

AM1* parameters for cobalt and nickel

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Abstract: We report the parameterization of AM1* for the elements Co and Ni. The basis sets for both metals contain one set each of s-, p- and d orbitals. AM1* parameters are now available for H, C, N, O and F (which use the original AM1 parameters), Al, Si, P, S, Cl, Ti, V, Cr, Co, Ni, Cu, Zn, Br, Zr, Mo and I. The performance and typical errors of AM1* are discussed for Co and Ni and compared with available NDDO Hamiltonians.

Response to Reviewers: Dear Andrzej,

we have revised our manuscript in accord with the referees' comments as follows:

Reviewer 1:
1. "Phtalocyanine" has been corrected throughout
2. "Co#P" has been corrected to Co P
3. nickel dimethylglyoxime is now mentioned by name
4. The error for CoTi has been reduced to zero, but this cannot be done for CoZr. This is because the two variables are not independent (i.e. there is not necessarily a combination of the two that gives zero errors in Heat of Formation and Bond length)

I trust the paper will now be acceptable for publication.

Best wishes
Tim

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AM1* parameters for cobalt and nickel

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Abstract

We report the parameterization of AM1* for the elements Co and Ni. The basis sets for both metals contain one set each of *s*-, *p*- and *d*-orbitals. AM1* parameters are now available for H, C, N, O and F (which use the original AM1 parameters), Al, Si, P, S, Cl, Ti, V, Cr, Co, Ni, Cu, Zn, Br, Zr, Mo and I. The performance and typical errors of AM1* are discussed for Co and Ni and compared with available NDDO Hamiltonians.

Keywords AM1* · Cobalt parameters · Nickel parameters · Semiempirical MO-theory

Introduction

AM1* [1-5] is an extension of AM1 [6] that uses *d*-orbitals for the elements P, S, Cl, [1] Al, Si, Ti and Zr, [2] Cu and Zn, [3] Br and I, [4] V and Cr [5]. The AM1* molybdenum parameters are a slight modification of Voityuk and Rösch's AM1(d) parameter set [7]. AM1* retains the original AM1 parameters for the elements H, C, N, O and F. The intention is to provide a technique that has the advantages of AM1 for first-row elements, such as good energies for hydrogen bonds, higher rotation barriers for π-systems than MNDO [8, 9] or PM3 [10-12] but performs better for heavier elements and to be applicable to the first row transition metals. As a continuation of this work, we now report AM1* parameters for cobalt and nickel. Both cobalt and nickel are important in the chemistry of organometallic and biological catalysts [13, 14]. Because the experimental data for heats of formation of compounds of these two metals are relatively sparse, we have also used a series of model compounds whose heats of formation we have derived from DFT calculations [15].

Theory

AM1* for the two new elements uses the same basic theory as outlined previously [1, 2]. As for other element-H interactions, the core-core repulsion potential for the Co-H and Ni-H interactions used a distance-dependent term δ_{ij}, rather than the constant term used for core-core potentials for most other interactions in AM1* [1]. This distance-dependent δ_{ij} was also used for the Mo-H and interaction in AM1(d) [7] and for Ti-H, V-H, Cr-H, Cu-H, Zn-H, Br-H, Zr-H, Mo-H and I-H in AM1* [2-5]. The core-core terms for Co-H and Ni-H are thus:

$$E^{core}(i-j) = Z_i Z_j \rho_{ss}^0 \left[1 + r_{ij}\delta_{ij} \exp\left(-\alpha_{ij} r_{ij}\right)\right] \qquad (1)$$

where all terms have the same meaning as given in reference [1].

The standard MNDO/d formula is used for all other core-core interactions:

$$E^{core}(i-j) = Z_i Z_j \rho_{ss}^0 \left[1 + \delta_{ij} \exp\left(-\alpha_{ij} r_{ij}\right)\right] \qquad (2)$$

The parameterization techniques were those reported in references [1] and [2] and will not be described further here.

Parameterization data

The target values used for parameterization and their sources are defined in Table S1 of the Supplementary Material. We have used both reaction energies and heats of formation as we did for the Ti, Zr, Cu, Zn, Br, I, V and Cr parameterizations [2-5] and have also used a small series of model compounds whose heats of formation we have derived from DFT calculations. As before, [1-5] we checked that experimental values for heats of formation were reasonable using DFT calculations.

DFT calculations used the Gaussian 03 suite of programs [16] with the LANL2DZ basis set and standard effective core potentials [17-20] augmented by a set of polarization functions [21] (designated LANL2DZ+pol) and the B3LYP hybrid functional [22-24].

Experimental parameterization data for cobalt and nickel were taken largely from the NIST Webbook, [25] but also from the OpenMopac collection [26] and the other experimental and theoretical sources given in the Supplementary Material.

The energetic parameterization data and their sources are given in Table S1 of the Supplementary Material. In addition to the energetic data, geometries, dipole moments and ionization potentials taken from the above sources, crystal structures from the Cambridge Structural Database (CSD) [27] were used in the parameterization to ensure that not only the energetic and electronic properties for the "prototype" compounds, but also the structures of large cobalt and nickel compounds are well produced.

Results

The optimized AM1* parameters are shown in Table 1. Geometries were optimized with the new AM1* parameterization using VAMP 10.0, [28] while the PM5 calculations used LinMOPAC2.0 [29] and those with PM6 used MOPAC2007 [30]. The three programs give essentially identical results for the Hamiltonians that are available in all three.

- Table 1 about here -

Cobalt

Heats of formation

The calculated heats of formation for our training set of cobalt compounds are shown in Table 2. We have compared our results with Stewart's recently published PM6 method [31] and also unpublished PM5 method implemented in LinMopac [29].

- Table 2 about here -

AM1* reproduces the heats of formation of the training set of cobalt compounds used in parameterization better than either PM6 or PM5. The mean unsigned error (MUE) for the AM1* parameterization dataset is 20.5 kcal mol^{-1}, compared with 61.9 and 84.3 kcal mol^{-1} for PM6 and PM5, respectively. PM6 produces large errors for the compounds that were not included in its original training set. The parameterization data set for PM5 has not been published, but clearly does not cover the range of compounds used for AM1*. All three methods tend to underestimate heats of formation to cobalt-containing compounds. However, this tendency is less pronounced for AM1* (mean signed error (MSE) -7.4 kcal mol^{-1}) than PM6 and PM5 (MSEs of -48.6 and -70.8 kcal mol^{-1}, respectively).

