# SUPPORTING INFORMATION

## Rhodamine based turn-on dual mode chemosensor for the selective recognition of nickel ions: practical and theoretical applications

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**CONTENTS**



### 1. Characterization Data of the synthesized compound P1

**Synthesis of 3',6'-bis(diethylamino)-2-((2-(((E)-thiophen-2-ylmethylene)hydrazono)ethylidene)amino)spiro[isoindoline-1,9'-xanthen]-3-one (P1);** pure yellow product in 78% yield: m.p. 234-236 °C. $^{1}$H NMR (400 MHz, DMSO) δ 8.76 (s, 1H), 8.04 (d, *J* = 8.3 Hz, 1H), 7.95 (d, *J* = 7.7 Hz, 2H), 7.83 (d, *J* = 4.9 Hz, 1H), 7.62 (d, *J* = 7.4 Hz, 2H), 7.56 (s, 1H), 7.22 – 7.19 (m, 1H), 7.06 (d, *J* = 7.3 Hz, 1H), 6.43 (d, *J* = 8.9 Hz, 4H), 6.36 (d, *J* = 9.0 Hz, 2H),

3.31 (s, 7H), 1.08 (s, 11H). $^{13}$C NMR (100 MHz, DMSO) δ 164.91, 160.16, 152.57, 149.18, 145.20, 138.34, 135.27, 128.89, 127.89, 124.25, 123.89, 121.47, 118.91, 112.02, 108.72, 104.60, 97.84, 88.56, 44.14, 12.87. HRMS data: calculated mass $(M + H)^+$, 604.77; found, 604.77.

A $^1$H NMR titration experiment was conducted to investigate the binding relationship between P1 and $Ni^{2+}$ by adding 1 equivalent of $Ni^{2+}$ to P1 (Fig. **S3**). The introduction of $Ni^{2+}$ led to a downfield shift of aromatic proton signals, suggesting that the spirolactam ring of P1 opens upon coordination with $Ni^{2+}$ ions.

Supporting evidence for this interaction is supplied by the IR spectroscopy data (Fig. **S4** and **S5**). The distinctive carbonyl amide stretching frequency at 1692 $cm^{-1}$ in free P1 was shown to disappear in the P1-$Ni^{2+}$ complex, indicating the participation of the carbonyl oxygen in coordination with $Ni^{2+}$. The results clearly confirm the proposed ring-opening mechanism and validate the 1:1 binding stoichiometry between P1 and $Ni^{2+}$.

