Site Symmetry in crystals : basis of the theory and applications for the electron and phonon states.

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RUSSIA

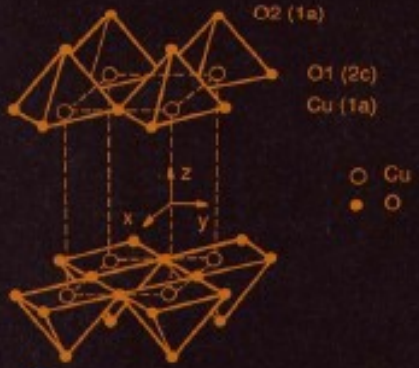
Solid-State Sciences

R. A. Evarestov V. P. Smirnov

Site Symmetry in Crystals

Theory and Applications

Second Enlarged Edition



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The LCAO First Principles Treatment of Crystals

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Site symmetry approach establishes symmetry relations between the localized states (atomic electron states and atomic displacements) and extended molecular or crystalline states (symmetry of molecular or crystalline orbitals and phonons). The localized states transform according to the irreducible representations (irreps) of the site symmetry point groups (in crystals- point symmetry groups of Wyckoff positions occupied by atoms). The extended states transform according to the irreps of the space group of the crystal (point group of the molecule). The extended states are induced from the localized states.

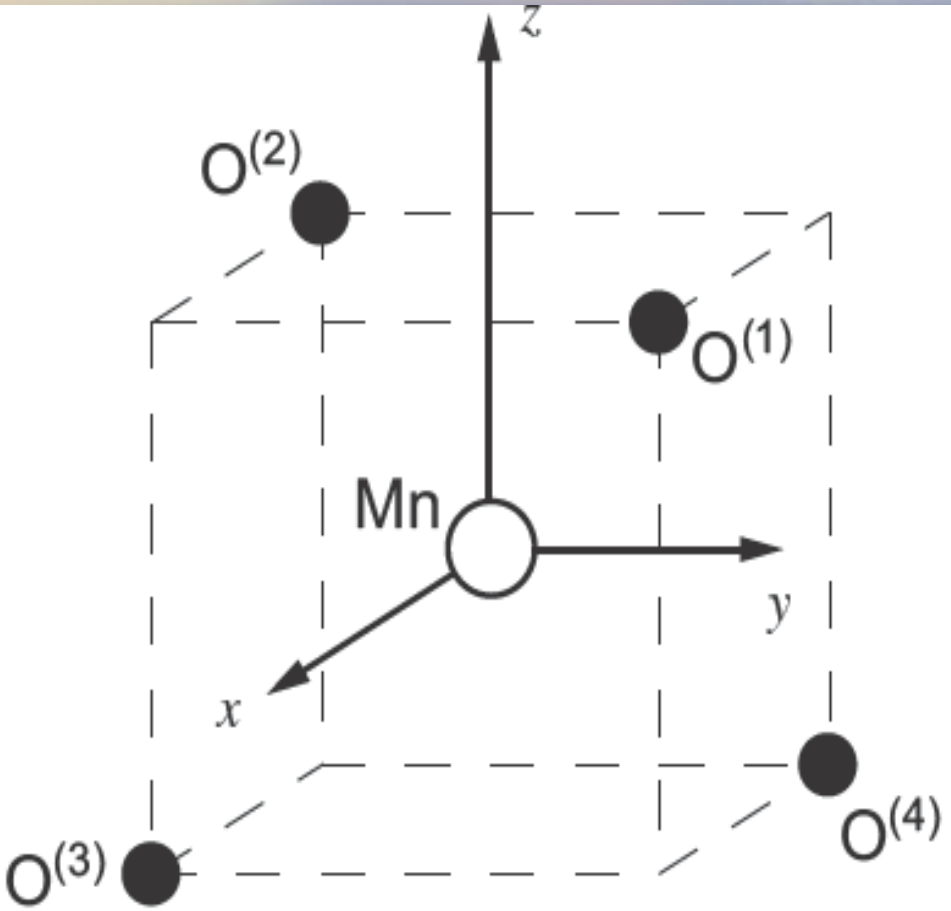


Fig. 3.8. MnO_4^- ion

$KMnO_4$ Pnma ($62\text{-}D_{2h}^{16}$) Z=4

4c .m. x 0.25 z 8d 1 x y z

K, Mn –4c O-4c,4c,8d

(MnO_4)$^-$ Mn-T_d O-C_{3v}

Point Group Tables of T_d(-43m)

Character Table

T_d(-43m)	#	E	3	2	-4	m	functions
Mult.	-	1	8	3	6	6	·
A_1	Γ_1	1	1	1	1	1	$x^2+y^2+z^2$
A_2	Γ_2	1	1	1	-1	-1	·
E	Γ_3	2	-1	2	0	0	$(2z^2-x^2-y^2, x^2-y^2)$
T_1	Γ_4	3	0	-1	1	-1	(J_x, J_y, J_z)
T_2	Γ_5	3	0	-1	-1	1	(x,y,z),(xy,xz,yz)

Point Group Tables of C_{3v}(3m)

Character Table

C_{3v}(3m)	#	1	3	m	functions
Mult.	-	1	2	3	·
A_1	Γ_1	1	1	1	z, x^2+y^2, z^2
A_2	Γ_2	1	1	-1	J_z
E	Γ_3	2	-1	0	$(x,y),(xz,yz),(x^2-y^2,xy),(J_x,J_y)$

$G=T_d=H_{Mn}$ $H_O=C_{3v}$

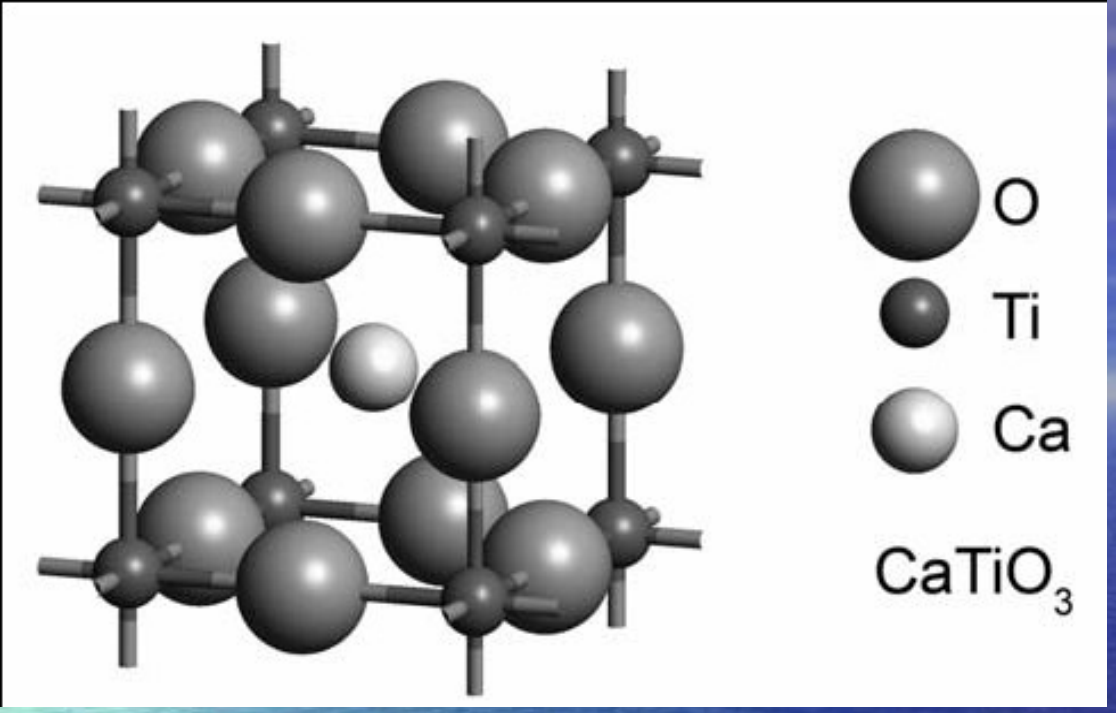
Subduced irreps of T_d (correlation table)

