

# Contenu du paquet `mes_macros.sty`

Germain Vallverdu

`<germain.vallverdu@univ-pau.fr>`

`http://gvallver.perso.univ-pau.fr/`

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## Résumé

Ce paquet contient un ensemble de commandes simples qui sont de simples raccourcis. Il contient également des commandes plus complexes, en lien avec la chimie physique et plus précisément la chimie quantique, permettant de dessiner des diagrammes d'orbitales moléculaires, de représenter certaines orbitales atomiques ou d'afficher une configuration électronique.

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# 1 Commandes simples

## Énumération – Nombres

<code>1\er</code>	1 <sup>er</sup>
<code>1\ere</code>	1 <sup>ère</sup>
<code>2\de</code>	2 <sup>de</sup>
<code>4\eme</code>	4 <sup>ème</sup>
<code>90\degre</code>	90°
<code>1.6\ex{-19}</code>	$1.6 \times 10^{-19}$
<code>\\$1.6\exm{-19}\\$</code>	$1.6 \times 10^{-19}$

## Vecteurs

<code>\\$vu\\$</code>	$\vec{u}$
<code>\\$vR\\$</code>	$\vec{R}$
<code>\\$vr\\$</code>	$\vec{r}$
<code>\\$vi\\$</code>	$\vec{i}$
<code>\\$vj\\$</code>	$\vec{j}$
<code>\\$vk\\$</code>	$\vec{k}$
<code>\\$fd\\$</code>	$\rightarrow$
<code>\\$ve{abc}\\$</code>	$\overrightarrow{abc}$

*divers*

`\etal` *et al*

## Constantes – unités

<code>\\$na\\$</code>	$\mathcal{N}_a$
<code>\\$kb\\$</code>	$k_B$
<code>\\$kt\\$</code>	$k_B T$
<code>\\$eps0\\$</code>	$\epsilon_0$
<code>\cmi</code>	$\text{cm}^{-1}$
<code>\\$eps\\$</code>	$\epsilon$

## Coordonnées

<code>\\$spheric\\$</code>	$(r, \theta, \phi)$
<code>\\$angulaire\\$</code>	$(\theta, \phi)$

## Mécanique Quantique

<code>\\$opH\\$</code>	$\hat{\mathcal{H}}$
<code>\\$opT\\$</code>	$\hat{T}$
<code>\\$opV\\$</code>	$\hat{V}$

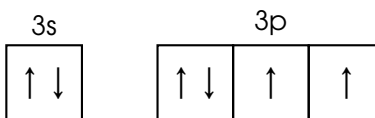
## Intégrales

<code>\\$tint\\$</code>	$\iiint_V$
<code>\\$tint[espace]\\$</code>	$\iiint_{\text{espace}}$
<code>\\$sphericint\\$</code>	$\int_0^\infty \int_0^\pi \int_0^{2\pi}$
<code>\\$radint\\$</code>	$\int_0^\infty$

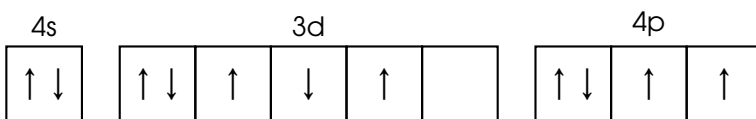
# 2 Boîtes quantiques avec Tikz

Ces commandes permettent de représenter les électrons avec leur spin dans des boîtes quantiques. Elles doivent être placées dans un environnement TikZ.

```
\begin{tikzpicture}
  \OAbxs{(0,0)}{updown}{3s}
  \OAbxp{(2,0)}{updown}{up}{up}{3p}
\end{tikzpicture}
```



```
\begin{tikzpicture}
  \OAbxs{(0,0)}{updown}{4s}
  \OAbxd{(1.5,0)}{updown}{up}{down}{up}{}{3d}
  \OAbxp{(7,0)}{updown}{up}{up}{4p}
\end{tikzpicture}
```



### 3 Configurations électroniques

J'en avais un peu assez de recopier sans arrêt les configurations électroniques des atomes et d'écrire celles que je n'avais pas. J'ai donc créé une commande `\configElectronique` qui prend comme argument le nombre d'électrons et écrit la configuration électronique correspondante. On peut également passer à cette commande deux options. L'option `valence` aura pour effet que la commande n'affiche que la structure électronique de valence. L'option `courte` aura pour effet de remplacer les couches complètes de la configuration électronique par le gaz rare correspondant.

Paramètres de la commande `\configElectronique` :

- #1 (Optionnel) `valence` ou `courte`
- #2 Un nombre entre 1 et 86.

Exemple pour le Fer (Z=26) :

```
\configElectronique{26}          1s22s22p63s23p64s23d6
\configElectronique[courte]{26}  [Ar] 4s23d6
\configElectronique[valence]{26} 4s23d6
```

Exemple pour l'étain (Z=50) :

```
\configElectronique{50}          1s22s22p63s23p64s23d104p65s24d105p2
\configElectronique[courte]{50}  [Kr] 5s24d105p2
\configElectronique[valence]{50}  5s25p2
```

Si vous regardez le fichier source (ou la fin de ce document), vous verrez que la fonction `\configElectronique` est écrite sans aucune finesse. Si quelqu'un sait (en  $\LaTeX$  ou  $\TeX$ ) écrire un code plus intelligent je suis preneur. La fonction est entre les lignes 71 et 1011 du fichier source ... le nombre de ligne vous donne un aperçu de la finesse de la macro. Sur ma page perso, il y a un script python (plus fin) qui donne la configuration électronique en fonction du nombre d'électrons.

### 4 Dessin de paires libres avec Tikz

Les deux commandes concernées sont : `\orbital` et `\Atom` elles permettent de dessiner des orbitales dans un style proche de la théorie de l'hybridation. Le code original provient de [TeXample.net](http://www.texample.net).

<http://www.texample.net/tikz/examples/atoms-and-orbitals/>

La commande `\Atom` sert simplement à placer de façon efficace plusieurs paires autour d'un atome. Elle place le symbole de l'atome au centre d'un cercle de couleur.

#### Description des commandes

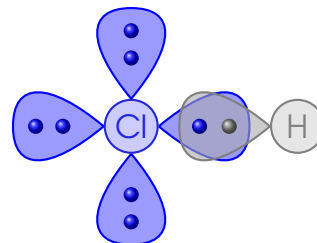
- Paramètres de la commande `\orbital` :
  - #1 (Optionnel) Couleur de l'orbitale. (Pas de mélange de couleur, `blue!40` est interdit)
  - #2 Rotation de l'orbitale, 0° correspond à une orbitale sur un axe vertical orienté vers le haut.
  - #3 Coordonnées pour placer l'orbitale.
  - #4 Nombre d'électron à dessiner à l'intérieur de l'orbitale.
- Paramètres de la commande `\Atom` :
  - #1 (Optionnel) Nom du noeud tikz.
  - #2 Symbole de l'atome (texte du centre du noeud).
  - #3 Couleur de l'atome.
  - #4 Une liste du genre `couleur/angle/position/nombre d'electron`.

## Exemples

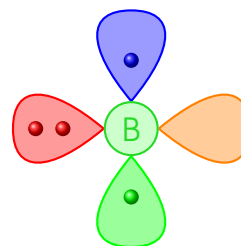
```
\begin{tikzpicture}
  \node at (0,0) (S) {S};
  \orbital[orange]{270}{S.east}{2}
\end{tikzpicture}
```



```
\begin{tikzpicture}
  \Atom{Cl}{blue}{blue/90/west/2,blue/0/north/2,%
    blue/270/east/1,blue/180/south/2}
  \begin{scope}[xshift=2.2cm]
    \Atom{H}{gray}{gray/90/west/1}
  \end{scope}
\end{tikzpicture}
```



```
\begin{tikzpicture}
  \Atom{B}{green}{red/90/west/2,blue/0/north/1,%
    orange/270/east/0,green/180/south/1}
\end{tikzpicture}
```



## 5 Dessin d'orbitales atomiques avec Tikz

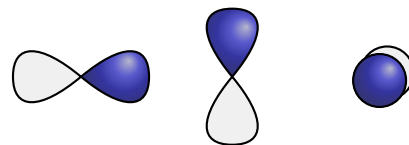
Les nouvelles commandes sont `\orbitalP`, `\orbitalPz` et `orbitals`. Elles permettent respectivement de dessiner une orbitale atomique de type np dans le plan de la page, une orbitale atomique np perpendiculaire à la page et une orbitale de type ns.

### Description des commandes

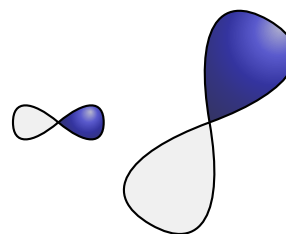
- Paramètres de la commande `\orbitalP` :
  - #1 (Optionnel) Facteur d'échelle pour contrôler la taille.
  - #2 Position du centre de l'orbitale atomique.
  - #3 Rotation de l'orbitale atomique.
- Paramètres de la commande `\orbitalPz` :
  - #1 (Optionnel) Facteur d'échelle pour contrôler la taille.
  - #2 Position du centre de l'orbitale atomique.
- Paramètres de la commande `\orbitals` :
  - #1 (Optionnel) p pour une couleur bleuté ou m pour blanc.
  - #2 Position du centre de l'orbitale atomique.
  - #3 Facteur d'échelle pour contrôler la taille.

