

**Appendix A. Character Tables for selected point groups.**

$C_s$	E	h		
A'	1	1	x,y,R <sub>z</sub>	x <sup>2</sup> ,y <sup>2</sup> ,z <sup>2</sup> ,xy
A''	1	-1	z,R <sub>x</sub> ,R <sub>y</sub>	yz,xz

$C_i$	E	i		
A <sub>g</sub>	1	1	R <sub>x</sub> ,R <sub>y</sub> ,R <sub>z</sub>	x <sup>2</sup> ,y <sup>2</sup> ,z <sup>2</sup> ,xy,xz,yz
A <sub>u</sub>	1	-1	x,y,z	

$C_2$	E	$C_2$		
A	1	1	z,R <sub>z</sub>	x <sup>2</sup> +y <sup>2</sup> ,z <sup>2</sup>
B	1	-1	x,y,R <sub>x</sub> ,R <sub>y</sub>	yz,xz

$D_2$	E	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1		x <sup>2</sup> ,y <sup>2</sup> ,z <sup>2</sup> , xy
B <sub>1</sub>	1	1	-1	-1	z,R <sub>z</sub>	xy
B <sub>2</sub>	1	-1	1	-1	y,R <sub>y</sub>	xz
B <sub>3</sub>	1	-1	-1	1	x,R <sub>x</sub>	yz

$D_3$	E	2C <sub>3</sub>	3C <sub>2</sub>		
A <sub>1</sub>	1	1	1		x <sup>2</sup> +y <sup>2</sup> , z <sup>2</sup>
A <sub>2</sub>	1	1	-1	z,R <sub>z</sub>	
E	2	-1	0	(x,y);(R <sub>x</sub> ,R <sub>y</sub> )	(xz,yz); (x <sup>2</sup> -y <sup>2</sup> ,xy)

$C_{2v}$	E	C <sub>2</sub>	$\sigma_v(xz)$	$\sigma_v(yz)$		
A <sub>1</sub>	1	1	1	1	z	x <sup>2</sup> ,y <sup>2</sup> ,z <sup>2</sup>
A <sub>2</sub>	1	1	-1	-1	R <sub>z</sub>	xy
B <sub>1</sub>	1	-1	1	-1	x,R <sub>x</sub>	xz
B <sub>2</sub>	1	-1	-1	1	y,R <sub>y</sub>	yz

$C_{3v}$	E	2C <sub>3</sub>	3 $\sigma_v$		
A <sub>1</sub>	1	1	1	z	x <sup>2</sup> +y <sup>2</sup> , z <sup>2</sup>
A <sub>2</sub>	1	1	-1	R <sub>z</sub>	
E	2	-1	0	(x,y), (R <sub>x</sub> ,R <sub>y</sub> )	(x <sup>2</sup> -y <sup>2</sup> ,xy), (xz,yz)

$C_{4v}$	E	2C <sub>4</sub>	C <sub>2</sub>	2 $\sigma_v$	2 $\sigma_d$		
A <sub>1</sub>	1	1	1	1	1	z	x <sup>2</sup> +y <sup>2</sup> , z <sup>2</sup>
A <sub>2</sub>	1	1	1	-1	-1	R <sub>z</sub>	
B <sub>1</sub>	1	-1	1	1	-1		x <sup>2</sup> -y <sup>2</sup>
B <sub>2</sub>	1	-1	1	-1	1		xy
E	2	0	-2	0	0	(x,y) (R <sub>x</sub> ,R <sub>y</sub> )	(xz,yz)

$C_{2h}$	E	C <sub>2</sub>	i	h		
A <sub>g</sub>	1	1	1	1	R <sub>z</sub>	x <sup>2</sup> ,y <sup>2</sup> , z <sup>2</sup> , xy
B <sub>g</sub>	1	-1	1	-1	R <sub>x</sub> , R <sub>y</sub>	xz, yz
A <sub>u</sub>	1	1	-1	-1	z	
B <sub>u</sub>	1	-1	-1	1	x, y	