The largest single positive error for AM1* is found for Co^{+} (108.4 kcal mol^{-1}). This is potentially disturbing as the ionization potential of Co is an important determinant of the reactivity of cobalt centers. However, we cannot detect serious systematic trends caused by this error. Molecules that give the largest positive errors are $C_{10}H_{15}NS_2CoI$ (GECVEP) (52.0 kcal mol^{-1}), $CoC_9N_4H_{19}O_5$ (AMGXCO01) (39.3 kcal mol^{-1}) and $CoCl_2$ (33.8 kcal mol^{-1}). The largest negative errors are found for $Co(H_2O)_6^{2+}$ (-110.0 kcal mol^{-1}), CoO^{-} (-75.5 kcal mol^{-1}),

CoOBr (-68.6 kcal mol^{-1}) and $HCoPH_2$ (-53.2 kcal mol^{-1}). The large negative errors with oxygen-containing compounds are not surprising as we have pointed out in our previous parameterizations [5]. AM1* uses the unchanged AM1 parameterization for the elements H, C, N, O and F, which limits the possible accuracy of the parameterization. In this respect, the heats of formation of $Co(H_2O)_6^{2+}$ and $Co(H_2O)_4^{4+}$ agree remarkably well with experiment considering the large AM1* errors for Co^{2+} and Co^{4+} (see below). As found for other metals, the large errors in pure AM1* element-containing compounds is likely to be a consequence of our sequential parameterization strategy, in contrast to the simultaneous parameterization used for PM6 [31].

Not only AM1* gives very large errors for cobalt di-, tri-, tetra- and penta-cations (not shown in Table 2 and not included in the statistics), but also PM6 and PM5. AM1* errors are found to be 143.0 kcal mol^{-1} (-96.5 and 119.6 kcal mol^{-1} for PM6 and PM5, respectively) for Co^{2+}, 131.8 kcal mol^{-1} (-545.6 and -126.7 kcal mol^{-1} for PM6 and PM5, respectively) for Co^{3+}, -56.8 kcal mol^{-1} (-1356.1 and -335.6 kcal mol^{-1} for PM6 and PM5, respectively) for Co^{4+} and -704.5 kcal mol^{-1} (-2758.8 and -902.8 kcal mol^{-1} for PM6 and PM5, respectively) for Co^{5+}. Experimental heats of formation of these cations are given in Table S1 of the Supplementary Material. Nonetheless, on aggregate AM1* performs better than the other available methods for the heats of formation of cobalt compounds.

Table 2, however, also shows the performance of the three methods for only the PM6 parameterization dataset [31]. These data demonstrate the influence of the extent of the training data. AM1* performs approximately equally well for its own training set and for the subset used to parameterize PM6, whereas PM6 performs significantly better for the subset for which it was trained. This situation is unavoidable and is a direct consequence of the relative paucity of data for parameterizing semiempirical MO techniques for transition metals.

Ionization potentials and dipole moments

A comparison of the calculated and experimental Koopmans' theorem ionization potentials and dipole moments for AM1*, PM6 and PM5 are shown in Table 3.

- Table 3 about here -

The performance of the three methods is comparable. The mean unsigned errors vary in a relatively small range from 0.99 (PM5) to 1.50 eV (PM6). The AM1* MUE, 1.23 eV, lies in the middle of this range. With an MSE of -0.16 eV, AM1* tends to underestimate ionization potentials slightly, whereas PM6 and PM5 overestimate them by 0.80 and 0.41 eV, respectively.

Large AM1* errors are found for $CoCl_2$ (-2.10 eV), $CoCH_3$ (1.88 eV), $CoC_{10}H_{10}$ (1.87 eV) and $Co(CO)_8$ (-1.54 eV). The large error for $CoCl_2$ may originate from a general weakness in the original chlorine parameterization, whereas the others may be an indirect result of using the original AM1 parameters for hydrogen, carbon and oxygen.

AM1* and PM5 show positive systematic errors for the dipole moments of cobalt compounds, whereas PM6 with 0.03 Debye (MSE) shows no tendency to systematic errors. AM1* and PM5 overestimate dipole moments by 0.34 and 1.13 Debye (MSE), respectively. AM1* performs well, with an MUE of 0.69 Debye for the dipole moments of the training set of cobalt compounds. The largest AM1* errors are found for CoI (2.76 Debye) and CoBr (-1.77 Debye). These errors may be a consequence of our sequential parameterization strategy. The MUEs for PM6 and PM5 are found to be 1.03 and 1.76 Debye, respectively.

Geometries

Table 4 shows a comparison of AM1*, PM6 and PM5 results in reproducing the geometries of the cobalt-containing compounds.

- Table 4 about here -

AM1* and PM5 overestimate bond lengths to cobalt-containing compounds systematically by 0.04 and 0.36 Å, respectively, whereas PM6 underestimates them by 0.03 Å. AM1*, with an MUE of 0.08 Å performs quite well for bond lengths, compared with MUEs of 0.16 Å and 0.51 Å for PM6 and PM5, respectively. On the other hand, PM6 (MUE=7.1°) performs slightly better than AM1* (MUE=9.3°) and far better than PM5 (MUE=16.7°) for the bond angles. In general, AM1* gives bond angles for cobalt-containing that are on average 1.5° too small, whereas PM6 and PM5 give bond angles are too large by 4.0° and 5.1°, respectively.

Nickel

Heats of formation

The results obtained for heats of formation of nickel-containing compounds are shown in Table 5.

- Table 5 about here -

Table 5 shows that, for the training set used, AM1* reproduces heats of formation of nickel-containing compounds slightly better than PM6 and far better than PM5. The mean unsigned error between target and AM1*-calculated heats of formation is 21.5 kcal mol^{-1}. For PM6 and PM5, the MUEs are found 27.3 and 53.0 kcal mol^{-1}, respectively. AM1* and PM6 underestimate heats of formation to nickel compounds by 6.7 and 4.3 kcal mol^{-1}, respectively (MSEs). PM5 systematically predicts heats of formation to be too positive with a mean signed error of 21.0 kcal mol^{-1}. The largest positive errors for AM1* are found for the compounds $NiC_{11}N_2H_{21}S_2O_2^+$ (53.6 kcal mol^{-1}), $Ni(H_2S)_4^{2+}$ (53.1 kcal mol^{-1}), NiH^+ (50.6 kcal mol^{-1}), NiCO (48.0 kcal mol^{-1}) and nickel dimethylglyoxime ($NiC_8N_4H_{14}O_4$, NIMGLO01) (42.0 kcal mol^{-1}). The largest negative errors for AM1* are found for $Ni(CN)_5^{3-}$ (-108.4 kcal mol^{-1}), $NiC_2N_3S_3^{2-}$ (CUSJUV) (-79.1 kcal mol^{-1}), $Ni(CN)_4^{2-}$ (-73.7 kcal mol^{-1}). AM1* also gives negative errors for the chlorinated compounds $NiCH_3Cl$, $NiCl_2O$, *cis*- and *trans*-$NiCl_2.(H_2O)_2$ and *cis*- and *trans*-$Ni((CH_3)_2S)_2Cl_2$ more than 30 kcal mol^{-1}. Large errors in AM1* are given by the compounds that contain original AM1 elements or AM1 elements with sulfur, and also from the chlorinated compounds. We attribute this to a weakness in the AM1* parameterization for the chlorine and the sulfur, and also general weakness of the original AM1 parameterization.