## Exemples

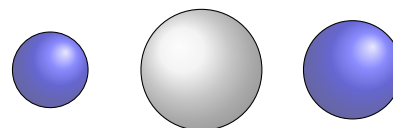
```
\begin{tikzpicture}
  \path (0,0) node (OA1) {} (2,0) node (OA2) {}
    (4,0) node (OA3) {} ;
  \orbitalP{OA1.center}{0.}
  \orbitalP{OA2.center}{90.}
  \orbitalPz{OA3.center}
\end{tikzpicture}
```



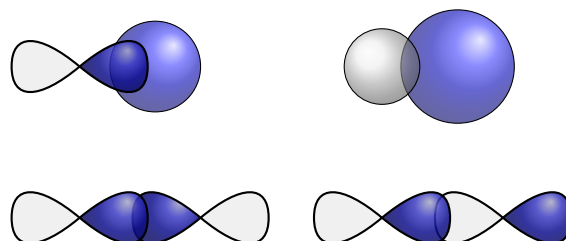
```
\begin{tikzpicture}
  \path (0,0) node (OA1) {} (2,0) node (OA2) {} ;
  \orbitalP[0.5]{OA1.center}{0.}
  \orbitalP[1.3]{OA2.center}{60.}
\end{tikzpicture}
```



```
\begin{tikzpicture}
  \orbitalS{0,0}{1.}
  \orbitalS[m]{2,0}{1.6}
  \orbitalS[p]{4,0}{1.3}
\end{tikzpicture}
```



```
\begin{tikzpicture}
  \path (0,2) node (OA1) {} (1,2) node (OA2) {} ;
  \orbitalS{OA2.center}{1.2}
  \orbitalP{OA1.center}{0.}
  \path (4,2) node (OA1) {} (5,2) node (OA2) {} ;
  \orbitalS[p]{OA2.center}{1.5}
  \orbitalS[m]{OA1.center}{1.}
  \path (0,0) node (OA1) {} (1.6,0) node (OA2) {} ;
  \orbitalP{OA2.center}{180.}
  \orbitalP{OA1.center}{0.}
  \path (4,0) node (OA1) {} (5.6,0) node (OA2) {} ;
  \orbitalP{OA2.center}{0.}
  \orbitalP{OA1.center}{0.}
\end{tikzpicture}
```



## 6 Diagramme d'orbitales moléculaires avec Tikz

La nouvelle commande est `\drawLevel`. Elle permet de placer un niveau d'énergie en indiquant le nombre d'électron à l'intérieur. Elle définit pour ce niveau, trois ancre : au centre, à gauche et à droite.

Paramètres de la commande `drawLevel` :

- #1 (Optionnel) donne le nombre d'électrons dans l'orbitale. Les valeurs sont : up, down ou updown
- #2 Coordonnées du point à gauche pour placer l'orbitale.
- #3 un nom qui permettra de définir les ancres : left#3, right#3 et middle#3.

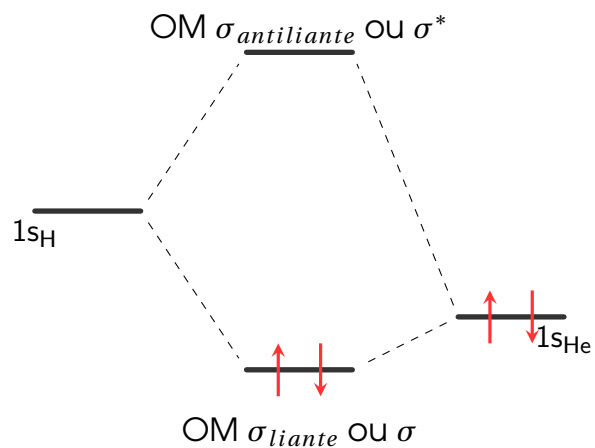
```

\begin{tikzpicture}
  % niveau
  \drawLevel{(0,0)}{1sH}
  \drawLevel[updown]{(8,-2)}{1sHe}
  \drawLevel[updown]{(4,-3)}{liante}
  \drawLevel{(4,3)}{antiliante}

  % traits reliant les niveaux
  \draw[dashed] (right1sH) -- (leftliante)
    (right1sH) -- (leftantiliante)
    (left1sHe) -- (rightantiliante)
    (left1sHe) -- (rightliante) ;

  % label
  \node[anchor=north] at (left1sH) {$1s_H$} ;
  \node[anchor=north] at (right1sHe) {$1s_{He}$} ;
  \node[anchor=north,yshift=-5mm] at (middleliante)
    {OM  $\sigma_{liante}$  ou  $\sigma$ } ;
  \node[anchor=south,yshift=0mm] at (middleantiliante)
    {OM  $\sigma_{antiliante}$  ou  $\sigma^*$ } ;
\end{tikzpicture}

```



## 7 Code source du package

```
1 % * * * * *
2 % *
3 % * quelques macro et raccourcis utiles
4 % *
5 % * Libre d'utiliser, modifier, distribuer
6 % * Germain Vallverdu <germain.vallverdu@univ-pau.fr>
7 % * Octobre 2010
8 % *
9 % * * * * *
10
11 \RequirePackage{xspace}
12 \RequirePackage{tikz}
13 \RequirePackage{ifthen}
14 \RequirePackage{amsmath}
15
16 % enumeration
17 \newcommand{\eme}{\text{\eme}}\xspace % eme
18 \newcommand{\er}{\text{er}}\xspace % premier
19 \newcommand{\ere}{\text{ere}}\xspace % premiere
20 \newcommand{\de}{\text{de}}\xspace % second
21
22 % degre
23 \renewcommand{\degre}{\text{\circ}}\xspace % degre
24
25 % puissance de 10
26 \newcommand{\ex}[1]{\text{\times}\text{10}^{\text{\#1}}\xspace}
27 \newcommand{\exm}[1]{\text{\times}\text{10}^{\text{\#1}}\xspace}
28
29 % constante
30 \newcommand{\na}{\mathcal{N}_a} % avogadro
31 \newcommand{\kb}{k_{\text{B}}} % boltzman
32 \newcommand{\kt}{k_{\text{B}}T} % kBT
33 \newcommand{\epsO}{\varepsilon_0} % epsilon0
34 \newcommand{\cmi}{\text{cm}^{-1}}\xspace % cm^-1
35
36 % epsilon
37 \newcommand{\eps}{\varepsilon}
38
39 % vecteurs
40 \newcommand{\vu}{\vec{u}}
41 \newcommand{\vR}{\vec{R}}
42 \newcommand{\vr}{\vec{r}}
43 \newcommand{\vi}{\vec{i}}
44 \newcommand{\vj}{\vec{j}}
45 \newcommand{\vk}{\vec{k}}
46 \newcommand{\ve}[1]{\overrightarrow{\#1}}
47 \newcommand{\fd}{\rightarrow}
48
49 % integrale
50 \newcommand{\tint}[1][V]{\int\!\!\!\int\int_{\#1}}
51 \newcommand{\sphericint}{\int_0^{\infty}\!\!\int_0^{\pi}\!\!\int_0^{2\pi}}
52 \newcommand{\radint}{\int_0^{\infty}}
53
54 % divers
55 \newcommand{\etal}{\textit{et al}}\xspace % et al
56 \newcommand{\Ncal}{\mathcal{N}}
57
58 % meca Q
59 \newcommand{\opH}{\hat{\mathcal{H}}}\xspace % operateur hamiltonien
```

```

60 \newcommand{\opT}{\hat{T}} % operateur E cinetique
61 \newcommand{\opV}{\hat{V}} % operateur E potentielle
62 \newcommand{\spheric}{(r,\theta,\phi)} % (r, theta, phi)
63 \newcommand{\angulaire}{(\theta,\phi)} % (theta, phi)
64
65 % * * * * *
66 % *
67 % * configuration electronique
68 % *
69 % * * * * *
70
71 % -----
72 % \configElectronique[2]
73 % -----
74 % affiche la configuration electronique complete, en remplaçant les sous couches completes
75 % par le gaz rare si #1 = courte ou la configuration electronique de valence si #1 = valence
76 % parametres #1 : (optionnel) courte ou valence
77 % #2 : nombre d'electrons <= 86
78 % -----
79 \newcommand{\configElectronique}[2][None]{%
80   \ifthenelse{\equal{#2}{1}}{%
81     $\text{1s}^{\text{1}}$%
82   }{%
83     \ifthenelse{\equal{#2}{2}}{%
84       $\text{1s}^{\text{2}}$%
85     }{%
86       \ifthenelse{\equal{#2}{3}}{%
87         \ifthenelse{\equal{#1}{valence}}{%
88           $\text{2s}^{\text{1}}$%
89         }{%
90           \ifthenelse{\equal{#1}{courte}}{%
91             $\left[\text{He}\right],\text{2s}^{\text{1}}$%
92           }{%
93             $\text{1s}^{\text{2}},\text{2s}^{\text{1}}$%
94           }%
95         }%
96       }{%
97         \ifthenelse{\equal{#2}{4}}{%
98           \ifthenelse{\equal{#1}{valence}}{%
99             $\text{2s}^{\text{2}}$%
100          }{%
101            \ifthenelse{\equal{#1}{courte}}{%
102              $\left[\text{He}\right],\text{2s}^{\text{2}}$%
103            }{%
104              $\text{1s}^{\text{2}},\text{2s}^{\text{2}}$%
105            }%
106          }%
107        }{%
108          \ifthenelse{\equal{#2}{5}}{%
109            \ifthenelse{\equal{#1}{valence}}{%
110              $\text{2s}^{\text{2}},\text{2p}^{\text{1}}$%
111            }{%
112              \ifthenelse{\equal{#1}{courte}}{%
113                $\left[\text{He}\right],\text{2s}^{\text{2}},\text{2p}^{\text{1}}$%
114              }{%
115                $\text{1s}^{\text{2}},\text{2s}^{\text{2}},\text{2p}^{\text{1}}$%
116              }%
117            }%
118          }{%
119            \ifthenelse{\equal{#2}{6}}{%
120              \ifthenelse{\equal{#1}{valence}}{%
121                $\text{2s}^{\text{2}},\text{2p}^{\text{2}}$%