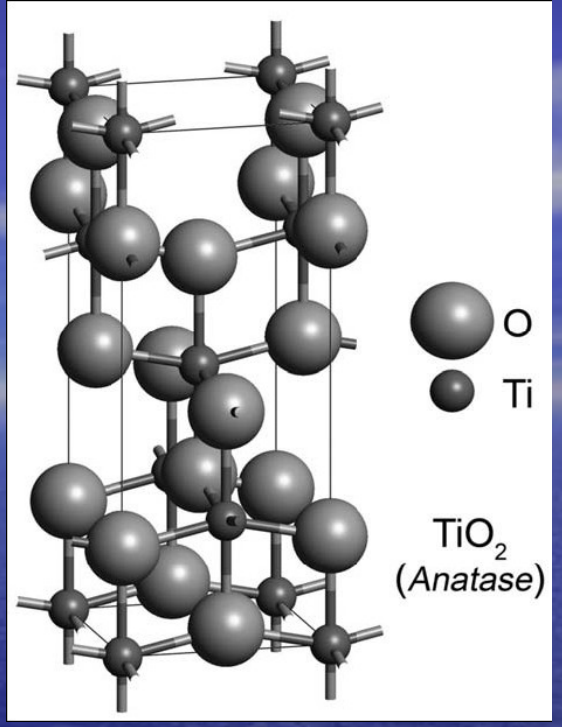
Induced irreps of T_d

T_d	C_{3v}
a_1	a_1
a_2	a_2
e	e
t_1	a_2e
t_2 (x,y,z)	a_1e

C_{3v}	T_d
a_1 (z)	a_1 t_2
a_2	a_2 t_1
e (x,y)	e t_1 t_2

The Frobenius reciprocity theorem is proved [13]: the multiplicity of an irrep $D^{(\alpha)}(g)$ of G in a rep $d^{[\gamma]} \uparrow$ G induced by an irrep $d^{(\gamma)}$ of H $\subset$ G is equal to the multiplicity of an irrep $d^{(\gamma)}$ of H in the rep $D^{(\alpha)} \downarrow$ H subduced by $D^{(\alpha)}$ of H.





Perovskite $CaTiO_3$

Ca 1b (0.5 ,0.5, 0.5)
Ti 1a (0 ,0, 0)
O 3d (0.5, 0, 0; 0,0.5,0; 0, 0, 0.5)
(abd)= (bac)

$Z=1$, Pm-3m

$(221\text{-}O_h^1)$

Anatase TiO_2

two Ti atoms 2a(0 ,0 ,0; 0, 1/2, 1/4), four oxygen atoms 4e (0, 0, u; 1/2, 0,–u + 1/2; 0, 1/2, u +1/4;1/2, 1/2,–u+1/2). The anatase structure is defined by three parameters: a, c, u.

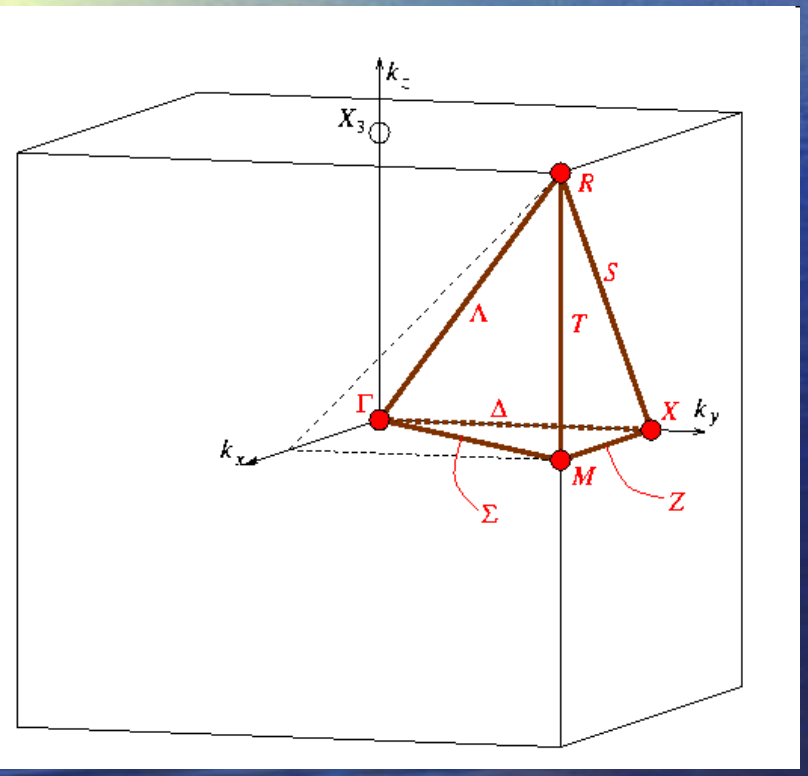
(a e) =(b e)