Once again, Table 5 shows the results obtained with the three methods for the PM6 training set [31]. AM1* systematically gives heats of formation that are too negative (MSE = -12 kcal mol^{-1}), but otherwise performs similarly for the PM6 subset and the complete dataset. PM6 clearly gives some additional outliers with the AM1* training set that decrease its statistical performance a little, whereas PM5 actually performs slightly better for the AM1* dataset than for the PM6 subset (but worse than the other two methods).

Ionization potentials and dipole moments

A comparison of the calculated and experimental Koopmans' theorem ionization potentials and dipole moments for the compounds containing nickel are shown in Table 6.

- Table 6 about here -

AM1* shows no systematic error-trend in the reproduction of Koopmans' theorem ionization potentials of nickel-containing compounds for the dataset used. PM6 underestimates ionization potentials to nickel compounds by 1.09 eV, whereas PM5 overestimates them by 0.73 eV. AM1* performs slightly better than PM6 (MUE=1.43 eV) and PM5 (1.83 eV) with an MUE of 1.17 eV.

The performance of the three methods is comparable for dipole moments. The mean unsigned errors vary in a narrow range from 1.73 (PM6) to 1.89 Debye (AM1*). The PM5 MUE is found to be 1.82 Debye. All three methods systematically underestimate dipole moments of nickel compounds. Mean signed errors are found to be -0.52, -0.82 and –0.89 Debye for PM5, AM1* and PM6, respectively. All the large AM1* errors are found for the compounds either contain original AM1 elements or chlorine.

Geometries

The geometrical parameters used to parameterize AM1* for nickel and a comparison of the AM1*, PM6 and PM5 results are shown in Table 7.

- Table 7 about here -

AM1* with a mean unsigned error of 0.09 Å performs slightly better than PM6 (MUE=0.11 Å) and far better than PM5 (MUE=0.33 Å) for bond lengths to nickel compounds. PM6 (MSE=0.01 Å) and AM1* (MSE=0.04 Å) show no significant systematic trend, whereas PM5 (MSE=0.24) seriously overestimates bond lengths to nickel.

The performance of AM1* for bond angles to nickel compounds is comparable to PM6 and better than PM5. The MUEs for AM1* and PM6 are 10.2° and 10.7°, respectively, and for PM5 15.9°. AM1* shows no significant systematic error with an MSE of 0.2°, whereas PM6 (MSE=-5.1°) and PM5 (MSE=-4.6°) predict the bond angles to be too small.

Discussion

Our new AM1* parameters for cobalt and nickel provide important additional elements especially for catalytic chemistry applications based on organometallic compounds of the two metals. As for our previous parameterizations, we have extended the range of the parameterization dataset and made it more reliable by including results from DFT calculations. For the training set used, AM1* parameterizations for cobalt and nickel give good energetic and electronic results. Additionally, AM1* performs very well for the structural properties.

As published NDDO-based semiempirical molecular orbital techniques that use *d*-orbitals, both AM1* and PM6 have very similar theoretical frameworks and provide a good opportunity to carry out comparative calculations for many different applications and provide good starting points for the reaction-specific local parameterizations. As for all semiempirical methods, AM1* and PM6 are likely to give large errors that were not revealed during parameterization. This is illustrated well by comparing their performance for the dataset used to parameterize PM6. The additional compounds in the AM1* dataset give slightly larger errors with PM6. The availability of two independently parameterized techniques of similar quality should, however, provide an additional validation possibility for semiempirical MO calculations on transition metal species.

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Supplementary material

The values and the sources of the parameterization data.

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Table 1 AM1* parameters for the elements Co and Ni

Parameter	Co	Ni
U_{ss} [eV]	-147.9969721	-47.9262400
U_{pp} [eV]	-75.4376929	-33.5123050
U_{dd} [eV]	-85.9948020	-92.9262050
ζ_s [bohr^{-1}]	10.6559732	2.1694428
ζ_p [bohr^{-1}]	31.1355546	2.0212614
ζ_d [bohr^{-1}]	1.6662813	2.9999800
β_s [eV]	-94.1552039	-9.7800503
β_p [eV]	-126.5074725	-7.8215436
β_d [eV]	-15.8120720	-10.1277693
g_{ss} [eV]	5.7855014	4.0808760
g_{pp} [eV]	16.2498362	5.6217732
g_{sp} [eV]	10.4339713	6.0176787
g_{p2} [eV]	66.1182470	5.5014852
h_{sp} [eV]	2.9132649	2.1328830
z_{sn} [bohr^{-1}]	2.2158238	0.7464700
z_{pn} [bohr^{-1}]	1.4599934	0.4533270
z_{dn} [bohr^{-1}]	1.4576614	1.4613450
ρ(core) [bohr^{-1}]	1.6385615	1.3878582
$\Delta H°_f$(atom) [kcal mol^{-1}]	101.98	102.8
F^0_{sd} [eV]	7.9584630	4.6516640
G^2_{sd} [eV]	6.6939630	1.8805020
α(ij)		
H	3.7250884	3.9112954
C	3.3514488	3.0416771
N	3.2268224	3.3195694
O	3.9648169	2.6648814
F	4.7295078	2.8884516
Al	2.2854320	2.4006390
Si	2.5793441	3.8488001
P	1.9571093	1.9182580
S	2.4315562	1.2619302
Cl	2.5666738	3.7009365
Ti	2.5672155	2.2550000
V	1.8037355	2.8635660
Cr	1.8441671	2.5326653
Co	2.9455643	3.5988970
Ni	3.5988970	2.3078430
Cu	2.0999846	2.4949800
Zn	2.5946347	2.9100500
Br	3.2938616	2.5296864
Zr	1.9076098	2.1815542
Mo	1.7152160	2.3116050
I	2.9718264	2.6608247
δ(ij)		
H	-7.4149924	-14.3720184
C	8.8159639	4.8355503
N	4.5514730	8.3058789
O	12.7561475	1.8194408

F	36.8730508	2.1280313
Al	3.6287393	4.4492610
Si	3.6071357	37.3623757
P	1.9376263	1.2970389
S	1.8108567	0.1685772
Cl	2.4236274	21.3405907
Ti	3.4060864	4.7044000
V	2.4096866	11.2551742
Cr	1.5174067	3.0903718
Co	18.3120000	35.4531600
Ni	35.4531600	2.4076920
Cu	0.8291495	3.5090000
Zn	1.3844244	4.1615000
Br	12.7590650	3.2087055
Zr	1.3523255	6.9245885
Mo	1.8055727	3.7298645
I	11.9594831	2.9999300

Table 2 Calculated AM1*, PM6 and PM5 heats of formation and errors compared with our target values for the cobalt-containing compounds used to parameterize AM1* (all values kcal mol^{-1}). Errors are classified by coloring the boxes in which they appear. Green indicates errors lower than 10 kcal mol^{-1}, yellow 10-20 kcal mol^{-1} and pink those greater than 20 kcal mol^{-1}. The codenames within parentheses indicate the CSD-names of the compounds