```



```

122 }{%
123   \ifthenelse{\equal{#1}{courte}}{%
124     $\left[\text{He}\right]\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{2}}$%
125   }{%
126     $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{2}}$%
127   }%
128 }%
129 }{%
130 \ifthenelse{\equal{#2}{7}}{%
131   \ifthenelse{\equal{#1}{valence}}{%
132     $\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{3}}$%
133   }{%
134     \ifthenelse{\equal{#1}{courte}}{%
135       $\left[\text{He}\right]\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{3}}$%
136     }{%
137       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{3}}$%
138     }%
139   }%
140 }{%
141 \ifthenelse{\equal{#2}{8}}{%
142   \ifthenelse{\equal{#1}{valence}}{%
143     $\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{4}}$%
144   }{%
145     \ifthenelse{\equal{#1}{courte}}{%
146       $\left[\text{He}\right]\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{4}}$%
147     }{%
148       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{4}}$%
149     }%
150   }%
151 }{%
152 \ifthenelse{\equal{#2}{9}}{%
153   \ifthenelse{\equal{#1}{valence}}{%
154     $\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{5}}$%
155   }{%
156     \ifthenelse{\equal{#1}{courte}}{%
157       $\left[\text{He}\right]\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{5}}$%
158     }{%
159       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{5}}$%
160     }%
161   }%
162 }{%
163 \ifthenelse{\equal{#2}{10}}{%
164   \ifthenelse{\equal{#1}{valence}}{%
165     $\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}$%
166   }{%
167     \ifthenelse{\equal{#1}{courte}}{%
168       $\left[\text{He}\right]\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}$%
169     }{%
170       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}$%
171     }%
172   }%
173 }{%
174 \ifthenelse{\equal{#2}{11}}{%
175   \ifthenelse{\equal{#1}{valence}}{%
176     $\text{3s}^{\text{1}}$%
177   }{%
178     \ifthenelse{\equal{#1}{courte}}{%
179       $\left[\text{Ne}\right]\text{\,},\text{\,}\text{3s}^{\text{1}}$%
180     }{%
181       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{1}}$%
182     }%
183   }%