$D_{2h}$	E	C <sub>2(z)</sub>	C <sub>2(y)</sub>	C <sub>2(x)</sub>	i	(xy)	(xz)	(yz)		
A <sub>g</sub>	1	1	1	1	1	1	1	1		x <sup>2</sup> , y <sup>2</sup> ,z <sup>2</sup>
B <sub>1g</sub>	1	1	-1	-1	1	1	-1	-1	R <sub>z</sub>	xy
B <sub>2g</sub>	1	-1	1	-1	1	-1	1	-1	R <sub>y</sub>	xz
B <sub>3g</sub>	1	-1	-1	1	1	-1	-1	1	R <sub>x</sub>	yz
A <sub>u</sub>	1	1	1	1	-1	-1	-1	-1		
B <sub>1u</sub>	1	1	-1	-1	-1	-1	1	1	z	
B <sub>2u</sub>	1	-1	1	-1	-1	1	-1	1	y	
B <sub>3u</sub>	1	-1	-1	1	-1	1	1	-1	x	

Appendices

<b>D<sub>3h</sub></b>	E	2C <sub>3</sub>	3C <sub>2</sub>	h	2S <sub>3</sub>	3 <sub>v</sub>		
A <sub>1</sub> '	1	1	1	1	1	1		x <sup>2</sup> +y <sup>2</sup> , z <sup>2</sup>
A <sub>2</sub> '	1	1	-1	1	1	-1	R <sub>z</sub>	
E'	2	-1	0	2	-1	0	(x,y)	(x <sup>2</sup> -y <sup>2</sup> , xy)
A <sub>1</sub> "	1	1	1	-1	-1	-1		
A <sub>2</sub> "	1	1	-1	-1	-1	1	z	
E"	2	-1	0	-2	1	0	(R <sub>v</sub> ,R <sub>v</sub> )	(xz,yz)

<b>D<sub>4h</sub></b>	E	2C <sub>4</sub>	C <sub>2</sub>	2C <sub>2</sub> '	2C <sub>2</sub> "	i	2S <sub>4</sub>	h	2 <sub>v</sub>	2 <sub>d</sub>		
A <sub>1g</sub>	1	1	1	1	1	1	1	1	1	1		x <sup>2</sup> +y <sup>2</sup> , z <sup>2</sup>
A <sub>2g</sub>	1	1	1	-1	-1	1	1	1	-1	-1	R <sub>z</sub>	
B <sub>1g</sub>	1	-1	1	1	-1	1	-1	1	1	-1		x <sup>2</sup> -y <sup>2</sup>
B <sub>2g</sub>	1	-1	1	-1	1	1	-1	1	-1	1		xy
E <sub>g</sub>	2	0	-2	0	0	2	0	-2	0	0	(R <sub>v</sub> , R <sub>v</sub> )	(xz, yz)
A <sub>1u</sub>	1	1	1	1	1	-1	-1	-1	-1	-1		
A <sub>2u</sub>	1	1	1	-1	-1	-1	-1	-1	1	1	z	
B <sub>1u</sub>	1	-1	1	1	-1	-1	1	-1	-1	1		
B <sub>2u</sub>	1	-1	1	-1	1	-1	1	-1	1	-1		
E <sub>u</sub>	2	0	-2	0	0	-2	0	2	0	0	(x,y)	

<b>D<sub>5h</sub></b>	E	2C <sub>5</sub>	2C <sub>5</sub> <sup>2</sup>	5C <sub>2</sub>	h	2S <sub>5</sub>	2S <sub>5</sub> <sup>3</sup>	5 <sub>v</sub>		
A <sub>1</sub> '	1	1	1	1	1	1	1	1		x <sup>2</sup> +y <sup>2</sup> , z <sup>2</sup>
A <sub>2</sub> '	1	1	1	-1	1	1	1	-1	R <sub>z</sub>	
E <sub>1</sub> '	2	2cos72°	2cos144°	0	2	2cos72°	2cos144°	0	(x,y)	
E <sub>2</sub> '	2	2cos144°	2cos72°	0	2	2cos144°	2cos72°	0		(x <sup>2</sup> -y <sup>2</sup> , xy)
A <sub>1</sub> "	1	1	1	1	-1	-1	-1	-1		
A <sub>2</sub> "	1	1	1	-1	-1	-1	-1	1	z	
E <sub>1</sub> "	2	2cos72°	2cos144°	0	-2	-2cos72°	-2cos144°	0	(R <sub>v</sub> , R <sub>v</sub> )	(xz, yz)
E <sub>2</sub> "	2	2cos144°	2cos72°	0	-2	-2cos144°	-2cos72°	0		