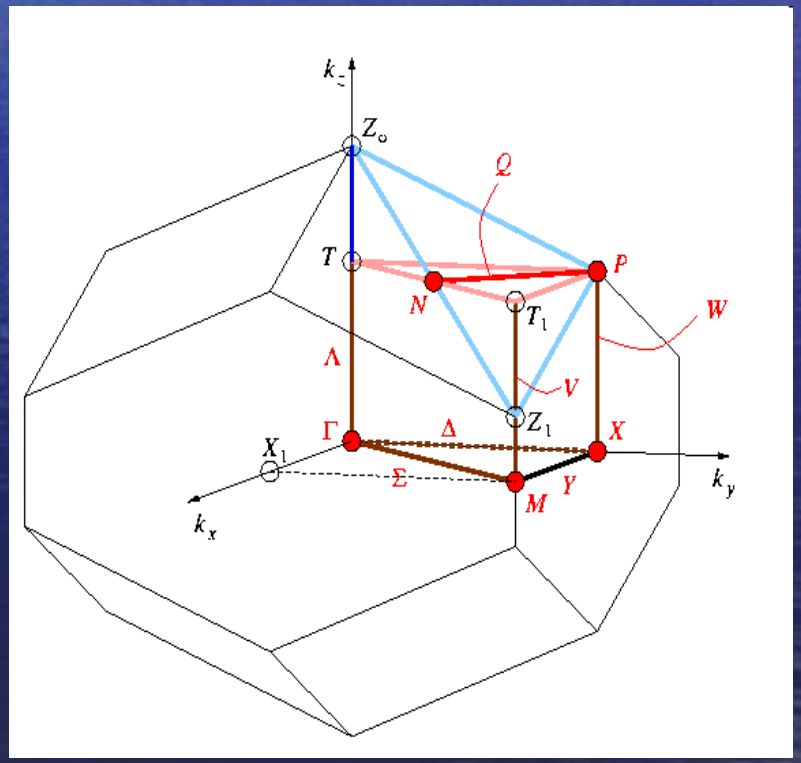
$Z=2$, $I4_1/amd$

$141\text{-}D_{4h}^{19}$

Brillouin Zones

- Simple cubic lattice Tetragonal bc lattice





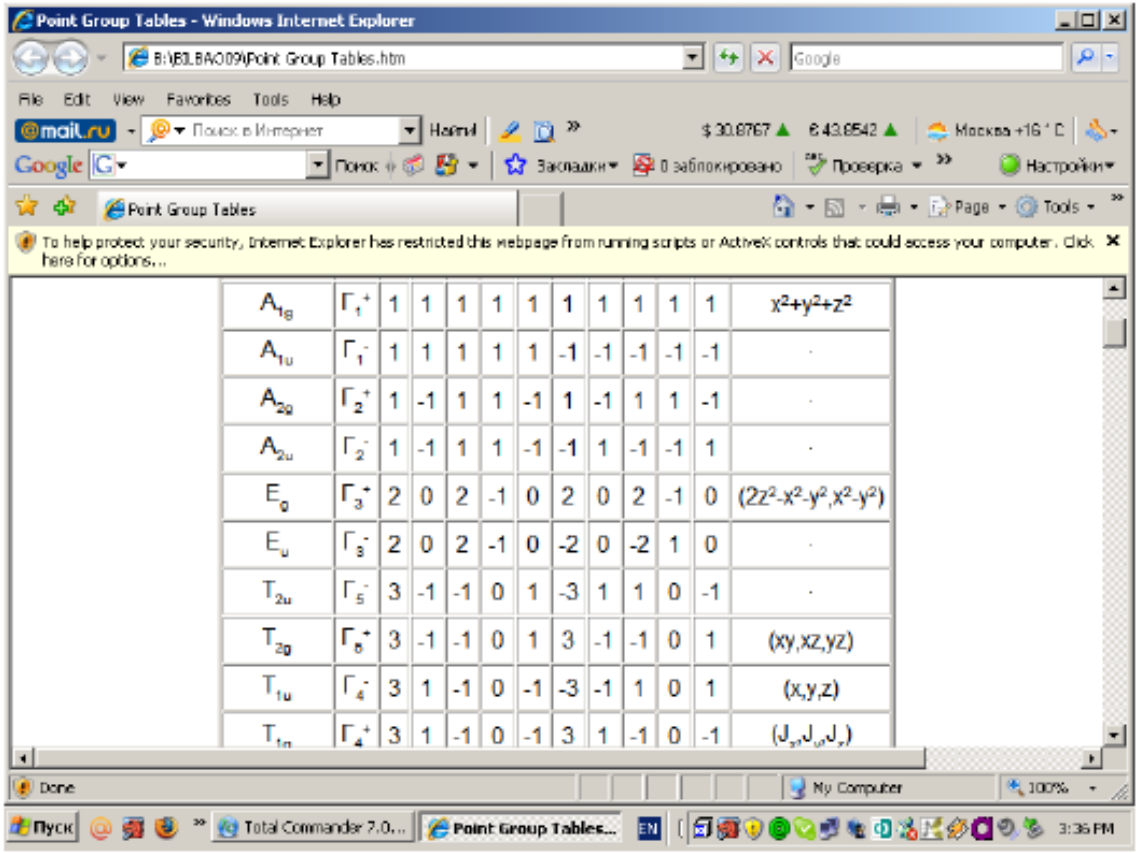
Γ(000) R(0.5 0.5 0.5)
3X(0.5 0 0) 3M(0.5 0.5 0)

Γ (000) M (0.5 0.5 0.5)
2P(0.25 0.25 0.25) 2X (0 0 0.5)
4N (0 0.5 0)

SYMMETRY OF LOCALIZED STATES IN PEROVSKITE AND ANATASE

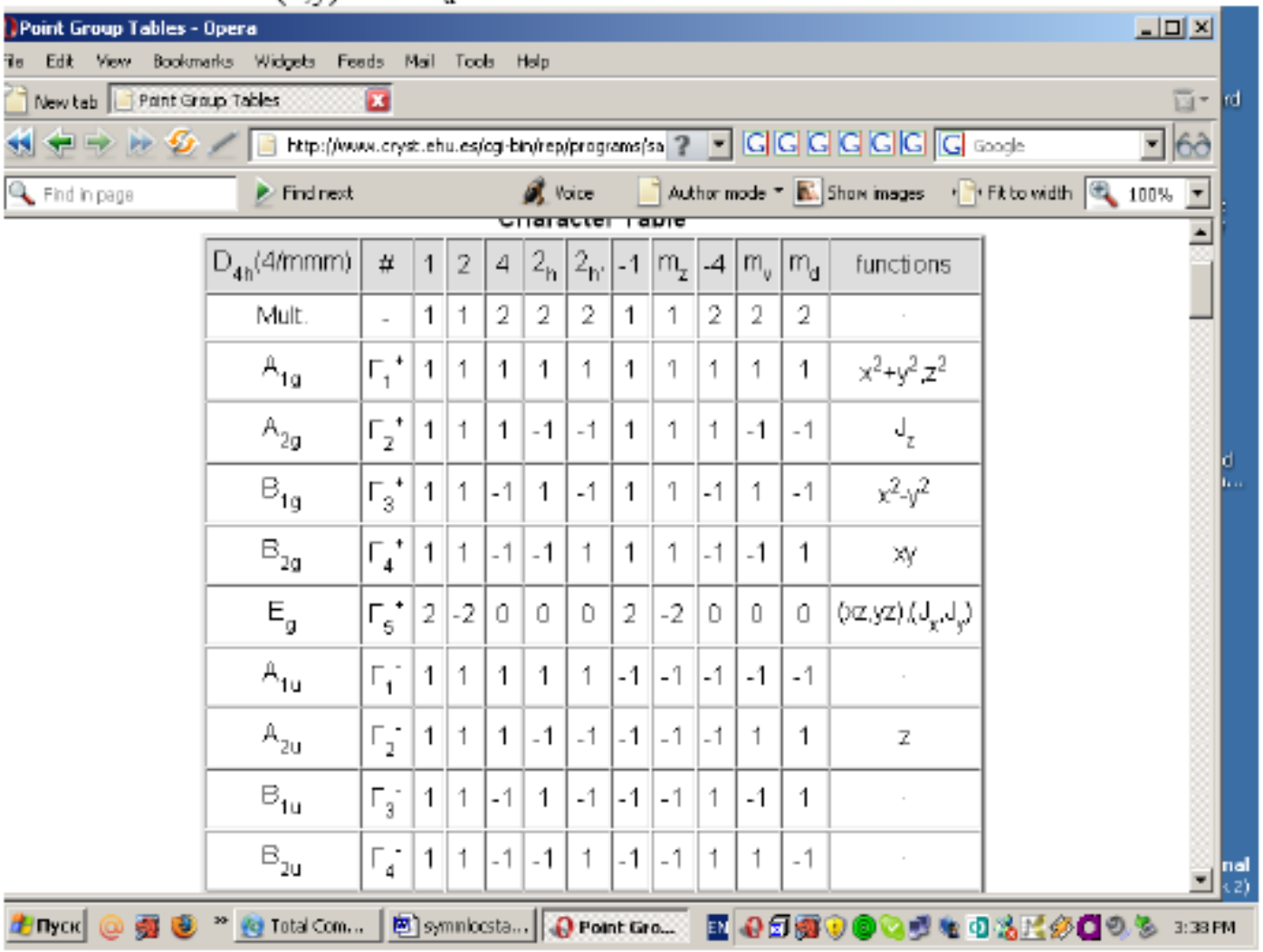
Perovskite $CaTiO_3$

Ti	a		s	a_{1g}
		Oh	(x, y, z)	t_{1u}
Ca	b		(z^2, x^2-y^2)	e_g
			(xy, xz, yz)	t_{2g}



A_{1g}	Γ_1^+	1	1	1	1	1	1	1	1	1	$x^2+y^2+z^2$
A_{1u}	Γ_1^-	1	1	1	1	1	-1	-1	-1	-1	·
A_{2g}	Γ_2^+	1	-1	1	1	-1	1	-1	1	1	-1	·
A_{2u}	Γ_2^-	1	-1	1	1	-1	-1	1	-1	-1	1	·
E_g	Γ_3^+	2	0	2	-1	0	2	0	2	-1	0	$(2z^2-x^2-y^2, x^2-y^2)$
E_u	Γ_3^-	2	0	2	-1	0	-2	0	-2	1	0	·
T_{2u}	Γ_5^-	3	-1	-1	0	1	-3	1	1	0	-1	·
T_{2g}	Γ_5^+	3	-1	-1	0	1	3	-1	-1	0	1	(xy,xz,yz)
T_{1u}	Γ_4^-	3	1	-1	0	-1	-3	-1	1	0	1	(x,y,z)
T_{1g}	Γ_4^+	3	1	-1	0	-1	3	1	-1	0	-1	(J_x,J_y,J_z)

