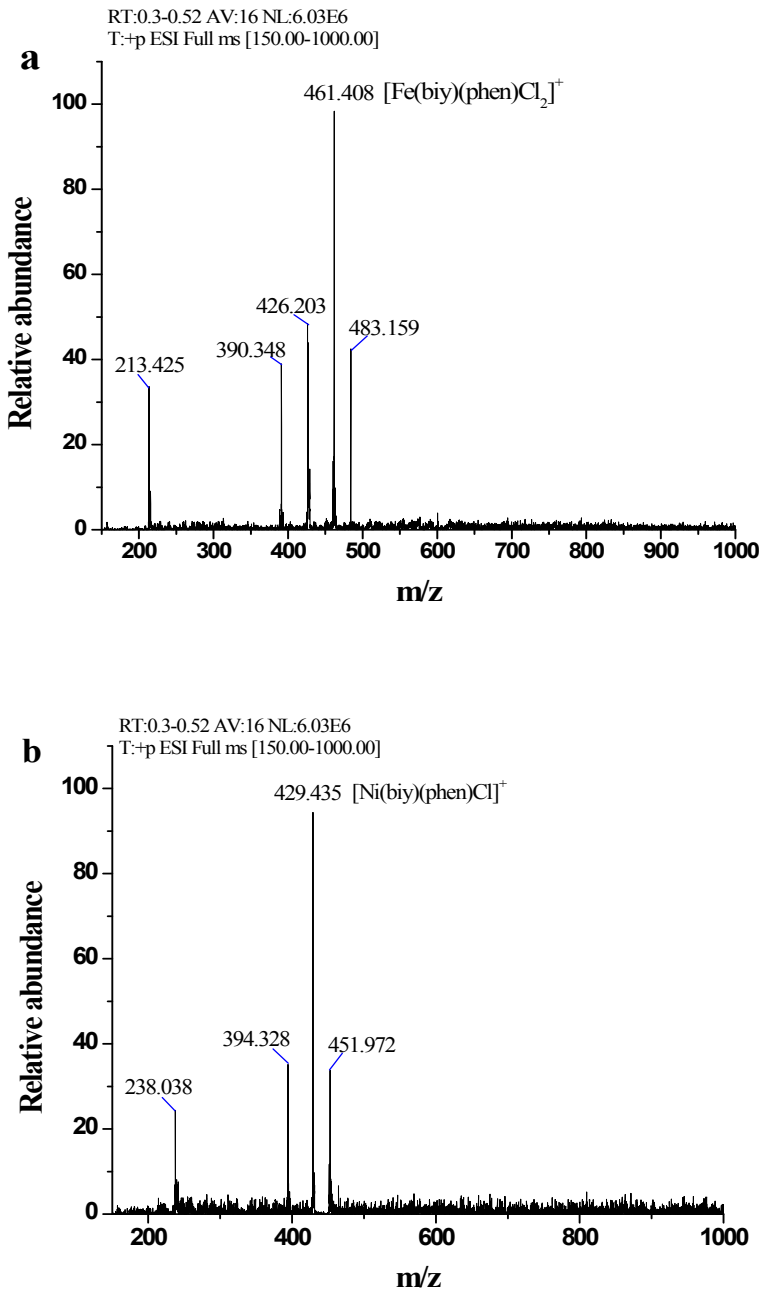



**Fig. S1.** ESI-MS for (a) $[Fe(bipy)(phen)Cl_2]^+$ & (b) $[Ni(bipy)(phen)Cl]^+$ complex

**Encapsulation and characterization of (2,2-bipy) or (1,10-Phen) iron(III) and nickel(II) complex in zeolite-Y**

To easily compare mixed bipy-phen liganded complex with simple bipy or phen ligand complexes encapsulated into the zeolite supper cage the same experimental procedure were used for both cases with exception of refluxing time and amount of ligand used. Besides, 1:2 mmol of metal to ligand ratio was used in the synthesis of the simple bipy or phen metal complexes with aiming to form the central metal attached to four nitrogen (i.e. to synthesis similar complexes with mixed ligands cases). The amount of bipy and phen used for encapsulation work is depends on the content of the metal ions in the metal exchanged zeolite (i.e. $Fe^{3+}$-Y and $Ni^{2+}$-Y).

1 g of the corresponding metal exchanged zeolite (i.e. iron(III) and nickel(II) exchanged zeolite) and 2 mmol of simple ligands (i.e.1,10-Phenanthroline or 2,2'-bipyridine) was dissolved in 50 mL of methanol and refluxed under constant stirring for 24 h at constant temperature of 150 $^{o}$C in oil bath. Subsequently the solution was kept for two consecutive days for proper formation of complexes in the zeolite supercage. Then the solid product was subjected to Soxhlet extraction for removing surface adsorbed ligands and metal complexes. The extraction was done with acetonitrile, dichloromethane and diethyl ether till the washings were colorless. Finally, any uncomplexed metal ions, remaining in surface or inside the zeolite cage after complex formation, was removed by back exchanged process by stirring zeolite encapsulated metal complex with 0.01 M of NaCl solution for 3 h. Then the solid product was washed with hot water to remove the chloride ion and dried at 100 $^{o}$C overnight.

Then to accurately differentiate the simple vs mixed liganded complexes metal and CHN analysis were used to characterize the synthesized simple bipy and phen-iron (III) and nickel (II) complexes.

**Table S1**

Physical and chemical analytical composition (molar ratio) of metal complex encapsulated into the zeolite superacge

| Sample | Color of the catalyst | Elemental Analysis | | | |
|---|---|---|---|---|---|
| | | Metal % | C % | N % | C/N |
| $[Fe(bipy)(phen)Cl_2]^+$-Y | Light orange | 0.03 | 0.67 | 0.12 | 5.58 |
| $[Ni(bipy)(phen)Cl]^+$-Y | Light blue | 0.03 | 0.62 | 0.11 | 5.63 |
| $[Fe(bipy)_2Cl_2]^+$-Y | Light pink | 0.02 | 0.51 | 0.12 | 4.25 |
| $[Ni(bipy)_2Cl_2]^+$-Y | Bluish green | 0.01 | 0.28 | 0.06 | 4.67 |
| $[Fe(phen)_2Cl_2]^+$-Y | Brick red | 0.02 | 0.41 | 0.08 | 5.12 |
| $[Ni(phen)_2Cl]^+$-Y | Light green | 0.02 | 0.36 | 0.07 | 5.14 |

In contrast to $[Fe(bipy)(phen)Cl_2]^+$-Y (Light orange) and $[Ni(bipy)(phen)Cl]^+$-Y (Light blue) the color of the final catalyst for $[Fe(bipy)_2Cl_2]^+$-Y, $[Ni(bipy)_2Cl_2]^+$-Y, $[Fe(phen)_2Cl_2]^+$-Y and $[Ni(phen)_2Cl]^+$-Y is light pink, blush green, brick red and light green respectively. As presented in Table S1, the elemental composition analyses also confirmed the purity of simple bipy or phen iron and nickel encapsulated complexes into zeolite supercage. The chemical analyses of encapsulated samples indicates the presence of organic matter with a C/N ratio roughly similar to the theoretical value and its indicating the successful formation of intended Fe(III) and Ni(II) complexes into the zeolite supercage. However in comparison to iron(III) and nickel(II) bipy-phen mixed liganded complexes they have different in C/N value. Moreover, all catalysts has the metal to carbon ratio is different from we reported for the mixed bipy-phen metal complexes.

Therefore, the above physical and elemental analysis comparison data is a good supporting evidence for the formation of zeolite encapsulated 1,10-phenanthroline and 2,2'-bipyridine iron(III) or nickel (II) mixed ligand complexes not the simple bipy or phen in the zeolite supercage during the original manuscript paper.

To compare the catalytic activity of simple iron(III) and nickel(II) bipy or phen ligand based catalyst with iron(III) and nickel(II) mixed bipy-phen ligand based catalyst an experiment on batch oxidation of 2-Phenyl Phenol (OPP) was carried out with similar experimental conditions

as mixed ligand cases. In a 250 mL conical flask, 50 mL of 25 mg/L 2-Phenyl Phenol (OPP) solution was treated with 0.10 M $H_2O_2$ and 0.15 g of respective catalyst. The experiments were conducted at room temperature (29±2 $^oC$) in dynamic condition on a universal shaker (80 rpm) for a period of 120 min.

The residual concentration of 2-Phenyl Phenol (OPP) after 120 min oxidation time was 8.19 mg/L, 8.75 mg/L, 10.81 mg/L and 11.66 mg/L for $[Fe(phen)_2Cl_2]^+$-Y, $[Ni(phen)_2Cl]^+$-Y, $[Fe(bipy)_2Cl_2]^+$-Y and $[Ni(bipy)_2Cl_2]^+$-Y catalysts respectively. As compared to mixed ligand based catalysts such as $[Fe(bipy)(phen)Cl_2]^+$-Y (5.46 mg/L) and $[Ni(bipy)(phen)Cl]^+$-Y (7.13 mg/L), simple bipy or phen metal complex based catalyst shows lower catalytic activity. The increase of the catalytic efficiency of the mixed ligand based metal complexes is owing to the existence of the central metal ions in two different coordination atmospheres and it enables them to show good oxidation properties.