<b>D<sub>6h</sub></b>	E	2C <sub>6</sub>	2C <sub>3</sub>	C <sub>2</sub>	3C <sub>2</sub> '	3C <sub>2</sub> "	i	2S <sub>3</sub>	2S <sub>6</sub>	h	3 <sub>d</sub>	3 <sub>v</sub>		
A <sub>1g</sub>	1	1	1	1	1	1	1	1	1	1	1	1		x <sup>2</sup> +y <sup>2</sup> , z <sup>2</sup>
A <sub>2g</sub>	1	1	1	1	-1	-1	1	1	1	1	-1	-1	R <sub>z</sub>	
B <sub>1g</sub>	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1		x <sup>2</sup> -y <sup>2</sup>
B <sub>2g</sub>	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1		xy
E <sub>1g</sub>	2	1	-1	-2	0	0	2	1	-1	-2	0	0	(R <sub>v</sub> ,R <sub>v</sub> )	(xz,yz)
E <sub>2g</sub>	2	-1	-1	2	0	0	2	-1	-1	2	0	0		
A <sub>1u</sub>	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1		
A <sub>2u</sub>	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	z	
B <sub>1u</sub>	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1		
B <sub>2u</sub>	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1		
E <sub>1u</sub>	2	1	-1	-2	0	0	-2	-1	1	2	0	0	(x,y)	
E <sub>2u</sub>	2	-1	-1	2	0	0	-2	1	1	-2	0	0		

<b>D<sub>2d</sub></b>	E	2S <sub>4</sub>	C <sub>2</sub>	2C <sub>2</sub> '	2 <sub>d</sub>		
A <sub>1</sub>	1	1	1	1	1		x <sup>2</sup> +y <sup>2</sup> , z <sup>2</sup>
A <sub>2</sub>	1	1	1	-1	-1	R <sub>z</sub>	
B <sub>1</sub>	1	-1	1	1	-1		x <sup>2</sup> -y <sup>2</sup>
B <sub>2</sub>	1	-1	1	-1	1	z	xy
E	2	0	-2	0	0	(x,y); (R <sub>v</sub> ,R <sub>v</sub> )	(xz,yz)

Appendices

<b>D<sub>3d</sub></b>	E	2C <sub>3</sub>	3C <sub>2</sub>	i	2S <sub>6</sub>	3 d		
A <sub>1g</sub>	1	1	1	1	1	1		$x^2+y^2, z^2$
A <sub>2g</sub>	1	1	-1	1	1	-1	R <sub>z</sub>	
E <sub>g</sub>	2	-1	0	2	-1	0	(R <sub>x</sub> , R <sub>y</sub> )	( $x^2-y^2, xy$ ); (xz, yz)
A <sub>1u</sub>	1	1	1	-1	-1	-1		
A <sub>2u</sub>	1	1	-1	-1	-1	1	z	
E <sub>u</sub>	2	-1	0	-2	1	0	(x, y)	

<b>S<sub>4</sub></b>	E	S <sub>4</sub>	C <sub>2</sub>	S <sub>4</sub> <sup>3</sup>		
A	1	1	1	1	R <sub>z</sub>	$x^2+y^2, z^2$
B	1	-1	1	-1	z	$x^2-y^2, xy$
E	1	±i	-1	-(-i)	(x, y); (R <sub>x</sub> , R <sub>y</sub> )	(xz, yz)

<b>T<sub>d</sub></b>	E	8C <sub>3</sub>	3C <sub>2</sub>	6S <sub>4</sub>	6 d		
A <sub>1</sub>	1	1	1	1	1		$x^2+y^2+z^2$
A <sub>2</sub>	1	1	1	-1	-1		
E	2	-1	2	0	0		( $2z^2-x^2-y^2, x^2-y^2$ )
T <sub>1</sub>	3	0	-1	1	-1	(R <sub>x</sub> , R <sub>y</sub> , R <sub>z</sub> )	
T <sub>2</sub>	3	0	-1	-1	1	(x, y, z)	(xz, yz, xy)

<b>O<sub>h</sub></b>	E	8C <sub>3</sub>	6C <sub>2</sub>	6C <sub>4</sub>	3C <sub>2</sub> (=C <sub>4</sub> <sup>2</sup> )	i	6S <sub>4</sub>	8S <sub>6</sub>	3 h	6 d		
A <sub>1g</sub>	1	1	1	1	1	1	1	1	1	1		$x^2+y^2+z^2$
A <sub>2g</sub>	1	1	-1	-1	1	1	-1	1	1	-1		
E <sub>g</sub>	2	-1	0	0	2	2	0	-1	2	0		( $2z^2-x^2-y^2, x^2-y^2$ )
T <sub>1g</sub>	3	0	-1	1	-1	3	1	0	-1	-1	(R <sub>x</sub> , R <sub>y</sub> , R <sub>z</sub> )	
T <sub>2g</sub>	3	0	1	-1	-1	3	-1	0	-1	1		(xz, yz, xy)
A <sub>1u</sub>	1	1	1	1	1	-1	-1	-1	-1	-1		
A <sub>2u</sub>	1	1	-1	-1	1	-1	1	-1	-1	1		
E <sub>u</sub>	2	-1	0	0	2	-2	0	1	-2	0		
T <sub>1u</sub>	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z)	
T <sub>2u</sub>	3	0	1	-1	-1	-3	1	0	1	-1		

