Diagrammes potentiel-pH (à compléter)

Figure A  Diagrammes potentiel-pH de l'aluminium et de l'or ($T = 298 \text{ K}$)
Données

Constante des gaz parfaits : \( R = 8,314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1} \).

Températures : \( T(\text{K}) = t(\circ \text{C}) + 273,15 \).

Produit ionique de l’eau (à 25 °C) : \( pK_w = 14 \).

Approximation à 298 K : \( \frac{RT}{F} \ln(10) \approx 0,06 \text{ V} \).

Densité de solutions de soude à 20 °C

\[
\begin{array}{cccccccccc}
\% \text{ masse d’hydroxyde de sodium} & 0,16 & 0,19 & 1,37 & 3 & 18,26 & 19,16 & 20,07 & 20,98 & 21,90 & 22,82 \\
\text{densité} & 1,00 & 1,10 & 1,15 & 1,20 & 1,21 & 1,22 & 1,23 & 1,24 & 1,25 \\
\end{array}
\]

Potentiels standard d’oxydoréduction à 25 °C

\[
\begin{array}{cccccccccc}
\text{Au(OH)}_3(\text{s})/\text{Au(0)} & \text{O}_2(\text{g})/\text{H}_2\text{O}(\text{aq}) & \text{NO}_3^-/\text{NO}_2^- & \text{Ag}^+/\text{Ag(0)} & \text{Asc}^-/\text{AscH}_2(\text{aq}) & \text{H}^+/\text{H}_2(\text{g}) & \text{Al}^{3+}/\text{Al(0)} \\
1,45 \text{ V} & 1,23 \text{ V} & 0,96 \text{ V} & 0,80 \text{ V} & 0,48 \text{ V} & 0,00 \text{ V} & −1,66 \text{ V} \\
\end{array}
\]

AscH₂ est l’acide ascorbique, Asc l’acide déshydrorascorbique.

Constantes d’acidité à 25 °C

Acide ascorbique AscH₂ : \( pK_A1 = 4,1 \); \( pK_A2 = 11,8 \).

Acide phosphorique \( H_3PO_4 \) : \( pK_A1 = 2,1 \); \( pK_A2 = 7,2 \); \( pK_A3 = 12,3 \).

Masse molaire

Acide ascorbique : \( M = 176 \text{ g mol}^{-1} \).