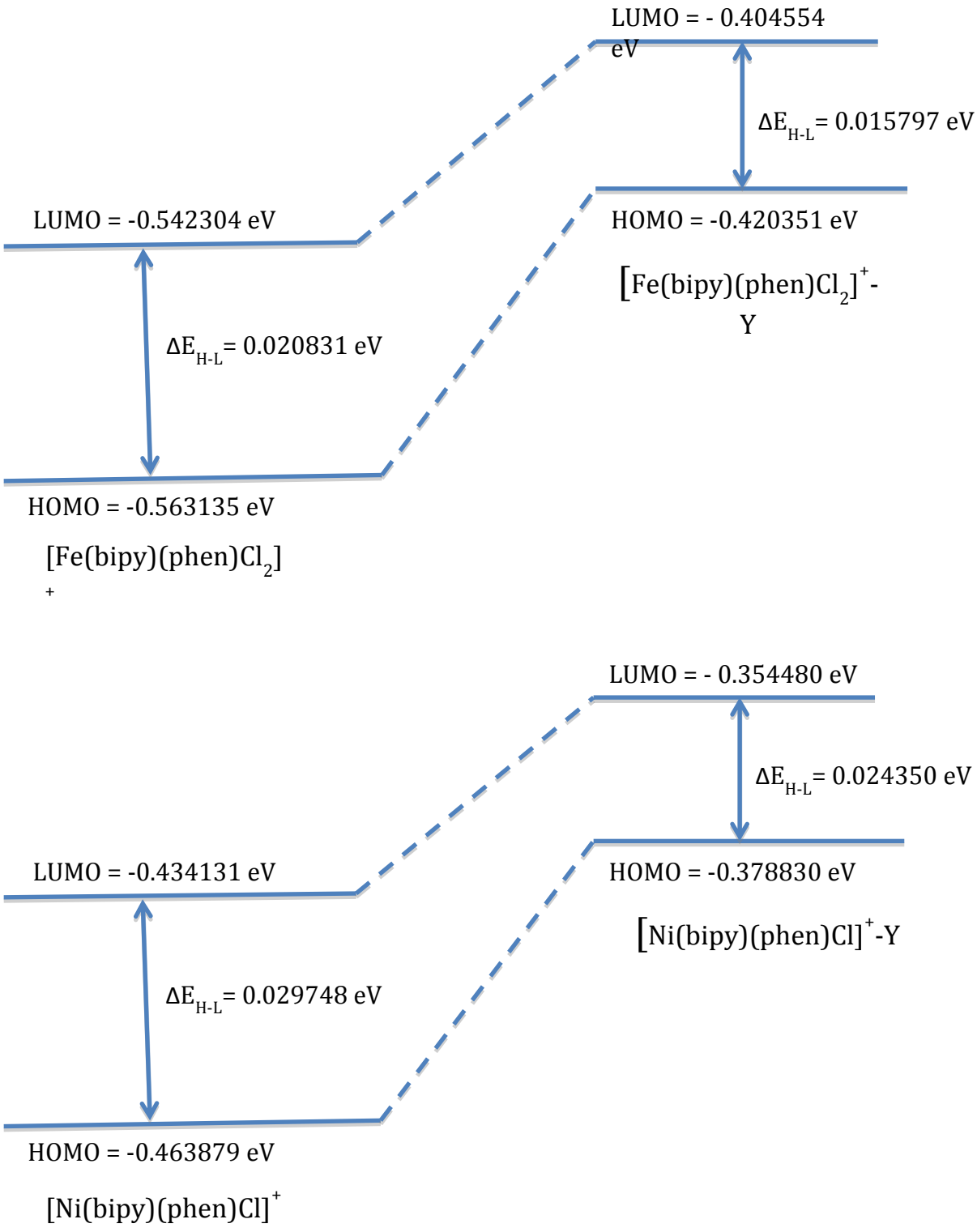
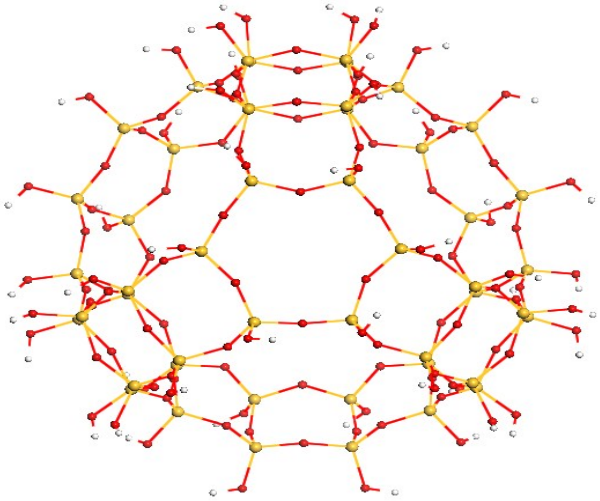
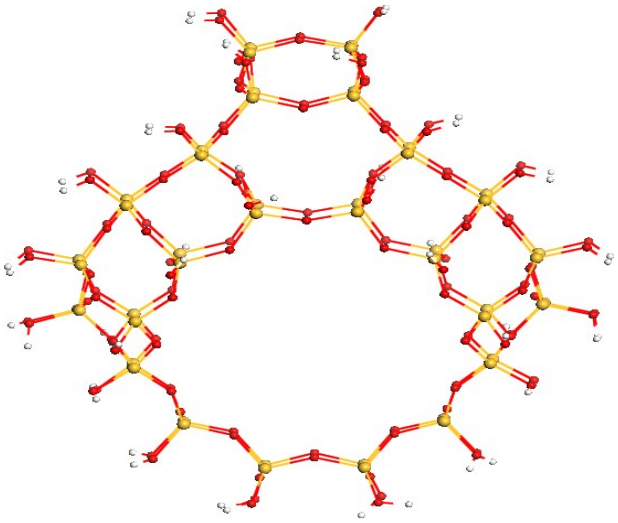


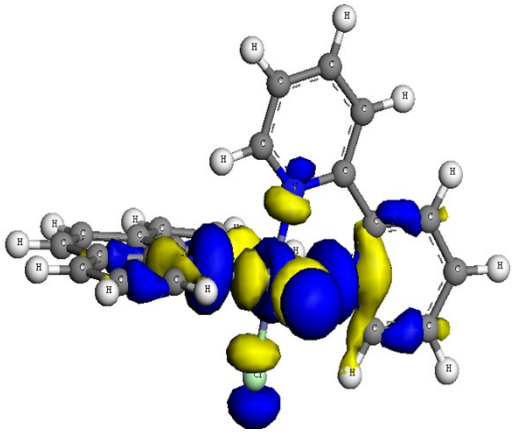

**Fig. S2.** Pictorial representation of the change in the HOMO-LUMO gap for Fe(III) and Ni(II) complexes of 1,10-phenanthroline and 2,2'-bipyridine ligands



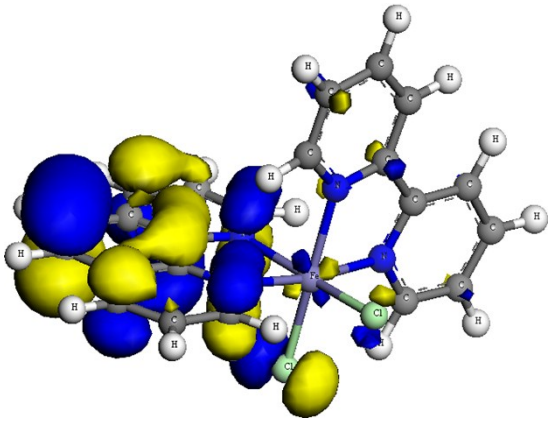
Neat zeolite



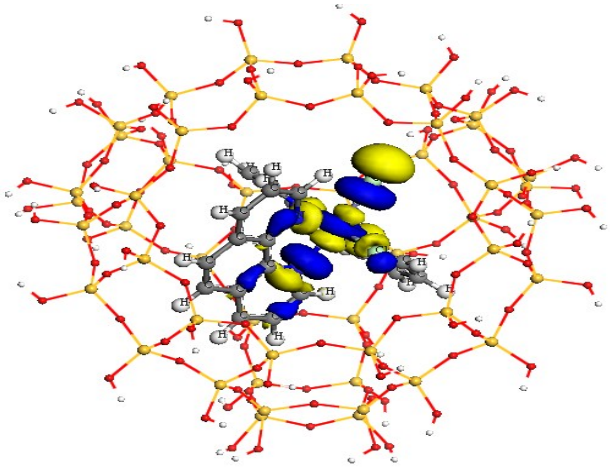
Neat zeolite



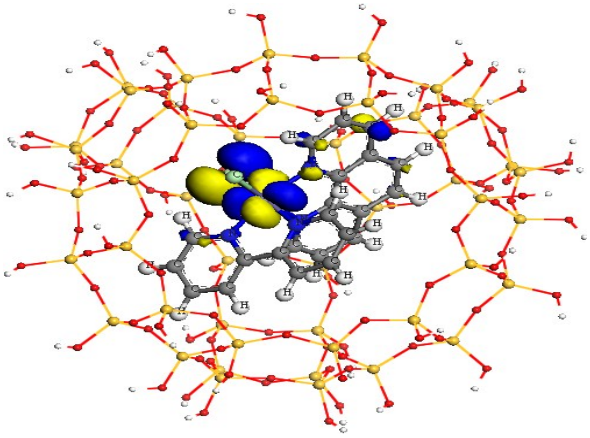
HOMO ([Fe(bipy)(phen)$Cl_2$]$^+$)



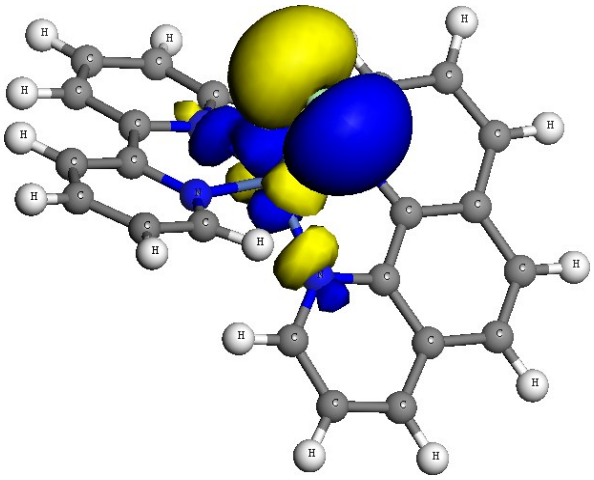
LUMO ([Fe(bipy)(phen)$Cl_2$]$^+$)



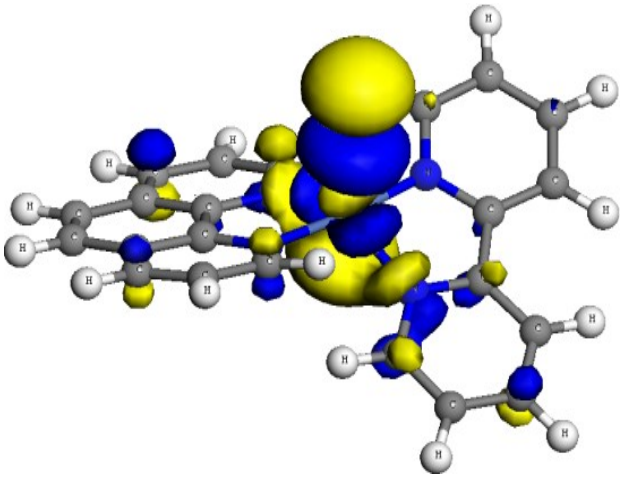
HOMO ([Fe(bipy)(phen)$Cl_2$]$^+$-Y)