```

```

184 }{%
185 \ifthenelse{\equal{#2}{12}}{%
186   \ifthenelse{\equal{#1}{valence}}{%
187     $\text{3s}^\text{2}$%
188   }{%
189     \ifthenelse{\equal{#1}{courte}}{%
190       $\left[\text{Ne}\right], \text{3s}^\text{2}$%
191     }{%
192       $\text{1s}^\text{2}\text{2s}^\text{2}\text{2p}^\text{6}\text{3s}^\text{2}$%
193     }%
194   }%
195 }{%
196 \ifthenelse{\equal{#2}{13}}{%
197   \ifthenelse{\equal{#1}{valence}}{%
198     $\text{3s}^\text{2}\text{3p}^\text{1}$%
199   }{%
200     \ifthenelse{\equal{#1}{courte}}{%
201       $\left[\text{Ne}\right], \text{3s}^\text{2}\text{3p}^\text{1}$%
202     }{%
203       $\text{1s}^\text{2}\text{2s}^\text{2}\text{2p}^\text{6}\text{3s}^\text{2}\text{3p}^\text{1}$%
204     }%
205   }%
206 }{%
207 \ifthenelse{\equal{#2}{14}}{%
208   \ifthenelse{\equal{#1}{valence}}{%
209     $\text{3s}^\text{2}\text{3p}^\text{2}$%
210   }{%
211     \ifthenelse{\equal{#1}{courte}}{%
212       $\left[\text{Ne}\right], \text{3s}^\text{2}\text{3p}^\text{2}$%
213     }{%
214       $\text{1s}^\text{2}\text{2s}^\text{2}\text{2p}^\text{6}\text{3s}^\text{2}\text{3p}^\text{2}$%
215     }%
216   }%
217 }{%
218 \ifthenelse{\equal{#2}{15}}{%
219   \ifthenelse{\equal{#1}{valence}}{%
220     $\text{3s}^\text{2}\text{3p}^\text{3}$%
221   }{%
222     \ifthenelse{\equal{#1}{courte}}{%
223       $\left[\text{Ne}\right], \text{3s}^\text{2}\text{3p}^\text{3}$%
224     }{%
225       $\text{1s}^\text{2}\text{2s}^\text{2}\text{2p}^\text{6}\text{3s}^\text{2}\text{3p}^\text{3}$%
226     }%
227   }%
228 }{%
229 \ifthenelse{\equal{#2}{16}}{%
230   \ifthenelse{\equal{#1}{valence}}{%
231     $\text{3s}^\text{2}\text{3p}^\text{4}$%
232   }{%
233     \ifthenelse{\equal{#1}{courte}}{%
234       $\left[\text{Ne}\right], \text{3s}^\text{2}\text{3p}^\text{4}$%
235     }{%
236       $\text{1s}^\text{2}\text{2s}^\text{2}\text{2p}^\text{6}\text{3s}^\text{2}\text{3p}^\text{4}$%
237     }%
238   }%
239 }{%
240 \ifthenelse{\equal{#2}{17}}{%
241   \ifthenelse{\equal{#1}{valence}}{%
242     $\text{3s}^\text{2}\text{3p}^\text{5}$%
243   }{%
244     \ifthenelse{\equal{#1}{courte}}{%
245       $\left[\text{Ne}\right], \text{3s}^\text{2}\text{3p}^\text{5}$%

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246     }{%
247     $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3p}^\text{6}\, \text{3d}^\text{1}\, \text{4s}^\text{1}
248     }{%
249     }{%
250   }{%
251   \ifthenelse{\equal{#2}{18}}{%
252     \ifthenelse{\equal{#1}{valence}}{%
253       $ \text{3s}^\text{2}\, \text{3p}^\text{6}\, \text{3d}^\text{1}\, \text{4s}^\text{1}
254     }{%
255       \ifthenelse{\equal{#1}{courte}}{%
256         $ \left[\text{Ne}\right]\, \text{3s}^\text{2}\, \text{3p}^\text{6}\, \text{3d}^\text{1}\, \text{4s}^\text{1}
257       }{%
258         $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3p}^\text{6}\, \text{3d}^\text{1}\, \text{4s}^\text{1}
259       }{%
260     }{%
261   }{%
262   \ifthenelse{\equal{#2}{19}}{%
263     \ifthenelse{\equal{#1}{valence}}{%
264       $ \text{4s}^\text{1}
265     }{%
266       \ifthenelse{\equal{#1}{courte}}{%
267         $ \left[\text{Ar}\right]\, \text{4s}^\text{1}
268       }{%
269         $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3p}^\text{6}\, \text{3d}^\text{1}\, \text{4s}^\text{1}
270       }{%
271     }{%
272   }{%
273   \ifthenelse{\equal{#2}{20}}{%
274     \ifthenelse{\equal{#1}{valence}}{%
275       $ \text{4s}^\text{2}
276     }{%
277       \ifthenelse{\equal{#1}{courte}}{%
278         $ \left[\text{Ar}\right]\, \text{4s}^\text{2}
279       }{%
280         $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3p}^\text{6}\, \text{3d}^\text{1}\, \text{4s}^\text{2}
281       }{%
282     }{%
283   }{%
284   \ifthenelse{\equal{#2}{21}}{%
285     \ifthenelse{\equal{#1}{valence}}{%
286       $ \text{4s}^\text{2}\, \text{3d}^\text{1}\, \text{4s}^\text{1}
287     }{%
288       \ifthenelse{\equal{#1}{courte}}{%
289         $ \left[\text{Ar}\right]\, \text{4s}^\text{2}\, \text{3d}^\text{1}\, \text{4s}^\text{1}
290       }{%
291         $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3p}^\text{6}\, \text{3d}^\text{1}\, \text{4s}^\text{2}\, \text{3d}^\text{1}\, \text{4s}^\text{1}
292       }{%
293     }{%
294   }{%
295   \ifthenelse{\equal{#2}{22}}{%
296     \ifthenelse{\equal{#1}{valence}}{%
297       $ \text{4s}^\text{2}\, \text{3d}^\text{2}\, \text{4s}^\text{2}
298     }{%
299       \ifthenelse{\equal{#1}{courte}}{%
300         $ \left[\text{Ar}\right]\, \text{4s}^\text{2}\, \text{3d}^\text{2}\, \text{4s}^\text{2}
301       }{%
302         $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3p}^\text{6}\, \text{3d}^\text{1}\, \text{4s}^\text{2}\, \text{3d}^\text{2}\, \text{4s}^\text{2}
303       }{%
304     }{%
305   }{%
306   \ifthenelse{\equal{#2}{23}}{%
307     \ifthenelse{\equal{#1}{valence}}{%

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308     $\text{4s}^\text{2}\,\,\text{3d}^\text{3}$%
309   }{%
310     \ifthenelse{\equal{#1}{courte}}{%
311       $\left[\text{Ar}\right]\,\,\text{4s}^\text{2}\,\,\text{3d}^\text{3}$%
312     }{%
313       $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}$%
314     }%
315   }%
316 }{%
317 \ifthenelse{\equal{#2}{24}}{%
318   \ifthenelse{\equal{#1}{valence}}{%
319     $\text{4s}^\text{2}\,\,\text{3d}^\text{4}$%
320   }{%
321     \ifthenelse{\equal{#1}{courte}}{%
322       $\left[\text{Ar}\right]\,\,\text{4s}^\text{2}\,\,\text{3d}^\text{4}$%
323     }{%
324       $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}$%
325     }%
326   }%
327 }{%
328 \ifthenelse{\equal{#2}{25}}{%
329   \ifthenelse{\equal{#1}{valence}}{%
330     $\text{4s}^\text{2}\,\,\text{3d}^\text{5}$%
331   }{%
332     \ifthenelse{\equal{#1}{courte}}{%
333       $\left[\text{Ar}\right]\,\,\text{4s}^\text{2}\,\,\text{3d}^\text{5}$%
334     }{%
335       $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}$%
336     }%
337   }%
338 }{%
339 \ifthenelse{\equal{#2}{26}}{%
340   \ifthenelse{\equal{#1}{valence}}{%
341     $\text{4s}^\text{2}\,\,\text{3d}^\text{6}$%
342   }{%
343     \ifthenelse{\equal{#1}{courte}}{%
344       $\left[\text{Ar}\right]\,\,\text{4s}^\text{2}\,\,\text{3d}^\text{6}$%
345     }{%
346       $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}$%
347     }%
348   }%
349 }{%
350 \ifthenelse{\equal{#2}{27}}{%
351   \ifthenelse{\equal{#1}{valence}}{%
352     $\text{4s}^\text{2}\,\,\text{3d}^\text{7}$%
353   }{%
354     \ifthenelse{\equal{#1}{courte}}{%
355       $\left[\text{Ar}\right]\,\,\text{4s}^\text{2}\,\,\text{3d}^\text{7}$%
356     }{%
357       $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}$%
358     }%
359   }%
360 }{%
361 \ifthenelse{\equal{#2}{28}}{%
362   \ifthenelse{\equal{#1}{valence}}{%
363     $\text{4s}^\text{2}\,\,\text{3d}^\text{8}$%
364   }{%
365     \ifthenelse{\equal{#1}{courte}}{%
366       $\left[\text{Ar}\right]\,\,\text{4s}^\text{2}\,\,\text{3d}^\text{8}$%
367     }{%
368       $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}$%
369     }%

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370     }%
371 }{%
372 \ifthenelse{\equal{#2}{29}}{%
373   \ifthenelse{\equal{#1}{valence}}{%
374     $\text{4s}^{\text{2}}\text{,}\text{3d}^{\text{9}}$%
375   }{%
376     \ifthenelse{\equal{#1}{courte}}{%
377       $\left[\text{Ar}\right]\text{,}\text{4s}^{\text{2}}\text{,}\text{3d}^{\text{9}}$%
378     }{%
379       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
380     }%
381   }%
382 }{%
383 \ifthenelse{\equal{#2}{30}}{%
384   \ifthenelse{\equal{#1}{valence}}{%
385     $\text{4s}^{\text{2}}$%
386   }{%
387     \ifthenelse{\equal{#1}{courte}}{%
388       $\left[\text{Ar}\right]\text{,}\text{4s}^{\text{2}}\text{,}\text{3d}^{\text{10}}$%
389     }{%
390       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
391     }%
392   }%
393 }{%
394 \ifthenelse{\equal{#2}{31}}{%
395   \ifthenelse{\equal{#1}{valence}}{%
396     $\text{4s}^{\text{2}}\text{,}\text{4p}^{\text{1}}$%
397   }{%
398     \ifthenelse{\equal{#1}{courte}}{%
399       $\left[\text{Ar}\right]\text{,}\text{4s}^{\text{2}}\text{,}\text{3d}^{\text{10}}\text{,}\text{4p}^{\text{1}}$%
400     }{%
401       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
402     }%
403   }%
404 }{%
405 \ifthenelse{\equal{#2}{32}}{%
406   \ifthenelse{\equal{#1}{valence}}{%
407     $\text{4s}^{\text{2}}\text{,}\text{4p}^{\text{2}}$%
408   }{%
409     \ifthenelse{\equal{#1}{courte}}{%
410       $\left[\text{Ar}\right]\text{,}\text{4s}^{\text{2}}\text{,}\text{3d}^{\text{10}}\text{,}\text{4p}^{\text{2}}$%
411     }{%
412       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
413     }%
414   }%
415 }{%
416 \ifthenelse{\equal{#2}{33}}{%
417   \ifthenelse{\equal{#1}{valence}}{%
418     $\text{4s}^{\text{2}}\text{,}\text{4p}^{\text{3}}$%
419   }{%
420     \ifthenelse{\equal{#1}{courte}}{%
421       $\left[\text{Ar}\right]\text{,}\text{4s}^{\text{2}}\text{,}\text{3d}^{\text{10}}\text{,}\text{4p}^{\text{3}}$%
422     }{%
423       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