O	d	D_{4h}	s, z^2	a_{1g}
			z	a_{2u}
			x^2-y^2	b_{1g}
			xy	b_{2g}
			(xz,yz)	e_g
			(x,y)	e_u



D_{4h}(4/mmm)	#	1	2	4	2_h	$2_{h'}$	-1	m_z	-4	m_v	m_d	functions
Mult.	-	1	1	2	2	2	1	1	2	2	2	
A_{1g}	Γ_1^+	1	1	1	1	1	1	1	1	1	1	x^2+y^2, z^2
A_{2g}	Γ_2^+	1	1	1	-1	-1	1	1	1	-1	-1	J_z
B_{1g}	Γ_3^+	1	1	-1	1	-1	1	1	-1	1	-1	x^2-y^2
B_{2g}	Γ_4^+	1	1	-1	-1	1	1	1	-1	-1	1	xy
E_g	Γ_5^+	2	-2	0	0	0	2	-2	0	0	0	(xz,yz) (J_x,J_y)
A_{1u}	Γ_1^-	1	1	1	1	1	-1	-1	-1	-1	-1	
A_{2u}	Γ_2^-	1	1	1	-1	-1	-1	-1	-1	1	1	z
B_{1u}	Γ_3^-	1	1	-1	1	-1	-1	-1	1	-1	1	
B_{2u}	Γ_4^-	1	1	-1	-1	1	-1	-1	1	1	-1	

Table 3.8. Simple induced representations of the O_h^1 - $Pm\bar{3}m$ space group

q	β	Γ	R		M		X	
			a	b	a	b	a	b
	a_{1g}	1^+	1^+	2^-	1^+	4^+	1^+	3^-
	a_{1u}	1^-	1^-	2^+	1^-	4^-	1^-	3^+
	a_{2g}	2^+	2^+	1^-	2^+	3^+	2^+	4^-
a	a_{2u}	2^-	2^-	1^+	2^-	3^-	2^-	4^+
	e_g	3^+	3^+	3^-	1^+2^+	3^+4^+	1^+2^+	3^-4^-
b	e_u	3^-	3^-	3^+	1^-2^-	3^-4^-	1^-2^-	3^+4^+
	t_{1g}	4^+	4^+	5^-	3^+5^+	2^+5^+	3^+5^+	1^-5^-
	t_{1u}	4^-	4^-	5^+	3^-5^-	2^-5^-	3^-5^-	1^+5^+
	t_{2g}	5^+	5^+	4^-	4^+5^+	1^+5^+	4^+5^+	2^-5^-
	t_{2u}	5^-	5^-	4^+	4^-5^-	1^-5^-	4^-5^-	2^+5^+
			c	d	c	d	c	d
	a_{1g}	1^+3^+	5^+	4^-	4^+5^-	1^+5^-	$1^+3^-4^-$	$1^+2^+3^-$
	a_{1u}	1^-3^-	5^-	4^+	4^-5^+	1^-5^+	$1^-3^+4^+$	$1^-2^-3^+$
	b_{2g}	2^+3^+	4^+	5^-	3^+5^-	2^+5^-	$2^+3^-4^-$	$1^+2^+4^-$
c	b_{2u}	2^-3^-	4^-	5^+	3^-5^+	2^-5^+	$2^-3^+4^+$	$1^-2^-4^+$
	a_{2g}	4^+	2^+3^+	1^-3-	$2^+3^-4^-$	$1^-2^-3^+$	3^+5^-	1^-5^+
d	a_{2u}	4^-	2^-3^-	1^+3+	$2^-3^+4^+$	$1^+2^+3^-$	3^-5^+	1^+5^-
	b_{1g}	5^+	1^+3^+	2^-3-	$1^+3^-4^-$	$1^-2^-4^+$	4^+5^-	2^-5^+
	b_{1u}	5^-	1^-3^-	2^+3+	$1^-3^+4^+$	$1^+2^+4^-$	4^-5^+	2^+5^-
	e_g	4^+5^+	4^+5^+	4^-5-	$1^-2^-5^+5^-$	$3^-4^-5^+5^-$	$1^-2^-5^+5^-$	$3^+4^+5^+5^-$
	e_u	4^-5^-	4^-5^-	4^+5+	$1^+2^+5^-5^+$	$3^+4^+5^-5^+$	$1^+2^+5^-5^+$	$3^-4^-5^-5^+$

In (aaa) units: $\mathrm{a_1}(100)$, $\mathrm{a_2}(010)$, $\mathrm{a_3}(001)$

Q: $O_h(m\bar{3}m)$ – $a(000)$, $b(1/2,1/2,1/2)$;

$D_{4h}(4/mmm)$ – $c(1/2,1/2,0)$, $d(1/2,0,0)$

In $(2\pi/a, 2\pi/a, 2\pi/a)$ units: $\mathrm{b_1}(100)$, $\mathrm{b_2}(010)$, $\mathrm{b_3}(001)$

K: O_h – $\Gamma(000)$, $R(1/2,1/2,1/2)$; D_{4h} – $M(1/2,1/2,0)$, $X(1/2,0,0)$

Induced site-symmetry representations of space group: P m -3 m (221)

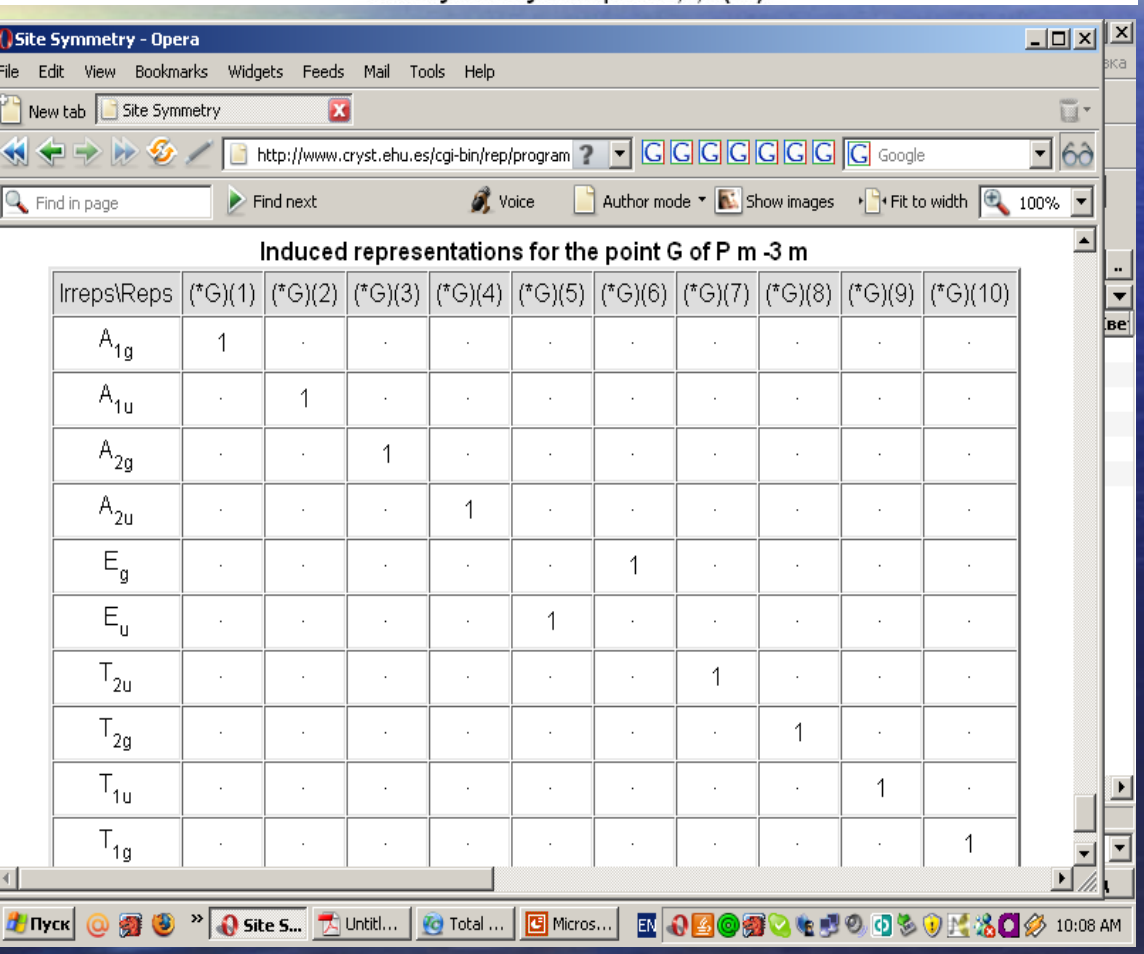
with K-vector: G=(0, 0, 0)