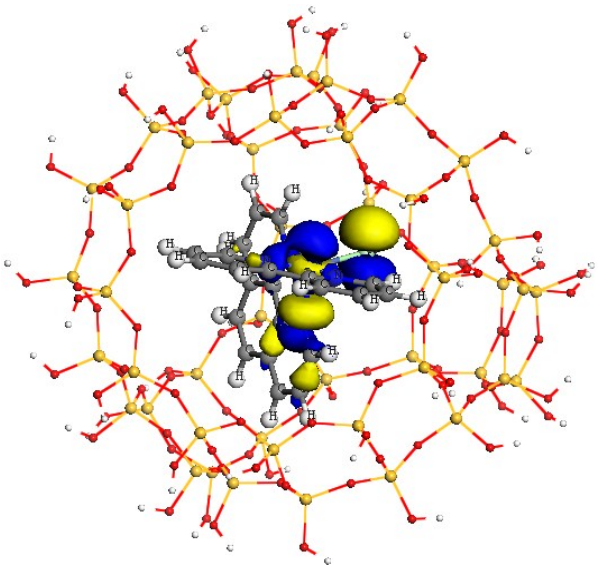
LUMO ([Fe(bipy)(phen)$Cl_2$]$^+$-Y)



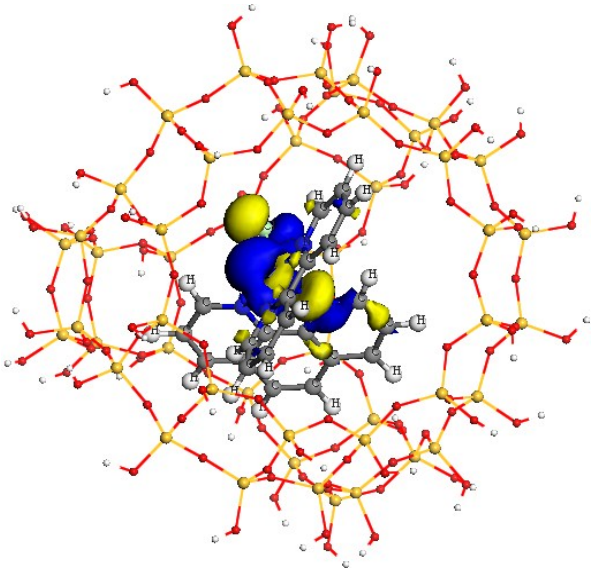
HOMO ([Ni(bipy)(phen)Cl]$^{+}$)



LUMO ([Ni(bipy)(phen)Cl]$^{+}$)



HOMO ([Ni(bipy)(phen)Cl]$^{+}$-Y)



LUMO ([Ni(bipy)(phen)Cl]$^{+}$-Y)

**Fig.S3.** Schematic representation for neat zeolite and the HOMO and LUMO level of the neat and encapsulated complexes Fe(III) and Ni(II) complexes of 1,10-phenanthroline and 2,2'-bipyridine ligands

**Table S2**

The optimized XYZ coordinates

**Neat zeolite-Y**

| | | | |
|---|---|---|---|
| O | -6.99880000 | 1.43990000 | 1.92990000 |
| O | 5.70190000 | -2.27060000 | 4.07560000 |
| O | 4.93200000 | 5.05430000 | 2.05690000 |
| O | -1.45000000 | 2.14830000 | -6.71910000 |
| O | -4.35070000 | -0.05050000 | 5.76730000 |
| O | 1.85840000 | 5.58630000 | 4.39620000 |
| O | 4.15980000 | -0.51420000 | -5.91360000 |
| O | 6.76860000 | -2.20750000 | -2.19880000 |
| O | -5.38690000 | 2.92740000 | -3.99760000 |
| O | -5.03120000 | -5.09330000 | -1.35210000 |
| O | -0.82160000 | 7.11310000 | 0.47120000 |
| O | -5.15360000 | 5.15210000 | -0.81900000 |
| O | -7.24230000 | -0.80120000 | -1.24560000 |
| O | 2.23320000 | 6.62290000 | -1.82360000 |
| O | -3.17360000 | -6.37390000 | 1.80010000 |
| O | 0.08130000 | 1.92850000 | 6.94650000 |
| O | -2.78400000 | -3.59360000 | 5.71710000 |
| O | 0.92280000 | -7.01050000 | -0.97640000 |
| O | 1.65270000 | -1.58880000 | 6.79550000 |
| O | 0.84240000 | -2.26430000 | -6.90010000 |
| O | 1.89440000 | 3.96310000 | -5.82900000 |
| O | 6.96270000 | 0.65670000 | 1.84530000 |
| O | 5.34260000 | -5.09500000 | 0.02560000 |
| O | -0.94930000 | -5.81750000 | -4.14950000 |

| | | | |
|---|---|---|---|
| O | -8.39140000 | 1.46180000 | -0.37190000 |
| O | 7.88530000 | -1.75680000 | 2.58750000 |
| O | 3.47890000 | 7.14720000 | 2.92470000 |
| O | 0.91420000 | 2.58020000 | -7.92190000 |
| O | -3.21530000 | -1.69080000 | 7.56750000 |
| O | 7.66850000 | -3.75760000 | -0.19970000 |
| O | -7.12140000 | 4.02400000 | -2.26890000 |
| O | -3.96030000 | -7.41620000 | -0.55220000 |
| O | 1.60730000 | 8.23270000 | 0.23050000 |
| O | -0.15350000 | -0.34800000 | 8.34720000 |
| O | -1.14070000 | -7.89410000 | -2.44870000 |
| O | 2.50360000 | -0.45940000 | -8.01330000 |
| O | 3.12490000 | -3.00140000 | -5.74550000 |
| O | -3.87240000 | 5.01160000 | -3.15060000 |
| O | -6.93490000 | -1.17660000 | 1.42220000 |
| O | -0.42130000 | 6.77190000 | -2.15550000 |
| O | -5.27330000 | -4.81020000 | 1.32110000 |
| O | 2.54240000 | 0.93760000 | 6.58010000 |
| O | -4.95070000 | -2.43220000 | 4.68960000 |
| O | 4.09540000 | 4.15770000 | 4.42140000 |
| O | 5.03760000 | -4.28090000 | -2.52060000 |
| O | 5.67960000 | 0.41550000 | 4.21760000 |
| O | -0.71460000 | 4.46230000 | -5.56730000 |
| O | 1.59650000 | -6.03300000 | -3.38720000 |
| O | -6.88720000 | 3.56460000 | 0.37320000 |
| O | 6.36320000 | -3.91990000 | 2.13720000 |
| O | 3.81310000 | 6.67200000 | 0.29240000 |

| | | | |
|---|---|---|---|
| O | -0.10300000 | 0.08100000 | -7.65470000 |
| O | -2.30300000 | 0.82510000 | 7.20230000 |
| O | 0.80130000 | 7.15810000 | 2.56830000 |
| O | 5.21210000 | -2.31950000 | -4.29740000 |
| O | 7.69170000 | -1.05970000 | -0.02190000 |
| O | -7.09270000 | 1.36110000 | -2.74310000 |
| O | -3.15540000 | 3.52550000 | -5.22570000 |
| O | -3.23780000 | -6.26880000 | -2.89900000 |
| O | -6.44670000 | -3.11690000 | -0.32150000 |
| O | -2.80790000 | 6.34650000 | -1.11960000 |
| O | 1.09890000 | 5.69310000 | -4.02640000 |
| O | -4.02840000 | -4.69300000 | 3.65640000 |
| O | 1.98280000 | 3.43030000 | 5.90020000 |
| O | -0.74230000 | -2.66960000 | 7.10770000 |
| O | 5.83860000 | 2.74690000 | 2.99620000 |
| O | -1.38550000 | -7.50030000 | 0.21850000 |
| O | 3.99170000 | -1.05470000 | 5.65750000 |
| O | 3.16700000 | 1.81340000 | -6.69230000 |
| O | -6.06280000 | -0.23490000 | 3.74800000 |
| O | 0.93630000 | -4.45910000 | -5.42160000 |
| O | 3.33400000 | -5.98870000 | -1.39930000 |
| Si | -7.86710000 | 2.35930000 | 0.89070000 |
| Si | 6.97860000 | -2.93160000 | 3.28660000 |
| Si | 4.50350000 | 6.60720000 | 1.77380000 |
| Si | -0.43050000 | 1.66100000 | -7.90450000 |
| Si | -3.61810000 | -0.14780000 | 7.22410000 |
| Si | 2.01840000 | 7.03380000 | 3.65650000 |

| | | | |
|---|---|---|---|
| Si | 4.49290000 | -2.12050000 | -5.74250000 |
| Si | 7.88030000 | -2.36280000 | -1.00370000 |
| Si | -6.90600000 | 2.85810000 | -3.38510000 |
| Si | -4.41700000 | 4.18600000 | -4.43500000 |
| Si | -4.45450000 | -6.54450000 | -1.83980000 |
| Si | 0.34180000 | 7.97550000 | 1.23030000 |
| Si | -6.71850000 | 4.67120000 | -0.82100000 |
| Si | -7.40190000 | -1.84580000 | 0.02000000 |
| Si | -8.04940000 | 0.55620000 | -1.68140000 |
| Si | -4.19730000 | 5.98490000 | -1.87310000 |
| Si | 1.01730000 | 6.87980000 | -2.91440000 |
| Si | -4.51750000 | -5.68530000 | 2.47320000 |
| Si | 1.69890000 | 2.26720000 | 7.00170000 |
| Si | -2.34080000 | -3.01680000 | 7.17890000 |
| Si | -4.26420000 | -3.87130000 | 5.03300000 |
| Si | -0.86940000 | 1.06380000 | 7.95430000 |
| Si | -6.03490000 | -4.67500000 | -0.10950000 |
| Si | 5.37790000 | 4.23870000 | 3.41980000 |
| Si | 6.04800000 | -3.24210000 | -3.25390000 |
| Si | -0.39910000 | -7.97230000 | -0.99580000 |
| Si | 5.50210000 | -0.97300000 | 5.06480000 |
| Si | 0.42070000 | -1.79260000 | 7.84990000 |
| Si | 3.67580000 | 0.35220000 | -7.21610000 |
| Si | 2.82430000 | 7.58240000 | -0.64000000 |
| Si | -5.55140000 | -0.97350000 | 5.10020000 |
| Si | 0.99530000 | -1.08120000 | -8.01440000 |
| Si | 0.77230000 | 5.13270000 | -5.50740000 |