Extrait du tableau périodique des éléments

<table>
<thead>
<tr>
<th>Numéro atomique</th>
<th>Symbole chimique</th>
<th>Nom de l’élément</th>
<th>Masse atomique</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H</td>
<td>Hydrogène</td>
<td>1,0080</td>
</tr>
<tr>
<td>2</td>
<td>He</td>
<td>Béryllium</td>
<td>9,0122</td>
</tr>
<tr>
<td>3</td>
<td>Li</td>
<td>Lithium</td>
<td>6,9985</td>
</tr>
<tr>
<td>4</td>
<td>Be</td>
<td>Béryllium</td>
<td>9,0122</td>
</tr>
<tr>
<td>5</td>
<td>B</td>
<td>Boron</td>
<td>10,814</td>
</tr>
<tr>
<td>6</td>
<td>C</td>
<td>Carbone</td>
<td>12,011</td>
</tr>
<tr>
<td>7</td>
<td>N</td>
<td>Azote</td>
<td>14,007</td>
</tr>
<tr>
<td>8</td>
<td>O</td>
<td>Oxygène</td>
<td>15,999</td>
</tr>
<tr>
<td>9</td>
<td>F</td>
<td>fluor</td>
<td>18,998</td>
</tr>
<tr>
<td>10</td>
<td>Ne</td>
<td>néon</td>
<td>20,180</td>
</tr>
<tr>
<td>11</td>
<td>Na</td>
<td>Sodium</td>
<td>22,990</td>
</tr>
<tr>
<td>12</td>
<td>Mg</td>
<td>Magnésium</td>
<td>24,306</td>
</tr>
<tr>
<td>13</td>
<td>Al</td>
<td>Aluminium</td>
<td>26,982</td>
</tr>
<tr>
<td>14</td>
<td>Si</td>
<td>Silicium</td>
<td>28,085</td>
</tr>
<tr>
<td>15</td>
<td>P</td>
<td>Phosphore</td>
<td>30,974</td>
</tr>
<tr>
<td>16</td>
<td>S</td>
<td>Sulfure</td>
<td>32,068</td>
</tr>
<tr>
<td>17</td>
<td>Cl</td>
<td>Chlorure</td>
<td>35,452</td>
</tr>
<tr>
<td>18</td>
<td>Ar</td>
<td>Argon</td>
<td>39,948</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Numéro atomique</th>
<th>Symbole chimique</th>
<th>Nom de l’élément</th>
<th>Masse atomique</th>
</tr>
</thead>
<tbody>
<tr>
<td>19</td>
<td>K</td>
<td>potassium</td>
<td>39,098</td>
</tr>
<tr>
<td>20</td>
<td>Ca</td>
<td>Calcium</td>
<td>40,078</td>
</tr>
<tr>
<td>21</td>
<td>Sc</td>
<td>Scandium</td>
<td>44,956</td>
</tr>
<tr>
<td>22</td>
<td>Ti</td>
<td>Titane</td>
<td>47,867</td>
</tr>
<tr>
<td>23</td>
<td>V</td>
<td>Vanadine</td>
<td>50,941</td>
</tr>
<tr>
<td>24</td>
<td>Cr</td>
<td>Chrome</td>
<td>52,005</td>
</tr>
<tr>
<td>25</td>
<td>Mn</td>
<td>Manganèse</td>
<td>54,938</td>
</tr>
<tr>
<td>26</td>
<td>Fe</td>
<td>Fer</td>
<td>55,845</td>
</tr>
<tr>
<td>27</td>
<td>Co</td>
<td>Cobalt</td>
<td>58,933</td>
</tr>
<tr>
<td>28</td>
<td>Ni</td>
<td>Nickel</td>
<td>63,546</td>
</tr>
<tr>
<td>29</td>
<td>Cu</td>
<td>Cuivre</td>
<td>65,381</td>
</tr>
<tr>
<td>30</td>
<td>Zn</td>
<td>Zinc</td>
<td>69,723</td>
</tr>
<tr>
<td>31</td>
<td>Ga</td>
<td>Gélement</td>
<td>72,630</td>
</tr>
<tr>
<td>32</td>
<td>Ge</td>
<td>Géle</td>
<td>74,921</td>
</tr>
<tr>
<td>33</td>
<td>As</td>
<td>Astat</td>
<td>78,971</td>
</tr>
<tr>
<td>34</td>
<td>Se</td>
<td>Sélénium</td>
<td>79,904</td>
</tr>
<tr>
<td>35</td>
<td>Br</td>
<td>Bromure</td>
<td>83,798</td>
</tr>
<tr>
<td>36</td>
<td>Kr</td>
<td>Kripton</td>
<td>85,467</td>
</tr>
<tr>
<td>37</td>
<td>Rb</td>
<td>Rubidium</td>
<td>85,508</td>
</tr>
<tr>
<td>38</td>
<td>Sr</td>
<td>Strontium</td>
<td>88,467</td>
</tr>
<tr>
<td>39</td>
<td>Y</td>
<td>yttrium</td>
<td>88,906</td>
</tr>
<tr>
<td>40</td>
<td>Zr</td>
<td>Zirconium</td>
<td>91,224</td>
</tr>
<tr>
<td>41</td>
<td>Nb</td>
<td>Nébium</td>
<td>92,906</td>
</tr>
<tr>
<td>42</td>