	Target	AM1*		PM6		PM5	
Compound	**$\Delta H°_f$**	**$\Delta H°_f$**	**Error**	**$\Delta H°_f$**	**Error**	**$\Delta H°_f$**	**Error**
Co^-	86.2	83.3	-2.9	-84.2	-170.4	43.8	-42.4
Co	102.0	102.0	0.0	82.3	-19.7	91.4	-10.6
Co^+	281.5	389.9	108.4	304.1	22.6	292.6	11.1
Co_2	183.5	179.5	-4.0	-72.1	-255.6	114.5	-69.0
Co_2^-	137.6	146.8	9.2	-263.1	-400.7	121.1	-16.5
HCo	102.8	79.0	-23.8	50.5	-52.3	14.8	-87.9
HCo^-	98.5	67.6	-30.9	-52.0	-150.5	16.9	-81.6
$C_5H_5Co^-$	114.8	111.1	-3.7	10.0	-104.8	95.8	-19.0
$CoC_{10}H_{10}$	73.9	72.1	-1.8	52.4	-21.5	72.2	-1.7
$CoCp_2$ (DCYPCO)	52.0	72.2	20.2	51.2	-0.8	71.4	19.4
$CoC_6N_6H_{24}^{3+}$ (COTENC01)	587.5	587.8	0.3	557.2	-30.3	531.6	-55.9
$CoC_6N_6H_{24}^{2+}$ (QICSOK)	280.9	263.3	-17.6	284.9	4.0	228.4	-52.5
$CoC_9N_6H_{15}$ (FEFRUD)	58.2	85.3	27.1	68.4	10.2	-24.8	-83.0
CoO^-	36.6	-38.9	-75.5	-130.2	-166.8	-81.4	-118.0
CoO_2^-	-34.0	-5.0	29.1	-57.7	-23.7	-109.1	-75.1
$Co_2(H_2O)_4^{4+}$	1052.6	1009.7	-42.8	857.5	-195.1	839.0	-213.5
$Co(H_2O)_6^{2+}$	58.3	-51.7	-110.0	36.0	-22.3	-19.0	-77.3
$Co(CO)_4$	-134.3	-153.2	-18.9	-136.8	-2.5	-62.5	71.8
$CoH(CO)_4$	-136.0	-147.2	-11.2	-114.1	21.9	-152.2	-16.2
$Co(CO)_5^+$	4.1	-39.8	-43.9	33.4	29.3	38.2	34.1
$CoC_6O_{12}^{3-}$ (Co(iii)(ox)$_3$)	-542.2	-515.7	26.5	-532.3	9.9	-751.5	-209.3
$Co_2(CO)_8$	-283.0	-286.5	-3.5	-278.8	4.2	-253.6	29.4
$CoN_6H_{15}O_2^{2+}$ (FAMYEX)	252.3	211.0	-41.3	247.2	-5.1	254.2	1.9
$CoC_6N_4H_{16}O_4^+$ (AETXCO)	-93.9	-71.5	22.4	-68.0	25.9	-153.2	-59.3
$CoC_6N_4H_{16}O_4^+$ (OXENCO)	-96.0	-77.7	18.3	-74.8	21.2	-159.3	-63.3

$CoC_6N_6H_{18}O_4^+$ (NIXGEG)	27.9	26.3	-1.6	48.2	20.3	20.8	-7.1
$CoC_9N_4H_{19}O_5$ (AMGXCO01)	-131.7	-92.4	39.3	-123.3	8.4	-158.5	-26.8
$CoC_6N_6H_{20}O_6^+$ (NITNCO)	-39.2	-39.7	-0.5	-21.5	17.7	-123.3	-84.1
CoOF	-70.8	-85.9	-15.1	-32.6	38.2	-128.8	-58.0
CoF_2	-85.2	-85.2	0.0	-66.1	19.1	-85.4	-0.2
CoF_3	-139.6	-180.7	-41.1	-137.1	2.5	-95.3	44.3
CoF_4^-	-302.0	-297.9	4.1	-253.8	48.2	-238.7	63.3
$CoAlH_2$	125.9	92.4	-33.6	33.8	-92.1	49.7	-76.2
$HCoAlH_2$	160.3	131.7	-28.6	80.3	-80.0	10.6	-149.7
$CoSiH_3$	109.6	97.1	-12.5	32.2	-77.3	41.2	-68.4
CoP	131.2	131.3	0.0	79.3	-51.9	41.8	-89.5
$CoPH_2$	100.3	72.5	-27.8	17.0	-83.3	-127.9	-228.2
$HCoPH_2$	111.1	57.9	-53.2	38.6	-72.6	-68.1	-179.3
CoS	117.5	83.7	-33.8	20.8	-96.7	117.4	-0.1
CoSH	82.7	81.6	-1.1	4.7	-78.0	90.8	8.1
HCoSH	87.4	61.6	-25.8	4.9	-82.5	19.9	-67.4
$CoC_{10}H_{14}S_4$ (TACACO10)	-11.8	-1.9	9.9	-22.1	-10.3	-5.3	6.5
$CoC_9H_{21}S_6$ (MEDTCO10)	-65.7	-105.0	-39.3	-65.2	0.5	-72.6	-6.9
$CoC_3N_3H_6S_6$ (TDTCCO)	-24.9	-25.1	-0.2	-7.1	17.8	30.9	55.8
CoCl	46.1	45.6	-0.5	51.6	5.5	35.3	-10.8
CoClO	13.8	7.9	-5.9	0.3	-13.5	-44.5	-58.3
$CoCl_2$	-22.4	11.4	33.8	10.1	32.5	-38.8	-16.4
$CoCl_3$	-39.1	-37.1	2.0	-24.5	14.6	-49.1	-10.0
Co_2Cl_4	-83.8	-81.4	2.4	-89.7	-5.9	63.5	147.3
$CoC_4N_5H_{19}Cl^{2+}$ (ADETCO)	254.0	262.4	8.4	250.2	-3.8	224.5	-29.5
$Co(NH_3)_2(H_2O)_2ClF^+$	-104.6	-147.8	-43.2	-113.3	-8.7	-128.2	-23.6
$CoC_2N_4H_8S_2Cl_2$ (COTUCL11)	-61.2	-54.2	7.0	-99.5	-38.3	-83.5	-22.3
$CoC_6N_3H_{17}Cl_3$ (AMPRCO)	-159.2	-150.9	8.3	-138.4	20.8	-214.5	-55.3
$CoC_4N_2H_{12}SCl_3$ (CATBAA)	-128.2	-118.7	9.5	-117.8	10.4	-159.5	-31.3
CoTi	116.0	116.0	0.0	66.4	-49.6	147.4	31.4
CoV	161.5	161.5	0.0	59.3	-102.2	-72.4	-233.9
CoCr	217.7	191.2	-26.5	89.3	-128.4	-347.4	-565.1
CoNi	108.1	108.2	0.1	1.4	-106.6	-118.0	-226.1
CoCu	143.1	141.8	-1.3	36.7	-106.4	-108.7	-251.9
HCoCu	150.9	150.9	0.0	79.2	-71.6	-127.7	-278.6