| | | | |
|---|---|---|---|
| Si | 1.77690000 | -3.55980000 | -6.47560000 |
| Si | 2.27000000 | 3.10270000 | -7.16560000 |
| Si | 2.13940000 | -6.85310000 | -2.08520000 |
| Si | -1.48770000 | 7.29220000 | -1.03290000 |
| Si | -7.18530000 | -0.05870000 | 2.59120000 |
| Si | 8.01010000 | -0.55800000 | 1.49950000 |
| Si | 4.89620000 | -5.54450000 | -1.48790000 |
| Si | 6.63240000 | 1.36030000 | 3.29830000 |
| Si | 6.75780000 | -4.71990000 | 0.76280000 |
| Si | 2.85430000 | 4.67380000 | 5.34430000 |
| Si | 0.61800000 | -5.86590000 | -4.68120000 |
| Si | -1.92360000 | -6.98850000 | -3.55950000 |
| Si | -1.93630000 | 3.66380000 | -6.28440000 |
| Si | 2.98570000 | -0.61100000 | 6.85540000 |
| Si | -2.94420000 | -7.57240000 | 0.71710000 |
| O | -4.72260000 | 0.37170000 | 8.33270000 |
| H | -4.36460000 | 0.76420000 | 9.14150000 |
| O | -6.73970000 | -1.25410000 | 6.20600000 |
| H | -6.85840000 | -0.56240000 | 6.87480000 |
| O | -8.72760000 | -0.19960000 | 3.16410000 |
| H | -9.22840000 | -0.91800000 | 2.74710000 |
| O | -5.18610000 | -4.68550000 | 6.13560000 |
| H | -6.04320000 | -4.26980000 | 6.31420000 |
| O | -2.52840000 | -4.14320000 | 8.36300000 |
| H | -3.33360000 | -4.67730000 | 8.28450000 |
| O | -5.51010000 | -6.89590000 | 2.99820000 |
| H | -6.40950000 | -6.84510000 | 2.64050000 |

| | | | |
|---|---|---|---|
| O | -3.15830000 | -9.05600000 | 1.39470000 |
| H | -3.89420000 | -9.11290000 | 2.02260000 |
| O | 0.13240000 | -9.51610000 | -0.76270000 |
| H | -0.45110000 | -10.09100000 | -0.24740000 |
| O | 2.60350000 | -8.33240000 | -2.64510000 |
| H | 2.51060000 | -9.06490000 | -2.01660000 |
| O | 5.89370000 | -6.75830000 | -1.99540000 |
| H | 6.37910000 | -6.54470000 | -2.80770000 |
| O | 7.60580000 | -6.07220000 | 1.13030000 |
| H | 7.54670000 | -6.77900000 | 0.47070000 |
| O | 9.40030000 | -2.42410000 | -1.63910000 |
| H | 9.73990000 | -1.58770000 | -1.98570000 |
| O | 9.55910000 | 0.00940000 | 1.64110000 |
| H | 9.85730000 | 0.57200000 | 0.91290000 |
| O | 8.02690000 | 1.55620000 | 4.15890000 |
| H | 8.84520000 | 1.58170000 | 3.64050000 |
| O | 6.60310000 | 5.05130000 | 4.15850000 |
| H | 6.93090000 | 5.81870000 | 3.66560000 |
| O | 5.90560000 | 7.47020000 | 1.86000000 |
| H | 5.86260000 | 8.40320000 | 1.60730000 |
| O | -0.31840000 | 9.43580000 | 1.61730000 |
| H | -0.06270000 | 9.80000000 | 2.47680000 |
| O | 1.84970000 | 8.28890000 | 4.70570000 |
| H | 2.28470000 | 8.15940000 | 5.56220000 |
| O | 3.36920000 | 5.63380000 | 6.58330000 |
| H | 3.37430000 | 5.22140000 | 7.45930000 |
| O | 2.14150000 | 2.76450000 | 8.51990000 |

| | | | |
|---|---|---|---|
| H | 2.75680000 | 2.15000000 | 8.95140000 |
| O | -1.19710000 | 1.89250000 | 9.33820000 |
| H | -0.44100000 | 2.35850000 | 9.72480000 |
| O | 5.42070000 | -2.63160000 | -7.00730000 |
| H | 5.84600000 | -1.91910000 | -7.50990000 |
| O | 5.00320000 | 0.46140000 | -8.18980000 |
| H | 4.98450000 | 1.13890000 | -8.88060000 |
| O | 3.17620000 | 3.96950000 | -8.22820000 |
| H | 2.88340000 | 4.88380000 | -8.36000000 |
| O | 0.65650000 | -1.62990000 | -9.52680000 |
| H | 0.94300000 | -2.54080000 | -9.69350000 |
| O | 2.16950000 | -4.35740000 | -7.86690000 |
| H | 3.10660000 | -4.58880000 | -7.94790000 |
| O | -1.25660000 | 1.93190000 | -9.30850000 |
| H | -0.91230000 | 1.51750000 | -10.11210000 |
| O | 0.92840000 | 6.32720000 | -6.63520000 |
| H | 1.06570000 | 7.21670000 | -6.27750000 |
| O | -2.47420000 | 4.48350000 | -7.61330000 |
| H | -2.41070000 | 3.98500000 | -8.44410000 |
| O | -5.23440000 | 5.25470000 | -5.40220000 |
| H | -4.97800000 | 5.21320000 | -6.33660000 |
| O | -8.06350000 | 3.01610000 | -4.54520000 |
| H | -8.09760000 | 3.88060000 | -4.97930000 |
| O | -9.16710000 | 3.01420000 | 1.64890000 |
| H | -9.57590000 | 2.43490000 | 2.30910000 |
| O | -9.45380000 | 0.05560000 | -2.38130000 |
| H | -9.89930000 | 0.70020000 | -2.94930000 |

| | | | |
|---|---|---|---|
| O | -8.99150000 | -2.24300000 | 0.23910000 |
| H | -9.52960000 | -2.26000000 | -0.56650000 |
| O | -7.32090000 | -5.70790000 | -0.05600000 |
| H | -7.53990000 | -6.13490000 | -0.89850000 |
| O | -5.70610000 | -7.33690000 | -2.56280000 |
| H | -5.47370000 | -7.90240000 | -3.31300000 |
| O | -2.47430000 | -7.97410000 | -4.75670000 |
| H | -1.81280000 | -8.19420000 | -5.43020000 |
| O | 0.79000000 | -7.17340000 | -5.67790000 |
| H | 1.46030000 | -7.80410000 | -5.37230000 |
| O | -7.70630000 | 5.94910000 | -0.52820000 |
| H | -7.38720000 | 6.79080000 | -0.88570000 |
| O | -5.02170000 | 7.32230000 | -2.38160000 |
| H | -5.06900000 | 7.42040000 | -3.34440000 |
| O | -1.75890000 | 8.88250000 | -1.36810000 |
| H | -1.98800000 | 9.43860000 | -0.60740000 |
| O | 1.02960000 | -2.59170000 | 9.15670000 |
| H | 0.44190000 | -3.24510000 | 9.56230000 |
| O | 3.64480000 | -0.62420000 | 8.36590000 |
| H | 3.58160000 | -1.46520000 | 8.84420000 |
| O | 6.65250000 | -1.03350000 | 6.24910000 |
| H | 7.22410000 | -0.25070000 | 6.27410000 |
| O | 7.91930000 | -3.79150000 | 4.31620000 |
| H | 7.99380000 | -3.41280000 | 5.20480000 |
| O | 7.17650000 | -4.21440000 | -3.97360000 |
| H | 8.02840000 | -3.80740000 | -4.18470000 |
| O | 3.73620000 | 8.80370000 | -1.25980000 |

| | | | |
|---|---|---|---|
| H | 3.37810000 | 9.21550000 | -2.06000000 |
| O | 1.18080000 | 8.36750000 | -3.62830000 |
| H | 0.45380000 | 8.97270000 | -3.41060000 |

**$[Fe(bipy)(phen)Cl_2]^+$**

| | | | |
|---|---|---|---|
| C | 2.29600000 | -0.58870000 | 1.37110000 |
| C | 0.29160000 | -1.73680000 | 1.84200000 |
| C | 0.81480000 | -2.21850000 | 3.04570000 |
| C | 2.11240000 | -1.86700000 | 3.41460000 |
| C | 2.85520000 | -1.04640000 | 2.57050000 |
| C | 2.99170000 | 0.23570000 | 0.40900000 |
| C | 2.79850000 | 1.36590000 | -1.64620000 |
| C | 4.14620000 | 1.74850000 | -1.59300000 |
| C | 4.92550000 | 1.35770000 | -0.50540000 |
| C | 4.34210000 | 0.59630000 | 0.50590000 |
| H | -0.71370000 | -2.00650000 | 1.50890000 |
| H | 0.20380000 | -2.87200000 | 3.67620000 |
| H | 2.54570000 | -2.23560000 | 4.35040000 |
| H | 3.87590000 | -0.76620000 | 2.84550000 |
| H | 2.16490000 | 1.64320000 | -2.49450000 |
| H | 4.56860000 | 2.33960000 | -2.41230000 |
| H | 5.98330000 | 1.63610000 | -0.44880000 |
| H | 4.94740000 | 0.27020000 | 1.35650000 |
| N | 2.23620000 | 0.62900000 | -0.66640000 |
| N | 1.01410000 | -0.94140000 | 1.03170000 |
| H | 1.01520000 | 2.49490000 | 0.48760000 |
| C | -0.05680000 | 2.37040000 | 0.66350000 |
| C | -0.82360000 | 3.38190000 | 1.25140000 |

| | | | |
|---|---|---|---|
| C | -2.19080000 | 3.20430000 | 1.41980000 |
| H | -0.33670000 | 4.31270000 | 1.55840000 |
| C | -1.94540000 | 1.00640000 | 0.43490000 |
| C | -2.78720000 | 1.99310000 | 1.00340000 |
| H | -2.80540000 | 3.99840000 | 1.86020000 |
| C | -2.48780000 | -0.22420000 | -0.03020000 |
| C | -4.17850000 | 1.72190000 | 1.09380000 |
| C | -3.88110000 | -0.46770000 | 0.03940000 |
| C | -4.71270000 | 0.52610000 | 0.61830000 |
| H | -4.84280000 | 2.47580000 | 1.53330000 |
| C | -4.35870000 | -1.68480000 | -0.50180000 |
| C | -2.09110000 | -2.26800000 | -1.09610000 |
| H | -5.79360000 | 0.35130000 | 0.68110000 |
| C | -3.45760000 | -2.57470000 | -1.07180000 |
| H | -5.43060000 | -1.91500000 | -0.48040000 |
| H | -1.36130000 | -2.94820000 | -1.54790000 |
| H | -3.79940000 | -3.51700000 | -1.51200000 |
| N | -0.61360000 | 1.20690000 | 0.26530000 |
| N | -1.61690000 | -1.11170000 | -0.57390000 |
| Fe | 0.35080000 | -0.29520000 | -0.76620000 |
| Cl | -0.20580000 | 0.72650000 | -2.58900000 |
| Cl | 1.11920000 | -2.10760000 | -1.66030000 |

