Supplementary Information

Hydroxylation and sulfidation for nickel recovery from a spent catalyst containing the chelating agent, 2,2'-bipyridine

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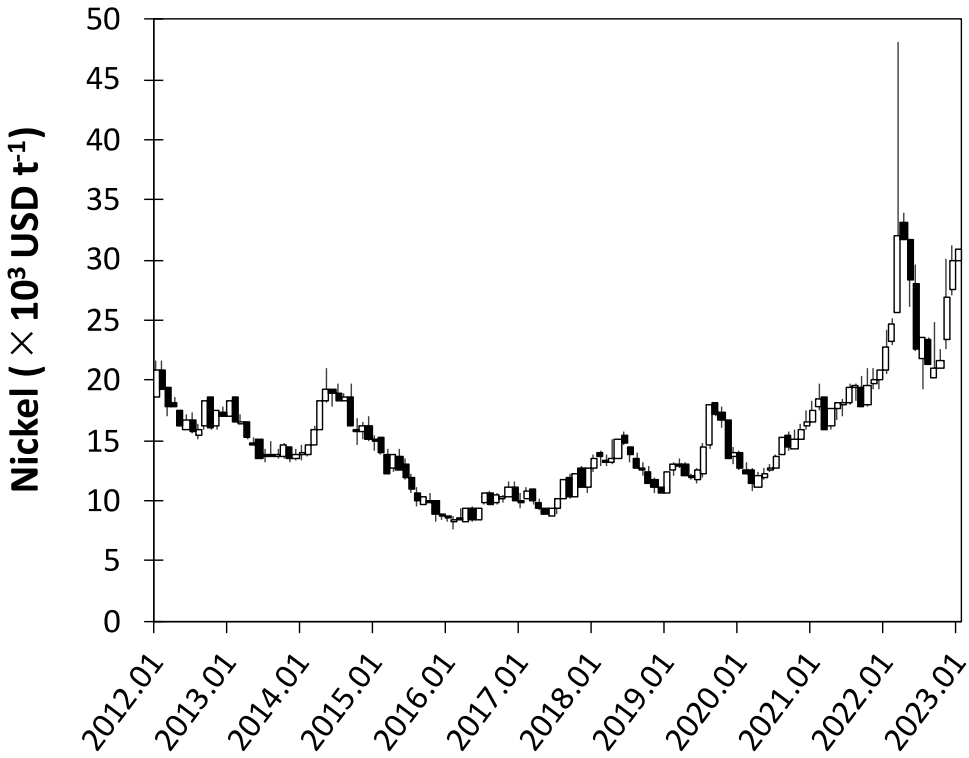

Figure S1. Candlestick chart of Ni market price at LME in the last 10 years. The monthly averaged values (Open–Close, and High–Low prices) were obtained from summarized data in TRADING ECONOMICS [https://tradingeconomics.com/commodity/nickel, (accessed on 15, 01, 2023)].