CoZn	124.6	114.3	-10.3	-158.1	-282.6	89.6	-34.9
HCoZn	121.4	91.7	-29.7	-78.0	-199.4	13.5	-107.9
CoBr	86.4	72.9	-13.5	61.0	-25.4	22.4	-64.0
CoOBr	19.9	-48.7	-68.6	17.6	-2.3	-129.4	-149.3
$CoBr_2$	29.0	52.6	23.6	63.2	34.2	-94.6	-123.6
$CoBr_3$	15.9	21.8	5.9	40.1	24.2	-149.5	-165.4
$CoBr_4$	19.3	-10.6	-29.9	38.9	19.6	-196.7	-216.0
$CoBr_4^{2-}$	-99.0	-100.3	-1.3	-169.9	-70.9	-286.5	-187.5
$C_4H_8N_4O_5CoBr$ (BUKPIG)	-99.6	-80.2	19.4	-121.0	-21.4	-152.7	-53.1
CoZr	209.8	172.1	-37.7	-10.4	-220.3	133.7	-76.2
CoMo	285.3	285.4	0.1	75.6	-209.6	288.2	3.0
HCoMo	280.4	261.9	-18.5	83.3	-197.1	222.7	-57.7
CoI	96.2	90.1	-6.2	49.9	-46.3	38.6	-57.6
ICoO	34.0	-2.7	-36.7	25.6	-8.4	-98.2	-132.2
CoI_3	19.5	42.7	23.2	38.1	18.6	-78.0	-97.5
CoI_4	39.0	40.0	0.9	-3.9	-42.9	-102.3	-141.3
$C_{10}H_{15}NS_2CoI$ (GECVEP)	-13.3	38.7	52.0	2.5	15.8	-71.7	-58.4
$C_4H_4N_4O_4CoI_2^-$ (FIRCOY01)	-16.8	-29.3	-12.5	-15.6	1.2	-135.0	-118.2

	AM1*	PM6	PM5
N=78			
Most positive error	108.4	48.2	147.3
Most negative error	-110.0	-400.7	-565.1
MSE	-7.4	-48.6	-70.8
MUE	20.5	61.9	84.3
RMSD	30.4	98.1	121.8

Results for the PM6 parameterization set (*N=42*)

MSE	-2.0	2.0	-32.4
MUE	22.9	15.7	52.5
RMSD	34.3	19.3	69.5

Table 3 Calculated AM1*, PM6 and PM5 Koopmans' theorem ionization potentials and dipole moments for cobalt-containing compounds. The errors are color coded as follows: green up to 0.5 eV or 0.5 Debye; yellow between 0.5 and 1.0; pink larger than 1.0

		AM1*		PM6		PM5	
Compound	**Target**		**Error**		**Error**		**Error**
Koopmans' Theorem Ionization Potentials for Cobalt Compounds (eV)							
$CoCH_3$	7.00	8.88	1.88	9.57	2.57	9.01	2.01
$CoC_{10}H_{10}$	5.55	7.42	1.87	7.08	1.53	7.94	2.39
$Co(CO)_4$	8.30	7.98	-0.32	8.97	0.67	8.04	-0.26
$Co_2(CO)_8$	8.30	6.76	-1.54	10.86	2.56	8.78	0.48
CoCl	8.90	8.78	-0.12	9.48	0.58	8.29	-0.61
$CoCl_2$	10.70	8.60	-2.10	8.27	-2.43	9.78	-0.92
$CoBr_2$	9.90	9.09	-0.81	10.05	0.15	9.67	-0.23
		AM1*		**PM6**		**PM5**	
N=7							
MSE		-0.16		0.80		0.41	
MUE		1.23		1.50		0.99	
Dipole Moments for Cobalt Compounds (Debye)							
CoO^-	1.07	1.42	0.35	3.72	2.65	3.61	2.54
$Co(CO)_4$	0.25	0.54	0.29	0.02	-0.23	4.35	4.10
$CoH(CO)_4$	0.42	1.18	0.76	0.61	0.19	0.95	0.53
$Co_2(CO)_8$	1.23	1.23	0.00	0.23	-1.01	0.02	-1.21
CoOF	0.16	0.57	0.41	0.34	0.18	1.26	1.10
CoClO	0.93	1.31	0.38	0.81	-0.12	1.51	0.58
CoBr	3.65	1.88	-1.77	0.77	-2.88	5.67	2.02
CoBrO	1.81	1.98	0.17	3.44	1.63	1.33	-0.48
CoI	2.32	5.08	2.76	1.58	-0.74	5.91	3.59
CoIO	2.40	2.40	0.00	3.04	0.64	0.97	-1.43
		AM1*		**PM6**		**PM5**	
N=10							
MSE		0.34		0.03		1.13	
MUE		0.69		1.03		1.76	

Table 4 Calculated AM1*, PM6 and PM5 bond lengths and angles for cobalt-containing compounds. The codenames within parentheses indicate the CSD-names of the compounds. The errors are color coded as follows: green up to 0.05 Å or 0.5°; yellow between 0.05-0.1 Å or 0.5-1.0°; pink larger than 0.1 Å or 1°

			AM1*		PM6		PM5	
Compound	**Variable**	**Target**		**Error**		**Error**		**Error**
Co_2	Co-Co	2.30	2.45	0.15	2.07	-0.23	2.11	-0.19
Co_2^-	Co-Co	2.63	2.56	-0.08	2.10	-0.53	2.26	-0.37
HCo	Co-H	1.55	1.59	0.04	1.71	0.16	1.40	-0.15
HCo^-	Co-H	1.66	1.62	-0.04	2.20	0.54	1.44	-0.23
$CoC_5H_5^-$	Co-C	1.93	2.00	0.07	2.07	0.14	2.27	0.34
$Co(Cp_2$ (DCYPCO)	Co-C	2.08	2.26	0.18	2.08	0.00	2.52	0.44
$Co(CN)_4^+$	Co-C	1.81	2.00	0.19	1.77	-0.04	2.08	0.27
	C-N	1.20	1.16	-0.04	1.16	-0.04	1.16	-0.04
$Co(CN)_6^{3-}$	Co-C	1.97	1.99	0.02	1.93	-0.04	2.16	0.19
$CoC_6N_6H_{24}$ ($Co(II)(en)_3$)	Co-N	2.06	2.10	0.04	2.02	-0.04	2.21	0.15
$CoC_6N_6H_{24}^{3+}$ (COTENC01)	Co-N	2.00	2.00	0.00	2.01	0.01	2.21	0.21
	N-Co-N	90.2	93.7	3.5	87.9	-2.3	81.4	-8.8
$CoC_6N_6H_{24}^{2+}$ (QICSOK)	Co-N	2.20	2.11	-0.09	2.24	0.04	2.26	0.06
	N-Co-N	78.7	83.3	4.7	85.5	6.8	80.8	2.1
$CoC_9N_6H_{15}$ (FEFRUD)	Co-N	2.01	2.00	-0.01	2.06	0.05	2.23	0.22
	N-Co-N	90.3	92.5	2.2	92.1	1.8	92.0	1.7
	Co-C	1.89	2.05	0.16	1.84	-0.05	2.11	0.22
CoO^-	Co=O	1.65	1.72	0.06	1.78	0.12	1.53	-0.13
CoO_2^-	Co=O	1.68	1.81	0.13	1.79	0.11	1.61	-0.07
$Co(H_2O)_4^{2+}$	Co-O	1.94	1.93	-0.02	1.91	-0.03	2.07	0.13
$Co(H_2O)_6^{3+}$	Co-O	2.03	1.94	-0.09	1.99	-0.04	1.99	-0.04
$Co_2(H_2O)_4^{4+}$	Co-O	2.17	1.96	-0.21	1.92	-0.25	1.95	-0.22
$Co(H_2O)_6^{2+}$ (NAZVOZ)	Co-O	2.06	1.97	-0.09	1.88	-0.18	1.52	-0.54
	Co-O'	2.12	2.02	-0.10	1.87	-0.25	2.23	0.11
$Co(H_2O)_6^{2+}$	Co-O	2.12	1.96	-0.16	1.99	-0.13	2.11	-0.02
	Co-O'	1.96	1.95	-0.01	2.01	0.05	2.09	0.13
$Co(CO)_4$	Co-C	1.85	1.89	0.04	1.98	0.13	2.18	0.33