## 2. $^1$H and $^{13}$C Spectra of the synthesized compound P1

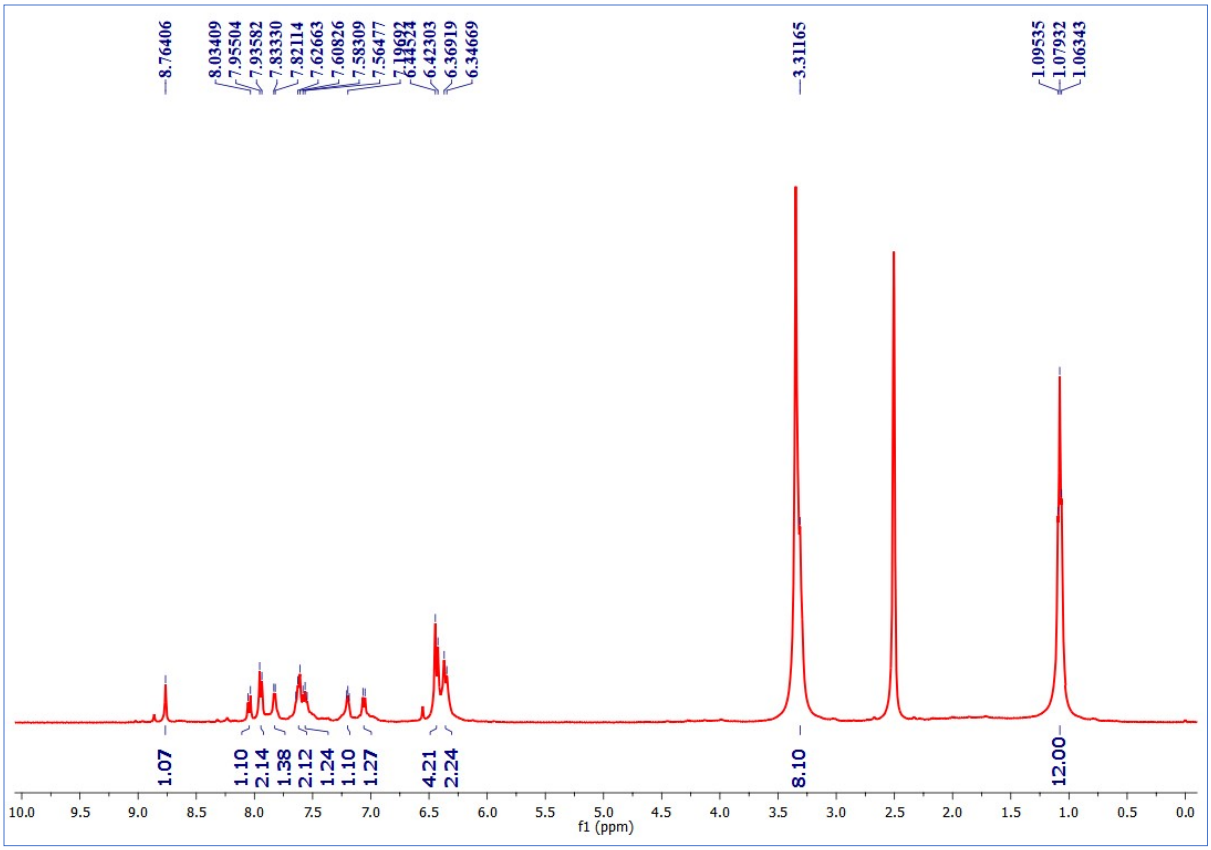



**Figure S1.** $^{1}$H NMR of chemosensor **P1** in DMSO 400MHz

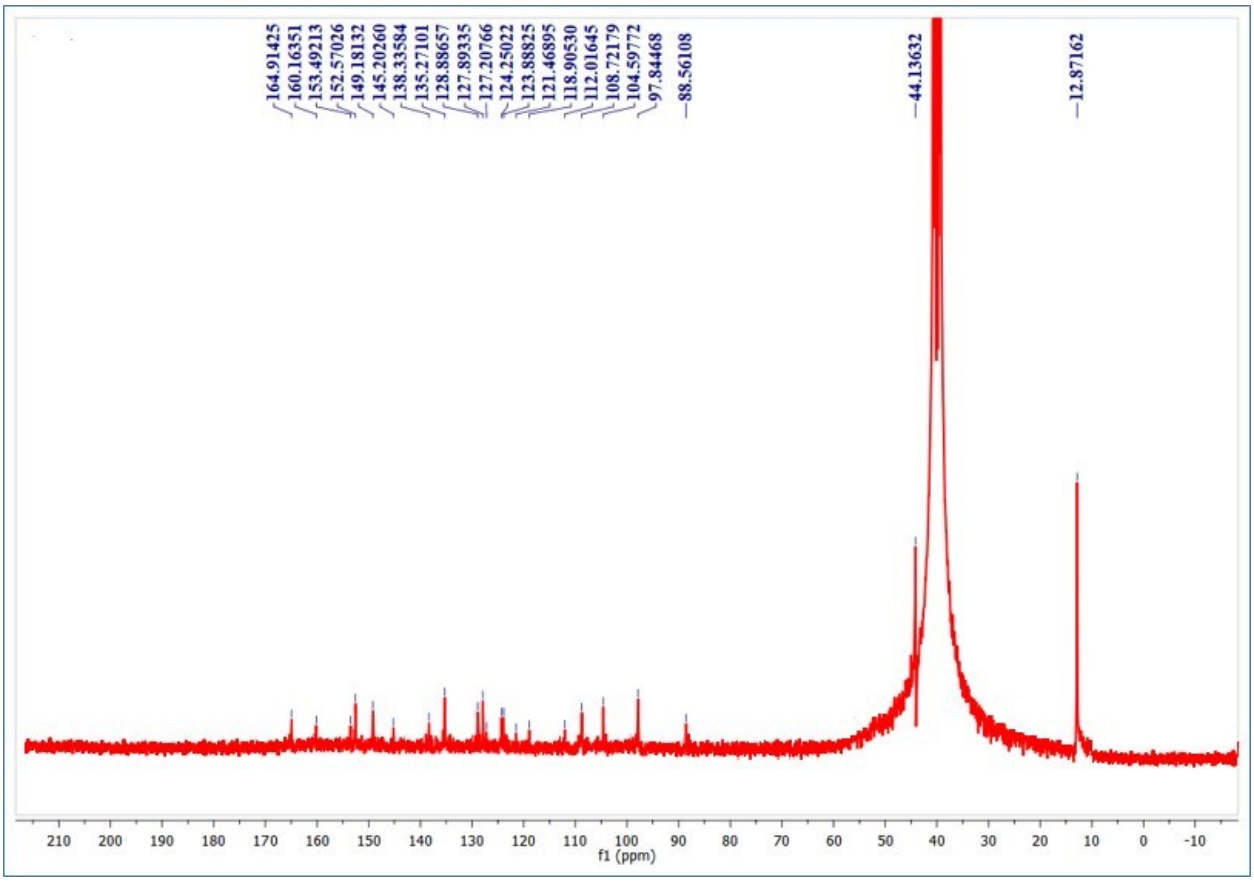



**Figure S2.** $^{13}C$ NMR of chemosensor **P1** in DMSO 100MHz

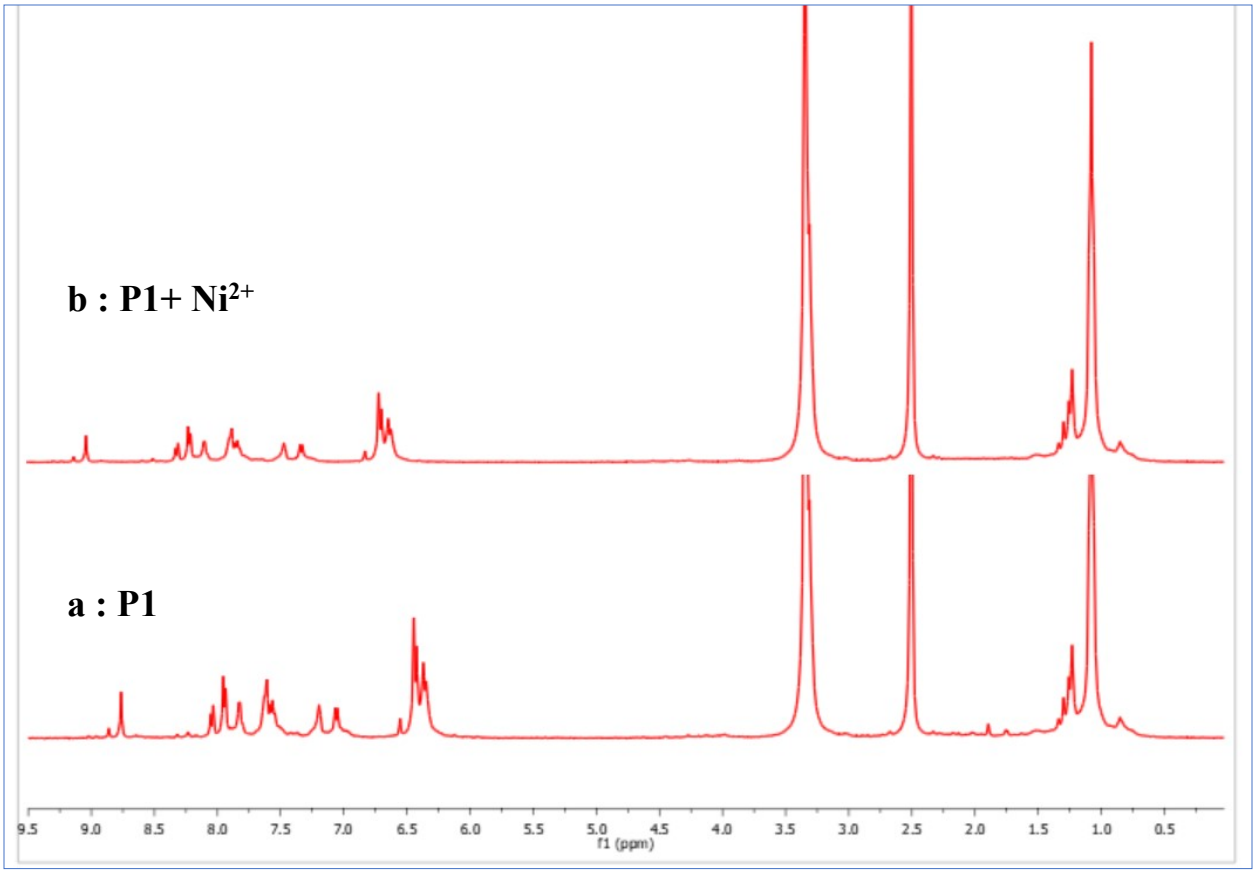



**Figure S3.** $^{1}$H NMR titration of chemosensor **P1** and **P1- $Ni^{2+}$** complex in DMSO 400MHz

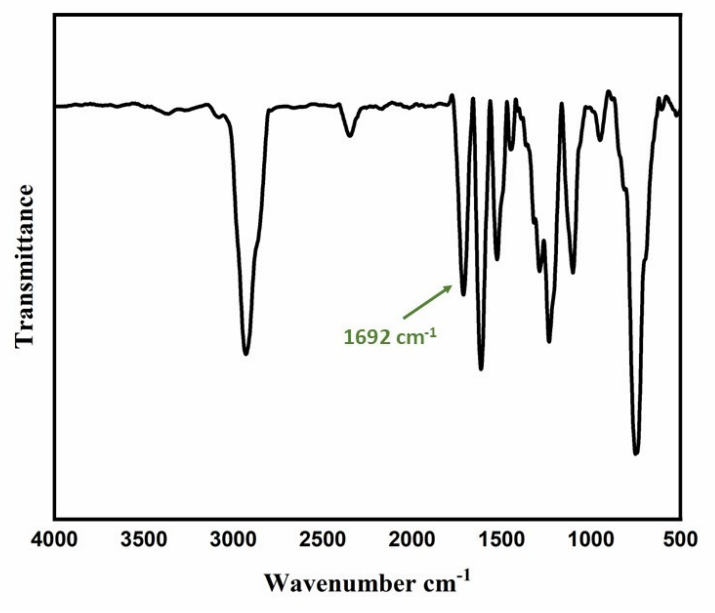



**Figure S4.** IR spectra of chemosensor **P1**

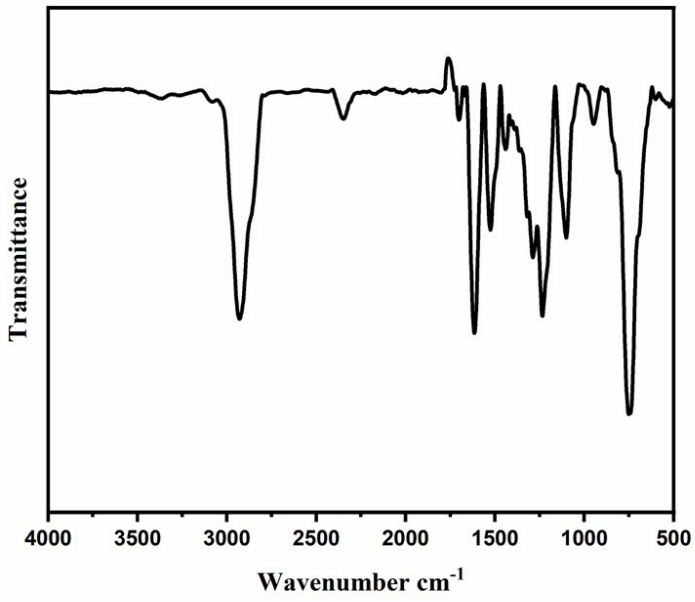
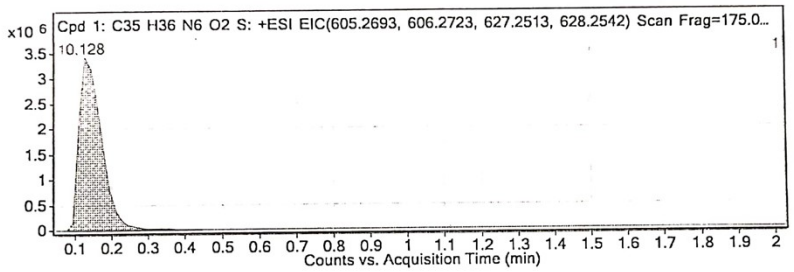



**Figure S5.** IR spectra of **P1- $Ni^{2+}$** complex

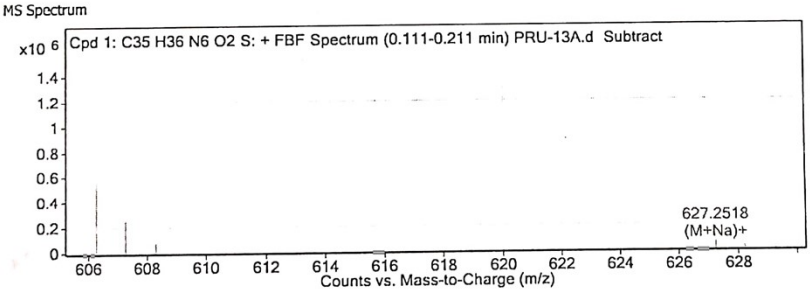
Compound Table

| Compound Label | RT | Mass | Abund | Formula | Tgt Mass | Diff (ppm) | MFG Formula | DB Formula |
|---|---|---|---|---|---|---|---|---|
| Cpd 1: C35 H36 N6 O2 S | 0.128 | 604.2638 | 1346666 | C35 H36 N6 O2 S | 604.262 | 2.97 | C35 H36 N6 O2 S | C35 H36 N6 O2 S |