424     }%
425   }%
426 }{%
427 \ifthenelse{\equal{#2}{34}}{%
428   \ifthenelse{\equal{#1}{valence}}{%
429     $\text{4s}^{\text{2}}\text{,}\text{4p}^{\text{4}}$%
430   }{%
431     \ifthenelse{\equal{#1}{courte}}{%

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432         $\left[\text{Ar}\right], \text{4s}^2, \text{3d}^{10}, \text{4p}^4$%
433     }%
434     $\text{1s}^2, \text{2s}^2, \text{2p}^6, \text{3s}^2, \text{3p}^4$%
435 }%
436 }%
437 }%
438 \ifthenelse{\equal{#2}{35}}{%
439     \ifthenelse{\equal{#1}{valence}}{%
440         $\text{4s}^2, \text{4p}^5$%
441     }%
442     \ifthenelse{\equal{#1}{courte}}{%
443         $\left[\text{Ar}\right], \text{4s}^2, \text{3d}^{10}, \text{4p}^5$%
444     }%
445     $\text{1s}^2, \text{2s}^2, \text{2p}^6, \text{3s}^2, \text{3p}^4$%
446 }%
447 }%
448 }%
449 \ifthenelse{\equal{#2}{36}}{%
450     \ifthenelse{\equal{#1}{valence}}{%
451         $\text{4s}^2, \text{4p}^6$%
452     }%
453     \ifthenelse{\equal{#1}{courte}}{%
454         $\left[\text{Ar}\right], \text{4s}^2, \text{3d}^{10}, \text{4p}^6$%
455     }%
456     $\text{1s}^2, \text{2s}^2, \text{2p}^6, \text{3s}^2, \text{3p}^4$%
457 }%
458 }%
459 }%
460 \ifthenelse{\equal{#2}{37}}{%
461     \ifthenelse{\equal{#1}{valence}}{%
462         $\text{5s}^1$%
463     }%
464     \ifthenelse{\equal{#1}{courte}}{%
465         $\left[\text{Kr}\right], \text{5s}^1$%
466     }%
467     $\text{1s}^2, \text{2s}^2, \text{2p}^6, \text{3s}^2, \text{3p}^4$%
468 }%
469 }%
470 }%
471 \ifthenelse{\equal{#2}{38}}{%
472     \ifthenelse{\equal{#1}{valence}}{%
473         $\text{5s}^2$%
474     }%
475     \ifthenelse{\equal{#1}{courte}}{%
476         $\left[\text{Kr}\right], \text{5s}^2$%
477     }%
478     $\text{1s}^2, \text{2s}^2, \text{2p}^6, \text{3s}^2, \text{3p}^4$%
479 }%
480 }%
481 }%
482 \ifthenelse{\equal{#2}{39}}{%
483     \ifthenelse{\equal{#1}{valence}}{%
484         $\text{5s}^2, \text{4d}^1$%
485     }%
486     \ifthenelse{\equal{#1}{courte}}{%
487         $\left[\text{Kr}\right], \text{5s}^2, \text{4d}^1$%
488     }%
489     $\text{1s}^2, \text{2s}^2, \text{2p}^6, \text{3s}^2, \text{3p}^4$%
490 }%
491 }%
492 }%
493 \ifthenelse{\equal{#2}{40}}{%

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494 \iffthenelse{\equal{#1}{valence}}{%
495   $\text{5s}^\text{2}\text{,}\text{4d}^\text{2}$%
496 }{%
497   \iffthenelse{\equal{#1}{courte}}{%
498     $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{2}$%
499   }{%
500     $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
501   }%
502 }%
503 }{%
504 \iffthenelse{\equal{#2}{41}}{%
505   \iffthenelse{\equal{#1}{valence}}{%
506     $\text{5s}^\text{2}\text{,}\text{4d}^\text{3}$%
507   }{%
508     \iffthenelse{\equal{#1}{courte}}{%
509       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{3}$%
510     }{%
511       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
512     }%
513   }%
514 }{%
515 \iffthenelse{\equal{#2}{42}}{%
516   \iffthenelse{\equal{#1}{valence}}{%
517     $\text{5s}^\text{2}\text{,}\text{4d}^\text{4}$%
518   }{%
519     \iffthenelse{\equal{#1}{courte}}{%
520       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{4}$%
521     }{%
522       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
523     }%
524   }%
525 }{%
526 \iffthenelse{\equal{#2}{43}}{%
527   \iffthenelse{\equal{#1}{valence}}{%
528     $\text{5s}^\text{2}\text{,}\text{4d}^\text{5}$%
529   }{%
530     \iffthenelse{\equal{#1}{courte}}{%
531       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{5}$%
532     }{%
533       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
534     }%
535   }%
536 }{%
537 \iffthenelse{\equal{#2}{44}}{%
538   \iffthenelse{\equal{#1}{valence}}{%
539     $\text{5s}^\text{2}\text{,}\text{4d}^\text{6}$%
540   }{%
541     \iffthenelse{\equal{#1}{courte}}{%
542       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{6}$%
543     }{%
544       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
545     }%
546   }%
547 }{%
548 \iffthenelse{\equal{#2}{45}}{%
549   \iffthenelse{\equal{#1}{valence}}{%
550     $\text{5s}^\text{2}\text{,}\text{4d}^\text{7}$%
551   }{%
552     \iffthenelse{\equal{#1}{courte}}{%
553       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{7}$%
554     }{%
555       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%

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556     }%
557   }%
558 }{%
559 \ifthenelse{\equal{#2}{46}}{%
560   \ifthenelse{\equal{#1}{valence}}{%
561     $\text{5s}^\text{2}\text{,}\text{4d}^\text{8}$%
562   }{%
563     \ifthenelse{\equal{#1}{courte}}{%
564       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{8}$%
565     }{%
566       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
567     }%
568   }%
569 }{%
570 \ifthenelse{\equal{#2}{47}}{%
571   \ifthenelse{\equal{#1}{valence}}{%
572     $\text{5s}^\text{2}\text{,}\text{4d}^\text{9}$%
573   }{%
574     \ifthenelse{\equal{#1}{courte}}{%
575       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{9}$%
576     }{%
577       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
578     }%
579   }%
580 }{%
581 \ifthenelse{\equal{#2}{48}}{%
582   \ifthenelse{\equal{#1}{valence}}{%
583     $\text{5s}^\text{2}$%
584   }{%
585     \ifthenelse{\equal{#1}{courte}}{%
586       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{10}$%
587     }{%
588       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
589     }%
590   }%
591 }{%
592 \ifthenelse{\equal{#2}{49}}{%
593   \ifthenelse{\equal{#1}{valence}}{%
594     $\text{5s}^\text{2}\text{,}\text{5p}^\text{1}$%
595   }{%
596     \ifthenelse{\equal{#1}{courte}}{%
597       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{10}\text{,}\text{5p}^\text{1}$%
598     }{%
599       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
600     }%
601   }%
602 }{%
603 \ifthenelse{\equal{#2}{50}}{%
604   \ifthenelse{\equal{#1}{valence}}{%
605     $\text{5s}^\text{2}\text{,}\text{5p}^\text{2}$%
606   }{%
607     \ifthenelse{\equal{#1}{courte}}{%
608       $\left[\text{Kr}\right]\text{,}\text{5s}^\text{2}\text{,}\text{4d}^\text{10}\text{,}\text{5p}^\text{2}$%
609     }{%
610       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
611     }%
612   }%
613 }{%
614 \ifthenelse{\equal{#2}{51}}{%
615   \ifthenelse{\equal{#1}{valence}}{%
616     $\text{5s}^\text{2}\text{,}\text{5p}^\text{3}$%
617   }{%

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618         \ifthenelse{\equal{#1}{courte}}{%
619             $\left[\text{Kr}\right]\text{\,},\text{\,}\text{5s}^{\text{2}}\text{\,},\text{\,}\text{4d}^{\text{10}}\text{\,},\text{\,}\text{5p}^{\text{3}}$%
620         }{%
621             $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{3}}$%
622         }%
623     }%
624 }{%
625 \ifthenelse{\equal{#2}{52}}{%
626     \ifthenelse{\equal{#1}{valence}}{%
627         $\text{5s}^{\text{2}}\text{\,},\text{\,}\text{5p}^{\text{4}}$%
628     }{%
629         \ifthenelse{\equal{#1}{courte}}{%
630             $\left[\text{Kr}\right]\text{\,},\text{\,}\text{5s}^{\text{2}}\text{\,},\text{\,}\text{4d}^{\text{10}}\text{\,},\text{\,}\text{5p}^{\text{4}}$%
631         }{%
632             $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{4}}$%
633         }%
634     }%
635 }{%
636 \ifthenelse{\equal{#2}{53}}{%
637     \ifthenelse{\equal{#1}{valence}}{%
638         $\text{5s}^{\text{2}}\text{\,},\text{\,}\text{5p}^{\text{5}}$%
639     }{%
640         \ifthenelse{\equal{#1}{courte}}{%
641             $\left[\text{Kr}\right]\text{\,},\text{\,}\text{5s}^{\text{2}}\text{\,},\text{\,}\text{4d}^{\text{10}}\text{\,},\text{\,}\text{5p}^{\text{5}}$%
642         }{%
643             $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{5}}$%
644         }%
645     }%
646 }{%
647 \ifthenelse{\equal{#2}{54}}{%
648     \ifthenelse{\equal{#1}{valence}}{%
649         $\text{5s}^{\text{2}}\text{\,},\text{\,}\text{5p}^{\text{6}}$%
650     }{%
651         \ifthenelse{\equal{#1}{courte}}{%
652             $\left[\text{Kr}\right]\text{\,},\text{\,}\text{5s}^{\text{2}}\text{\,},\text{\,}\text{4d}^{\text{10}}\text{\,},\text{\,}\text{5p}^{\text{6}}$%
653         }{%
654             $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{6}}$%
655         }%
656     }%
657 }{%
658 \ifthenelse{\equal{#2}{55}}{%
659     \ifthenelse{\equal{#1}{valence}}{%
660         $\text{6s}^{\text{1}}$%
661     }{%
662         \ifthenelse{\equal{#1}{courte}}{%
663             $\left[\text{Xe}\right]\text{\,},\text{\,}\text{6s}^{\text{1}}$%
664         }{%
665             $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{6}}$%
666         }%
667     }%
668 }{%
669 \ifthenelse{\equal{#2}{56}}{%
670     \ifthenelse{\equal{#1}{valence}}{%
671         $\text{6s}^{\text{2}}$%
672     }{%
673         \ifthenelse{\equal{#1}{courte}}{%
674             $\left[\text{Xe}\right]\text{\,},\text{\,}\text{6s}^{\text{2}}$%
675         }{%
676             $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{6}}$%
677         }%
678     }%
679 }%