$Co(CO)_4^-$ (FUBYOQ)	Co-C	1.75	1.95	0.20	1.90	0.15	2.04	0.29
$CoH(CO)_4$	Co-H	1.55	1.62	0.06	1.70	0.14	1.39	-0.17
	Co-C	1.81	1.90	0.09	1.83	0.02	2.02	0.21
$Co(CO)_5^+$	Co-C(eq)	1.83	2.00	0.17	1.82	-0.01	2.07	0.24
	Co-C(ax)	1.89	1.92	0.03	1.82	-0.07	2.92	1.03
$CoC_6O_{12}^{3-}$ ($Co(iii)(ox)_3$)	Co-O	1.95	1.95	0.00	1.98	0.03	2.00	0.05
$Co_2(CO)_8$	Co-Co	2.47	3.08	0.61	2.47	0.00	3.50	1.03
$Co(CO)_3NO$	Co-C	1.81	1.94	0.13	2.14	0.33	2.04	0.23
	C-Co-C	103.2	85.9	-17.3	81.0	-22.2	93.1	-10.2
	Co-N	1.67	1.74	0.07	1.60	-0.07	1.93	0.26
$Co(NO_3)_3$	Co-O	1.89	1.84	-0.05	1.88	-0.01	2.19	0.30
	O-Co-O	68.0	65.3	-2.7	71.1	3.1	176.0	108.0
	O-Co-O'	93.0	98.8	5.8	98.6	5.6	86.8	-6.2
$CoN_6H_{15}O_2^{2+}$ (FAMYEX)	Co-N(O2)	1.95	1.91	-0.04	1.79	-0.16	2.09	0.14
	Co-N(H3)	1.96	2.08	0.12	2.03	0.07	2.20	0.24
	N-Co-N	90.0	92.9	2.9	89.0	-1.0	88.8	-1.2
$CoC_6N_4H_{16}O_4^+$ (OXENCO)	Co-N	1.98	2.04	0.06	1.98	0.00	2.30	0.32
	N-Co-N	86.0	85.3	-0.7	89.7	3.6	81.2	-4.8
	Co-O	1.94	1.92	-0.02	1.95	0.01	1.91	-0.03
$CoC_6N_4H_{16}O_4^+$ (AETXCO)	Co-O	1.92	1.90	-0.02	1.93	0.01	1.91	-0.01
	O-Co-O	84.8	84.3	-0.5	87.8	3.0	85.9	1.1
	Co-N(H2C)	1.98	2.05	0.07	1.96	-0.02	2.21	0.23
	Co-N(H3)	1.95	2.04	0.09	2.00	0.05	2.27	0.32
	C-N(HC2)	1.92	2.07	0.15	1.94	0.02	2.23	0.31
$CoC_6N_6H_{18}O_4^+$ (NIXGEG)	Co-N(C3)	1.96	2.11	0.15	1.96	0.00	2.20	0.24
	Co-N(CH2)	1.96	2.09	0.13	2.04	0.08	2.20	0.24
	N-Co-N	86.8	87.7	0.9	85.4	-1.4	90.7	3.9
	Co-N(O2)	1.99	2.01	0.02	1.87	-0.12	2.13	0.14
	Co-N(O2)	1.93	1.90	-0.03	1.83	-0.10	2.08	0.15
$CoC_9N_4H_{19}O_5$ (AMGXCO01)	Co-N	1.89	1.99	0.10	1.88	-0.01	2.12	0.23
	N-Co-N	82.0	82.1	0.1	82.8	0.8	74.5	-7.5
	Co-C	1.98	2.04	0.06	2.01	0.03	2.15	0.17
	Co-O	2.06	2.03	-0.03	2.21	0.15	2.16	0.10
$CoC_{15}H_{21}O_6^-$ ($Co(II)(Acac)_3$(-) IKEYAY)	Co-O	2.06	1.95	-0.11	2.12	0.06	1.97	-0.09
	O-Co-O	88.0	87.0	-0.9	101.1	13.1	94.0	6.1

