Table 1 – Lattice parameters of Tetracene molecule calculated in VASP code

	D2	**D3**	**TS**	**TS-SCS**	**PBE***	**Exp**
a	7.54 (7.41)	7.92	7.71	7.70	9.25	7.90
b	5.96 (5.83)	6.00	5.99	6.08	7.21	6.03
c	13.28 (13.39)	13.38	13.38	13.47	16.62	13.53
α	102.10 (102.21)	101.21	101.36	100.97	101.36	100.30
β	114.33 (113.23)	113.26	113.61	114.39	112.14	113.20
γ	85.20 (85.11)	85.89	85.74	85.68	86.67	86.30
Volume (Å^3)	531.41 (519.01)	572.96	554.74	563.74	1007.16	582.85

* without dispersion correction
() Parenthesis values were calculated with CRYSTAL program
Exp Campbell, R. B *et al* Acta cryst, 15(3): 289-290, 1962.

Tetracene

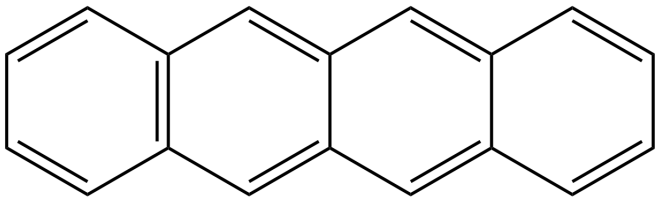

Figure 1 – Tetracene molecule

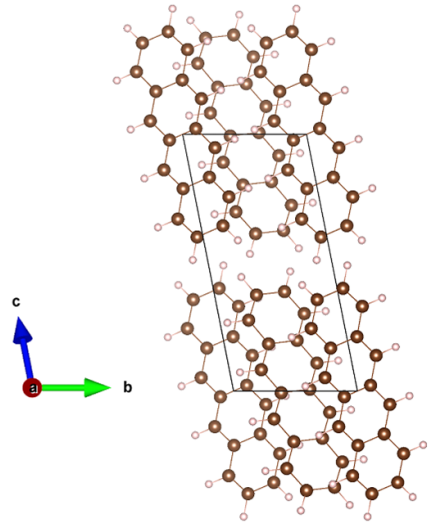

Figure 2 – The *bc* plane of Tetracene Crystal

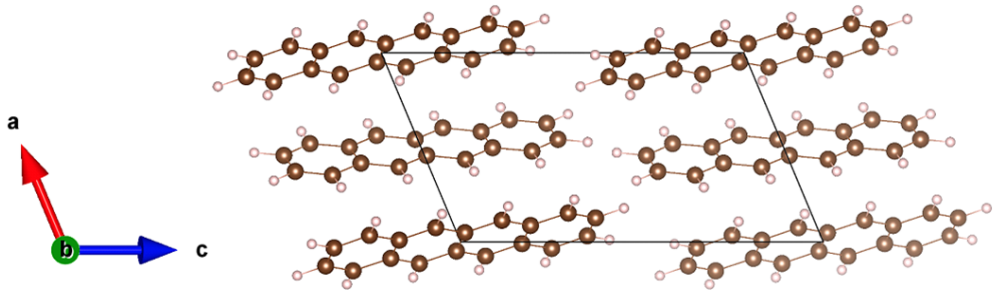

Figure 3 – The *ac* plane of Tetracene Crystal

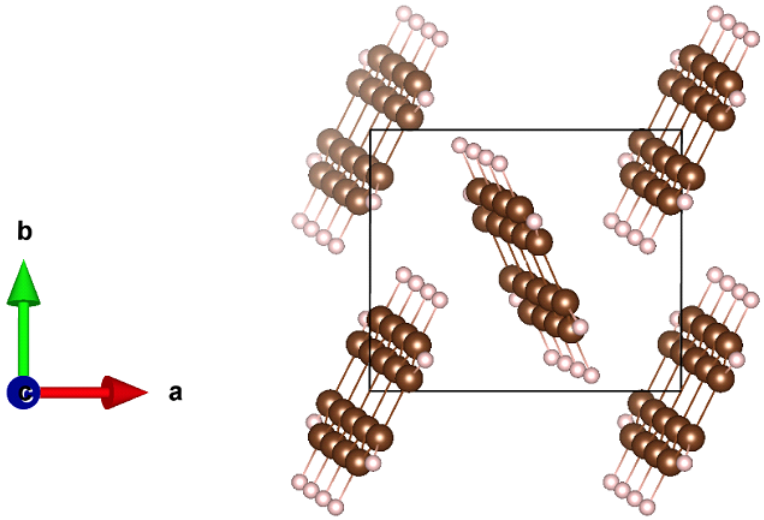

Figure 4 – The *ab* plane of Tetracene Crystal

Table 2 – Calculated vibrational frequencies (cm^{-1}) of the monomer, dimer and solid-state (PBE tetracene system).

Monomer		**Dimer**	**Experimental (P.A.) this work**	**VASP/CRYSTAL**
Assignment	ν(cm^{-1}) Int(km/mol)	ν(cm^{-1}) Int(km/mol)	ν(cm^{-1})	ω(cm^{-1}) Int(relative)
		15 (<0.01)		
		31 (0)		
		52 (0)		
ν_1	57 (0.8)	59 (0.6)		69.7 (8.2)
		80 (1.0)		
		87 (0.1)		
		94 (0)		
		112 (0)		
ν_2	93 (0)	117 (0.3)	106 (m) + sh	102.4 (2.1)
				105.7 (9.5)
		124 (0)		
$3\nu_1$	132 (<0.01)			
ν_3	153 (0.01)		142 (m)	128.5 (7.1)
				148 (0.1)
		162 (0)		
ν_4	164 (1.3)	168 (1.7)	166 (s) + sh	164.6 (15.5)
		169 (0)		
ν_5	199 (0.05)	176 (0.2)	197 (w)	170.1 (0.1)
$\nu_1 + \nu_3$	201 (<0.01)			
		208 (0)		
		212 (0.09)	217 (w)	
$\nu_1 + 2\nu_2$	228 (<0.01)			
$\nu_2 + \nu_3$	247 (0.01)		252 (vw)	
ν_6	275 (1.03)	282 (1.6)	271 (m)	267.4 (3.0)
		286 (0)		274.6 (2.6)
$\nu_2 + \nu_5$	293 (<0.01)		306 (vw)	
		316 (0)		
		316 (0.03)		
		324 (0)	322 (w)	320.8 (0.9)
ν_8	322 (<0.01)	325 (0.06)		323.8 (0.5)
		335 (0.03)	342 (w)	
		335 (0)		
$\nu_1 + 2\nu_3$	353 (<0.01)			
$\nu_1 + \nu_8$	379 (<0.01)			
ν_{10}	385 (0.04)	390 (0.02)	392 (w)	
$2\nu_1 + \nu_6$	380 (<0.01)			

Italic: Intermolecular modes