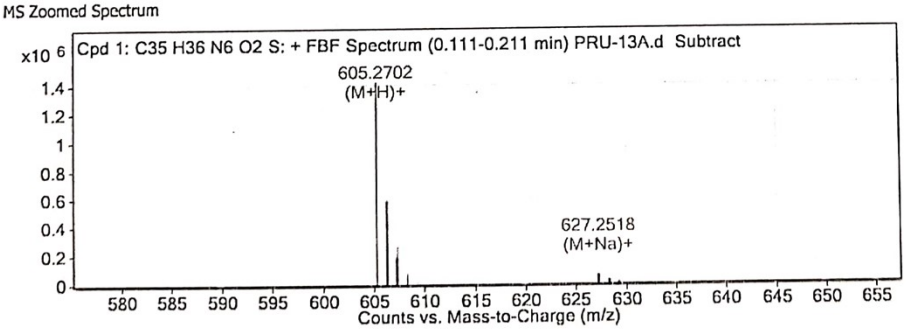
| Compound Label | m/z | RT | Algorithm | Mass |
|---|---|---|---|---|
| Cpd 1: C35 H36 N6 O2 S | 605.2702 | 0.128 | Find By Formula | 604.2638 |




MS Spectrum




MS Zoomed Spectrum




MS Spectrum Peak List

| m/z | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 605.2702 | 1 | 1346665.63 | C35H37N6O2S | (M+H)+ |
| 606.2731 | 1 | 561065.19 | C35H37N6O2S | (M+H)+ |
| 607.2781 | 1 | 264068.69 | C35H37N6O2S | (M+H)+ |
| 608.2818 | 1 | 72219.39 | C35H37N6O2S | (M+H)+ |
| 627.2518 | 1 | 52954.46 | C35H36N6NaO2S | (M+Na)+ |
| 628.2547 | 1 | 21726.07 | C35H36N6NaO2S | (M+Na)+ |
| 629.2605 | 1 | 11855.37 | C35H36N6NaO2S | (M+Na)+ |
| 630.2651 | 1 | 3973.69 | C35H36N6NaO2S | (M+Na)+ |

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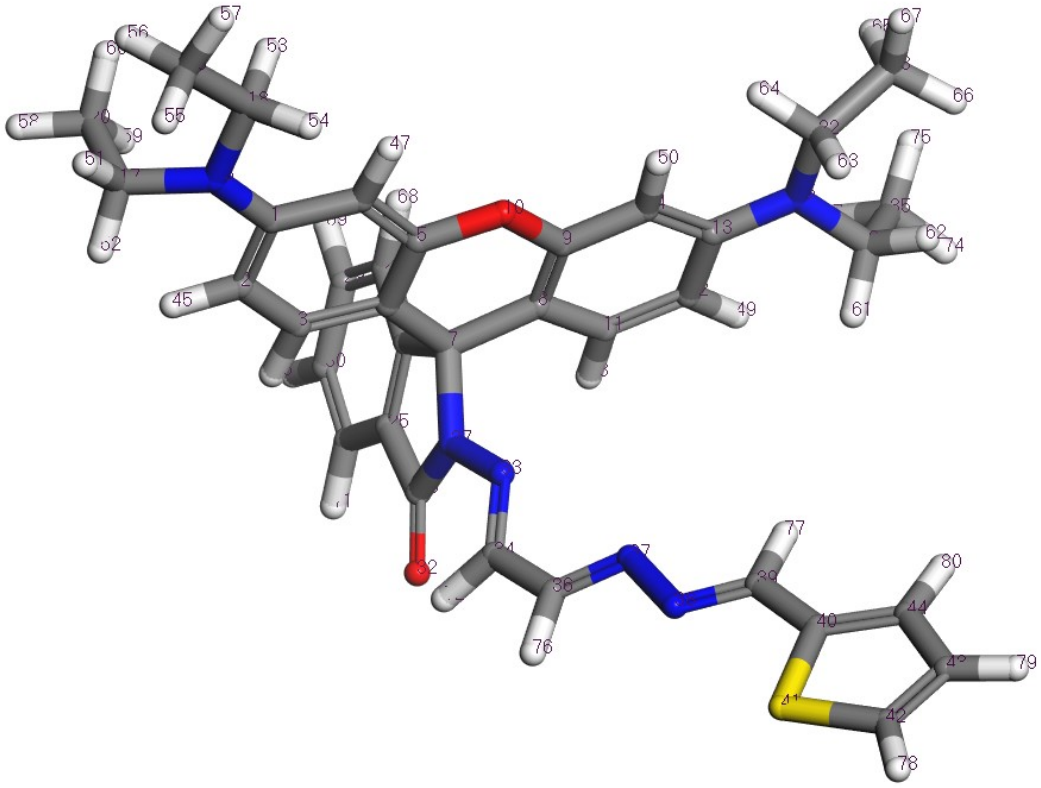
**Figure S6.** HRMS spectra of chemosensor **P1**