$CoC_6N_6H_{20}O_6^+$ (NITNCO)	Co-N	2.00	2.01	0.01	1.99	-0.01	2.23	0.23
	N-Co-N	87.7	89.6	1.9	89.0	1.3	95.0	7.3
	Co-O	1.90	1.87	-0.03	1.99	0.09	1.91	0.01
CoF	Co-F	1.91	1.91	0.00	1.84	-0.07	1.91	0.00
CoOF	Co=O	1.59	1.63	0.04	1.57	-0.02	1.44	-0.15
	Co-F	1.72	1.72	0.00	1.68	-0.04	1.53	-0.20
CoF_2	Co-F	1.72	1.76	0.04	1.70	-0.02	1.55	-0.17
CoF_3	Co-F	1.72	1.72	0.00	1.76	0.04	1.76	0.04
	F-Co-F	108.5	147.4	39.0	119.8	11.3	143.1	34.7
CoF_4^-	Co-F	1.79	1.81	0.02	1.75	-0.04	1.85	0.06
$CoAlH_2$	Co-Al	2.40	2.37	-0.03	2.28	-0.12	2.40	0.00
$HCoAlH_2$	Co-Al	2.53	2.57	0.04	2.29	-0.24	2.36	-0.16
$CoSiH_3$	Co-Si	2.33	2.33	0.00	2.50	0.17	2.30	-0.02
$CoSiC_4O_4F_3$ (FUZMAO)	Co-Si	2.23	2.46	0.23	2.23	0.00	2.27	0.04
	Si-F	1.50	1.71	0.21	1.56	0.06	1.59	0.09
	F-Si-Co	114.8	116.6	1.8	107.5	-7.3	117.2	2.4
	Co-C	1.79	1.91	0.12	1.82	0.03	2.15	0.36
	C-O	1.11	1.18	0.07	1.13	0.02	1.15	0.03
CoP	Co≡P	2.16	2.28	0.11	2.04	-0.13	1.87	-0.29
$CoPH_2$	Co-P	2.26	2.31	0.04	2.10	-0.16	1.91	-0.36
$HCoPH_2$	Co-P	2.32	2.34	0.02	2.26	-0.06	1.96	-0.36
CoS	Co=S	2.01	2.05	0.04	1.70	-0.31	1.96	-0.06
CoSH	Co-S	2.16	1.99	-0.17	1.91	-0.25	2.45	0.29
HCoSH	Co-S	2.23	2.24	0.01	2.01	-0.23	2.28	0.05
$CoC_{10}H_{14}S_4$ (TACACO10)	Co-S	2.17	2.18	0.01	2.13	-0.04	2.51	0.34
	S-Co-S	96.9	91.9	-4.9	94.8	-2.0	82.9	-14.0
$CoC_9H_{21}S_6$ (MEDTCO10)	Co-S	2.30	2.42	0.12	2.27	-0.03	2.68	0.38
	S-Co-S	89.8	50.2	-39.6	90.7	0.9	82.4	-7.4
$CoC_3N_3H_6S_6$ (TDTCCO)	Co-S	2.29	2.32	0.03	2.26	-0.03	2.56	0.27
	S-Co-S	76.3	74.2	-2.2	79.9	3.5	69.2	-7.1
CoCl	Co-Cl	2.07	2.02	-0.05	1.96	-0.11	1.97	-0.10
CoClO	Co=O	1.61	1.73	0.12	1.59	-0.02	1.56	-0.05
	Co-Cl	2.07	2.34	0.27	1.82	-0.25	2.15	0.08
$CoCl_2$	Co-Cl	2.11	2.07	-0.04	1.98	-0.12	2.07	-0.04
$CoCl_3$	Co-Cl	2.13	2.12	0.00	2.10	-0.03	2.06	-0.06

$CoCl_4^{2-}$ (DMDPCO)	Co-Cl	2.25	2.29	0.04	2.31	0.06	2.14	-0.11
Co_2Cl_4	Co-Cl	2.12	2.09	-0.04	2.01	-0.11	2.03	-0.09
	Co-Cl'	2.21	2.23	0.01	2.04	-0.17	2.18	-0.04
$CoCH_3ClOH$	Co-O	1.73	1.82	0.09	1.78	0.05	1.66	-0.07
	Co-C	1.91	2.06	0.15	1.87	-0.04	2.08	0.17
	Co-Cl	2.10	2.15	0.05	2.08	-0.02	2.23	0.13
$CoC_4N_5H_{19}Cl^{2+}$ (ADETCO)	Co-Cl	2.28	2.16	-0.12	2.29	0.01	2.27	-0.01
	Co-N(H3)	1.97	2.07	0.10	2.02	0.05	2.18	0.21
	N-Co-Cl	87.7	87.9	0.2	83.9	-3.8	86.2	-1.5
	Co-N(C2H)	1.94	2.14	0.20	1.93	-0.01	2.17	0.23
	N-Co-N	94.3	90.9	-3.4	93.7	-0.6	96.8	2.5
	Co-N(H2C)	1.99	2.07	0.08	1.98	-0.01	2.20	0.21
$Co(NH_3)_2(H_2O)_2ClF^{+}$	Co-Cl	2.23	2.16	-0.07	2.30	0.07	2.30	0.06
	Co-N	1.97	2.08	0.11	1.96	-0.01	2.15	0.18
	Co-F	1.85	1.81	-0.04	1.84	-0.01	1.84	-0.01
	Co-O	1.97	2.01	0.04	2.00	0.03	2.00	0.03
$CoC_9P_3H_{27}Cl$ (BUTDEZ)	Co-Cl	2.22	2.32	0.10	2.38	0.16	2.36	0.14
	Co-P	2.24	2.26	0.02	2.28	0.04	2.00	-0.24
	Cl-Co-P	113.8	82.8	-31.0	167.6	53.8	169.9	56.1
$CoC_2N_4H_8S_2Cl_2$ (COTUCL11)	Co-Cl	2.26	2.15	-0.11	2.29	0.03	2.32	0.06
	Co-Cl'	2.27	2.23	-0.04	2.44	0.17	2.33	0.06
	Cl-Co-Cl	107.7	74.2	-33.5	105.3	-2.4	90.7	-17.1
	Co-S	2.30	2.38	0.08	2.11	-0.19	2.66	0.36
	Co-C	3.31	3.32	0.01	3.15	-0.16	3.41	0.10
$CoC_6N_3H_{17}Cl_3$ (AMPRCO)	Co-Cl	2.24	2.10	-0.14	2.30	0.06	2.31	0.07
	Co-Cl'	2.31	2.18	-0.13	2.36	0.05	2.35	0.04
	Cl-Co-Cl	91.2	90.8	-0.4	93.7	2.5	92.3	1.1
	Co-N	1.97	2.09	0.12	1.95	-0.02	2.16	0.19
$CoC_4N_2H_{12}SCl_3$ (CATBAA)	Co-Cl	2.28	2.21	-0.07	2.32	0.04	2.29	0.01
	Cl-Co-Cl	91.7	86.4	-5.4	98.4	6.6	98.4	6.7
	Co-N	1.93	2.11	0.18	1.95	0.02	2.20	0.27
	Co-S	2.22	2.47	0.25	2.02	-0.20	2.78	0.56
CoTi	Co-Ti	2.35	2.35	0.00	2.50	0.15	36.49	34.14
CoV	Co-V	2.34	2.36	0.02	2.56	0.22	1.62	-0.72
CoCr	Co-Cr	2.35	2.35	0.00	2.79	0.44	1.29	-1.05