**[Ni(bipy)(phen)Cl]$^{+}$**

| | | | |
|---|---|---|---|
| C | 2.97520000 | 0.73110000 | 0.17130000 |
| C | 1.64110000 | 2.44100000 | 1.10460000 |
| C | 2.75470000 | 3.25100000 | 1.27570000 |
| C | 4.00600000 | 2.78550000 | 0.87260000 |

| | | | |
|---|---|---|---|
| C | 4.11600000 | 1.50950000 | 0.32860000 |
| C | 2.93590000 | -0.63510000 | -0.30390000 |
| C | 1.50290000 | -2.46480000 | -0.68590000 |
| C | 2.55030000 | -3.20830000 | -1.21370000 |
| C | 3.82470000 | -2.64770000 | -1.26830000 |
| C | 4.01380000 | -1.34350000 | -0.81910000 |
| H | 0.65430000 | 2.72730000 | 1.47770000 |
| H | 2.63970000 | 4.22960000 | 1.74880000 |
| H | 4.89720000 | 3.40530000 | 1.00710000 |
| H | 5.09460000 | 1.11130000 | 0.04780000 |
| H | 0.48800000 | -2.86510000 | -0.64750000 |
| H | 2.36080000 | -4.21920000 | -1.58400000 |
| H | 4.66560000 | -3.21920000 | -1.67180000 |
| H | 5.00070000 | -0.87720000 | -0.88030000 |
| N | 1.69310000 | -1.20940000 | -0.22080000 |
| N | 1.75140000 | 1.22330000 | 0.52820000 |
| H | 0.07010000 | 2.93690000 | -0.73770000 |
| C | -0.92320000 | 2.48190000 | -0.70810000 |
| C | -2.04790000 | 3.17430000 | -1.17490000 |
| C | -3.30170000 | 2.58590000 | -1.13460000 |
| H | -1.91870000 | 4.18700000 | -1.56620000 |
| C | -2.25390000 | 0.62760000 | -0.22720000 |
| C | -3.43210000 | 1.26750000 | -0.65220000 |
| H | -4.18520000 | 3.13460000 | -1.47730000 |
| C | -2.28430000 | -0.69610000 | 0.23770000 |
| C | -4.65950000 | 0.54250000 | -0.55540000 |
| C | -3.49960000 | -1.39280000 | 0.36980000 |

| | | | |
|---|---|---|---|
| C | -4.69320000 | -0.73210000 | -0.05370000 |
| H | -5.58420000 | 1.03000000 | -0.88070000 |
| C | -3.43750000 | -2.68350000 | 0.93200000 |
| C | -1.04380000 | -2.44150000 | 1.17710000 |
| H | -5.64600000 | -1.26490000 | 0.02930000 |
| C | -2.21480000 | -3.19050000 | 1.34380000 |
| H | -4.35390000 | -3.26850000 | 1.06260000 |
| H | -0.07940000 | -2.78960000 | 1.55830000 |
| H | -2.14820000 | -4.17110000 | 1.82240000 |
| N | -1.02460000 | 1.23170000 | -0.22120000 |
| N | -1.07980000 | -1.23130000 | 0.59240000 |
| Ni | 0.34090000 | -0.00080000 | 0.43570000 |
| Cl | 0.37330000 | -0.00440000 | 2.70100000 |

**$[Fe(bipy)(phen)Cl_2]^+$-Y**

| | | | |
|---|---|---|---|
| O | -6.99880000 | 1.43990000 | 1.92990000 |
| O | 5.70190000 | -2.27060000 | 4.07560000 |
| O | 4.93200000 | 5.05430000 | 2.05690000 |
| O | -1.45000000 | 2.14830000 | -6.71910000 |
| O | -4.35070000 | -0.05050000 | 5.76730000 |
| O | 1.85840000 | 5.58630000 | 4.39620000 |
| O | 4.15980000 | -0.51420000 | -5.91360000 |
| O | 6.76860000 | -2.20750000 | -2.19880000 |
| O | -5.38690000 | 2.92740000 | -3.99760000 |
| O | -5.03120000 | -5.09330000 | -1.35210000 |
| O | -0.82160000 | 7.11310000 | 0.47120000 |
| O | -5.15360000 | 5.15210000 | -0.81900000 |

| | | | |
|---|---|---|---|
| O | -7.24230000 | -0.80120000 | -1.24560000 |
| O | 2.23320000 | 6.62290000 | -1.82360000 |
| O | -3.17360000 | -6.37390000 | 1.80010000 |
| O | 0.08130000 | 1.92850000 | 6.94650000 |
| O | -2.78400000 | -3.59360000 | 5.71710000 |
| O | 0.92280000 | -7.01050000 | -0.97640000 |
| O | 1.65270000 | -1.58880000 | 6.79550000 |
| O | 0.84240000 | -2.26430000 | -6.90010000 |
| O | 1.89440000 | 3.96310000 | -5.82900000 |
| O | 6.96270000 | 0.65670000 | 1.84530000 |
| O | 5.34260000 | -5.09500000 | 0.02560000 |
| O | -0.94930000 | -5.81750000 | -4.14950000 |
| O | -8.39140000 | 1.46180000 | -0.37190000 |
| O | 7.88530000 | -1.75680000 | 2.58750000 |
| O | 3.47890000 | 7.14720000 | 2.92470000 |
| O | 0.91420000 | 2.58020000 | -7.92190000 |
| O | -3.21530000 | -1.69080000 | 7.56750000 |
| O | 7.66850000 | -3.75760000 | -0.19970000 |
| O | -7.12140000 | 4.02400000 | -2.26890000 |
| O | -3.96030000 | -7.41620000 | -0.55220000 |
| O | 1.60730000 | 8.23270000 | 0.23050000 |
| O | -0.15350000 | -0.34800000 | 8.34720000 |
| O | -1.14070000 | -7.89410000 | -2.44870000 |
| O | 2.50360000 | -0.45940000 | -8.01330000 |
| O | 3.12490000 | -3.00140000 | -5.74550000 |
| O | -3.87240000 | 5.01160000 | -3.15060000 |
| O | -6.93490000 | -1.17660000 | 1.42220000 |

| | | | |
|---|---|---|---|
| O | -0.42130000 | 6.77190000 | -2.15550000 |
| O | -5.27330000 | -4.81020000 | 1.32110000 |
| O | 2.54240000 | 0.93760000 | 6.58010000 |
| O | -4.95070000 | -2.43220000 | 4.68960000 |
| O | 4.09540000 | 4.15770000 | 4.42140000 |
| O | 5.03760000 | -4.28090000 | -2.52060000 |
| O | 5.67960000 | 0.41550000 | 4.21760000 |
| O | -0.71460000 | 4.46230000 | -5.56730000 |
| O | 1.59650000 | -6.03300000 | -3.38720000 |
| O | -6.88720000 | 3.56460000 | 0.37320000 |
| O | 6.36320000 | -3.91990000 | 2.13720000 |
| O | 3.81310000 | 6.67200000 | 0.29240000 |
| O | -0.10300000 | 0.08100000 | -7.65470000 |
| O | -2.30300000 | 0.82510000 | 7.20230000 |
| O | 0.80130000 | 7.15810000 | 2.56830000 |
| O | 5.21210000 | -2.31950000 | -4.29740000 |
| O | 7.69170000 | -1.05970000 | -0.02190000 |
| O | -7.09270000 | 1.36110000 | -2.74310000 |
| O | -3.15540000 | 3.52550000 | -5.22570000 |
| O | -3.23780000 | -6.26880000 | -2.89900000 |
| O | -6.44670000 | -3.11690000 | -0.32150000 |
| O | -2.80790000 | 6.34650000 | -1.11960000 |
| O | 1.09890000 | 5.69310000 | -4.02640000 |
| O | -4.02840000 | -4.69300000 | 3.65640000 |
| O | 1.98280000 | 3.43030000 | 5.90020000 |
| O | -0.74230000 | -2.66960000 | 7.10770000 |
| O | 5.83860000 | 2.74690000 | 2.99620000 |

| | | | |
|---|---|---|---|
| O | -1.38550000 | -7.50030000 | 0.21850000 |
| O | 3.99170000 | -1.05470000 | 5.65750000 |
| O | 3.16700000 | 1.81340000 | -6.69230000 |
| O | -6.06280000 | -0.23490000 | 3.74800000 |
| O | 0.93630000 | -4.45910000 | -5.42160000 |
| O | 3.33400000 | -5.98870000 | -1.39930000 |
| Si | -7.86710000 | 2.35930000 | 0.89070000 |
| Si | 6.97860000 | -2.93160000 | 3.28660000 |
| Si | 4.50350000 | 6.60720000 | 1.77380000 |
| Si | -0.43050000 | 1.66100000 | -7.90450000 |
| Si | -3.61810000 | -0.14780000 | 7.22410000 |
| Si | 2.01840000 | 7.03380000 | 3.65650000 |
| Si | 4.49290000 | -2.12050000 | -5.74250000 |
| Si | 7.88030000 | -2.36280000 | -1.00370000 |
| Si | -6.90600000 | 2.85810000 | -3.38510000 |
| Si | -4.41700000 | 4.18600000 | -4.43500000 |
| Si | -4.45450000 | -6.54450000 | -1.83980000 |
| Si | 0.34180000 | 7.97550000 | 1.23030000 |
| Si | -6.71850000 | 4.67120000 | -0.82100000 |
| Si | -7.40190000 | -1.84580000 | 0.02000000 |
| Si | -8.04940000 | 0.55620000 | -1.68140000 |
| Si | -4.19730000 | 5.98490000 | -1.87310000 |
| Si | 1.01730000 | 6.87980000 | -2.91440000 |
| Si | -4.51750000 | -5.68530000 | 2.47320000 |
| Si | 1.69890000 | 2.26720000 | 7.00170000 |
| Si | -2.34080000 | -3.01680000 | 7.17890000 |
| Si | -4.26420000 | -3.87130000 | 5.03300000 |