## 3. Density Functional Theory (DFT) Studies

### Coordinates

**P1**



Final Coordinates (Angstroms)

| | ATOM | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -3.936287 | 1.419972 | 1.430051 |
| 2 | C | -4.392917 | 0.420215 | 0.522890 |
| 3 | C | -3.522506 | -0.180828 | -0.370691 |
| 4 | C | -2.154699 | 0.142499 | -0.433816 |
| 5 | C | -1.706512 | 1.105155 | 0.473928 |
| 6 | C | -2.560679 | 1.738800 | 1.384101 |
| 7 | C | -1.241485 | -0.488131 | -1.465473 |
| 8 | C | 0.135504 | 0.126119 | -1.408626 |
| 9 | C | 0.494574 | 1.060106 | -0.430538 |
| 10 | O | -0.389895 | 1.530669 | 0.527388 |
| 11 | C | 1.145109 | -0.239460 | -2.317457 |
| 12 | C | 2.428853 | 0.282294 | -2.260046 |
| 13 | C | 2.789904 | 1.227433 | -1.256125 |

| | | | | |
|---|---|---|---|---|
| 14 | C | 1.781003 | 1.596803 | -0.338469 |
| 15 | N | 4.065824 | 1.764586 | -1.210606 |
| 16 | N | -4.802678 | 2.037630 | 2.324921 |
| 17 | C | -6.247223 | 1.997990 | 2.052601 |
| 18 | C | -4.281759 | 3.180428 | 3.098510 |
| 19 | C | -5.229804 | 3.717138 | 4.164011 |
| 20 | C | -6.693367 | 2.909629 | 0.905662 |
| 21 | C | 5.174341 | 1.048698 | -1.862427 |
| 22 | C | 4.417021 | 2.750096 | -0.180604 |
| 23 | C | 5.514082 | 3.727990 | -0.598830 |
| 24 | C | -1.871563 | -0.441204 | -2.849539 |
| 25 | C | -2.149306 | -1.726890 | -3.322938 |
| 26 | C | -1.691960 | -2.728709 | -2.344855 |
| 27 | N | -1.177147 | -1.998134 | -1.259715 |
| 28 | C | -2.204328 | 0.681119 | -3.602398 |
| 29 | C | -2.823552 | 0.483856 | -4.842682 |
| 30 | C | -3.111263 | -0.809982 | -5.314455 |
| 31 | C | -2.773196 | -1.933971 | -4.557529 |
| 32 | O | -1.706825 | -3.963548 | -2.442798 |
| 33 | N | -0.417879 | -2.444344 | -0.237207 |
| 34 | C | -0.535081 | -3.687283 | 0.149991 |
| 35 | C | 5.506206 | 1.544092 | -3.272554 |
| 36 | C | 0.364914 | -4.243736 | 1.139003 |
| 37 | N | 1.533212 | -3.728660 | 1.407209 |
| 38 | N | 2.218330 | -4.460874 | 2.362925 |
| 39 | C | 3.482939 | -4.137567 | 2.423422 |
| 40 | C | 4.382001 | -4.789462 | 3.326359 |
| 41 | S | 3.844318 | -6.009228 | 4.451267 |
| 42 | C | 5.440442 | -6.233732 | 5.045014 |
| 43 | C | 6.359228 | -5.415231 | 4.412074 |
| 44 | C | 5.757129 | -4.589676 | 3.433274 |
| 45 | H | -5.438208 | 0.122707 | 0.503949 |
| 46 | H | -3.920096 | -0.929296 | -1.059343 |
| 47 | H | -2.121693 | 2.499621 | 2.023957 |
| 48 | H | 0.908466 | -0.958725 | -3.104249 |
| 49 | H | 3.151814 | -0.031473 | -3.010464 |
| 50 | H | 1.968568 | 2.285194 | 0.480912 |
| 51 | H | -6.767069 | 2.272449 | 2.977797 |
| 52 | H | -6.538616 | 0.958638 | 1.855879 |
| 53 | H | -3.989837 | 4.001734 | 2.416047 |
| 54 | H | -3.360316 | 2.845383 | 3.595972 |
| 55 | H | -5.554238 | 2.927515 | 4.856647 |
| 56 | H | -6.120402 | 4.194889 | 3.733737 |
| 57 | H | -4.697035 | 4.480670 | 4.747506 |
| 58 | H | -7.782236 | 2.840190 | 0.767080 |
| 59 | H | -6.207920 | 2.624852 | -0.038610 |
| 60 | H | -6.442711 | 3.959516 | 1.116095 |
| 61 | H | 4.936099 | -0.024940 | -1.883963 |
| 62 | H | 6.058544 | 1.146840 | -1.215966 |
| 63 | H | 4.708722 | 2.238864 | 0.757179 |
| 64 | H | 3.517092 | 3.336609 | 0.039905 |
| 65 | H | 5.226329 | 4.288367 | -1.499586 |
| 66 | H | 6.474582 | 3.230715 | -0.789006 |
| 67 | H | 5.671605 | 4.445879 | 0.218234 |
| 68 | H | -1.990676 | 1.686313 | -3.237297 |
| 69 | H | -3.089019 | 1.347431 | -5.453636 |
| 70 | H | -3.602186 | -0.933796 | -6.280004 |
| 71 | H | -2.987538 | -2.944065 | -4.907622 |
| 72 | H | -1.299374 | -4.360186 | -0.242517 |
| 73 | H | 4.640656 | 1.451316 | -3.943240 |
| 74 | H | 6.331464 | 0.950228 | -3.693299 |
| 75 | H | 5.813286 | 2.598513 | -3.261220 |
| 76 | H | 0.052648 | -5.182072 | 1.616385 |
| 77 | H | 3.900365 | -3.370191 | 1.756683 |

| | | | | |
|---|---|---|---|---|
| 78 | H | 5.620456 | -6.954476 | 5.838678 |
| 79 | H | 7.420659 | -5.413294 | 4.650103 |
| 80 | H | 6.294790 | -3.874582 | 2.813049 |

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**DMol3/COSMO Results**

| cosmo energy | [Hartree atomic units] | [eV] | [kcal/mol] |
|---|---|---|---|
| Total energy | = -2230.749921 | | |
| Total energy + OC corr. | = -2230.749921 | | |
| Dielectric (solvation) energy | = -0.042734 | -1.163 | -26.82 |
| Diel. energy + OC corr. | = -0.042734 | -1.163 | -26.82 |