```

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680 \ifthenelse{\equal{#2}{57}}{%
681   \ifthenelse{\equal{#1}{valence}}{%
682     $\text{6s}^\text{2}\text{,}\text{4f}^\text{1}$%
683   }{%
684     \ifthenelse{\equal{#1}{courte}}{%
685       $\left[\text{Xe}\right]\text{,}\text{6s}^\text{2}\text{,}\text{4f}^\text{1}$%
686     }{%
687       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
688     }%
689   }%
690 }{%
691 \ifthenelse{\equal{#2}{58}}{%
692   \ifthenelse{\equal{#1}{valence}}{%
693     $\text{6s}^\text{2}\text{,}\text{4f}^\text{2}$%
694   }{%
695     \ifthenelse{\equal{#1}{courte}}{%
696       $\left[\text{Xe}\right]\text{,}\text{6s}^\text{2}\text{,}\text{4f}^\text{2}$%
697     }{%
698       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
699     }%
700   }%
701 }{%
702 \ifthenelse{\equal{#2}{59}}{%
703   \ifthenelse{\equal{#1}{valence}}{%
704     $\text{6s}^\text{2}\text{,}\text{4f}^\text{3}$%
705   }{%
706     \ifthenelse{\equal{#1}{courte}}{%
707       $\left[\text{Xe}\right]\text{,}\text{6s}^\text{2}\text{,}\text{4f}^\text{3}$%
708     }{%
709       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
710     }%
711   }%
712 }{%
713 \ifthenelse{\equal{#2}{60}}{%
714   \ifthenelse{\equal{#1}{valence}}{%
715     $\text{6s}^\text{2}\text{,}\text{4f}^\text{4}$%
716   }{%
717     \ifthenelse{\equal{#1}{courte}}{%
718       $\left[\text{Xe}\right]\text{,}\text{6s}^\text{2}\text{,}\text{4f}^\text{4}$%
719     }{%
720       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
721     }%
722   }%
723 }{%
724 \ifthenelse{\equal{#2}{61}}{%
725   \ifthenelse{\equal{#1}{valence}}{%
726     $\text{6s}^\text{2}\text{,}\text{4f}^\text{5}$%
727   }{%
728     \ifthenelse{\equal{#1}{courte}}{%
729       $\left[\text{Xe}\right]\text{,}\text{6s}^\text{2}\text{,}\text{4f}^\text{5}$%
730     }{%
731       $\text{1s}^\text{2}\text{,}\text{2s}^\text{2}\text{,}\text{2p}^\text{6}\text{,}\text{3s}^\text{2}\text{,}\text{3p}^\text{6}$%
732     }%
733   }%
734 }{%
735 \ifthenelse{\equal{#2}{62}}{%
736   \ifthenelse{\equal{#1}{valence}}{%
737     $\text{6s}^\text{2}\text{,}\text{4f}^\text{6}$%
738   }{%
739     \ifthenelse{\equal{#1}{courte}}{%
740       $\left[\text{Xe}\right]\text{,}\text{6s}^\text{2}\text{,}\text{4f}^\text{6}$%
741     }{%

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742         $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}\,\,\text{3d}^\text{5}\,\,\text{4s}^\text{1}$
743     }%
744 }%
745 }%
746 \ifthenelse{\equal{#2}{63}}{%
747     \ifthenelse{\equal{#1}{valence}}{%
748         $\text{6s}^\text{2}\,\,\text{4f}^\text{7}$%
749     }%
750     \ifthenelse{\equal{#1}{courte}}{%
751         $\left[\text{Xe}\right]\,\,\text{6s}^\text{2}\,\,\text{4f}^\text{7}$%
752     }%
753     $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}\,\,\text{3d}^\text{5}\,\,\text{4s}^\text{1}$
754 }%
755 }%
756 }%
757 \ifthenelse{\equal{#2}{64}}{%
758     \ifthenelse{\equal{#1}{valence}}{%
759         $\text{6s}^\text{2}\,\,\text{4f}^\text{8}$%
760     }%
761     \ifthenelse{\equal{#1}{courte}}{%
762         $\left[\text{Xe}\right]\,\,\text{6s}^\text{2}\,\,\text{4f}^\text{8}$%
763     }%
764     $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}\,\,\text{3d}^\text{5}\,\,\text{4s}^\text{1}$
765 }%
766 }%
767 }%
768 \ifthenelse{\equal{#2}{65}}{%
769     \ifthenelse{\equal{#1}{valence}}{%
770         $\text{6s}^\text{2}\,\,\text{4f}^\text{9}$%
771     }%
772     \ifthenelse{\equal{#1}{courte}}{%
773         $\left[\text{Xe}\right]\,\,\text{6s}^\text{2}\,\,\text{4f}^\text{9}$%
774     }%
775     $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}\,\,\text{3d}^\text{5}\,\,\text{4s}^\text{1}$
776 }%
777 }%
778 }%
779 \ifthenelse{\equal{#2}{66}}{%
780     \ifthenelse{\equal{#1}{valence}}{%
781         $\text{6s}^\text{2}\,\,\text{4f}^\text{10}$%
782     }%
783     \ifthenelse{\equal{#1}{courte}}{%
784         $\left[\text{Xe}\right]\,\,\text{6s}^\text{2}\,\,\text{4f}^\text{10}$%
785     }%
786     $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}\,\,\text{3d}^\text{5}\,\,\text{4s}^\text{1}$
787 }%
788 }%
789 }%
790 \ifthenelse{\equal{#2}{67}}{%
791     \ifthenelse{\equal{#1}{valence}}{%
792         $\text{6s}^\text{2}\,\,\text{4f}^\text{11}$%
793     }%
794     \ifthenelse{\equal{#1}{courte}}{%
795         $\left[\text{Xe}\right]\,\,\text{6s}^\text{2}\,\,\text{4f}^\text{11}$%
796     }%
797     $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}\,\,\text{3d}^\text{5}\,\,\text{4s}^\text{1}$
798 }%
799 }%
800 }%
801 \ifthenelse{\equal{#2}{68}}{%
802     \ifthenelse{\equal{#1}{valence}}{%
803         $\text{6s}^\text{2}\,\,\text{4f}^\text{12}$%

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```

804 }{%
805   \ifthenelse{\equal{#1}{courte}}{%
806     $\left[\text{Xe}\right]\text{\,},\text{\,}\text{6s}^{\text{2}}\text{\,},\text{\,}\text{4f}^{\text{12}}$%
807   }{%
808     $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{6}}$%
809   }%
810 }%
811 }{%
812 \ifthenelse{\equal{#2}{69}}{%
813   \ifthenelse{\equal{#1}{valence}}{%
814     $\text{6s}^{\text{2}}\text{\,},\text{\,}\text{4f}^{\text{13}}$%
815   }{%
816     \ifthenelse{\equal{#1}{courte}}{%
817       $\left[\text{Xe}\right]\text{\,},\text{\,}\text{6s}^{\text{2}}\text{\,},\text{\,}\text{4f}^{\text{13}}$%
818     }{%
819       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{6}}$%
820     }%
821   }%
822 }%
823 \ifthenelse{\equal{#2}{70}}{%
824   \ifthenelse{\equal{#1}{valence}}{%
825     $\text{6s}^{\text{2}}$%
826   }{%
827     \ifthenelse{\equal{#1}{courte}}{%
828       $\left[\text{Xe}\right]\text{\,},\text{\,}\text{6s}^{\text{2}}\text{\,},\text{\,}\text{4f}^{\text{14}}$%
829     }{%
830       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{6}}$%
831     }%
832   }%
833 }%
834 \ifthenelse{\equal{#2}{71}}{%
835   \ifthenelse{\equal{#1}{valence}}{%
836     $\text{6s}^{\text{2}}\text{\,},\text{\,}\text{5d}^{\text{1}}$%
837   }{%
838     \ifthenelse{\equal{#1}{courte}}{%
839       $\left[\text{Xe}\right]\text{\,},\text{\,}\text{6s}^{\text{2}}\text{\,},\text{\,}\text{4f}^{\text{14}}\text{\,},\text{\,}\text{5d}^{\text{1}}$%
840     }{%
841       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{6}}$%
842     }%
843   }%
844 }%
845 \ifthenelse{\equal{#2}{72}}{%
846   \ifthenelse{\equal{#1}{valence}}{%
847     $\text{6s}^{\text{2}}\text{\,},\text{\,}\text{5d}^{\text{2}}$%
848   }{%
849     \ifthenelse{\equal{#1}{courte}}{%
850       $\left[\text{Xe}\right]\text{\,},\text{\,}\text{6s}^{\text{2}}\text{\,},\text{\,}\text{4f}^{\text{14}}\text{\,},\text{\,}\text{5d}^{\text{2}}$%
851     }{%
852       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{6}}$%
853     }%
854   }%
855 }%
856 \ifthenelse{\equal{#2}{73}}{%
857   \ifthenelse{\equal{#1}{valence}}{%
858     $\text{6s}^{\text{2}}\text{\,},\text{\,}\text{5d}^{\text{3}}$%
859   }{%
860     \ifthenelse{\equal{#1}{courte}}{%
861       $\left[\text{Xe}\right]\text{\,},\text{\,}\text{6s}^{\text{2}}\text{\,},\text{\,}\text{4f}^{\text{14}}\text{\,},\text{\,}\text{5d}^{\text{3}}$%
862     }{%
863       $\text{1s}^{\text{2}}\text{\,},\text{\,}\text{2s}^{\text{2}}\text{\,},\text{\,}\text{2p}^{\text{6}}\text{\,},\text{\,}\text{3s}^{\text{2}}\text{\,},\text{\,}\text{3p}^{\text{6}}$%
864     }%
865   }%

