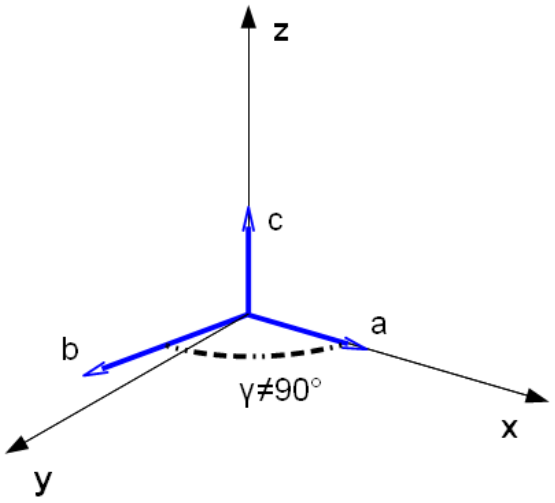
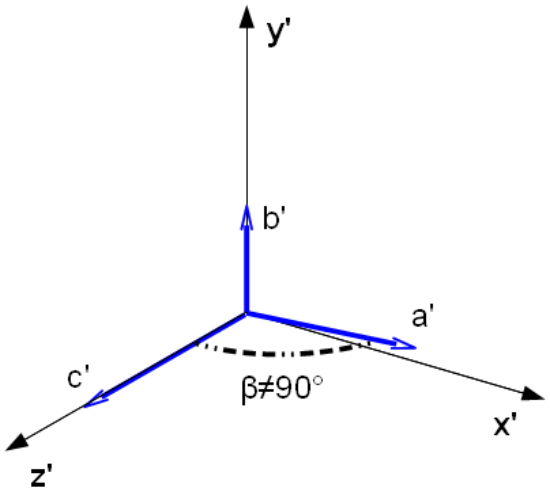
Table SI.1(a). The correspondence between the elastic constant computed using the monoclinic unit cell orientation in Quantum ESPRESSO and the elastic constants associated with the 'standard' monoclinic unit cell orientation

Quantum ESPRESSO (QE) crystallographic convention	Standard crystallographic (SC) convention (Cambridge Crystallographic Database)
	
Special axis: **c**	Special axis: **b**
Axis vectors for the monoclinic lattice: $\mathbf{R}_{QE} = \begin{pmatrix} a & 0 & 0 \\ b_x & b_y & 0 \\ 0 & 0 & c \end{pmatrix}$	Axis vectors for the monoclinic lattice: $\mathbf{R}_{SC} = \begin{pmatrix} a'_{x'} & 0 & a'_z \\ 0 & b & 0 \\ 0 & 0 & c' \end{pmatrix}$

Transformation from the crystallographic convention used in Quantum ESPRESSO for monoclinic lattices to the standard crystallographic convention:

$$\boldsymbol{a} \rightarrow \boldsymbol{c}' \ (x \rightarrow z')$$
$$\boldsymbol{b} \rightarrow \boldsymbol{a}' \ (y \rightarrow x')$$
$$\boldsymbol{c} \rightarrow \boldsymbol{b}' \ (z \rightarrow x')$$

Correspondence between the elastic constant computed using the monoclinic unit cell orientation used in Quantum ESPRESSO with the elastic constants associated with the standard monoclinic unit cell orientation.

C_{11}^{QE}	C_{33}^{SC}
C_{22}^{QE}	C_{11}^{SC}
C_{33}^{QE}	C_{22}^{SC}
C_{44}^{QE}	C_{66}^{SC}
C_{55}^{QE}	C_{44}^{SC}
C_{66}^{QE}	C_{55}^{SC}
C_{12}^{QE}	C_{13}^{SC}

C_{13}^{QE}	C_{23}^{SC}
C_{15}^{QE}	C_{34}^{SC}
C_{25}^{QE}	C_{14}^{SC}
C_{35}^{QE}	C_{24}^{SC}
C_{23}^{QE}	C_{12}^{SC}
C_{26}^{QE}	C_{15}^{SC}
C_{36}^{QE}	c_{25}^{SC}
C_{16}^{QE}	C_{35}^{SC}
C_{45}^{QE}	C_{46}^{SC}
C_{46}^{QE}	C_{56}^{SC}

Table SI.1(b). The calculated single crystal elastic constants (in GPa) of COA and COM computed using the monoclinic unit cell orientation in Quantum ESPRESSO. For DFT-D calculations, the term 'unrelaxed' refers to single point calculations of the deformed unit cell where the atomic coordinates followed linearly the linear elastic deformation imposed.