**Charge partitioning by Hirshfeld method: ( 0.00419)**

| | | | |
|---|---|---|---|
| C | 1 | charge | 0.0404 |
| C | 2 | charge | -0.0736 |
| C | 3 | charge | -0.0558 |
| C | 4 | charge | -0.0487 |
| C | 5 | charge | 0.0504 |
| C | 6 | charge | -0.0919 |
| C | 7 | charge | 0.0627 |
| C | 8 | charge | -0.0475 |
| C | 9 | charge | 0.0510 |
| O | 10 | charge | -0.1001 |
| C | 11 | charge | -0.0537 |
| C | 12 | charge | -0.0769 |
| C | 13 | charge | 0.0401 |
| C | 14 | charge | -0.0928 |
| N | 15 | charge | -0.0407 |
| N | 16 | charge | -0.0492 |
| C | 17 | charge | -0.0060 |
| C | 18 | charge | -0.0044 |
| C | 19 | charge | -0.0919 |
| C | 20 | charge | -0.1017 |
| C | 21 | charge | -0.0023 |
| C | 22 | charge | -0.0031 |
| C | 23 | charge | -0.0943 |
| C | 24 | charge | 0.0064 |
| C | 25 | charge | -0.0186 |
| C | 26 | charge | 0.1339 |
| N | 27 | charge | 0.0142 |
| C | 28 | charge | -0.0376 |
| C | 29 | charge | -0.0268 |
| C | 30 | charge | -0.0360 |
| C | 31 | charge | -0.0308 |
| O | 32 | charge | -0.3063 |
| N | 33 | charge | -0.1142 |
| C | 34 | charge | 0.0100 |
| C | 35 | charge | -0.1008 |
| C | 36 | charge | 0.0171 |
| N | 37 | charge | -0.1453 |
| N | 38 | charge | -0.1581 |
| C | 39 | charge | 0.0187 |
| C | 40 | charge | -0.0370 |
| S | 41 | charge | 0.1207 |
| C | 42 | charge | -0.0563 |
| C | 43 | charge | -0.0614 |
| C | 44 | charge | -0.0480 |
| H | 45 | charge | 0.0467 |
| H | 46 | charge | 0.0402 |
| H | 47 | charge | 0.0428 |
| H | 48 | charge | 0.0424 |
| H | 49 | charge | 0.0444 |

| | | | |
|---|---|---|---|
| H | 50 | charge | 0.0437 |
| H | 51 | charge | 0.0431 |
| H | 52 | charge | 0.0435 |
| H | 53 | charge | 0.0330 |
| H | 54 | charge | 0.0425 |
| H | 55 | charge | 0.0412 |
| H | 56 | charge | 0.0400 |
| H | 57 | charge | 0.0488 |
| H | 58 | charge | 0.0434 |
| H | 59 | charge | 0.0309 |
| H | 60 | charge | 0.0369 |
| H | 61 | charge | 0.0391 |
| H | 62 | charge | 0.0456 |
| H | 63 | charge | 0.0355 |
| H | 64 | charge | 0.0451 |
| H | 65 | charge | 0.0386 |
| H | 66 | charge | 0.0389 |
| H | 67 | charge | 0.0470 |
| H | 68 | charge | 0.0548 |
| H | 69 | charge | 0.0609 |
| H | 70 | charge | 0.0595 |
| H | 71 | charge | 0.0571 |
| H | 72 | charge | 0.0446 |
| H | 73 | charge | 0.0351 |
| H | 74 | charge | 0.0430 |
| H | 75 | charge | 0.0352 |
| H | 76 | charge | 0.0490 |
| H | 77 | charge | 0.0550 |
| H | 78 | charge | 0.0721 |
| H | 79 | charge | 0.0657 |
| H | 80 | charge | 0.0679 |

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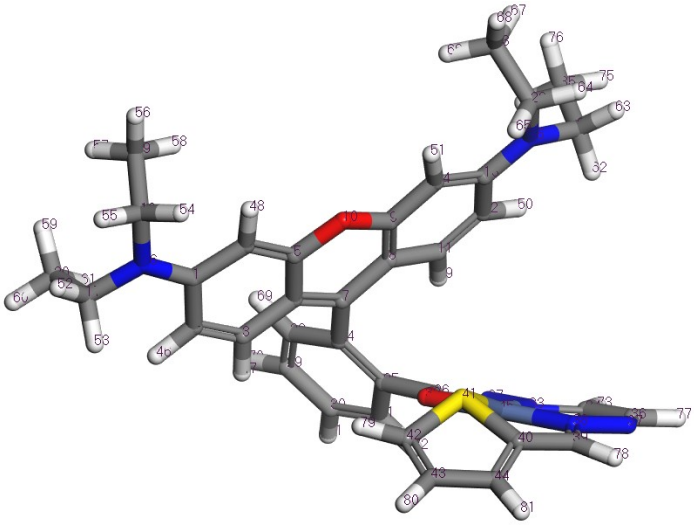
**P1-$Ni^{2+}$ complex (singlet)**



Final Coordinates (Angstroms)

| | ATOM | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -4.154427 | 0.083670 | 1.365438 |

| | | | | |
|---|---|---|---|---|
| 2 | C | -4.122776 | -1.000397 | 0.422463 |
| 3 | C | -3.028921 | -1.215567 | -0.377867 |
| 4 | C | -1.875472 | -0.375339 | -0.323836 |
| 5 | C | -1.872150 | 0.593642 | 0.721990 |
| 6 | C | -2.957607 | 0.826587 | 1.542154 |
| 7 | C | -0.801466 | -0.413430 | -1.243448 |
| 8 | C | 0.265555 | 0.504233 | -1.074690 |
| 9 | C | 0.278259 | 1.361806 | 0.065644 |
| 10 | O | -0.768949 | 1.374961 | 0.951678 |
| 11 | C | 1.352322 | 0.674338 | -1.980454 |
| 12 | C | 2.371318 | 1.564334 | -1.743577 |
| 13 | C | 2.398795 | 2.369333 | -0.552305 |
| 14 | C | 1.301889 | 2.247523 | 0.341019 |
| 15 | N | 3.425050 | 3.224044 | -0.300194 |
| 16 | N | -5.283867 | 0.388801 | 2.055416 |
| 17 | C | -6.552447 | -0.320084 | 1.802543 |
| 18 | C | -5.327963 | 1.554863 | 2.957106 |
| 19 | C | -5.450006 | 2.899458 | 2.233341 |
| 20 | C | -7.270549 | 0.128429 | 0.526586 |
| 21 | C | 4.505477 | 3.443729 | -1.279058 |
| 22 | C | 3.453614 | 4.035908 | 0.929235 |
| 23 | C | 2.630014 | 5.324739 | 0.858944 |
| 24 | C | -0.863768 | -1.312733 | -2.424423 |
| 25 | C | 0.137823 | -2.263144 | -2.744749 |
| 26 | C | 1.287958 | -2.518767 | -1.852449 |
| 27 | N | 2.493278 | -2.652546 | -2.398377 |
| 28 | C | -1.943337 | -1.152507 | -3.311079 |
| 29 | C | -2.040707 | -1.907671 | -4.481803 |
| 30 | C | -1.045555 | -2.837857 | -4.795384 |
| 31 | C | 0.038852 | -3.007132 | -3.933879 |
| 32 | O | 1.094391 | -2.589930 | -0.560263 |
| 33 | N | 3.411507 | -2.821530 | -1.406046 |
| 34 | C | 4.684395 | -2.877952 | -1.720794 |
| 35 | C | 4.129485 | 4.401945 | -2.411586 |
| 36 | C | 5.720824 | -3.048088 | -0.753269 |
| 37 | N | 5.629603 | -3.214389 | 0.542729 |
| 38 | N | 4.399930 | -3.199708 | 1.118664 |
| 39 | C | 4.398968 | -3.589799 | 2.394386 |
| 40 | C | 3.165627 | -3.580525 | 3.082023 |
| 41 | S | 1.906030 | -2.595527 | 2.347326 |
| 42 | C | 0.661386 | -3.516851 | 3.140549 |
| 43 | C | 1.209778 | -4.393196 | 4.049175 |
| 44 | C | 2.631916 | -4.447653 | 4.017410 |
| 45 | Ni | 2.729453 | -2.880525 | 0.304630 |
| 46 | H | -4.979900 | -1.660762 | 0.317877 |
| 47 | H | -3.049131 | -2.037117 | -1.092579 |
| 48 | H | -2.872854 | 1.617180 | 2.283144 |
| 49 | H | 1.370698 | 0.094581 | -2.902987 |
| 50 | H | 3.161269 | 1.653962 | -2.484905 |
| 51 | H | 1.211645 | 2.859800 | 1.234279 |
| 52 | H | -7.188013 | -0.140367 | 2.678594 |
| 53 | H | -6.356674 | -1.401364 | 1.778924 |
| 54 | H | -4.432966 | 1.537186 | 3.596374 |
| 55 | H | -6.187618 | 1.403092 | 3.621749 |
| 56 | H | -5.448472 | 3.710357 | 2.975981 |
| 57 | H | -6.384823 | 2.961604 | 1.659358 |
| 58 | H | -4.610068 | 3.067240 | 1.544227 |
| 59 | H | -7.539523 | 1.192781 | 0.570059 |
| 60 | H | -8.196056 | -0.453975 | 0.409896 |
| 61 | H | -6.648279 | -0.036010 | -0.364421 |
| 62 | H | 4.826147 | 2.472087 | -1.680757 |
| 63 | H | 5.358484 | 3.842145 | -0.714458 |
| 64 | H | 4.507746 | 4.275216 | 1.120478 |
| 65 | H | 3.118475 | 3.406727 | 1.766415 |