### Appendix B. Constants & Useful Energy Conversions

Planck's Constant,  $h = 6.626 \times 10^{-34}$  J-s  
 Boltzman's Constant,  $k = 1.381 \times 10^{-23}$  J/K = 0.6950 cm<sup>-1</sup>/K  
 speed of light,  $c = 2.998 \times 10^8$  m/s

$$1 \text{ eV} = 1.60219 \times 10^{-19} \text{ J} = 96.485 \text{ kJ/mol} = 22.58 \text{ kcal/mol} = 8065.5 \text{ cm}^{-1}$$

$$1 \text{ cm}^{-1} = 11.96 \text{ J/mol} = 2.859 \text{ cal/mol} = 0.1240 \text{ meV}$$

### Appendix C. Some Direct Products

Note that in some instances, g and u must be added ( $g \times g = u$ ;  $u \times u = g$ ;  $g \times u = u$ ), some subscripts must be omitted and ' and " must be added (' x ' = " x " = ' ; ' x " = ")

<b>D<sub>2</sub>, D<sub>2h</sub></b>	A	B <sub>1</sub>	B <sub>2</sub>	B <sub>3</sub>
A	A	B <sub>1</sub>	B <sub>2</sub>	B <sub>3</sub>
B <sub>1</sub>		A	B <sub>3</sub>	B <sub>2</sub>
B <sub>2</sub>			A	B <sub>1</sub>
B <sub>3</sub>				A

<b>C<sub>2v</sub></b>	A <sub>1</sub>	A <sub>2</sub>	B <sub>1</sub>	B <sub>2</sub>
A <sub>1</sub>	A <sub>1</sub>	A <sub>2</sub>	B <sub>1</sub>	B <sub>2</sub>
A <sub>2</sub>		A <sub>1</sub>	B <sub>2</sub>	B <sub>1</sub>
B <sub>1</sub>			A <sub>1</sub>	A <sub>2</sub>
B <sub>2</sub>				A <sub>1</sub>

<b>C<sub>3v</sub>, D<sub>3</sub>, D<sub>3d</sub>, D<sub>3h</sub></b>	A <sub>1</sub>	A <sub>2</sub>	E
A <sub>1</sub>	A <sub>1</sub>	A <sub>2</sub>	E
A <sub>2</sub>		A <sub>1</sub>	E
E			A <sub>1</sub> +A <sub>2</sub> +E

<b>C<sub>4</sub>, C<sub>4h</sub>, S<sub>4</sub></b>	A	B	E
A	A	B	E
B		A	E
E			[A]+A+E

<b>C<sub>4v</sub>, D<sub>4</sub>, D<sub>2d</sub>, D<sub>4h</sub></b>	A <sub>1</sub>	A <sub>2</sub>	B <sub>1</sub>	B <sub>2</sub>	E
A <sub>1</sub>	A <sub>1</sub>	A <sub>2</sub>	B <sub>1</sub>	B <sub>2</sub>	E
A <sub>2</sub>		A <sub>1</sub>	B <sub>2</sub>	B <sub>1</sub>	E
B <sub>1</sub>			A <sub>1</sub>	A <sub>2</sub>	E
B <sub>2</sub>				A <sub>1</sub>	E
E					A <sub>1</sub> +A <sub>2</sub> +B <sub>1</sub> +B <sub>2</sub>

<b>C<sub>5v</sub>, D<sub>5</sub>, D<sub>5h</sub>, D<sub>5d</sub></b>	A <sub>1</sub>	A <sub>2</sub>	E <sub>1</sub>	E <sub>2</sub>
A <sub>1</sub>	A <sub>1</sub>	A <sub>2</sub>	E <sub>1</sub>	E <sub>2</sub>
A <sub>2</sub>		A <sub>1</sub>	E <sub>1</sub>	E <sub>2</sub>
E <sub>1</sub>			A <sub>1</sub> +A <sub>2</sub> +E <sub>2</sub>	E <sub>1</sub> +E <sub>2</sub>
E <sub>2</sub>				A <sub>1</sub> +A <sub>2</sub> +E <sub>1</sub>