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```

866 }{%
867 \ifthenelse{\equal{#2}{74}}{%
868   \ifthenelse{\equal{#1}{valence}}{%
869     $\text{6s}^{\text{2}}\text{,}\text{5d}^{\text{4}}$%
870   }{%
871     \ifthenelse{\equal{#1}{courte}}{%
872       $\left[\text{Xe}\right]\text{,}\text{6s}^{\text{2}}\text{,}\text{4f}^{\text{14}}\text{,}\text{5d}^{\text{4}}$%
873     }{%
874       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
875     }%
876   }%
877 }{%
878 \ifthenelse{\equal{#2}{75}}{%
879   \ifthenelse{\equal{#1}{valence}}{%
880     $\text{6s}^{\text{2}}\text{,}\text{5d}^{\text{5}}$%
881   }{%
882     \ifthenelse{\equal{#1}{courte}}{%
883       $\left[\text{Xe}\right]\text{,}\text{6s}^{\text{2}}\text{,}\text{4f}^{\text{14}}\text{,}\text{5d}^{\text{5}}$%
884     }{%
885       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
886     }%
887   }%
888 }{%
889 \ifthenelse{\equal{#2}{76}}{%
890   \ifthenelse{\equal{#1}{valence}}{%
891     $\text{6s}^{\text{2}}\text{,}\text{5d}^{\text{6}}$%
892   }{%
893     \ifthenelse{\equal{#1}{courte}}{%
894       $\left[\text{Xe}\right]\text{,}\text{6s}^{\text{2}}\text{,}\text{4f}^{\text{14}}\text{,}\text{5d}^{\text{6}}$%
895     }{%
896       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
897     }%
898   }%
899 }{%
900 \ifthenelse{\equal{#2}{77}}{%
901   \ifthenelse{\equal{#1}{valence}}{%
902     $\text{6s}^{\text{2}}\text{,}\text{5d}^{\text{7}}$%
903   }{%
904     \ifthenelse{\equal{#1}{courte}}{%
905       $\left[\text{Xe}\right]\text{,}\text{6s}^{\text{2}}\text{,}\text{4f}^{\text{14}}\text{,}\text{5d}^{\text{7}}$%
906     }{%
907       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
908     }%
909   }%
910 }{%
911 \ifthenelse{\equal{#2}{78}}{%
912   \ifthenelse{\equal{#1}{valence}}{%
913     $\text{6s}^{\text{2}}\text{,}\text{5d}^{\text{8}}$%
914   }{%
915     \ifthenelse{\equal{#1}{courte}}{%
916       $\left[\text{Xe}\right]\text{,}\text{6s}^{\text{2}}\text{,}\text{4f}^{\text{14}}\text{,}\text{5d}^{\text{8}}$%
917     }{%
918       $\text{1s}^{\text{2}}\text{,}\text{2s}^{\text{2}}\text{,}\text{2p}^{\text{6}}\text{,}\text{3s}^{\text{2}}\text{,}\text{3p}^{\text{6}}$%
919     }%
920   }%
921 }{%
922 \ifthenelse{\equal{#2}{79}}{%
923   \ifthenelse{\equal{#1}{valence}}{%
924     $\text{6s}^{\text{2}}\text{,}\text{5d}^{\text{9}}$%
925   }{%
926     \ifthenelse{\equal{#1}{courte}}{%
927       $\left[\text{Xe}\right]\text{,}\text{6s}^{\text{2}}\text{,}\text{4f}^{\text{14}}\text{,}\text{5d}^{\text{9}}$%

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```

928     }{%
929     $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3}
930     }{%
931   }{%
932 }{%
933 \ifthenelse{\equal{#2}{80}}{%
934   \ifthenelse{\equal{#1}{valence}}{%
935     $ \text{6s}^\text{2}$%
936   }{%
937     \ifthenelse{\equal{#1}{courte}}{%
938       $ \left[\text{Xe}\right]\, \text{6s}^\text{2}\, \text{4f}^\text{14}\, \text{5d}^\text{10}$%
939     }{%
940       $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3}
941     }%
942   }%
943 }{%
944 \ifthenelse{\equal{#2}{81}}{%
945   \ifthenelse{\equal{#1}{valence}}{%
946     $ \text{6s}^\text{2}\, \text{6p}^\text{1}$%
947   }{%
948     \ifthenelse{\equal{#1}{courte}}{%
949       $ \left[\text{Xe}\right]\, \text{6s}^\text{2}\, \text{4f}^\text{14}\, \text{5d}^\text{10}\,
950     }{%
951       $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3}
952     }%
953   }%
954 }{%
955 \ifthenelse{\equal{#2}{82}}{%
956   \ifthenelse{\equal{#1}{valence}}{%
957     $ \text{6s}^\text{2}\, \text{6p}^\text{2}$%
958   }{%
959     \ifthenelse{\equal{#1}{courte}}{%
960       $ \left[\text{Xe}\right]\, \text{6s}^\text{2}\, \text{4f}^\text{14}\, \text{5d}^\text{10}\,
961     }{%
962       $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3}
963     }%
964   }%
965 }{%
966 \ifthenelse{\equal{#2}{83}}{%
967   \ifthenelse{\equal{#1}{valence}}{%
968     $ \text{6s}^\text{2}\, \text{6p}^\text{3}$%
969   }{%
970     \ifthenelse{\equal{#1}{courte}}{%
971       $ \left[\text{Xe}\right]\, \text{6s}^\text{2}\, \text{4f}^\text{14}\, \text{5d}^\text{10}\,
972     }{%
973       $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3}
974     }%
975   }%
976 }{%
977 \ifthenelse{\equal{#2}{84}}{%
978   \ifthenelse{\equal{#1}{valence}}{%
979     $ \text{6s}^\text{2}\, \text{6p}^\text{4}$%
980   }{%
981     \ifthenelse{\equal{#1}{courte}}{%
982       $ \left[\text{Xe}\right]\, \text{6s}^\text{2}\, \text{4f}^\text{14}\, \text{5d}^\text{10}\,
983     }{%
984       $ \text{1s}^\text{2}\, \text{2s}^\text{2}\, \text{2p}^\text{6}\, \text{3s}^\text{2}\, \text{3}
985     }%
986   }%
987 }{%
988 \ifthenelse{\equal{#2}{85}}{%
989   \ifthenelse{\equal{#1}{valence}}{%

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```

990     $\text{6s}^\text{2}\,\,\text{6p}^\text{5}$%
991   }{%
992     \ifthenelse{\equal{#1}{courte}}{%
993       $\left[\text{Xe}\right]\,\,\text{6s}^\text{2}\,\,\text{4f}^\text{14}\,\,\text{5d}^\text{10}\,\,
994     }{%
995       $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}$%
996     }%
997   }%
998 }{%
999 \ifthenelse{\equal{#2}{86}}{%
1000   \ifthenelse{\equal{#1}{valence}}{%
1001     $\text{6s}^\text{2}\,\,\text{6p}^\text{6}$%
1002   }{%
1003     \ifthenelse{\equal{#1}{courte}}{%
1004       $\left[\text{Xe}\right]\,\,\text{6s}^\text{2}\,\,\text{4f}^\text{14}\,\,\text{5d}^\text{10}\,\,
1005     }{%
1006       $\text{1s}^\text{2}\,\,\text{2s}^\text{2}\,\,\text{2p}^\text{6}\,\,\text{3s}^\text{2}\,\,\text{3p}^\text{6}$%
1007     }%
1008   }%
1009 }{%
1010   Apres le Radon j'en avais mare !!%
1011   }%
1012 }
1013
1014 % * * * * *
1015 % *
1016 % * boite quantique avec tikz
1017 % *
1018 % * * * * *
1019
1020 % commande interne teste le spin
1021 \newcommand{\testspin}[1]{%
1022   \ifthenelse{\equal{#1}{updown}}{ $\uparrow$ $ \downarrow$ }{%
1023     \ifthenelse{\equal{#1}{up}}{ $\uparrow$ }{%
1024       \ifthenelse{\equal{#1}{down}}{ $\downarrow$ }{%
1025         }%
1026       }%
1027     }%
1028 }
1029
1030 % style OA
1031 \tikzstyle{OAbox} = [draw,thick,minimum height=1cm,minimum width=1cm]
1032
1033 % -----
1034 % boite quantique ns : \OAboxs[3]
1035 % -----
1036 % cree une case quantique
1037 % parametres #1 : positions
1038 % #2 : remplissage = up, down ou updown
1039 % #3 : nom
1040 % -----
1041 \newcommand{\OAboxs}[3] {
1042   \path #1 node[OAbox] (OAs) {\Large \testspin{#2}} ;
1043   \node[anchor=south] at (OAs.north) {#3};
1044 }
1045
1046 % -----
1047 % boite quantique np : \OAboxp[5]
1048 % -----
1049 % cree trois cases quantiques accolees
1050 % parametres #1 : positions
1051 % #2-4 : remplissage = up, down ou updown