	COA			COM
	PBE	PBE-D	PBE-D unrelaxed	PBE-D
C_{11}^{QE}	109.5	104.0	968.0	144.2
C_{22}^{QE}		94.4	249.5	76.0
C_{33}^{QE}		97.8	138.7	89.6
C_{44}^{QE}		0.9	75.0	4.2
C_{55}^{QE}		27.4	75.0	29.2
C_{66}^{QE}	9.4	4.7	88.9	28.6
C_{12}^{QE}		39.1		29.0
C_{13}^{QE}		17.8		24.7
C_{23}^{QE}		18.5		8.2
C_{15}^{QE}		-2.3		-1.8
C_{25}^{QE}		0.6		-2.0
C_{35}^{QE}		-2.8		-1.9
C_{46}^{QE}		1.2		-1.6

Table SI.2. The value of C_{ij}^{QE} as a function of N_p, the number of energy points and P, the order of the polynomial fit (μ is the mean and σ is the standard deviation).

C_{11}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	106.7	106.7	108.3	108.3	109.0	109.0	109.9	109.9	107.8	107.8	108.2	108.2	102.7
	13	107.1	107.1	108.5	108.5	109.7	109.7	108.3	108.3	108.3	108.3	102.8		
	11	107.4	107.4	109.3	109.3	108.7	108.7	108.4	108.4	103.0				
	9	108.1	108.1	109.0	109.0	108.6	108.6	103.2						
	7	108.5	108.5	108.8	108.8	103.5								
	5	108.8	108.8	104.0										
	3	105.1												

C_{22}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	93.6	93.6	94.1	94.1	96.5	96.5	96.0	96.0	89.7	89.7	93.3	93.3	94.8
	13	93.6	93.6	95.2	95.2	96.8	96.8	91.0	91.0	92.8	92.8	94.8		
	11	93.9	93.9	96.5	96.5	92.7	92.7	92.5	92.5	94.7				
	9	95.0	95.0	94.2	94.2	92.5	92.5	94.7						
	7	94.7	94.7	92.9	92.9	94.5								
	5	93.7	93.7	94.4										
	3	94.2												

C_{33}^{QE}	P												
$\mathbf{N_p}$	2	3	4	5	6	7	8	9	10	11	12	13	14
15	88.3	88.3	87.4	87.4	90.7	90.7	92.8	92.8	91.0	91.0	87.9	87.9	100.5
13	87.9	87.9	88.7	88.7	92.1	92.1	91.7	91.7	88.1	88.1	100.2		
11	87.9	87.9	90.5	90.5	92.0	92.0	88.4	88.4	99.9				
9	88.7	88.7	91.6	91.6	88.8	88.8	99.4						
7	90.1	90.1	89.4	89.4	98.8								
5	89.5	89.5	97.8										
3	96.0												

C_{44}^{QE}	***P***												
$\boldsymbol{N_p}$	2	3	4	5	6	7	8	9	10	11	12	13	14
15	0.1	0.1	0.1	0.1	0.1	0.1	0.3	0.3	-0.1	-0.1	0.9	0.9	0.3
13	0.1	0.1	0.1	0.1	0.3	0.3	0.0	0.0	0.8	0.8	0.3		
11	0.1	0.1	0.2	0.2	0.0	0.0	0.7	0.7	0.3				
9	0.1	0.1	0.0	0.0	0.6	0.6	0.3						
7	0.1	0.1	0.4	0.4	0.4								
5	0.3	0.3	0.4										
3	0.3												

C_{55}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	24.5	24.5	24.8	24.8	24.8	24.8	25.2	25.2	25.8	25.8	23.8	23.8	28.2
	13	24.6	24.6	24.7	24.7	25.0	25.0	25.8	25.8	24.0	24.0	28.2		
	11	24.6	24.6	24.8	24.8	25.7	25.7	24.2	24.2	28.0				
	9	24.6	24.6	25.4	25.4	24.4	24.4	27.9						
	7	25.0	25.0	24.6	24.6	27.7								
	5	24.7	24.7	27.4										
	3	26.8												

C_{66}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	7.9	7.9	7.9	7.9	8.4	8.4	9.1	9.1	9.1	9.1	7.8	7.8	3.6
	13	7.9	7.9	8.0	8.0	8.8	8.8	9.2	9.2	8.0	8.0	3.7		
	11	7.9	7.9	8.4	8.4	9.1	9.1	8.3	8.3	3.8				
	9	8.0	8.0	8.9	8.9	8.6	8.6	4.0						
	7	8.4	8.4	8.8	8.8	4.2								
	5	8.7	8.7	4.7										
	3	5.6												