| | | | |
|---|---|---|---|
| Si | -0.86940000 | 1.06380000 | 7.95430000 |
| Si | -6.03490000 | -4.67500000 | -0.10950000 |
| Si | 5.37790000 | 4.23870000 | 3.41980000 |
| Si | 6.04800000 | -3.24210000 | -3.25390000 |
| Si | -0.39910000 | -7.97230000 | -0.99580000 |
| Si | 5.50210000 | -0.97300000 | 5.06480000 |
| Si | 0.42070000 | -1.79260000 | 7.84990000 |
| Si | 3.67580000 | 0.35220000 | -7.21610000 |
| Si | 2.82430000 | 7.58240000 | -0.64000000 |
| Si | -5.55140000 | -0.97350000 | 5.10020000 |
| Si | 0.99530000 | -1.08120000 | -8.01440000 |
| Si | 0.77230000 | 5.13270000 | -5.50740000 |
| Si | 1.77690000 | -3.55980000 | -6.47560000 |
| Si | 2.27000000 | 3.10270000 | -7.16560000 |
| Si | 2.13940000 | -6.85310000 | -2.08520000 |
| Si | -1.48770000 | 7.29220000 | -1.03290000 |
| Si | -7.18530000 | -0.05870000 | 2.59120000 |
| Si | 8.01010000 | -0.55800000 | 1.49950000 |
| Si | 4.89620000 | -5.54450000 | -1.48790000 |
| Si | 6.63240000 | 1.36030000 | 3.29830000 |
| Si | 6.75780000 | -4.71990000 | 0.76280000 |
| Si | 2.85430000 | 4.67380000 | 5.34430000 |
| Si | 0.61800000 | -5.86590000 | -4.68120000 |
| Si | -1.92360000 | -6.98850000 | -3.55950000 |
| Si | -1.93630000 | 3.66380000 | -6.28440000 |
| Si | 2.98570000 | -0.61100000 | 6.85540000 |
| Si | -2.94420000 | -7.57240000 | 0.71710000 |

| | | | |
|---|---|---|---|
| O | -4.72260000 | 0.37170000 | 8.33270000 |
| H | -4.36460000 | 0.76420000 | 9.14150000 |
| O | -6.73970000 | -1.25410000 | 6.20600000 |
| H | -6.85840000 | -0.56240000 | 6.87480000 |
| O | -8.72760000 | -0.19960000 | 3.16410000 |
| H | -9.22840000 | -0.91800000 | 2.74710000 |
| O | -5.18610000 | -4.68550000 | 6.13560000 |
| H | -6.04320000 | -4.26980000 | 6.31420000 |
| O | -2.52840000 | -4.14320000 | 8.36300000 |
| H | -3.33360000 | -4.67730000 | 8.28450000 |
| O | -5.51010000 | -6.89590000 | 2.99820000 |
| H | -6.40950000 | -6.84510000 | 2.64050000 |
| O | -3.15830000 | -9.05600000 | 1.39470000 |
| H | -3.89420000 | -9.11290000 | 2.02260000 |
| O | 0.13240000 | -9.51610000 | -0.76270000 |
| H | -0.45110000 | -10.09100000 | -0.24740000 |
| O | 2.60350000 | -8.33240000 | -2.64510000 |
| H | 2.51060000 | -9.06490000 | -2.01660000 |
| O | 5.89370000 | -6.75830000 | -1.99540000 |
| H | 6.37910000 | -6.54470000 | -2.80770000 |
| O | 7.60580000 | -6.07220000 | 1.13030000 |
| H | 7.54670000 | -6.77900000 | 0.47070000 |
| O | 9.40030000 | -2.42410000 | -1.63910000 |
| H | 9.73990000 | -1.58770000 | -1.98570000 |
| O | 9.55910000 | 0.00940000 | 1.64110000 |
| H | 9.85730000 | 0.57200000 | 0.91290000 |
| O | 8.02690000 | 1.55620000 | 4.15890000 |

| | | | |
|---|---|---|---|
| H | 8.84520000 | 1.58170000 | 3.64050000 |
| O | 6.60310000 | 5.05130000 | 4.15850000 |
| H | 6.93090000 | 5.81870000 | 3.66560000 |
| O | 5.90560000 | 7.47020000 | 1.86000000 |
| H | 5.86260000 | 8.40320000 | 1.60730000 |
| O | -0.31840000 | 9.43580000 | 1.61730000 |
| H | -0.06270000 | 9.80000000 | 2.47680000 |
| O | 1.84970000 | 8.28890000 | 4.70570000 |
| H | 2.28470000 | 8.15940000 | 5.56220000 |
| O | 3.36920000 | 5.63380000 | 6.58330000 |
| H | 3.37430000 | 5.22140000 | 7.45930000 |
| O | 2.14150000 | 2.76450000 | 8.51990000 |
| H | 2.75680000 | 2.15000000 | 8.95140000 |
| O | -1.19710000 | 1.89250000 | 9.33820000 |
| H | -0.44100000 | 2.35850000 | 9.72480000 |
| O | 5.42070000 | -2.63160000 | -7.00730000 |
| H | 5.84600000 | -1.91910000 | -7.50990000 |
| O | 5.00320000 | 0.46140000 | -8.18980000 |
| H | 4.98450000 | 1.13890000 | -8.88060000 |
| O | 3.17620000 | 3.96950000 | -8.22820000 |
| H | 2.88340000 | 4.88380000 | -8.36000000 |
| O | 0.65650000 | -1.62990000 | -9.52680000 |
| H | 0.94300000 | -2.54080000 | -9.69350000 |
| O | 2.16950000 | -4.35740000 | -7.86690000 |
| H | 3.10660000 | -4.58880000 | -7.94790000 |
| O | -1.25660000 | 1.93190000 | -9.30850000 |
| H | -0.91230000 | 1.51750000 | -10.11210000 |

| | | | |
|---|---|---|---|
| O | 0.92840000 | 6.32720000 | -6.63520000 |
| H | 1.06570000 | 7.21670000 | -6.27750000 |
| O | -2.47420000 | 4.48350000 | -7.61330000 |
| H | -2.41070000 | 3.98500000 | -8.44410000 |
| O | -5.23440000 | 5.25470000 | -5.40220000 |
| H | -4.97800000 | 5.21320000 | -6.33660000 |
| O | -8.06350000 | 3.01610000 | -4.54520000 |
| H | -8.09760000 | 3.88060000 | -4.97930000 |
| O | -9.16710000 | 3.01420000 | 1.64890000 |
| H | -9.57590000 | 2.43490000 | 2.30910000 |
| O | -9.45380000 | 0.05560000 | -2.38130000 |
| H | -9.89930000 | 0.70020000 | -2.94930000 |
| O | -8.99150000 | -2.24300000 | 0.23910000 |
| H | -9.52960000 | -2.26000000 | -0.56650000 |
| O | -7.32090000 | -5.70790000 | -0.05600000 |
| H | -7.53990000 | -6.13490000 | -0.89850000 |
| O | -5.70610000 | -7.33690000 | -2.56280000 |
| H | -5.47370000 | -7.90240000 | -3.31300000 |
| O | -2.47430000 | -7.97410000 | -4.75670000 |
| H | -1.81280000 | -8.19420000 | -5.43020000 |
| O | 0.79000000 | -7.17340000 | -5.67790000 |
| H | 1.46030000 | -7.80410000 | -5.37230000 |
| O | -7.70630000 | 5.94910000 | -0.52820000 |
| H | -7.38720000 | 6.79080000 | -0.88570000 |
| O | -5.02170000 | 7.32230000 | -2.38160000 |
| H | -5.06900000 | 7.42040000 | -3.34440000 |
| O | -1.75890000 | 8.88250000 | -1.36810000 |

| | | | |
|---|---|---|---|
| H | -1.98800000 | 9.43860000 | -0.60740000 |
| O | 1.02960000 | -2.59170000 | 9.15670000 |
| H | 0.44190000 | -3.24510000 | 9.56230000 |
| O | 3.64480000 | -0.62420000 | 8.36590000 |
| H | 3.58160000 | -1.46520000 | 8.84420000 |
| O | 6.65250000 | -1.03350000 | 6.24910000 |
| H | 7.22410000 | -0.25070000 | 6.27410000 |
| O | 7.91930000 | -3.79150000 | 4.31620000 |
| H | 7.99380000 | -3.41280000 | 5.20480000 |
| O | 7.17650000 | -4.21440000 | -3.97360000 |
| H | 8.02840000 | -3.80740000 | -4.18470000 |
| O | 3.73620000 | 8.80370000 | -1.25980000 |
| H | 3.37810000 | 9.21550000 | -2.06000000 |
| O | 1.18080000 | 8.36750000 | -3.62830000 |
| H | 0.45380000 | 8.97270000 | -3.41060000 |
| C | 1.63210000 | -0.58440000 | 1.78400000 |
| C | -0.35890000 | -1.84710000 | 1.75520000 |
| C | -0.19460000 | -2.19660000 | 3.09260000 |
| C | 0.92900000 | -1.73650000 | 3.78090000 |
| C | 1.84470000 | -0.91970000 | 3.11900000 |
| C | 2.53580000 | 0.20350000 | 0.96700000 |
| C | 3.06710000 | 0.82600000 | -1.25010000 |
| C | 4.16720000 | 1.54890000 | -0.80930000 |
| C | 4.42740000 | 1.63500000 | 0.55670000 |
| C | 3.61640000 | 0.93650000 | 1.44970000 |
| H | -1.20290000 | -2.21450000 | 1.16660000 |
| H | -0.93130000 | -2.84540000 | 3.58290000 |