[Symmetry elements Space Group P m -3 m (221)]

WP	Representative
1a	0,0,0

Site Symmetry Group

Site Symmetry Group for 0,0,0 (1a)



Induced representations for the point G of P m -3 m

Irreps\Reps	(*G)(1)	(*G)(2)	(*G)(3)	(*G)(4)	(*G)(5)	(*G)(6)	(*G)(7)	(*G)(8)	(*G)(9)	(*G)(10)
A_{1g}	1	·	·	·	·	·	·	·	·	·
A_{1u}	·	1	·	·	·	·	·	·	·	·
A_{2g}	·	·	1	·	·	·	·	·	·	·
A_{2u}	·	·	·	1	·	·	·	·	·	·
E_g	·	·	·	·	·	1	·	·	·	·
E_u	·	·	·	·	1	·	·	·	·	·
T_{2u}	·	·	·	·	·	·	1	·	·	·
T_{2g}	·	·	·	·	·	·	·	1	·	·
T_{1u}	·	·	·	·	·	·	·	·	1	·
T_{1g}	·	·	·	·	·	·	·	·	·	1

G(1) a_{1g} 1^{+} ;G(2) a_{1u} 1^{-}; G(3) a_{2g} 2^{+}; G(4) a_{2u} 2^{-};

G(5) e_u 3^{-}; G(6) e_g 3^{+}; G(7) t_{2u} 5^{-}; G(8) t_{2g} 5^{+};

G(9) t_{1u} 4^{-}; G(10) t_{2u} 4^{+}

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Induced site-symmetry representations of space group: P m -3 m (221)

with K-vector: R=(0.5, 0.5, 0.5)

[Symmetry elements Space Group P m -3 m (221)]

WP	Representative
1a	0,0,0

Site Symmetry Group

Site Symmetry Group for 0,0,0 (1a)

g_1	x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0.0 \\ 0 & 1 & 0 & 0.0 \\ 0 & 0 & 1 & 0.0 \end{pmatrix}$

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Induced representations for the point R of P m -3 m

Irreps\Reps	(*R)(1)	(*R)(2)	(*R)(3)	(*R)(4)	(*R)(5)	(*R)(6)	(*R)(7)	(*R)(8)	(*R)(9)	(*R)(10)
A_{1g}	1	.	.	.	.	.	.	.	.	.
A_{1u}	.	1	.	.	.	.	.	.	.	.
A_{2g}	.	.	1	.	.	.	.	.	.	.
A_{2u}	.	.	.	1	.	.	.	.	.	.
E_g	.	.	.	.	.	1	.	.	.	.
E_u	.	.	.	.	1	.	.	.	.	.
T_{2u}	.	.	.	.	.	.	1	.	.	.
T_{2g}	.	.	.	.	.	.	.	1	.	.
T_{1u}	.	.	.	.	.	.	.	.	1	.
T_{1g}	.	.	.	.	.	.	.	.	.	1

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R(1) a_{1g} 1^+ ;R(2) a_{1u} 1^-; R(3) a_{2g} 2^+; R(4) a_{2u} 2^-;

R(5) e_u 3^-; R(6) e_g 3^+; R(7) t_{2u} 5^-; R(8) t_{2g} 5^+;

R(9) t_{1u} 4^-; R(10) t_{2u} 4^+

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Induced site-symmetry representations of space group: P m -3 m (221)

with K-vector: R=(0.5, 0.5, 0.5)

[Symmetry elements Space Group P m -3 m (221)]

WP	Representative
1b	1/2,1/2,1/2

Site Symmetry Group

Site Symmetry Group for 1/2,1/2,1/2 (1b)

g_1	x,y,z	$\begin{pmatrix} 1. & 0. & 0. & 0.0 \\ 0. & 1. & 0. & 0.0 \\ 0. & 0. & 1. & 0.0 \end{pmatrix}$
		$\begin{pmatrix} -1 & 0 & 0 & 1.0 \end{pmatrix}$

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Induced representations for the point R of P m -3 m

Irreps\Reps	(*R)(1)	(*R)(2)	(*R)(3)	(*R)(4)	(*R)(5)	(*R)(6)	(*R)(7)	(*R)(8)	(*R)(9)	(*R)(10)
A_{1g}	.	.	.	1	.	.	.	.	.	.
A_{1u}	.	.	1	.	.	.	.	.	.	.
A_{2g}	.	1	.	.	.	.	.	.	.	.
A_{2u}	1	.	.	.	.	.	.	.	.	.
E_g	.	.	.	.	1	.	.	.	.	.
E_u	.	.	.	.	.	1	.	.	.	.
T_{2u}	.	.	.	.	.	.	.	.	.	1
T_{2g}	.	.	.	.	.	.	.	.	1	.
T_{1u}	.	.	.	.	.	.	.	1	.	.
T_{1g}	.	.	.	.	.	.	1	.	.	.

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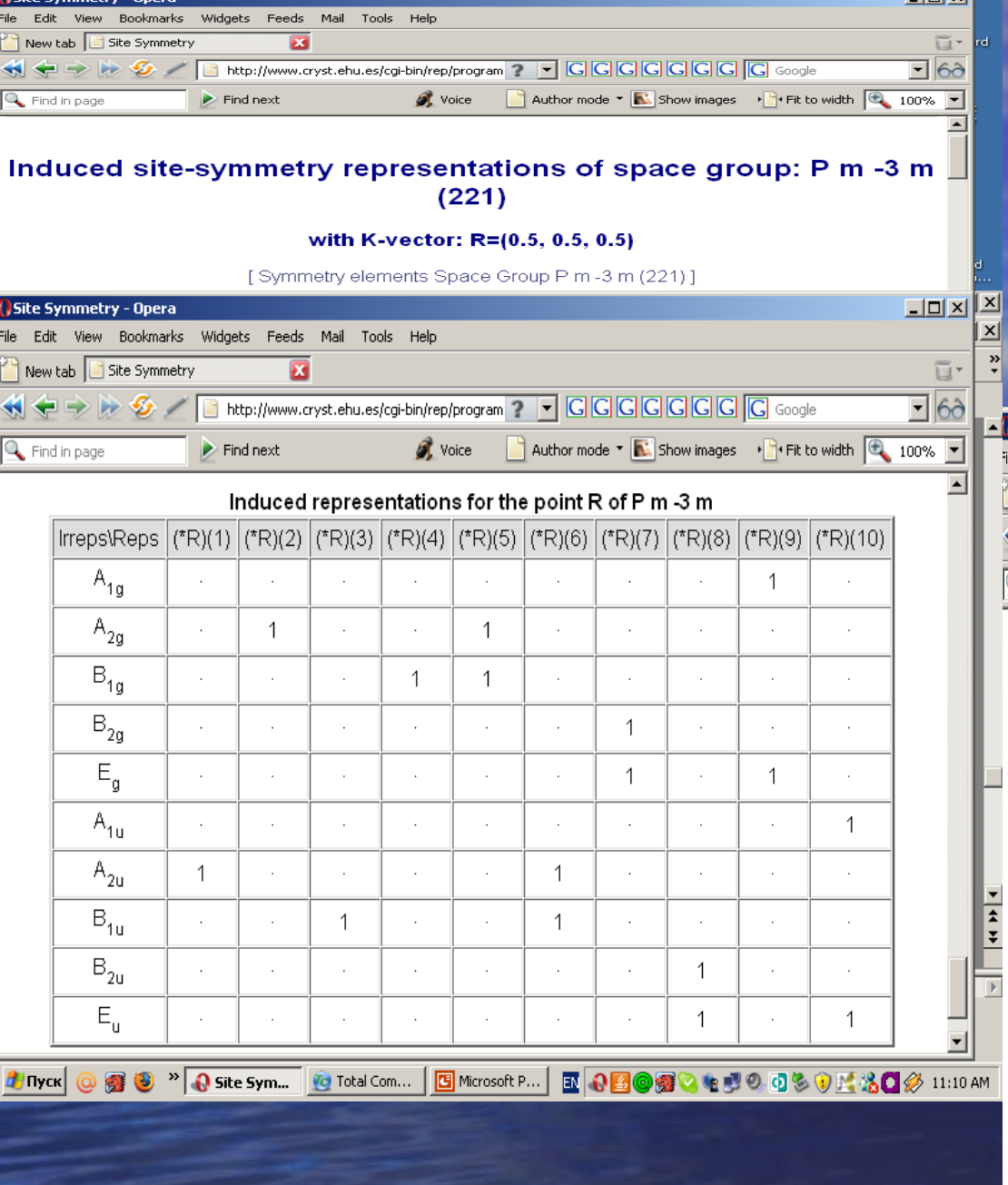