<td>Mo</td>
<td>Molybdéne</td>
<td>95,95</td>
</tr>
<tr>
<td>43</td>
<td>Tc</td>
<td>Térbium</td>
<td>98,719</td>
</tr>
<tr>
<td>44</td>
<td>Ru</td>
<td>Rutil</td>
<td>101,07</td>
</tr>
<tr>
<td>45</td>
<td>Rh</td>
<td>Rhodium</td>
<td>102,91</td>
</tr>
<tr>
<td>46</td>
<td>Pd</td>
<td>Pd</td>
<td>106,42</td>
</tr>
<tr>
<td>47</td>
<td>Ag</td>
<td>Argent</td>
<td>107,87</td>
</tr>
<tr>
<td>48</td>
<td>Cd</td>
<td>Cadmium</td>
<td>111,24</td>
</tr>
<tr>
<td>49</td>
<td>In</td>
<td>Indium</td>
<td>113,75</td>
</tr>
<tr>
<td>50</td>
<td>Sn</td>
<td>Sb</td>
<td>117,18</td>
</tr>
<tr>
<td>51</td>
<td>Sb</td>
<td>Sb</td>
<td>119,73</td>
</tr>
<tr>
<td>52</td>
<td>Te</td>
<td>Tellure</td>
<td>121,76</td>
</tr>
<tr>
<td>53</td>
<td>I</td>
<td>Iode</td>
<td>126,90</td>
</tr>
<tr>
<td>54</td>
<td>Xe</td>
<td>Xénon</td>
<td>126,90</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Numéro atomique</th>
<th>Symbole chimique</th>
<th>Nom de l’élément</th>
<th>Masse atomique</th>
</tr>
</thead>
<tbody>
<tr>
<td>55</td>
<td>Cs</td>
<td>Césium</td>
<td>132,91</td>
</tr>
<tr>
<td>56</td>
<td>Ba</td>
<td>Barium</td>
<td>137,33</td>
</tr>
<tr>
<td>57</td>
<td>La</td>
<td>Lanthane</td>
<td>138,91</td>
</tr>
<tr>
<td>58</td>
<td>Ce</td>
<td>Céterne</td>
<td>140,11</td>
</tr>
<tr>
<td>59</td>
<td>Pr</td>
<td>Praséne</td>
<td>140,91</td>
</tr>
<tr>
<td>60</td>
<td>Nd</td>
<td>Néodyne</td>
<td>144,24</td>
</tr>
<tr>
<td>61</td>
<td>Pm</td>
<td>Pm</td>
<td>145,01</td>
</tr>
<tr>
<td>62</td>
<td>Sm</td>
<td>Sm</td>
<td>150,36</td>
</tr>
<tr>
<td>63</td>
<td>Eu</td>
<td>Eu</td>
<td>151,96</td>
</tr>
<tr>
<td>64</td>
<td>Gd</td>
<td>Gd</td>
<td>157,25</td>
</tr>
<tr>
<td>65</td>
<td>Tb</td>
<td>Tb</td>
<td>158,93</td>
</tr>
<tr>
<td>66</td>
<td>Dy</td>
<td>Dy</td>
<td>162,50</td>
</tr>
<tr>
<td>67</td>
<td>Ho</td>
<td>Ho</td>
<td>164,93</td>
</tr>
<tr>
<td>68</td>
<td>Er</td>
<td>Er</td>
<td>167,25</td>
</tr>
<tr>
<td>69</td>
<td>Tm</td>
<td>Tm</td>
<td>168,93</td>
</tr>
<tr>
<td>70</td>
<td>Yb</td>
<td>Yb</td>
<td>173,04</td>
</tr>
<tr>
<td>71</td>
<td>Lu</td>
<td>Lu</td>
<td>174,96</td>
</tr>
<tr>
<td>72</td>
<td>Hf</td>
<td>Héféntium</td>
<td>178,49</td>
</tr>
<tr>
<td>73</td>
<td>Ta</td>
<td>Tantal</td>
<td>180,94</td>
</tr>
<tr>
<td>74</td>
<td>W</td>
<td>Tungsténe</td>
<td>186,21</td>
</tr>
<tr>
<td>75</td>
<td>Re</td>
<td>Rhenium</td>
<td>190,23</td>
</tr>
<tr>
<td>76</td>
<td>Os</td>
<td>Os</td>
<td>192,22</td>
</tr>
<tr>
<td>77</td>
<td>Ir</td>
<td>Ir</td>
<td>195,08</td>
</tr>
<tr>
<td>78</td>
<td>Pt</td>
<td>Pt</td>
<td>196,97</td>
</tr>
<tr>
<td>79</td>
<td>Au</td>
<td>Or</td>
<td>200,59</td>
</tr>
<tr>
<td>80</td>
<td>Hg</td>
<td>Plomb</td>
<td>204,38</td>
</tr>
<tr>
<td>81</td>
<td>Tl</td>
<td>Thallium</td>
<td>207,2</td>
</tr>
<tr>
<td>82</td>
<td>Pb</td>
<td>Plomb</td>
<td>208,98</td>
</tr>
<tr>
<td>83</td>
<td>Bi</td>
<td>Bi</td>
<td>209,00</td>
</tr>
<tr>
<td>84</td>
<td>Po</td>
<td>Po</td>
<td>209,00</td>
</tr>
<tr>
<td>85</td>
<td>At</td>
<td>At</td>
<td>209,00</td>
</tr>
<tr>
<td>86</td>
<td>Rn</td>
<td>Rn</td>
<td>222,00</td>
</tr>
</tbody>
</table>
Schéma de synthèse du Siméprévir