| | | | |
|---|---|---|---|
| H | 1.10910000 | -2.01340000 | 4.83140000 |
| H | 2.74620000 | -0.58770000 | 3.64710000 |
| H | 2.81560000 | 0.74780000 | -2.31120000 |
| H | 4.79950000 | 2.05600000 | -1.54220000 |
| H | 5.25210000 | 2.24340000 | 0.93990000 |
| H | 3.81710000 | 0.97720000 | 2.52710000 |
| N | 2.25110000 | 0.19540000 | -0.37420000 |
| N | 0.53690000 | -1.06220000 | 1.12020000 |
| H | 1.28470000 | 2.47350000 | 0.13930000 |
| C | 0.19110000 | 2.44030000 | 0.10910000 |
| C | -0.57420000 | 3.58510000 | 0.38260000 |
| C | -1.95590000 | 3.51930000 | 0.32140000 |
| H | -0.08480000 | 4.52820000 | 0.65010000 |
| C | -1.73260000 | 1.19200000 | -0.30200000 |
| C | -2.57230000 | 2.29710000 | -0.02050000 |
| H | -2.56640000 | 4.41270000 | 0.50750000 |
| C | -2.28970000 | -0.04330000 | -0.73150000 |
| C | -3.98170000 | 2.12750000 | -0.11290000 |
| C | -3.68260000 | -0.15870000 | -0.92740000 |
| C | -4.50700000 | 0.94570000 | -0.57330000 |
| H | -4.63830000 | 2.95310000 | 0.19490000 |
| C | -4.18100000 | -1.36380000 | -1.46590000 |
| C | -1.93750000 | -2.24090000 | -1.48870000 |
| H | -5.58410000 | 0.81390000 | -0.68400000 |
| C | -3.30600000 | -2.41000000 | -1.72240000 |
| H | -5.25220000 | -1.44700000 | -1.69410000 |
| H | -1.21080000 | -3.02820000 | -1.71440000 |

| | | | |
|---|---|---|---|
| H | -3.67990000 | -3.37220000 | -2.09960000 |
| N | -0.37960000 | 1.27110000 | -0.22380000 |
| N | -1.44280000 | -1.07750000 | -1.00760000 |
| Fe | 0.50740000 | -0.64460000 | -0.84500000 |
| Cl | 0.50280000 | 0.09940000 | -2.88880000 |
| Cl | 1.28350000 | -2.70750000 | -1.22940000 |

**$[Ni(bipy)(phen)Cl]^{+}$-Y**

| | | | |
|---|---|---|---|
| O | -7.22680000 | 1.39420000 | 1.92100000 |
| O | 5.75100000 | -2.23830000 | 4.09210000 |
| O | 5.01550000 | 5.08630000 | 2.11340000 |
| O | -1.49210000 | 2.08580000 | -6.76470000 |
| O | -4.45080000 | -0.03860000 | 5.71100000 |
| O | 1.90910000 | 5.59960000 | 4.41840000 |
| O | 4.15440000 | -0.52850000 | -6.01890000 |
| O | 6.77110000 | -2.15880000 | -2.21880000 |
| O | -5.48160000 | 2.84200000 | -3.99910000 |
| O | -5.16460000 | -5.10120000 | -1.38590000 |
| O | -0.83850000 | 7.02860000 | 0.48740000 |
| O | -5.23630000 | 5.06940000 | -0.80190000 |
| O | -7.48260000 | -0.84650000 | -1.24360000 |
| O | 2.22670000 | 6.54780000 | -1.82610000 |
| O | -3.28000000 | -6.36890000 | 1.76920000 |
| O | 0.07040000 | 1.95070000 | 6.90260000 |
| O | -2.86350000 | -3.59080000 | 5.65580000 |
| O | 0.87220000 | -6.96670000 | -0.98830000 |
| O | 1.64340000 | -1.58290000 | 6.74660000 |
| O | 0.84090000 | -2.29170000 | -6.98530000 |

| | | | |
|---|---|---|---|
| O | 1.85550000 | 3.91470000 | -5.88880000 |
| O | 7.06620000 | 0.70370000 | 1.90790000 |
| O | 5.32410000 | -5.05110000 | 0.01680000 |
| O | -0.99820000 | -5.79100000 | -4.18680000 |
| O | -8.59950000 | 1.44560000 | -0.39500000 |
| O | 7.93910000 | -1.74670000 | 2.59330000 |
| O | 3.50240000 | 7.16720000 | 2.92420000 |
| O | 0.86330000 | 2.55420000 | -7.99310000 |
| O | -3.26060000 | -1.67030000 | 7.49730000 |
| O | 7.66170000 | -3.71920000 | -0.21570000 |
| O | -7.21500000 | 3.97890000 | -2.28210000 |
| O | -4.03510000 | -7.40950000 | -0.59540000 |
| O | 1.59260000 | 8.16850000 | 0.21770000 |
| O | -0.19840000 | -0.34230000 | 8.27260000 |
| O | -1.19510000 | -7.85540000 | -2.47020000 |
| O | 2.48970000 | -0.48780000 | -8.12110000 |
| O | 3.12240000 | -3.01160000 | -5.80240000 |
| O | -3.92970000 | 4.90500000 | -3.13260000 |
| O | -7.16260000 | -1.22410000 | 1.42080000 |
| O | -0.44920000 | 6.66790000 | -2.14360000 |
| O | -5.41900000 | -4.83910000 | 1.29130000 |
| O | 2.54710000 | 0.94790000 | 6.58410000 |
| O | -5.06970000 | -2.43710000 | 4.66830000 |
| O | 4.17430000 | 4.19810000 | 4.47970000 |
| O | 5.02250000 | -4.23560000 | -2.53860000 |
| O | 5.77280000 | 0.45110000 | 4.27450000 |
| O | -0.76350000 | 4.38630000 | -5.57500000 |

| | | | |
|---|---|---|---|
| O | 1.55680000 | -6.00500000 | -3.40790000 |
| O | -7.05050000 | 3.51880000 | 0.36820000 |
| O | 6.37930000 | -3.88920000 | 2.13600000 |
| O | 3.84120000 | 6.64940000 | 0.29800000 |
| O | -0.12400000 | 0.04250000 | -7.74210000 |
| O | -2.35280000 | 0.85110000 | 7.12850000 |
| O | 0.81300000 | 7.12980000 | 2.57740000 |
| O | 5.20870000 | -2.29580000 | -4.34560000 |
| O | 7.73450000 | -1.01530000 | -0.01470000 |
| O | -7.26370000 | 1.31070000 | -2.75270000 |
| O | -3.21380000 | 3.42620000 | -5.22680000 |
| O | -3.31640000 | -6.24720000 | -2.93980000 |
| O | -6.65330000 | -3.16150000 | -0.33110000 |
| O | -2.84890000 | 6.23670000 | -1.09250000 |
| O | 1.07020000 | 5.60810000 | -4.03390000 |
| O | -4.15240000 | -4.70110000 | 3.62420000 |
| O | 2.02210000 | 3.45180000 | 5.91940000 |
| O | -0.78390000 | -2.66700000 | 7.03180000 |
| O | 5.96390000 | 2.79880000 | 3.09420000 |
| O | -1.45640000 | -7.47360000 | 0.19690000 |
| O | 4.02870000 | -1.02990000 | 5.66890000 |
| O | 3.14230000 | 1.78780000 | -6.80120000 |
| O | -6.24390000 | -0.26250000 | 3.73360000 |
| O | 0.91530000 | -4.45860000 | -5.47030000 |
| O | 3.29990000 | -5.94260000 | -1.41120000 |
| Si | -8.07420000 | 2.33890000 | 0.87800000 |
| Si | 7.01650000 | -2.91760000 | 3.29150000 |

| | | | |
|---|---|---|---|
| Si | 4.54520000 | 6.62590000 | 1.78330000 |
| Si | -0.47880000 | 1.62270000 | -7.97280000 |
| Si | -3.67530000 | -0.12440000 | 7.15570000 |
| Si | 2.04030000 | 7.04390000 | 3.66210000 |
| Si | 4.49720000 | -2.13150000 | -5.80590000 |
| Si | 7.88770000 | -2.31940000 | -1.01660000 |
| Si | -7.01620000 | 2.80350000 | -3.39990000 |
| Si | -4.47740000 | 4.08650000 | -4.42700000 |
| Si | -4.54290000 | -6.53930000 | -1.88510000 |
| Si | 0.32750000 | 7.91560000 | 1.22730000 |
| Si | -6.82000000 | 4.62370000 | -0.82470000 |
| Si | -7.63800000 | -1.90650000 | 0.01910000 |
| Si | -8.26210000 | 0.52570000 | -1.70350000 |
| Si | -4.24620000 | 5.88250000 | -1.85010000 |
| Si | 0.99070000 | 6.78650000 | -2.90920000 |
| Si | -4.63720000 | -5.70110000 | 2.44230000 |
| Si | 1.69510000 | 2.27710000 | 6.99940000 |
| Si | -2.38960000 | -3.00540000 | 7.10950000 |
| Si | -4.36180000 | -3.87210000 | 5.00320000 |
| Si | -0.91140000 | 1.07890000 | 7.88550000 |
| Si | -6.19000000 | -4.71400000 | -0.13980000 |
| Si | 5.47690000 | 4.29600000 | 3.49640000 |
| Si | 6.04200000 | -3.20050000 | -3.27570000 |
| Si | -0.45290000 | -7.93390000 | -1.01180000 |
| Si | 5.55560000 | -0.95120000 | 5.10080000 |
| Si | 0.38390000 | -1.79110000 | 7.77850000 |
| Si | 3.66740000 | 0.33070000 | -7.33130000 |