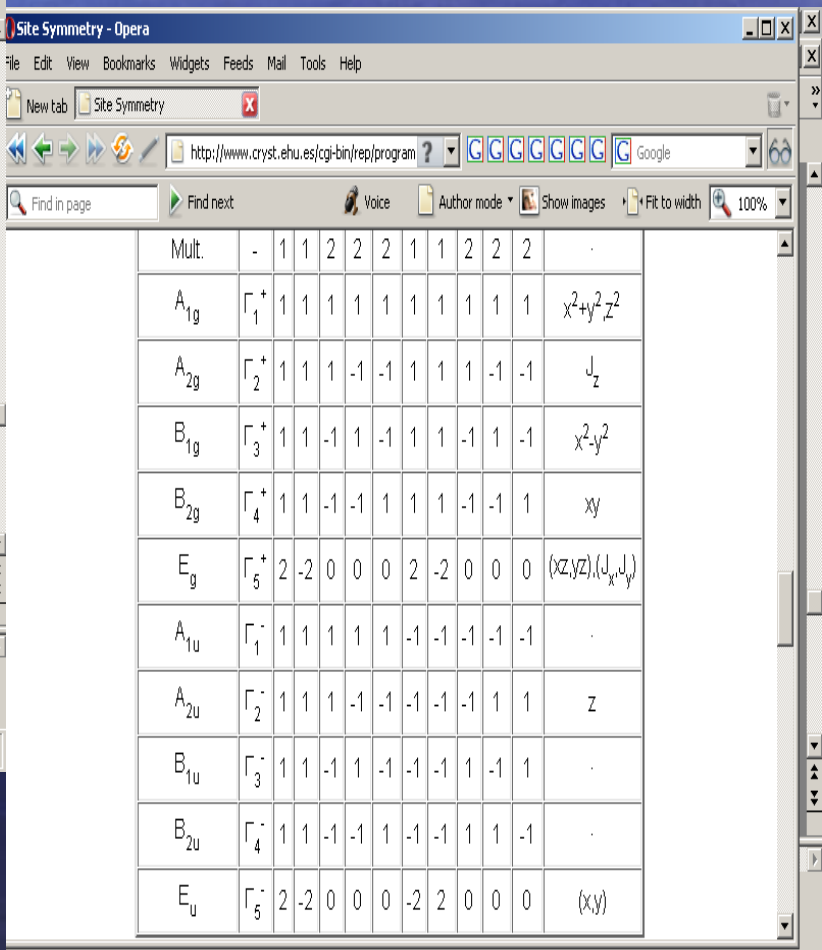
Induced site-symmetry representations of space group: P m -3 m (221)

with K-vector: R=(0.5, 0.5, 0.5)

[Symmetry elements Space Group P m -3 m (221)]

Induced representations for the point R of P m -3 m

Irreps\Reps	(*R)(1)	(*R)(2)	(*R)(3)	(*R)(4)	(*R)(5)	(*R)(6)	(*R)(7)	(*R)(8)	(*R)(9)	(*R)(10)
A_{1g}	.	.	.	.	.	.	.	.	1	.
A_{2g}	.	1	.	.	1	.	.	.	.	.
B_{1g}	.	.	.	1	1	.	.	.	.	.
B_{2g}	.	.	.	.	.	.	1	.	.	.
E_g	.	.	.	.	.	.	1	.	1	.
A_{1u}	.	.	.	.	.	.	.	.	.	1
A_{2u}	1	.	.	.	.	1	.	.	.	.
B_{1u}	.	.	1	.	.	1	.	.	.	.
B_{2u}	.	.	.	.	.	.	.	1	.	.
E_u	.	.	.	.	.	.	.	1	.	1



Mult.	-	1	1	2	2	2	1	1	2	2	2	.
A_{1g}	Γ_1^+	1	1	1	1	1	1	1	1	1	1	x^2+y^2,z^2
A_{2g}	Γ_2^+	1	1	1	-1	-1	1	1	1	-1	-1	J_z
B_{1g}	Γ_3^+	1	1	-1	1	-1	1	1	-1	1	-1	x^2-y^2
B_{2g}	Γ_4^+	1	1	-1	-1	1	1	1	-1	-1	1	xy
E_g	Γ_5^+	2	-2	0	0	0	2	-2	0	0	0	$(xz,yz),(J_x,J_y)$
A_{1u}	Γ_1^-	1	1	1	1	1	-1	-1	-1	-1	-1	.
A_{2u}	Γ_2^-	1	1	1	-1	-1	-1	-1	-1	1	1	z
B_{1u}	Γ_3^-	1	1	-1	1	-1	-1	-1	1	-1	1	.
B_{2u}	Γ_4^-	1	1	-1	-1	1	-1	-1	1	1	-1	.
E_u	Γ_5^-	2	-2	0	0	0	-2	2	0	0	0	(x,y)

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Induced site-symmetry representations of space group: P m -3 m (221)

with K-vector: M=(0.5, 0.5, 0)

[Symmetry elements Space Group P m -3 m (221)]

WP	Representative
3d	1/2,0,0

Site Symmetry Group

Site Symmetry Group for 1/2,0,0 (3d)

g_1	x,y,z	$\begin{pmatrix} 1. & 0. & 0. & 0.0 \\ 0. & 1. & 0. & 0.0 \\ 0. & 0. & 1. & 0.0 \end{pmatrix}$
g_2	-x+1,-y,z	$\begin{pmatrix} -1. & 0. & 0. & 1.0 \\ 0. & -1. & 0. & 0.0 \end{pmatrix}$

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Induced representations for the point M of P m -3 m

Irreps\Reps	(*M)(1)	(*M)(2)	(*M)(3)	(*M)(4)	(*M)(5)	(*M)(6)	(*M)(7)	(*M)(8)	(*M)(9)	(*M)(10)
A_{1g}	1	.	.	.	.	.	.	.	1	.
A_{2g}	.	1	1	.	.	1	.	.	.	.
B_{1g}	.	1	.	.	.	1	1	.	.	.
B_{2g}	.	.	.	.	1	.	.	.	1	.
E_g	.	.	.	1	.	.	.	1	1	1
A_{1u}	.	1	.	.	.	.	.	.	.	1
A_{2u}	1	.	.	1	1	.	.	.	.	.
B_{1u}	1	.	.	.	1	.	.	1	.	.
B_{2u}	.	.	.	.	.	1	.	.	.	1
E_u	.	.	1	.	.	.	1	.	1	1