| | | | | |
|---|---|---|---|---|
| 66 | H | 1.571660 | 5.121010 | 0.643552 |
| 67 | H | 3.014436 | 6.006062 | 0.088043 |
| 68 | H | 2.687450 | 5.839486 | 1.829571 |
| 69 | H | -2.701483 | -0.400075 | -3.089133 |
| 70 | H | -2.891039 | -1.758588 | -5.148693 |
| 71 | H | -1.113749 | -3.433331 | -5.706962 |
| 72 | H | 0.814417 | -3.737757 | -4.165244 |
| 73 | H | 4.956059 | -2.792495 | -2.774450 |
| 74 | H | 3.282459 | 4.019471 | -2.999930 |
| 75 | H | 4.989437 | 4.522000 | -3.086782 |
| 76 | H | 3.859013 | 5.392981 | -2.022430 |
| 77 | H | 6.741754 | -3.064852 | -1.136761 |
| 78 | H | 5.326131 | -3.953694 | 2.840997 |
| 79 | H | -0.382495 | -3.245978 | 3.001514 |
| 80 | H | 0.599388 | -4.990476 | 4.725078 |
| 81 | H | 3.232948 | -5.157624 | 4.583466 |

## DMol3/COSMO Results

| cosmo energy | [Hartree atomic units] | [eV] | [kcal/mol] |
|---|---|---|---|
| Total energy | = | -2424.027514 | |
| Total energy + OC corr. | = | -2424.027514 | |
| Dielectric (solvation) energy | = -0.181222 | -4.931 | -113.72 |
| Diel. energy + OC corr. | = -0.181222 | -4.931 | -113.72 |

**Charge partitioning by Hirshfeld method: ( 2.0016 0.0000)**

| | | | | |
|---|---|---|---|---|
| C | 1 | charge | 0.0740 | -0.0000 |
| C | 2 | charge | -0.0395 | -0.0000 |
| C | 3 | charge | -0.0241 | -0.0000 |
| C | 4 | charge | -0.0143 | 0.0000 |
| C | 5 | charge | 0.0840 | 0.0000 |
| C | 6 | charge | -0.0675 | -0.0000 |
| C | 7 | charge | 0.0396 | 0.0000 |
| C | 8 | charge | -0.0182 | -0.0000 |
| C | 9 | charge | 0.0827 | 0.0000 |
| O | 10 | charge | -0.0476 | -0.0000 |
| C | 11 | charge | -0.0316 | -0.0000 |
| C | 12 | charge | -0.0406 | -0.0000 |
| C | 13 | charge | 0.0720 | -0.0000 |
| C | 14 | charge | -0.0691 | -0.0000 |
| N | 15 | charge | 0.0084 | -0.0000 |
| N | 16 | charge | 0.0094 | 0.0000 |
| C | 17 | charge | 0.0040 | 0.0000 |
| C | 18 | charge | 0.0039 | 0.0000 |
| C | 19 | charge | -0.0989 | 0.0000 |
| C | 20 | charge | -0.0990 | 0.0000 |
| C | 21 | charge | 0.0036 | 0.0000 |
| C | 22 | charge | 0.0033 | -0.0000 |
| C | 23 | charge | -0.0982 | 0.0000 |
| C | 24 | charge | 0.0127 | 0.0000 |
| C | 25 | charge | -0.0011 | -0.0000 |
| C | 26 | charge | 0.1285 | 0.0000 |
| N | 27 | charge | -0.1420 | 0.0000 |
| C | 28 | charge | -0.0248 | -0.0000 |
| C | 29 | charge | -0.0205 | 0.0000 |
| C | 30 | charge | -0.0242 | 0.0000 |
| C | 31 | charge | -0.0278 | -0.0000 |
| O | 32 | charge | -0.1852 | -0.0000 |
| N | 33 | charge | 0.0183 | -0.0000 |

| | | | | | |
|---|---|---|---|---|---|
| C | 34 | charge | spin | 0.0462 | -0.0000 |
| C | 35 | charge | spin | -0.0990 | -0.0000 |
| C | 36 | charge | spin | 0.0413 | 0.0000 |
| N | 37 | charge | spin | -0.0877 | 0.0000 |
| N | 38 | charge | spin | -0.0003 | 0.0000 |
| C | 39 | charge | spin | 0.0808 | 0.0000 |
| C | 40 | charge | spin | -0.0052 | 0.0000 |
| S | 41 | charge | spin | 0.2554 | 0.0000 |
| C | 42 | charge | spin | -0.0113 | 0.0000 |
| C | 43 | charge | spin | -0.0067 | 0.0000 |
| C | 44 | charge | spin | 0.0079 | 0.0000 |
| Ni | 45 | charge | spin | 0.0975 | -0.0000 |
| H | 46 | charge | spin | 0.0648 | 0.0000 |
| H | 47 | charge | spin | 0.0585 | -0.0000 |
| H | 48 | charge | spin | 0.0622 | -0.0000 |
| H | 49 | charge | spin | 0.0505 | 0.0000 |
| H | 50 | charge | spin | 0.0641 | -0.0000 |
| H | 51 | charge | spin | 0.0613 | 0.0000 |
| H | 52 | charge | spin | 0.0618 | 0.0000 |
| H | 53 | charge | spin | 0.0562 | -0.0000 |
| H | 54 | charge | spin | 0.0559 | 0.0000 |
| H | 55 | charge | spin | 0.0621 | -0.0000 |
| H | 56 | charge | spin | 0.0542 | 0.0000 |
| H | 57 | charge | spin | 0.0450 | 0.0000 |
| H | 58 | charge | spin | 0.0395 | 0.0000 |
| H | 59 | charge | spin | 0.0450 | -0.0000 |
| H | 60 | charge | spin | 0.0542 | 0.0000 |
| H | 61 | charge | spin | 0.0396 | -0.0000 |
| H | 62 | charge | spin | 0.0552 | -0.0000 |
| H | 63 | charge | spin | 0.0614 | 0.0000 |
| H | 64 | charge | spin | 0.0613 | -0.0000 |
| H | 65 | charge | spin | 0.0543 | -0.0000 |
| H | 66 | charge | spin | 0.0413 | -0.0000 |
| H | 67 | charge | spin | 0.0453 | -0.0000 |
| H | 68 | charge | spin | 0.0544 | 0.0000 |
| H | 69 | charge | spin | 0.0602 | 0.0000 |
| H | 70 | charge | spin | 0.0703 | -0.0000 |
| H | 71 | charge | spin | 0.0695 | -0.0000 |
| H | 72 | charge | spin | 0.0579 | -0.0000 |
| H | 73 | charge | spin | 0.0918 | -0.0000 |
| H | 74 | charge | spin | 0.0411 | 0.0000 |
| H | 75 | charge | spin | 0.0540 | 0.0000 |
| H | 76 | charge | spin | 0.0444 | 0.0000 |
| H | 77 | charge | spin | 0.0885 | 0.0000 |
| H | 78 | charge | spin | 0.1015 | -0.0000 |
| H | 79 | charge | spin | 0.0949 | -0.0000 |
| H | 80 | charge | spin | 0.0940 | 0.0000 |
| H | 81 | charge | spin | 0.0983 | 0.0000 |