| | | | |
|---|---|---|---|
| Si | 2.82300000 | 7.52570000 | -0.64990000 |
| Si | -5.67190000 | -0.97640000 | 5.08210000 |
| Si | 0.97880000 | -1.11630000 | -8.11450000 |
| Si | 0.72440000 | 5.06790000 | -5.52320000 |
| Si | 1.77310000 | -3.58250000 | -6.53380000 |
| Si | 2.22880000 | 3.07960000 | -7.24750000 |
| Si | 2.09860000 | -6.81100000 | -2.09310000 |
| Si | -1.52000000 | 7.18330000 | -1.01690000 |
| Si | -7.40140000 | -0.10380000 | 2.59930000 |
| Si | 8.08250000 | -0.53330000 | 1.51680000 |
| Si | 4.86770000 | -5.49800000 | -1.49860000 |
| Si | 6.75430000 | 1.39910000 | 3.37850000 |
| Si | 6.74960000 | -4.68600000 | 0.75010000 |
| Si | 2.90530000 | 4.70060000 | 5.38180000 |
| Si | 0.57870000 | -5.85160000 | -4.70790000 |
| Si | -1.98370000 | -6.95840000 | -3.59140000 |
| Si | -1.99430000 | 3.58960000 | -6.29190000 |
| Si | 2.98320000 | -0.60750000 | 6.84740000 |
| Si | -3.02160000 | -7.56310000 | 0.68330000 |
| O | -4.76950000 | 0.39790000 | 8.28080000 |
| H | -4.40860000 | 0.79580000 | 9.08900000 |
| O | -6.82760000 | -1.25700000 | 6.22980000 |
| H | -6.93980000 | -0.56200000 | 6.90070000 |
| O | -8.93880000 | -0.25020000 | 3.19870000 |
| H | -9.45140000 | -0.97350000 | 2.79750000 |
| O | -5.25710000 | -4.68560000 | 6.13630000 |
| H | -6.11600000 | -4.27770000 | 6.33900000 |

| | | | |
|---|---|---|---|
| O | -2.56590000 | -4.12890000 | 8.30560000 |
| H | -3.37340000 | -4.66740000 | 8.24720000 |
| O | -5.61020000 | -6.93430000 | 2.96900000 |
| H | -6.51640000 | -6.90600000 | 2.61790000 |
| O | -3.21890000 | -9.05800000 | 1.35420000 |
| H | -3.95840000 | -9.13810000 | 1.97980000 |
| O | 0.09000000 | -9.47900000 | -0.77700000 |
| H | -0.48760000 | -10.06690000 | -0.26440000 |
| O | 2.56440000 | -8.29920000 | -2.64450000 |
| H | 2.47280000 | -9.03570000 | -2.01580000 |
| O | 5.86400000 | -6.72190000 | -2.00330000 |
| H | 6.35690000 | -6.52080000 | -2.81790000 |
| O | 7.59040000 | -6.05270000 | 1.10520000 |
| H | 7.52500000 | -6.76270000 | 0.44530000 |
| O | 9.40750000 | -2.39560000 | -1.66490000 |
| H | 9.76260000 | -1.56310000 | -2.01330000 |
| O | 9.64910000 | 0.00260000 | 1.64930000 |
| H | 9.95890000 | 0.57220000 | 0.92760000 |
| O | 8.15150000 | 1.56300000 | 4.25140000 |
| H | 8.98030000 | 1.58660000 | 3.74410000 |
| O | 6.68230000 | 5.13820000 | 4.24630000 |
| H | 7.01100000 | 5.91110000 | 3.75620000 |
| O | 5.93270000 | 7.52270000 | 1.85330000 |
| H | 5.87850000 | 8.45270000 | 1.58190000 |
| O | -0.35320000 | 9.37780000 | 1.59310000 |
| H | -0.10250000 | 9.76910000 | 2.44540000 |
| O | 1.84930000 | 8.31730000 | 4.69360000 |

| | | | |
|---|---|---|---|
| H | 2.28630000 | 8.21850000 | 5.55650000 |
| O | 3.39400000 | 5.67280000 | 6.62900000 |
| H | 3.39210000 | 5.27070000 | 7.51300000 |
| O | 2.10030000 | 2.75660000 | 8.53970000 |
| H | 2.70180000 | 2.13710000 | 8.99010000 |
| O | -1.25240000 | 1.90100000 | 9.27660000 |
| H | -0.50200000 | 2.36480000 | 9.68360000 |
| O | 5.43690000 | -2.67100000 | -7.05730000 |
| H | 5.86970000 | -1.97360000 | -7.58050000 |
| O | 4.99560000 | 0.44300000 | -8.31190000 |
| H | 4.98000000 | 1.11760000 | -9.00950000 |
| O | 3.11860000 | 3.97080000 | -8.31210000 |
| H | 2.82290000 | 4.88850000 | -8.43460000 |
| O | 0.63300000 | -1.67170000 | -9.62860000 |
| H | 0.92040000 | -2.58380000 | -9.80440000 |
| O | 2.17390000 | -4.40710000 | -7.91360000 |
| H | 3.11190000 | -4.64790000 | -7.99280000 |
| O | -1.32750000 | 1.90600000 | -9.36680000 |
| H | -0.99490000 | 1.50860000 | -10.18710000 |
| O | 0.85680000 | 6.28660000 | -6.63620000 |
| H | 0.99370000 | 7.17720000 | -6.27320000 |
| O | -2.55490000 | 4.43180000 | -7.60420000 |
| H | -2.49920000 | 3.95540000 | -8.45210000 |
| O | -5.28030000 | 5.17300000 | -5.39610000 |
| H | -5.02540000 | 5.14000000 | -6.33430000 |
| O | -8.15650000 | 2.99020000 | -4.58010000 |
| H | -8.16850000 | 3.85460000 | -5.02210000 |

| | | | |
|---|---|---|---|
| O | -9.37230000 | 3.02500000 | 1.62290000 |
| H | -9.80940000 | 2.46030000 | 2.28210000 |
| O | -9.67160000 | 0.04930000 | -2.42160000 |
| H | -10.10400000 | 0.69630000 | -3.00180000 |
| O | -9.22730000 | -2.32050000 | 0.24660000 |
| H | -9.77830000 | -2.34400000 | -0.55380000 |
| O | -7.45150000 | -5.78540000 | -0.09350000 |
| H | -7.66720000 | -6.21740000 | -0.93790000 |
| O | -5.78080000 | -7.35240000 | -2.62010000 |
| H | -5.54270000 | -7.91420000 | -3.37510000 |
| O | -2.52630000 | -7.95510000 | -4.79050000 |
| H | -1.86470000 | -8.18190000 | -5.46590000 |
| O | 0.74900000 | -7.17790000 | -5.68920000 |
| H | 1.41480000 | -7.81540000 | -5.37820000 |
| O | -7.78060000 | 5.93260000 | -0.54900000 |
| H | -7.43880000 | 6.77180000 | -0.89950000 |
| O | -5.05150000 | 7.23610000 | -2.36450000 |
| H | -5.09750000 | 7.34320000 | -3.32940000 |
| O | -1.80070000 | 8.77500000 | -1.36500000 |
| H | -2.03000000 | 9.34540000 | -0.61120000 |
| O | 0.98060000 | -2.59840000 | 9.09240000 |
| H | 0.39230000 | -3.25620000 | 9.49680000 |
| O | 3.60420000 | -0.64270000 | 8.37950000 |
| H | 3.53230000 | -1.48950000 | 8.85230000 |
| O | 6.69370000 | -1.04350000 | 6.30280000 |
| H | 7.28080000 | -0.26980000 | 6.35470000 |
| O | 7.95200000 | -3.80610000 | 4.31030000 |

| | | | |
|---|---|---|---|
| H | 8.04410000 | -3.44340000 | 5.20710000 |
| O | 7.17450000 | -4.18600000 | -3.98350000 |
| H | 8.03360000 | -3.79010000 | -4.19950000 |
| O | 3.71580000 | 8.75690000 | -1.29200000 |
| H | 3.35340000 | 9.16030000 | -2.09800000 |
| O | 1.13580000 | 8.28090000 | -3.62620000 |
| H | 0.40680000 | 8.88820000 | -3.40760000 |
| C | 2.51510000 | 0.82620000 | -0.45810000 |
| C | 2.25830000 | 0.32280000 | 1.83500000 |
| C | 3.41440000 | 1.03490000 | 2.13730000 |
| C | 4.12640000 | 1.65450000 | 1.11110000 |
| C | 3.67530000 | 1.53880000 | -0.19830000 |
| C | 1.93870000 | 0.63910000 | -1.76970000 |
| C | 0.13400000 | -0.32240000 | -2.94210000 |
| C | 0.63240000 | 0.14630000 | -4.15320000 |
| C | 1.81870000 | 0.87900000 | -4.15280000 |
| C | 2.47420000 | 1.12590000 | -2.95230000 |
| H | 1.68010000 | -0.21510000 | 2.59310000 |
| H | 3.75750000 | 1.08360000 | 3.17850000 |
| H | 5.02780000 | 2.23170000 | 1.33540000 |
| H | 4.22800000 | 2.01050000 | -1.01390000 |
| H | -0.78430000 | -0.91180000 | -2.90030000 |
| H | 0.08340000 | -0.07450000 | -5.07820000 |
| H | 2.26920000 | 1.27030000 | -5.07020000 |
| H | 3.40640000 | 1.69520000 | -2.94780000 |
| N | 0.77720000 | -0.08330000 | -1.77730000 |
| N | 1.81720000 | 0.23180000 | 0.56030000 |

| | | | |
|---|---|---|---|
| H | 0.19570000 | 2.34470000 | 1.12970000 |
| C | -0.79840000 | 2.11520000 | 0.73410000 |
| C | -1.83720000 | 3.06320000 | 0.74530000 |
| C | -3.08950000 | 2.73070000 | 0.25120000 |
| H | -1.64250000 | 4.06370000 | 1.14840000 |
| C | -2.21670000 | 0.54180000 | -0.25090000 |
| C | -3.30690000 | 1.43420000 | -0.26670000 |
| H | -3.90990000 | 3.46570000 | 0.26010000 |
| C | -2.34340000 | -0.77420000 | -0.74790000 |
| C | -4.53090000 | 0.96360000 | -0.82800000 |
| C | -3.55830000 | -1.21990000 | -1.29850000 |
| C | -4.64800000 | -0.30100000 | -1.33910000 |
| H | -5.38650000 | 1.64880000 | -0.84280000 |
| C | -3.59830000 | -2.54350000 | -1.78340000 |
| C | -1.28250000 | -2.83360000 | -1.14090000 |
| H | -5.60050000 | -0.63350000 | -1.76960000 |
| C | -2.46070000 | -3.33240000 | -1.71460000 |
| H | -4.52490000 | -2.96410000 | -2.19240000 |
| H | -0.38110000 | -3.44520000 | -1.03240000 |
| H | -2.47980000 | -4.34480000 | -2.13450000 |
| N | -0.99590000 | 0.88940000 | 0.23600000 |
| N | -1.23860000 | -1.57310000 | -0.68390000 |
| Ni | 0.24890000 | -0.64270000 | -0.02390000 |
| Cl | 0.02710000 | -1.79470000 | 1.78950000 |