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Irreps		Mult.										
A_{1g}	Γ_1^+	1	1	1	1	1	1	1	1	1	1	x^2+y^2,z^2
A_{2g}	Γ_2^+	1	1	1	-1	-1	1	1	1	-1	-1	J_z
B_{1g}	Γ_3^+	1	1	-1	1	-1	1	1	-1	1	-1	x^2-y^2
B_{2g}	Γ_4^+	1	1	-1	-1	1	1	1	-1	-1	1	xy
E_g	Γ_5^+	2	-2	0	0	0	2	-2	0	0	0	(xz,yz),(J_x,J_y)
A_{1u}	Γ_1^-	1	1	1	1	1	-1	-1	-1	-1	-1	.
A_{2u}	Γ_2^-	1	1	1	-1	-1	-1	-1	-1	1	1	z
B_{1u}	Γ_3^-	1	1	-1	1	-1	-1	-1	1	-1	1	.
B_{2u}	Γ_4^-	1	1	-1	-1	1	-1	-1	1	1	-1	.
E_u	Γ_5^-	2	-2	0	0	0	-2	2	0	0	0	(x,y)

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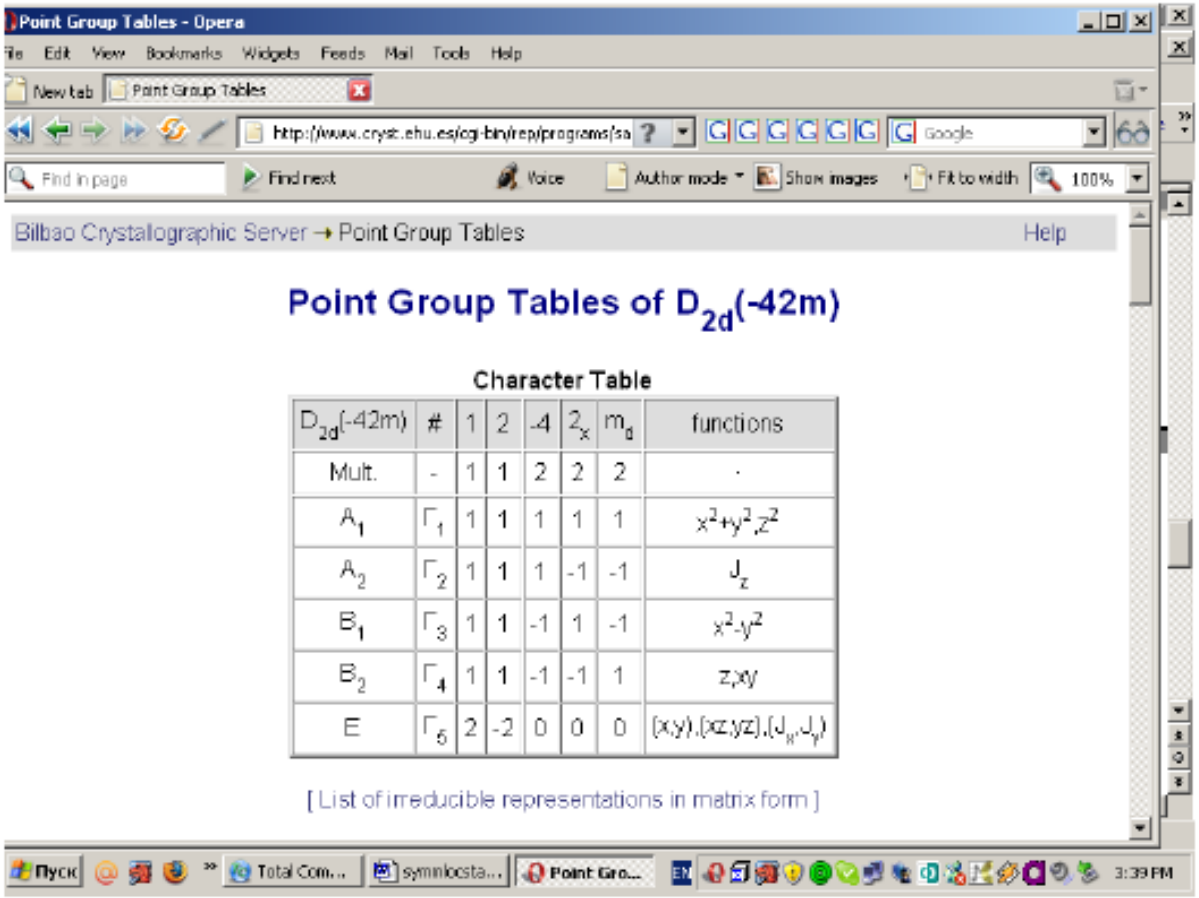
M(1) 1^+ ; M(2) 1^- ; M(3) 3^+ ; M(4) 3^- ; M(5) 2^+; M(6) 2^-

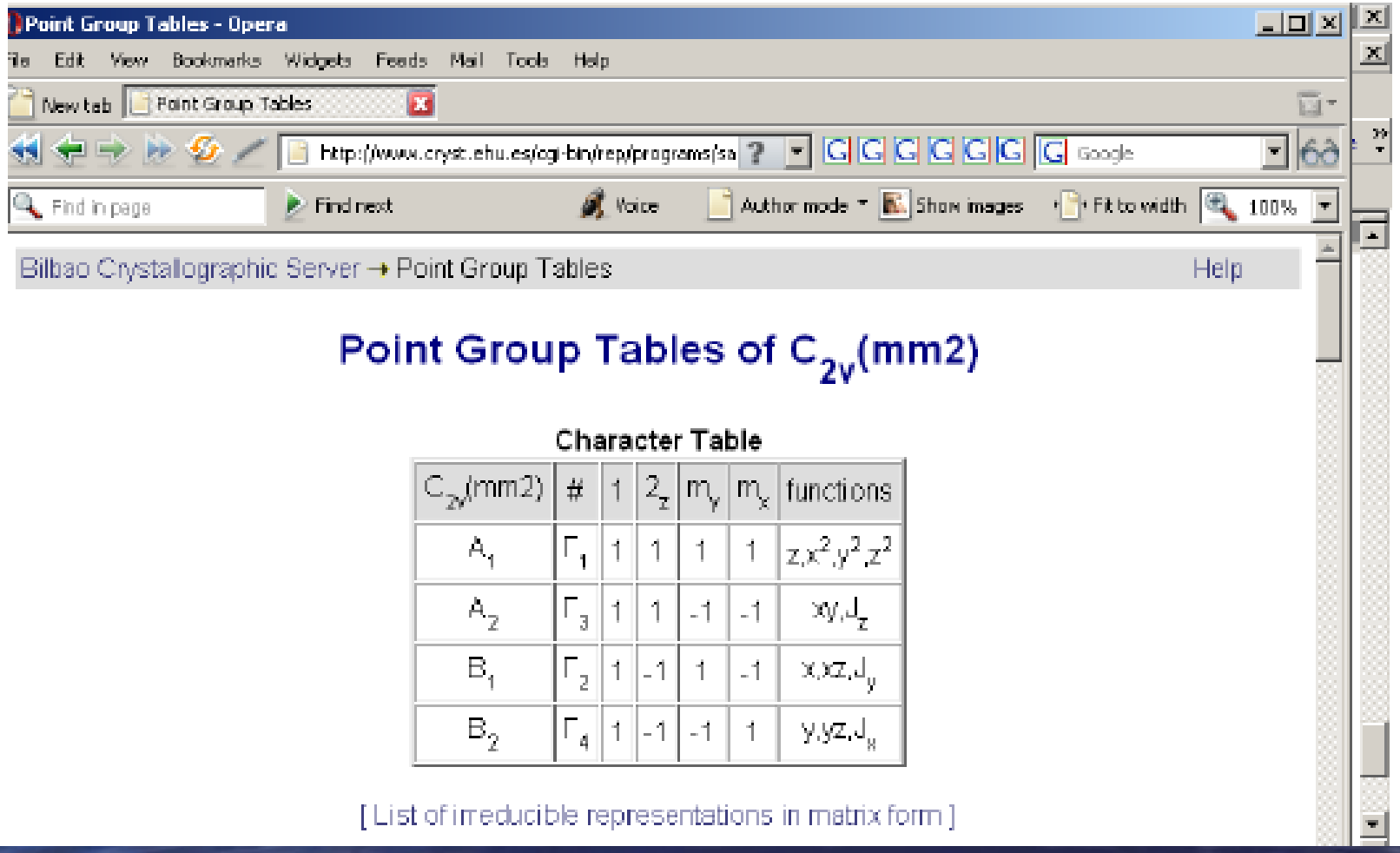
M(7) 4^+ ; M(8) 4^- ; M(9) 5^- ; M(10) 5^+