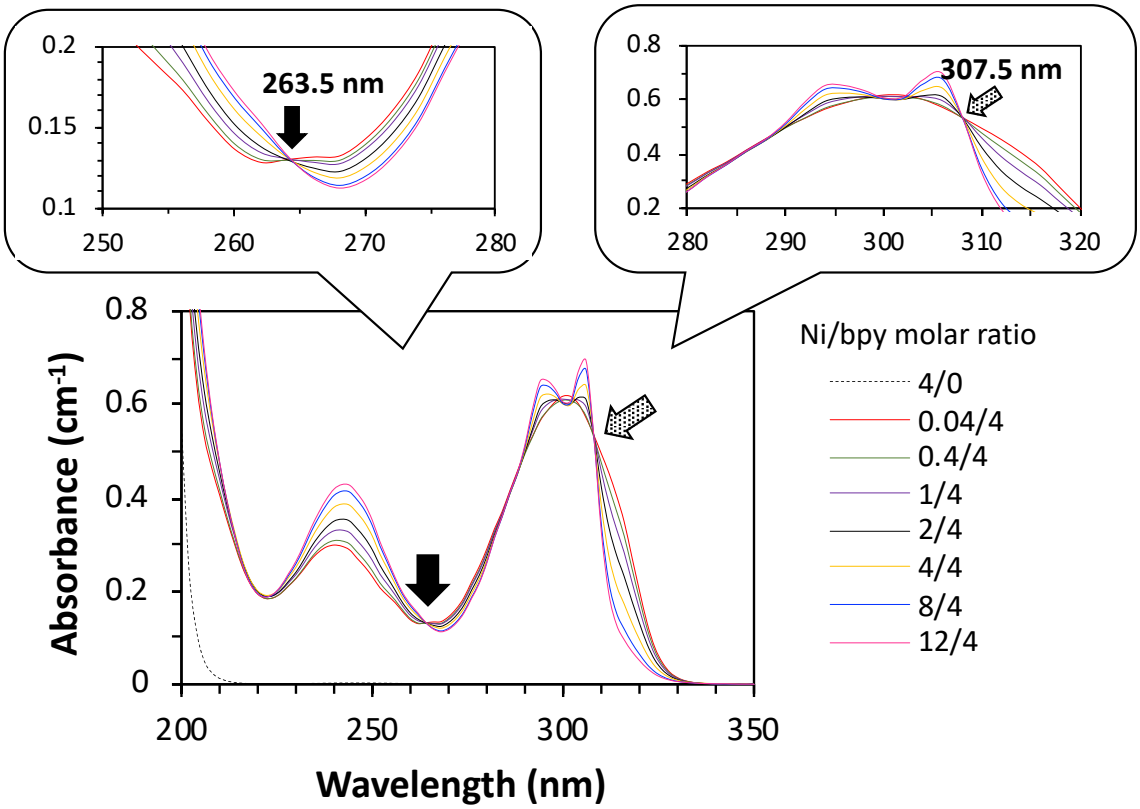

Figure S2. UV-Vis spectra of bpy (40 μM) with a various concentrations of Ni^{2+} (0–120 μM).