<b>C<sub>6</sub>, C<sub>6h</sub></b>	A	B	E <sub>1</sub>	E <sub>2</sub>
A	A	B	E <sub>1</sub>	E <sub>2</sub>
B		A	E <sub>2</sub>	E <sub>1</sub>
E <sub>1</sub>			[A]+A+E <sub>2</sub>	2B+E <sub>1</sub>
E <sub>2</sub>				[A]+A+E <sub>2</sub>

<b>C<sub>6v</sub>, D<sub>6</sub>, D<sub>6h</sub></b>	A <sub>1</sub>	A <sub>2</sub>	B <sub>1</sub>	B <sub>2</sub>	E <sub>1</sub>	E <sub>2</sub>
A <sub>1</sub>	A <sub>1</sub>	A <sub>2</sub>	B <sub>1</sub>	B <sub>2</sub>	E <sub>1</sub>	E <sub>2</sub>
A <sub>2</sub>		A <sub>1</sub>	B <sub>2</sub>	B <sub>1</sub>	E <sub>1</sub>	E <sub>2</sub>
B <sub>1</sub>			A <sub>1</sub>	A <sub>2</sub>	E <sub>2</sub>	E <sub>1</sub>
B <sub>2</sub>				A <sub>1</sub>	E <sub>2</sub>	E <sub>1</sub>
E <sub>1</sub>					A <sub>1</sub> +A <sub>2</sub> +E <sub>2</sub>	B <sub>1</sub> +B <sub>2</sub> +E <sub>1</sub>
E <sub>2</sub>						A <sub>1</sub> +A <sub>2</sub> +E <sub>2</sub>

<b>O<sub>h</sub>, T<sub>d</sub></b>	A <sub>1</sub>	A <sub>2</sub>	E	T <sub>1</sub>	T <sub>2</sub>
A <sub>1</sub>	A <sub>1</sub>	A <sub>2</sub>	E	T <sub>1</sub>	T <sub>2</sub>
A <sub>2</sub>		A <sub>1</sub>	E	T <sub>2</sub>	T <sub>1</sub>
E			A <sub>1</sub> +A <sub>2</sub> +E	T <sub>1</sub> +T <sub>2</sub>	T <sub>1</sub> +T <sub>2</sub>
T <sub>1</sub>				A <sub>1</sub> +E+[T <sub>1</sub> ]+T <sub>2</sub>	A <sub>2</sub> +E+T <sub>1</sub> +T <sub>2</sub>
T <sub>2</sub>					A <sub>1</sub> +E+[T <sub>1</sub> ]+T <sub>2</sub>

**Appendix D. Standard Valence Orbital  $H_{ij}$  values (eV).**

Atom	ns	np	(n-1)d	n
H	-13.6			1
B	-15.2	-8.5		2
C	-21.4	-11.4		
N	-26.0	-13.4		
O	-32.3	-14.8		
F	-40.0	-18.1		
Si	-17.3	-9.2		3
P	-18.7	-14.0		
S	-20.0	-13.3		
Cl	-26.3	-14.2		
Sc	-8.9	-2.8	-8.5	4
Ti	-9.0	-5.4	-10.8	
V	-8.8	-5.5	-11.0	
Cr	-8.7	-5.2	-11.2	
Mn	-9.8	-5.9	-11.7	
Fe	-9.1	-5.3	-12.6	
Co	-9.2	-5.3	-13.2	
Ni	-9.2	-5.2	-13.5	
Cu	-11.4	-6.1	-14.0	
Zn	-12.4	-6.5		
Ga	-14.6	-6.8		
Ge	-16.0	-9.0		
As	-16.2	-12.2		
Se	-20.5	-13.2		
Br	-22.7	-13.1		
Mo	-8.3	-5.2	-10.5	5
Ru	-10.4	-6.9	-14.9	
Rh	-3.09	-4.6	-12.5	
Pd	-7.3	-3.8	-12.0	
Sb	-18.8	-11.7		
I	-18.0	-12.7		
Te	-20.8	-13.2		6
W	-8.3	-5.2	-10.4	
Re	-9.36	-6.0	-12.7	
Os	-8.5	3.5	-11.0	
Pt	-9.1	-5.5	-12.6	
Au	-10.9	-5.6	-15.1	