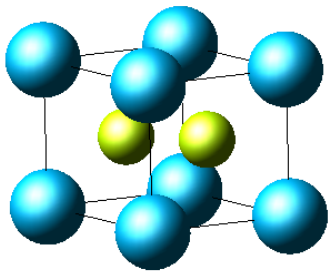
I. Elastic Constants of TiB_2

This application shows the calculation of the elastic constants of TiB_2, a hexagonal structure.

1. Retrieve structure from database



The structure of TiB_2 is taken from ICSD #30418.

2. Optimization of unit cell

The unit cell of TiB_2 is optimized using the following parameters (taken directly from the *Job.out* file as displayed by the JobServer): **Structure Optimization**: **☑ Relax Atom Positions**, **☑ Allow cell volume to change**, **☑ Allow cell shape to change**, **Convergence** of **0.001 eV/Ang**, **☑ Increase Plane wave cutoff** with **Normal** **Precision**. In the **SCF** panel put **set spacing between k-points** to **0.25 /Ång**, with **☑ Use odd size grids**, increase the **SCF convergence** to **1.0e-07**
The resulting cell parameters are:

Parameter	Original	change	Final	%
a	3.030000	0.004963	3.034963	0.2
b	3.030000	0.004963	3.034963	0.2
c	3.230000	-0.004577	3.225423	-0.1
alpha	90.000000	0.000000	90.000000	0.0
beta	90.000000	0.000000	90.000000	0.0
gamma	120.000000	0.000000	120.000000	0.0

3. Calculation of Elastic Constants

Load the optimized structure with **File**≫**Open**≫**Previous Calculation** and keep the computational parameters from the lattice optimization, change the type of calculation to **MT – Elastic Properties** and **Strains** of 1%, with **☐ Relax atoms of strained structures** unchecked.

Strain	Spacegroup	DOF	degrees of freedom
unstrained:	P6/mmm	0	
plus for each strain			
+e1:	Cmmm	1	degree of freedom for relaxation of atoms
-e1:	Cmmm	1	
+e3:	P6/mmm	0	
-e3:	P6/mmm	0	
+e4:	C2/m	2	

Checking **☑ Relax atoms of strained structures** includes relaxation of atoms in strained cells, where changes of the space group allow atoms to move, in the example of TiB_2 these are strains +e1, -e1, and +e4.

Experimental and computed elastic constants of TiB_2	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
Gilman and Roberts [1]	690	410	320	440	250
Spoor et al [2]	660	48	93	432	260
relaxed atoms of strained structures	649	72	102	457	258
This calculation	651	70	102	457	258

Note: The large value of C_{12} given by Gilman and Roberts appears not to be a simple typographical error.

The total computing time of this calculation was 7 minutes on an Intel Core 2 Duo with 2 GHz, including relaxation of atoms in strained structures requires 10 minutes total.

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1. **Gilman, J J and Robert, B W.** *J Appl Phys.* 1961, Vol. 32, p. 1405.

2. **Spoor, P S, et al.** *Appl. Phys. Lett.* 1997, Vol. 70, p. 1959.