Anatase TiO_2

Ti	a	D_{2d}	s, z^2	a_1
			x^2-y^2	b_1
			z, xy	b_2
			(x, y), (xz, yz)	e



O	e	C_{2v}	s, z, z^2	a_1
			xy, x^2-y^2	a_2
			x, xz	b_1
			y, yz	b_2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Point Group Tables of C_{2v}(mm2)
Character Table
C_{2v}(mm2) # 1 2_z m_y m_x functions
A_1 Γ_1 1 1 1 1 z,x^2,y^2,z^2
A_2 Γ_3 1 1 -1 -1 xy,J_z
B_1 Γ_2 1 -1 1 -1 x,xz,J_y
B_2 Γ_4 1 -1 -1 1 y,yz,J_x
[List of irreducible representations in matrix form]

Table 4.21. Simple induced representations of the $D_{4h}^{19} - I4_1/amd$ space group

q	β	Γ	M	X	P		N	
					a	b		
a	a_1	1^+4^-	1	1	2	1	1^+2^-	
	a_2	3^+2^-	2	2	2	1	1^-2^+	
b	b_2	3^-2^+	1	2	1	2	1^+2^-	
	b_1	1^-4^+	2	1	1	2	1^-2^+	
	e	5^+5^-	3 4	1 2	1 2	1 2	$1^+1^-2^+2^-$	
							c	d
c	a_g	$1^+2^+5^+$	1 4	1 2	1 2		$1^+1^+2^+2^-$	$1^+1^-2^-2^-$
	a_u	$1^-2^-5^-$	2 4	1 2	1 2		$1^-1^-2^+2^-$	$1^+1^-2^+2^+$
d	b_g	$3^+4^+5^+$	2 3	1 2	1 2		$1^+1^-2^+2^+$	$1^-1^-2^+2^-$
	b_u	$3^-4^-5^-$	1 3	1 2	1 2		$1^+1^-2^-2^-$	$1^+1^+2^+2^-$

The basis translations vectors of direct and reciprocal lattices and coordinates of K-set points are in Table 4.20.

Q: $D_{2d}(\bar{4}m2)$ – $a(000)$, $b(1/2, 1/2, 0)$;

$C_{2h}(.2/m.)$ – $c(3/8, 1/8, 1/4)$, $d(-1/8, -3/8, 1/4)$.

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Induced site-symmetry representations of space group: I 4_1/a m d (141)

with K-vector: M=(0.5, 0.5, 0.5)

[Symmetry elements Space Group I 4_1/a m d (141)]

WP	Representative
8e	0,1/4,z

Site Symmetry Group

Site Symmetry Group for 0,1/4,z (8e)

g_1	x,y,z	$\begin{pmatrix} 1. & 0. & 0. & 0.0 \\ 0. & 1. & 0. & 0.0 \\ 0. & 0. & 1. & 0.0 \end{pmatrix}$

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Irreducible representations

Character table for mm2

C_{2v}(mm2)	#	1	2_z	m_y	m_x	functions
A_1	Γ_1	1	1	1	1	z,x^2,y^2,z^2
A_2	Γ_3	1	1	-1	-1	xy,J_z
B_1	Γ_2	1	-1	1	-1	x,xz,J_y
B_2	Γ_4	1	-1	-1	1	y,yz,J_x

Subduced representations

Character table for the subduced representations (*M↓mm2) for Wyckoff position 8e

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(*M)(3)	2	·	·	·
(*M)(4)	·	2	·	·

Induced representations

Induced representations for the point M of I 4_1/a m d

Irreps\Reps	(*M)(1)	(*M)(2)	(*M)(3)	(*M)(4)
A_1	·	·	2	·
A_2	·	·	·	2
B_1	1	1	·	·
B_2	1	1	·	·

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M(1) 3; M(2) 4; M(3) 1 ; M(4) 2

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Induced site-symmetry representations of space group: I 4_1/a m d (141)

with K-vector: N=(0, 0.5, 0)

[Symmetry elements Space Group I 4_1/a m d (141)]

WP	Representative
4a	0,3/4,1/8

Site Symmetry Group

Site Symmetry Group for 0,3/4,1/8 (4a)

g_1	x,y,z	$\begin{pmatrix} 1. & 0. & 0. & 0.0 \\ 0. & 1. & 0. & 0.0 \\ 0. & 0. & 1. & 0.0 \end{pmatrix}$

Irreducible representations

Character table for -42m

D_{2d}(-42m)	#	1	2	-4	2_x	m_d	functions
Mult.	-	1	1	2	2	2	.
A_1	Γ_1	1	1	1	1	1	x^2+y^2,z^2
A_2	Γ_2	1	1	1	-1	-1	J_z
B_1	Γ_3	1	1	-1	1	-1	x^2-y^2
B_2	Γ_4	1	1	-1	-1	1	z,xy
E	Γ_5	2	-2	0	0	0	(x,y),(xz,yz),(J_x,J_y)

Subduced representations

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(*N)(4) . 1 1 . 1

Induced representations

Induced representations for the point N of I 4_1/a m d

Irreps\Reps	(*N)(1)	(*N)(2)	(*N)(3)	(*N)(4)
A_1	.	1	1	.
A_2	1	.	.	1
B_1	1	.	.	1
B_2	.	1	1	.
E	1	1	1	1

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N(1) 1^+; N(2) 1^-; N(3) 2^+ ; N(4) 2^-

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Induced site-symmetry representations of space group: I 4_1/a m d (141)

with K-vector: N=(0, 0.5, 0)

[Symmetry elements Space Group I 4_1/a m d (141)]

WP	Representative
8e	0,1/4,z

Site Symmetry Group

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Irreducible representations

Character table for mm2

C_{2v}(mm2)	#	1	2_z	m_y	m_x	functions
A_1	Γ_1	1	1	1	1	z,x^2,y^2,z^2
A_2	Γ_3	1	1	-1	-1	xy,J_z
B_1	Γ_2	1	-1	1	-1	x,xz,J_y
B_2	Γ_4	1	-1	-1	1	y,yz,J_x

Subduced representations

Character table for the subduced representations (*N↓mm2) for Wyckoff

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Reps\Irreps	A_1	A_2	B_1	B_2
(*N)(1)	·	2	1	1
(*N)(2)	2	·	1	1
(*N)(3)	2	·	1	1
(*N)(4)	·	2	1	1

Induced representations

Induced representations for the point N of I 4_1/a m d

Irreps\Reps	(*N)(1)	(*N)(2)	(*N)(3)	(*N)(4)
A_1	·	2	2	·
A_2	2	·	·	2
B_1	1	1	1	1
B_2	1	1	1	1

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N(1) 1^+; N(2) 1^-; N(3) 2^+ ; N(4) 2^-

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