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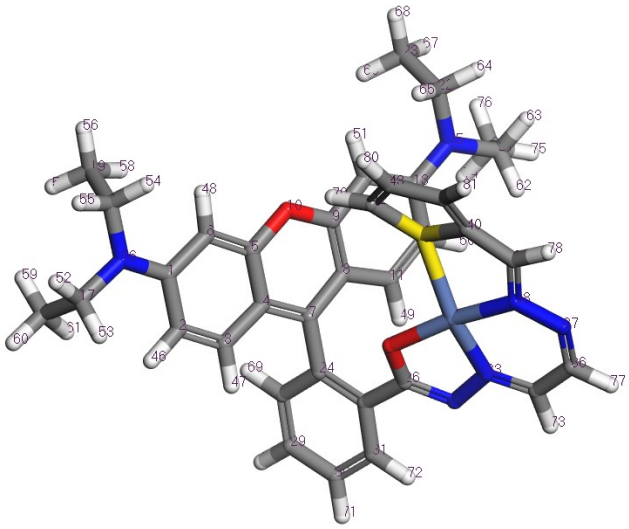
**P1-$Ni^{2+}$ complex (triplet)**



Final Coordinates (Angstroms)

| | ATOM | X | Y | Z |
|---|---|---|---|---|
| 1 | C | -4.179804 | -0.168847 | 1.187979 |
| 2 | C | -4.217120 | -1.017116 | 0.025724 |
| 3 | C | -3.162832 | -1.066414 | -0.849575 |
| 4 | C | -1.988002 | -0.278010 | -0.665329 |
| 5 | C | -1.951150 | 0.516324 | 0.521594 |
| 6 | C | -2.989769 | 0.570058 | 1.427525 |
| 7 | C | -0.892847 | -0.252052 | -1.559863 |
| 8 | C | 0.210953 | 0.581220 | -1.247618 |
| 9 | C | 0.223853 | 1.305664 | -0.019757 |
| 10 | O | -0.845284 | 1.263326 | 0.837614 |
| 11 | C | 1.354112 | 0.746384 | -2.081786 |
| 12 | C | 2.435417 | 1.494179 | -1.690739 |
| 13 | C | 2.458863 | 2.160110 | -0.417084 |
| 14 | C | 1.293231 | 2.074725 | 0.393117 |
| 15 | N | 3.554994 | 2.847822 | -0.005087 |
| 16 | N | -5.241350 | -0.079166 | 2.028137 |
| 17 | C | -6.503057 | -0.798077 | 1.763945 |
| 18 | C | -5.208466 | 0.819094 | 3.198841 |
| 19 | C | -5.433780 | 2.294473 | 2.855993 |
| 20 | C | -7.405239 | -0.096689 | 0.744792 |
| 21 | C | 4.766458 | 2.947598 | -0.841681 |
| 22 | C | 3.578381 | 3.544323 | 1.294140 |
| 23 | C | 2.979713 | 4.952550 | 1.248612 |
| 24 | C | -0.943075 | -1.019571 | -2.830080 |
| 25 | C | -0.034103 | -2.059694 | -3.154832 |
| 26 | C | 0.998495 | -2.519729 | -2.203254 |
| 27 | N | 2.102335 | -3.085861 | -2.708523 |
| 28 | C | -1.913322 | -0.643867 | -3.775150 |
| 29 | C | -1.992684 | -1.274530 | -5.018854 |
| 30 | C | -1.096759 | -2.299323 | -5.337875 |
| 31 | C | -0.124516 | -2.681479 | -4.414604 |
| 32 | O | 0.814448 | -2.352367 | -0.922512 |
| 33 | N | 2.987212 | -3.318113 | -1.708712 |
| 34 | C | 4.080941 | -4.012013 | -1.968406 |
| 35 | C | 4.698015 | 4.042978 | -1.907642 |
| 36 | C | 5.018542 | -4.377791 | -0.964305 |
| 37 | N | 5.014714 | -4.169497 | 0.339679 |
| 38 | N | 3.995838 | -3.467269 | 0.893558 |
| 39 | C | 4.152895 | -3.245831 | 2.208647 |
| 40 | C | 3.204257 | -2.456926 | 2.881002 |

| | | | | |
|---|---|---|---|---|
| 41 | S | 2.166524 | -1.461288 | 1.867357 |
| 42 | C | 1.064928 | -1.183413 | 3.172129 |
| 43 | C | 1.546407 | -1.731734 | 4.349500 |
| 44 | C | 2.756658 | -2.443802 | 4.201664 |
| 45 | Ni | 2.435790 | -2.773861 | 0.017115 |
| 46 | H | -5.087236 | -1.637486 | -0.171800 |
| 47 | H | -3.220784 | -1.730033 | -1.711054 |
| 48 | H | -2.866868 | 1.205960 | 2.299839 |
| 49 | H | 1.369915 | 0.266293 | -3.059650 |
| 50 | H | 3.279607 | 1.577364 | -2.369504 |
| 51 | H | 1.204961 | 2.597968 | 1.341285 |
| 52 | H | -7.016621 | -0.885194 | 2.728800 |
| 53 | H | -6.263574 | -1.818926 | 1.438870 |
| 54 | H | -4.248117 | 0.676976 | 3.714123 |
| 55 | H | -5.988586 | 0.466336 | 3.883093 |
| 56 | H | -5.375604 | 2.885689 | 3.781371 |
| 57 | H | -6.424529 | 2.453479 | 2.408651 |
| 58 | H | -4.674207 | 2.673203 | 2.158906 |
| 59 | H | -7.686582 | 0.908933 | 1.084610 |
| 60 | H | -8.324850 | -0.686051 | 0.621029 |
| 61 | H | -6.916599 | -0.009783 | -0.235838 |
| 62 | H | 4.956196 | 1.966565 | -1.298959 |
| 63 | H | 5.599672 | 3.142736 | -0.155004 |
| 64 | H | 4.629227 | 3.587274 | 1.606247 |
| 65 | H | 3.057488 | 2.919980 | 2.032432 |
| 66 | H | 1.938005 | 4.941173 | 0.898389 |
| 67 | H | 3.558888 | 5.610479 | 0.587985 |
| 68 | H | 2.995840 | 5.378191 | 2.262144 |
| 69 | H | -2.598172 | 0.171808 | -3.538910 |
| 70 | H | -2.752688 | -0.958782 | -5.734227 |
| 71 | H | -1.152547 | -2.803470 | -6.303575 |
| 72 | H | 0.570091 | -3.487729 | -4.648531 |
| 73 | H | 4.244076 | -4.363776 | -2.990857 |
| 74 | H | 3.859316 | 3.883532 | -2.599966 |
| 75 | H | 5.632302 | 4.027452 | -2.488555 |
| 76 | H | 4.590499 | 5.037981 | -1.454882 |
| 77 | H | 5.866761 | -4.974968 | -1.305832 |
| 78 | H | 4.996754 | -3.709623 | 2.722532 |
| 79 | H | 0.191722 | -0.552426 | 3.026347 |
| 80 | H | 1.030328 | -1.603651 | 5.299883 |
| 81 | H | 3.255102 | -2.983973 | 5.005212 |