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```

1052 % #5 : nom
1053 % -----
1054 \newcommand{\OAboxp}[5]{
1055   \path #1 node[OAbox] {\Large \testspin{#2}}
1056   ++ (1,0) node[OAbox] (OAp) {\Large \testspin{#3}}
1057   ++ (1,0) node[OAbox] {\Large \testspin{#4}} ;
1058   \node[anchor=south] at (OAp.north) {#5};
1059 }
1060
1061 % -----
1062 % boite quantique nd : \OAboxp[7]
1063 % -----
1064 % cree trois cases quantiques accolées
1065 % parametres #1 : positions
1066 % #2-6 : remplissage = up, down ou updown
1067 % #7 : nom
1068 % -----
1069 \newcommand{\OAboxd}[7]{
1070   \path #1 node[OAbox] {\Large \testspin{#2}}
1071   ++ (1,0) node[OAbox] {\Large \testspin{#3}}
1072   ++ (1,0) node[OAbox] (OAd) {\Large \testspin{#4}}
1073   ++ (1,0) node[OAbox] {\Large \testspin{#5}}
1074   ++ (1,0) node[OAbox] {\Large \testspin{#6}} ;
1075   \node[anchor=south] at (OAd.north) {#7};
1076 }
1077
1078 % * * * * *
1079 % *
1080 % * Diagramme d'OM avec tikz
1081 % *
1082 % * * * * *
1083
1084 % styles
1085 \tikzstyle{drawOAelectron} = [very thick,color=red!80,-stealth]
1086 \tikzstyle{levelstyle} = [line width=2pt,color=black!80,line cap=round]
1087
1088 % -----
1089 % commande \drawLevel[3]
1090 % -----
1091 % trace un niveau et rajoute des noeuds
1092 % Parameters: #1 (optional) Nombre de d'electron, par défaut 0
1093 % #2 position du point a gauche de l'orbitale
1094 % #3 base du nom du noeud : donne les label left#3 et right#3 et middle#3
1095 % -----
1096 \newcommand{\drawLevel}[3][no]{%
1097   \draw[levelstyle]
1098     #2 node (left#3) {} -- ++ (2,0)
1099     node (right#3) {}
1100     node[pos=0.5] (middle#3) {}
1101     node[pos=0.3] (pos1) {}
1102     node[pos=0.7] (pos2) {} ;
1103
1104   \ifthenelse{\equal{#1}{updown}}{
1105     \draw[drawOAelectron] (pos1.center) ++(0,-0.5) -- ++(0,1) ;
1106     \draw[drawOAelectron] (pos2.center) ++(0, 0.5) -- ++(0,-1) ;
1107   }{
1108     \ifthenelse{\equal{#1}{up}}{
1109       \draw[drawOAelectron] (middle#3.center) ++(0,-0.5) -- ++(0,1) ;
1110     }{
1111       \ifthenelse{\equal{#1}{down}}{
1112         \draw[drawOAelectron] (posm.center) ++(0, 0.5) -- ++(0,-1) ;
1113       }{

```



```

1114     }
1115   }
1116 }
1117 }
1118
1119 % * * * * *
1120 % *
1121 % * Dessins d'orbitales atomiques avec tikz
1122 % *
1123 % *   a partir de :
1124 % *   http://www.texample.net/tikz/examples/atoms-and-orbitals/
1125 % *   Berteun Damman, Arne Rohrs
1126 % *
1127 % * * * * *
1128
1129 \pgfdeclarelayer{background}
1130 \pgfdeclarelayer{main}
1131 \pgfdeclarelayer{foreground}
1132 \pgfsetlayers{background,main,foreground}
1133
1134 % style general pour les orbitales
1135 \tikzstyle{orbital}=[thick,fill opacity=.60]
1136
1137 % la commande \defOrbitalCurve permet de definir les points necessaires pour le tracer de
1138 % l'orbitale. C'est une commande ``interne''. A priori elle n'est pas utile en dehors des
1139 % macros definies ici.
1140 \def\orbheight{1.2}
1141 \def\orbwidth{.6}
1142 \newcommand{\defOrbitalCurve}{
1143   % These points define the curve for the orbital.
1144   \coordinate (c1) at (-\orbwidth, .6 * \orbheight);
1145   \coordinate (c2) at (-\orbwidth, \orbheight);
1146   \coordinate (c3) at (\orbwidth, \orbheight);
1147   \coordinate (c4) at (\orbwidth, .6 * \orbheight);
1148   \coordinate (top) at (0,\orbheight);
1149 }
1150
1151 % -----
1152 % commande \orbital[4]
1153 % -----
1154 % Parameters: #1 (optional) Orbital color (no mixing color ie. blue!50 is forbidden, put blue only)
1155 %             #2 Rotation of the orbital
1156 %             #3 Coordinate where the orbital should be attached
1157 %             #4 Number of electrons to draw in the orbital
1158 % -----
1159 \newcommand{\orbital}[4][blue]{
1160   % definit le tracer de l'orbitale
1161   \begin{scope}[rotate=#2,shift=(#3)]
1162     \defOrbitalCurve
1163
1164     %Coordinates of the electrons
1165     \coordinate (e1) at (0, 0.45*\orbheight);
1166     \coordinate (e2) at (0, 0.75*\orbheight);
1167   \end{scope}
1168
1169   % These are drawn on a background layer, so orbitals
1170   % can overlap without covering the electrons, which
1171   % visualises the role electrons play in chemical bonds.
1172   \begin{pgfonlayer}{background}
1173     \draw[orbital,fill=#1!66,draw=#1] (#3) .. controls (c1) and (c2) .. (top) ..
1174     controls (c3) and (c4) .. (#3);
1175   \end{pgfonlayer}

```

```

1176
1177 % Draw the electrons
1178 \ifnum#4>0
1179   \foreach \n in {1,...,#4} {
1180     \shade[ball color=#1] (e\n) circle (1mm);
1181   }
1182   \fi
1183 }
1184
1185 % -----
1186 % commande \atom[4]
1187 % -----
1188 % This allows to quickly place an atom.
1189 % Parameters: #1 (Optional) Name of the center node
1190 %             #2 Text for the center node
1191 %             #3 Atom color
1192 %             #4 orbital parameters : A list of color/rotation-angle/anchor/number of electrons
1193 % -----
1194 \tikzstyle{atomcore}=[shape=circle,thick,minimum size=7mm,inner sep=0pt]
1195 \newcommand{\Atom}[4][AtomNode]{
1196   \node[atomcore,draw=#3!40,color=#3!70!gray,fill=#3!20] (#1) {\large#2};
1197   \foreach \color/\ang/\anchor/\n in {#4} {
1198     \orbital[\color]{\ang}{#1.\anchor}{\n}
1199   }
1200 }
1201
1202 % -----
1203 % Dessins d'orbitales atomiques de type p
1204 %   on considere que x et y sont dans le plan de la feuille
1205 %   \orbitalP[3]   pour npx, npy
1206 %   \orbitalPz[3]  pour npz
1207 %   \orbitals[3]   pour ns
1208 % -----
1209
1210 % shading pour les OA p
1211 \pgfdeclare radialshading{shadeOAp}{\pgfpoint{10bp}{12bp}}
1212 {color(0bp)=(blue!15!white); color(9bp)=(blue!75!white);
1213 color(18bp)=(blue!70!black); color(25bp)=(blue!50!black); color(50bp)=(black) }
1214
1215 % -----
1216 % commande \orbitalP[3]
1217 % -----
1218 % dessine une OA p dans le plan (px ou py)
1219 % parametres #1 : (optionel) facteur de scaling
1220 %             #2 : position du centre de l'OA
1221 %             #3 : rotation de l'OA
1222 % -----
1223 \newcommand{\orbitalP}[3][0.75]{
1224   \begin{scope}[scale=#1,rotate=#3]
1225     \begin{scope}[rotate=270,shift=(#2)]
1226       \defOrbitalCurve
1227     \end{scope}
1228     \draw[orbital,fill=black!80,draw=black,shading=shadeOAp] (#2) .. controls (c1) and
1229       (c2) .. (top) .. controls (c3) and (c4) .. (#2);
1230
1231     \begin{scope}[rotate=90,shift=(#2)]
1232       \defOrbitalCurve
1233     \end{scope}
1234     \draw[orbital,fill=black!10,draw=black] (#2) .. controls (c1) and (c2) .. (top) ..
1235       controls (c3) and (c4) .. (#2);
1236   \end{scope}
1237 }

```

```

1238
1239 % -----
1240 % commande \orbitalPz[2]
1241 % -----
1242 % dessine une OA p perpendiculaire a la feuille (pz)
1243 % parametres #1 : (optionel) facteur de scaling
1244 %           #2 : position du centre de l'OA
1245 % -----
1246 \newcommand{\orbitalPz}[2][1.]{
1247   \node[xshift=-0.5mm,yshift=-0.5mm] at (#2) (circle1) {} ;
1248   \node[xshift=0.5mm,yshift=0.5mm] at (#2) (circle2) {} ;
1249   \draw[orbital,fill=black!10,draw=black] (circle2.center) circle (.35*#1) ;
1250   \draw[fill=white] (circle1.center) circle (.35*#1) ;
1251   \draw[orbital,fill=black!80,draw=black,shading=shadeOAp] (circle1.center) circle (.35*#1) ;
1252 }
1253
1254 % -----
1255 % commande \orbitalS[3]
1256 % -----
1257 % Dessins d'orbitales atomiques de type s
1258 %   #1 : (optionel) p pour bleu m pour blanc
1259 %   #2 : position, soit x,y soit nom d'un noeud
1260 %   #3 : facteur de scaling sur le rayon
1261 % -----
1262 \newcommand{\orbitalS}[3][p]{
1263   \ifthenelse{\equal{#1}{p}}{
1264     \draw[fill opacity=.60,shading=shadeOAp] (#2) circle (0.5*#3) ;
1265   }{
1266     \ifthenelse{\equal{#1}{m}}{
1267       \draw[fill opacity=.60,ball color=black!10] (#2) circle (0.5*#3) ;
1268     }{
1269       \draw[fill opacity=.60,ball color=black!10] (#2) circle (0.5*#3) ;
1270     }
1271   }
1272 }
1273
1274 %% end of file %%

```