C_{12}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	42.4	42.4	43.8	43.8	43.6	43.6	46.2	46.2	43.5	43.5	46.7	46.7	37.1
	13	42.8	42.8	43.5	43.5	45.5	45.5	43.9	43.9	46.5	46.5	37.3		
	11	42.9	42.9	44.6	44.6	44.2	44.2	46.3	46.3	37.6				
	9	43.5	43.5	44.3	44.3	46.0	46.0	37.9						
	7	43.7	43.7	45.7	45.7	38.4								
	5	44.9	44.9	39.1										
	3	40.5												

C_{13}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	19.1	19.1	18.8	18.8	18.9	18.9	21.1	21.1	19.4	19.4	15.9	15.9	17.9
	13	19.1	19.1	18.6	18.6	20.4	20.4	20.0	20.0	16.3	16.3	17.9		
	11	18.8	18.8	19.6	19.6	20.4	20.4	16.9	16.9	17.8				
	9	19.0	19.0	20.3	20.3	17.6	17.6	17.8						
	7	19.6	19.6	18.3	18.3	17.8								
	5	19.0	19.0	17.8										
	3	18.1												

C_{23}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	11.7	11.7	11.6	11.6	12.6	12.6	14.1	14.1	15.6	15.6	17.6	17.6	19.2
	13	11.6	11.6	11.9	11.9	13.4	13.4	15.1	15.1	17.3	17.3	19.1		
	11	11.6	11.6	12.5	12.5	14.5	14.5	17.0	17.0	19.1				
	9	11.9	11.9	13.5	13.5	16.4	16.4	19.0						
	7	12.4	12.4	15.5	15.5	18.8								
	5	14.0	14.0	18.5										
	3	17.5												

C_{15}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	-3.3	-3.3	-1.3	-1.3	-1.5	-1.5	-1.6	-1.6	-2.2	-2.2	-0.7	-0.7	-2.6
	13	-2.7	-2.7	-1.4	-1.4	-1.5	-1.5	-2.1	-2.1	-0.9	-0.9	-2.6		
	11	-2.4	-2.4	-1.4	-1.4	-2.0	-2.0	-1.0	-1.0	-2.5				
	9	-2.0	-2.0	-1.8	-1.8	-1.2	-1.2	-2.5						
	7	-1.9	-1.9	-1.3	-1.3	-2.4								
	5	-1.6	-1.6	-2.3										
	3	-2.1												

C_{25}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	-4.0	-4.0	-1.4	-1.4	-3.6	-3.6	-1.3	-1.3	-1.7	-1.7	-1.9	-1.9	1.4
	13	-3.1	-3.1	-2.6	-2.6	-2.1	-2.1	-1.6	-1.6	-1.9	-1.9	1.4		
	11	-3.0	-3.0	-2.4	-2.4	-1.7	-1.7	-1.9	-1.9	1.3				
	9	-2.8	-2.8	-2.0	-2.0	-2.0	-2.0	1.1						
	7	-2.5	-2.5	-2.1	-2.1	1.0								
	5	-2.3	-2.3	0.6										
	3	0.0												

C_{35}^{QE}														
		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	-7.2	-7.2	-4.9	-4.9	-5.1	-5.1	-5.2	-5.2	-4.8	-4.8	-4.6	-4.6	-2.1
	13	-6.6	-6.6	-5.0	-5.0	-5.2	-5.2	-4.9	-4.9	-4.7	-4.7	-2.2		
	11	-6.1	-6.1	-5.1	-5.1	-5.0	-5.0	-4.8	-4.8	-2.3				
	9	-5.8	-5.8	-5.0	-5.0	-4.9	-4.9	-2.4						
	7	-5.5	-5.5	-5.0	-5.0	-2.5								
	5	-5.3	-5.3	-2.8										
	3	-3.3												

C_{35}^{QE}		P												
	N_p	2	3	4	5	6	7	8	9	10	11	12	13	14
	15	1.3	1.3	1.0	1.0	1.1	1.1	1.3	1.3	1.1	1.1	1.0	1.0	1.2
	13	1.2	1.2	1.0	1.0	1.2	1.2	1.2	1.2	1.0	1.0	1.2		
	11	1.1	1.1	1.1	1.1	1.2	1.2	1.0	1.0	1.2				
	9	1.1	1.1	1.2	1.2	1.0	1.0	1.2						
	7	1.2	1.2	1.1	1.1	1.2								
	5	1.1	1.1	1.2										
	3	1.2												