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## DMol3/COSMO Results

| cosmo energy | [Hartree atomic units] | [eV] | [kcal/mol] |
|---|---|---|---|
| Total energy | = -2424.004268 | | |
| Total energy + OC corr. | = -2424.004268 | | |
| Dielectric (solvation) energy | = -0.185840 | -5.057 | -116.62 |
| Diel. energy + OC corr. | = -0.185840 | -5.057 | -116.62 |

**Charge partitioning by Hirshfeld method: ( 2.0016 2.0000)**

| | | | | |
|---|---|---|---|---|
| C | 1 charge | spin | 0.0829 | 0.0108 |
| C | 2 charge | spin | -0.0253 | 0.0376 |
| C | 3 charge | spin | -0.0152 | -0.0033 |
| C | 4 charge | spin | 0.0010 | 0.0469 |
| C | 5 charge | spin | 0.0916 | -0.0002 |
| C | 6 charge | spin | -0.0524 | 0.0324 |
| C | 7 charge | spin | 0.0506 | -0.0043 |
| C | 8 charge | spin | -0.0030 | 0.0522 |
| C | 9 charge | spin | 0.0867 | 0.0007 |

| | | | | | |
|---|---|---|---|---|---|
| O | 10 | charge | spin | -0.0394 | -0.0031 |
| C | 11 | charge | spin | -0.0202 | -0.0026 |
| C | 12 | charge | spin | -0.0258 | 0.0409 |
| C | 13 | charge | spin | 0.0792 | 0.0119 |
| C | 14 | charge | spin | -0.0576 | 0.0339 |
| N | 15 | charge | spin | 0.0314 | 0.1068 |
| N | 16 | charge | spin | 0.0323 | 0.1002 |
| C | 17 | charge | spin | 0.0088 | 0.0066 |
| C | 18 | charge | spin | 0.0085 | 0.0065 |
| C | 19 | charge | spin | -0.0948 | 0.0083 |
| C | 20 | charge | spin | -0.0946 | 0.0085 |
| C | 21 | charge | spin | 0.0083 | 0.0069 |
| C | 22 | charge | spin | 0.0080 | 0.0069 |
| C | 23 | charge | spin | -0.0941 | 0.0090 |
| C | 24 | charge | spin | 0.0111 | 0.0064 |
| C | 25 | charge | spin | -0.0015 | 0.0032 |
| C | 26 | charge | spin | 0.1176 | 0.0258 |
| N | 27 | charge | spin | -0.1481 | 0.0232 |
| C | 28 | charge | spin | -0.0253 | -0.0005 |
| C | 29 | charge | spin | -0.0198 | 0.0093 |
| C | 30 | charge | spin | -0.0246 | -0.0008 |
| C | 31 | charge | spin | -0.0279 | 0.0080 |
| O | 32 | charge | spin | -0.2012 | 0.0449 |
| N | 33 | charge | spin | -0.0053 | 0.0887 |
| C | 34 | charge | spin | 0.0284 | 0.0279 |
| C | 35 | charge | spin | -0.0944 | 0.0088 |
| C | 36 | charge | spin | 0.0188 | 0.0299 |
| N | 37 | charge | spin | -0.1083 | 0.0247 |
| N | 38 | charge | spin | -0.0194 | 0.0367 |
| C | 39 | charge | spin | 0.0516 | 0.0739 |
| C | 40 | charge | spin | -0.0163 | 0.0145 |
| S | 41 | charge | spin | 0.2079 | 0.0304 |
| C | 42 | charge | spin | -0.0375 | 0.0816 |
| C | 43 | charge | spin | -0.0276 | 0.0148 |
| C | 44 | charge | spin | -0.0192 | 0.0786 |
| Ni | 45 | charge | spin | 0.1276 | 0.7908 |
| H | 46 | charge | spin | 0.0709 | 0.0022 |
| H | 47 | charge | spin | 0.0632 | -0.0003 |
| H | 48 | charge | spin | 0.0690 | 0.0019 |
| H | 49 | charge | spin | 0.0594 | -0.0001 |
| H | 50 | charge | spin | 0.0706 | 0.0024 |
| H | 51 | charge | spin | 0.0682 | 0.0021 |
| H | 52 | charge | spin | 0.0666 | 0.0017 |
| H | 53 | charge | spin | 0.0615 | 0.0033 |
| H | 54 | charge | spin | 0.0609 | 0.0038 |
| H | 55 | charge | spin | 0.0668 | 0.0013 |
| H | 56 | charge | spin | 0.0582 | 0.0010 |
| H | 57 | charge | spin | 0.0478 | 0.0003 |
| H | 58 | charge | spin | 0.0425 | 0.0006 |
| H | 59 | charge | spin | 0.0476 | 0.0003 |
| H | 60 | charge | spin | 0.0582 | 0.0010 |
| H | 61 | charge | spin | 0.0435 | 0.0007 |
| H | 62 | charge | spin | 0.0604 | 0.0037 |
| H | 63 | charge | spin | 0.0667 | 0.0017 |
| H | 64 | charge | spin | 0.0665 | 0.0020 |
| H | 65 | charge | spin | 0.0584 | 0.0033 |
| H | 66 | charge | spin | 0.0444 | 0.0006 |
| H | 67 | charge | spin | 0.0481 | 0.0003 |
| H | 68 | charge | spin | 0.0583 | 0.0012 |
| H | 69 | charge | spin | 0.0618 | 0.0001 |
| H | 70 | charge | spin | 0.0704 | 0.0006 |
| H | 71 | charge | spin | 0.0691 | -0.0001 |
| H | 72 | charge | spin | 0.0525 | 0.0010 |
| H | 73 | charge | spin | 0.0791 | 0.0065 |

| | | | | | |
|---|---|---|---|---|---|
| H | 74 | charge | spin | 0.0444 | 0.0006 |
| H | 75 | charge | spin | 0.0583 | 0.0011 |
| H | 76 | charge | spin | 0.0478 | 0.0003 |
| H | 77 | charge | spin | 0.0764 | 0.0024 |
| H | 78 | charge | spin | 0.0879 | 0.0051 |
| H | 79 | charge | spin | 0.0720 | 0.0057 |
| H | 80 | charge | spin | 0.0847 | 0.0017 |
| H | 81 | charge | spin | 0.0872 | 0.0052 |

*****