Figure B  Schéma de synthèse du Siméprévir
## Données sur les orbitales du butadiène et du dioxyde de soufre

<table>
<thead>
<tr>
<th>Énergie (eV)</th>
<th>HO</th>
<th>BV</th>
</tr>
</thead>
<tbody>
<tr>
<td>−9,22</td>
<td></td>
<td>0,67</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Tableau A</th>
<th>Orbitales frontalières du butadiène</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numéro OM</td>
<td>1</td>
</tr>
<tr>
<td>Énergie (eV)</td>
<td>−37,92</td>
</tr>
<tr>
<td>Soufre</td>
<td>3s</td>
</tr>
<tr>
<td></td>
<td>3p_x</td>
</tr>
<tr>
<td></td>
<td>3p_y</td>
</tr>
<tr>
<td></td>
<td>3p_z</td>
</tr>
<tr>
<td>Oxygène</td>
<td>2s</td>
</tr>
<tr>
<td></td>
<td>2p_x</td>
</tr>
<tr>
<td></td>
<td>2p_y</td>
</tr>
<tr>
<td></td>
<td>2p_z</td>
</tr>
<tr>
<td>Oxygène</td>
<td>2s</td>
</tr>
<tr>
<td></td>
<td>2p_x</td>
</tr>
<tr>
<td></td>
<td>2p_y</td>
</tr>
<tr>
<td></td>
<td>2p_z</td>
</tr>
</tbody>
</table>

| Numéro OM | 7 | 8 | 9 | 10 | 11 | 12 |
| Énergie (eV) | −12,97 | −12,50 | −10,10 | −1,03 | 1,64 | 2,40 |
| Soufre | 3s | 0,00000 | 0,00000 | 0,51398 | 0,00000 | 0,38048 | 0,00000 |
| | 3p_x | −0,06446 | 0,00000 | 0,00000 | 0,00000 | 0,00000 | 0,78303 |
| | 3p_y | 0,00000 | 0,00000 | 0,00000 | 0,75580 | 0,00000 | 0,00000 |
| | 3p_z | 0,00000 | 0,00000 | −0,46052 | 0,00000 | 0,64468 | 0,00000 |
| Oxygène | 2s | 0,05773 | 0,00000 | 0,04150 | 0,00000 | −0,10676 | −0,15384 |
| | 2p_x | 0,55789 | 0,00000 | 0,10302 | 0,00000 | 0,45623 | 0,28761 |
| | 2p_y | 0,00000 | 0,70711 | 0,00000 | −0,46302 | 0,00000 | 0,00000 |
| | 2p_z | −0,42819 | 0,00000 | 0,49954 | 0,00000 | 0,01620 | 0,29504 |
| Oxygène | 2s | −0,05773 | 0,00000 | 0,04150 | 0,00000 | −0,10676 | 0,15384 |
| | 2p_x | 0,55789 | 0,00000 | −0,10302 | 0,00000 | −0,45623 | 0,28761 |
| | 2p_y | 0,00000 | −0,70711 | 0,00000 | −0,46302 | 0,00000 | 0,00000 |
| | 2p_z | 0,42819 | 0,00000 | 0,49954 | 0,00000 | 0,01620 | −0,29504 |

<table>
<thead>
<tr>
<th>Tableau B</th>
<th>Orbitales moléculaires (OM) du dioxyde de soufre</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tableaux construits à l’aide des orbitales fournies dans la base de donnée d’Orbimol (<a href="http://www.lct.jussieu.fr/pagesperso/">http://www.lct.jussieu.fr/pagesperso/</a> orbimol/fr/index-fr.shtml)</td>
<td></td>
</tr>
</tbody>
</table>