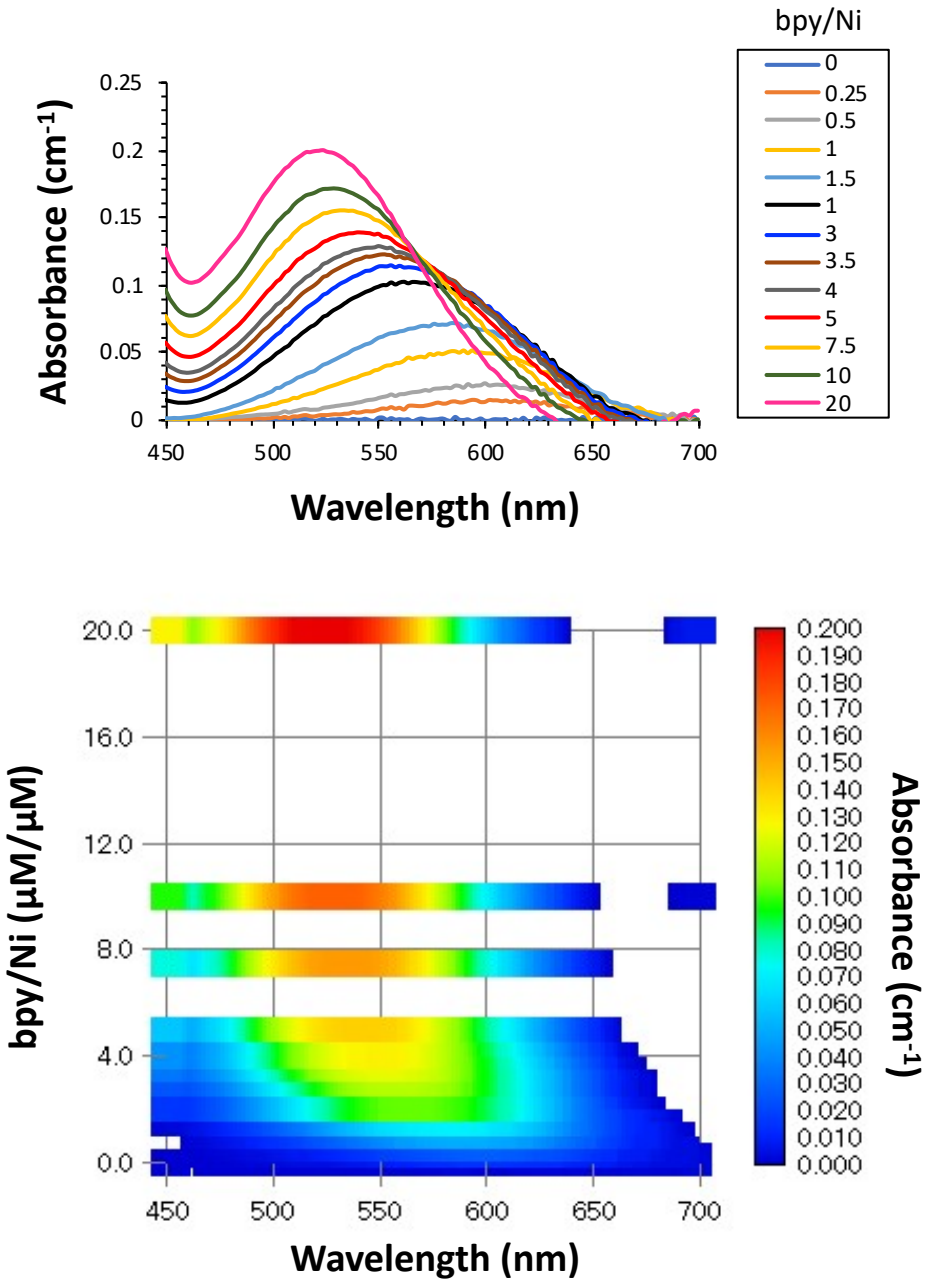

Figure S3. Visible range spectra of the Ni-bpy complex (upper) and the counter graph to show the blue shift with the formation of $Ni(bpy)_3$ from $Ni(bpy)_1$ (lower). The concentration of Ni^{2+} was fixed at 20 µM and that of bpy was varied between 0 and 200 µM (bpy/Ni concentration ratio of 0–20 µM/µM).

Table S1. The PHREEQC code for calculation of $Ni(OH)_2$ precipitate[α]

```
PHASES
Fix_H+
   H+ = H+
   log_k 0.0
SOLUTION 1
   temp      25
   pH        -0.5 charge
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Cl        3000
   Ni        20
   -water    1 # kg
EQUILIBRIUM_PHASES 1
Ni(OH)2 0.0 0.0
SELECTED_OUTPUT
-file Ni_S
-reset false
USER_PUNCH 1
   -headings
   -start
10 FOR i = 0 to 14 STEP 0.25
20 a$ = EOL$ + " USE SOLUTION 1 " + EOL$
30 a$ = a$ + " EQUILIBRIUM_PHASES 1 " + EOL$
40 a$ = a$ + " Ni(OH)2 0.0 0.0 " + EOL$
50 a$ = a$ + " Fix_H+ " + STR$(-i) + " NaOH 100 " + EOL$
60 a$ = a$ + " END " + EOL$
70 PUNCH a$
80 NEXT i
   -end
```

```
END
USER_PUNCH 1
   -headings
   -start
   -end
END
USER_GRAPH 1
   -headings              pH total_Ni NiCl+ Ni2OH+3 Ni(OH)2
   -axis_titles           "pH" "Ni" "amount"
   -chart_title           "Ni_S"
   -initial_solutions     false
   -connect_simulations   true
   -plot_concentration_vs  x
  -start
10 GRAPH_X  -la("H+")
20 GRAPH_Y tot("Ni"), mol("NiCl+"), mol("Ni2OH+3"), equi("Ni(OH)2")
  -end
   -active                true
INCLUDE$ Ni_S
END
```

[α] The llnl database was used for it.

Table S2. The PHREEQC code for calculation of NiS precipitate[α]

```
PHASES
Millerite
    NiS +1.0000 H+  =  + 1.0000 HS- + 1.0000 Ni++
    log_k          -8.0345
SOLUTION 1
  temp      25
  pH        3
  pe        3
  redox     pe
  units     mmol/kgw
  density   1
  Cl        3000
  Ni        40
  -water    1 # kg
EQUILIBRIUM_PHASES 1
Ni(OH)2 0.0 0.0
Millerite 0.0 0.0
H2S(g) 0.0 0.0
USER_GRAPH 1
-headings Na2S pH Millerite H2S(g) Ni S(-2) Na
-chart_title " NiS Equilibrium "
-axis_titles " Na2S " " pH " " Amount "
#-axis_scale x_axis 0 14 1
#-axis_scale y_axis -25 0 -5
#-initial_solutions true
-start
10 graph_x RXN
20 graph_y -la("H+")
30 graph_sy EQUI("Millerite") EQUI("H2S(g)") tot("Ni") tot("S(-2)") tot("Na")
-end
REACTION 1
```

Na2S 1

0.08 moles per 100 steps

END

[α] The llnl database was used for it.

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