symbols

'CH3Cl', ['C', 'H', 'H', 'H', 'Cl'], Atom('CH3Cl', (x,y,z))

positions

Atoms

cell

[ [a<sub>1</sub>, a<sub>2</sub>, a<sub>3</sub>], [b<sub>1</sub>, b<sub>2</sub>, b<sub>3</sub>], [c<sub>1</sub>, c<sub>2</sub>, c<sub>3</sub>] ], [|**a**|, |**b**|, |**c**|,  $\alpha$ ,  $\beta$ ,  $\gamma$ ]

pbc

(True, True, False)

calculator