	5.03
c (Å)	9.34	9.57	10.17	22.90	22.65	20.54
α (°)	65.9	65.9	60.5	90	90	90
β (°)	70.0	69.2	63.0	96.0	96.7	90.7
γ (°)	77.4	76.1	70.9	90	90	90
V (Å^3)	504.2	494.7	375.8	988.0	969.7	739.8
Relative stability / atom (meV)		0.9	2.9		0.0	0.0
CH-π H-bond distance (Å)	2.79	2.60	2.45			
Vertical stacking distance between the two anthracene planes (Å)				3.60	3.53	2.95
Dihedral angle (°)	64.5	52.0	31.0	67.5	53.4	52.3
Band Gap PBE (eV)		1.61	0.92		1.41	0.87
Band Gap B3LYP (eV)		2.74	2.01		2.47	1.94

Table S2. Dimer exciton couplings for C1 at 0 GPa

Cl (0 GPa)	S1	f	S2	f	*J* (meV)
D1	2.96	1.48	3.02	0.00	32
D2	2.96	0.00	3.01	1.07	28
1	2.98	0.00	3.02	1.22	18
6	3.00	0.00	3.04	1.19	18
4	2.98	1.34	3.00	0.00	10
5	3.00	1.33	3.02	0.00	10
0	3.01	0.00	3.01	1.22	3

Table S3. Dimer exciton couplings for C1 at 6 GPa

Cl (6 GPa)	S1	f	S2	f	*J* (meV)
D2	2.56	0.00	2.67	1.23	56
D1	2.67	1.80	2.74	0.00	38
4	2.66	1.71	2.71	0.00	26
5	2.70	1.71	2.75	0.00	23
14	2.69	0.00	2.72	1.55	17
20	2.72	0.00	2.74	1.54	13
0	2.71	0.00	2.73	1.54	7

Table S4. Dimer exciton couplings for C2 at 0 GPa

C2 (0 GPa)	S1	f	S2	f	*J* (meV)
D3	2.90	1.39	2.95	0.07	26
D4	2.90	0.00	2.95	1.21	25
14	2.92	1.46	2.96	0.03	21
2	2.90	0.00	2.93	1.33	15
0	2.83	0.00	2.86	0.90	15
4	2.93	1.33	2.94	0.03	6
10	2.93	1.32	2.94	0.03	5

Table S5. Dimer exciton couplings for C2 at 6 GPa

C2 (6 GPa)	S1	f	S2	f	*J* (meV)
D4	2.64	0.58	2.82	0.00	94
D3	2.89	1.38	2.96	0.09	33
1	2.90	0.00	2.96	1.15	30
2	2.91	0.00	2.96	1.29	24
18	2.93	1.45	2.97	0.01	22
0	2.93	0.00	2.97	1.19	21
3	2.94	0.00	2.96	1.26	7