CoNi	Co-Ni	2.38	2.38	0.00	2.49	0.10	1.28	-1.10
CoCu	Co-Cu	2.29	2.33	0.04	2.59	0.29	1.69	-0.61
HCoCu	Co-Cu	2.35	2.35	0.00	2.60	0.26	1.70	-0.65
CoZn	Co-Zn	2.54	2.49	-0.06	1.89	-0.65	2.55	0.00
HCoZn	Co-Zn	2.49	2.49	0.00	2.03	-0.46	2.41	-0.08
CoBr	Co-Br	2.21	2.23	0.02	2.00	-0.21	2.26	0.05
BrCoO	Co=O	1.60	1.62	0.02	1.60	0.00	1.36	-0.24
	Co-Br	2.19	2.27	0.08	1.63	-0.56	2.08	-0.11
$CoBr_2$	Co-Br	2.27	2.31	0.04	2.01	-0.25	2.17	-0.10
$CoBr_3$	Co-Br	2.28	2.28	0.00	2.44	0.15	2.11	-0.17
$CoBr_4$	Co-Br	2.43	2.33	-0.10	2.25	-0.18	2.27	-0.16
$CoBr_4^{2-}$	Co-Br	2.40	2.45	0.05	2.70	0.30	2.43	0.03
$C_4H_8N_4O_5CoBr$ (BUKPIG)	Co-Br	2.36	2.40	0.04	2.14	-0.22	2.35	-0.01
	Co-O	1.96	2.06	0.10	2.11	0.15	2.07	0.11
	Co-N	1.91	1.98	0.07	1.85	-0.06	2.16	0.25
CoZr	Co-Zr	2.16	2.16	0.00	2.47	0.31	3.28	1.12
CoMo	Co-Mo	2.33	2.33	0.00	2.23	-0.11	10.82	8.49
CoI_2	Co-I	2.57	2.51	-0.06	1.73	-0.84	2.39	-0.19
CoI_4	Co-I	2.61	2.68	0.07	1.63	-0.98	2.44	-0.17
CoI	Co-I	2.39	2.44	0.05	1.66	-0.73	2.37	-0.02
ICoO	Co=O	1.60	1.62	0.02	1.60	0.00	1.37	-0.23
	Co-I	2.40	2.49	0.09	1.67	-0.73	2.24	-0.16
$C_{10}H_{15}NS_2CoI$ (GECVEP)	Co-I	2.60	2.61	0.01	2.96	0.36	2.82	0.22
	Co-S	2.25	2.40	0.15	2.17	-0.08	2.60	0.35
	I-Co-S	95.6	92.2	-3.3	96.5	1.0	58.5	-37.1
	S-Co-S	76.5	70.4	-6.1	77.6	1.0	48.9	-27.6
$C_4H_4N_4O_4CoI_2^-$ (FIRCOY01)	Co-I	2.58	2.57	-0.01	3.31	0.73	2.67	0.09
	Co-N	1.88	2.01	0.13	1.90	0.02	2.14	0.26
CoI_3	Co-I	2.42	2.48	0.06	4.13	1.71	2.36	-0.06
$CoCH_3ICl$	Co-I	2.47	2.53	0.06	1.68	-0.79	2.55	0.07
	Co-C	1.95	2.07	0.12	1.89	-0.06	1.91	-0.04
	Co-Cl	2.14	2.13	-0.01	2.11	-0.03	2.17	0.03
	C-Co-I	101.5	120.1	18.7	109.9	8.4	90.2	-11.3
	C-Co-Cl	97.1	124.4	27.3	125.2	28.1	168.4	71.3
			AM1*		**PM6**		**PM5**	

N=138			
MSE bond length	0.04	-0.03	0.36
MUE bond length	0.08	0.16	0.51
N=28			
MSE bond angle	-1.5	4.0	5.1
MUE bond angle	9.3	7.1	16.7

Table 5 Calculated AM1*, PM6 and PM5 heats of formation and errors compared with our target values for the nickel-containing compounds used to parameterize AM1* (all values kcal mol^{-1}). Errors are classified by coloring the boxes in which they appear. Green indicates errors lower than 10 kcal mol^{-1}. yellow 10-20 kcal mol^{-1} and pink those greater than 20 kcal mol^{-1}. The codenames within parentheses indicate the CSD-names of the compounds

	Target	AM1*		PM6		PM5	
Compound	**$\Delta H°_f$**	**$\Delta H°_f$**	**Error**	**$\Delta H°_f$**	**Error**	**$\Delta H°_f$**	**Error**
Ni	102.8	102.8	0.0	93.5	-9.3	102.8	0.0
Ni^-	76.0	65.3	-10.8	20.2	-55.8	21.8	-54.2
Ni^+	276.7	281.8	5.1	266.1	-10.6	319.5	42.8
Ni^{2+}	697.2	694.9	-2.3	685.2	-12.0	760.9	63.7
Ni_2^-	128.6	87.1	-41.6	49.4	-79.2	148.6	20.0
Ni_2^+	428.3	371.6	-56.7	127.7	-300.6	413.7	-14.6
NiH	85.6	85.0	-0.6	87.0	1.4	175.6	90.0
NiH^+	254.5	305.0	50.6	292.5	38.0	394.9	140.5
NiH_2	83.5	65.0	-18.5	133.1	49.6	231.0	147.5
NiH_3	36.1	36.1	0.0	54.1	18.0	160.4	124.3
$Ni(C_5H_5)_2$	79.7	87.4	7.7	61.1	-18.7	17.8	-61.9
$Ni_2(C_5H_5)_2(CO)_2$	-27.0	12.9	39.9	-20.9	6.1	-95.6	-68.6
NiCO	35.1	83.1	48.0	23.2	-11.9	64.4	29.3
$NiCO^-$	17.2	-18.7	-35.9	-0.9	-18.1	-22.1	-39.3
$Ni(CO)_2$	-39.0	-3.4	35.6	-50.1	-11.1	-12.2	26.8
$Ni(CO)_2^-$	-53.0	-88.7	-35.7	-65.0	-12.0	-56.4	-3.4
$Ni(CO)_3$	-93.0	-80.5	12.5	-80.0	13.0	-78.9	14.1
$Ni(CO)_3^-$	-118.8	-150.1	-31.3	-106.9	11.9	-169.6	-50.8
$Ni(CO)_4$	-144.0	-142.2	1.8	-107.1	36.9	-143.6	0.4
NiO	75.0	85.4	10.4	154.0	79.0	71.8	-3.2
NiO^-	41.1	20.1	-21.0	44.3	3.2	-21.1	-62.2
NiO_2^-	-28.3	-28.5	-0.2	15.3	43.6	-51.3	-23.0
$Ni(OH)_2.(H_2O)_2$ cis	-180.9	-201.9	-21.0	-174.5	6.4	-210.2	-29.3
$Ni(OH)_2.(H_2O)_2$ trans	-177.6	-211.1	-33.5	-165.3	12.3	-218.1	-40.5
$Ni(OH).(H_2O)_3^+$	-36.3	-29.5	6.8	-31.2	5.1	-36.0	0.3

$Ni(H_2O)_4^{2+}$	221.9	214.7	-7.2	207.4	-14.5	217.1	-4.8
$Ni(H_2O)_6^{2+}$	55.7	54.9	-0.9	45.9	-9.8	11.1	-44.6
$NiH_{12}O_6^{2+}$ (JERNID)	54.4	55.2	0.8	49.0	-5.4	11.1	-43.3
$Ni(NH_2)_2$	39.4	37.1	-2.3	85.1	45.7	187.9	148.6
$Ni(NH_3)_4^{2+}$	319.5	325.0	5.5	309.3	-10.2	587.0	267.5
$Ni(NH_3)_6^{2+}$	271.4	266.6	-4.8	268.3	-3.1	485.8	214.4
$Ni(CN)_4^{2-}$	99.1	25.4	-73.7	57.8	-41.3	26.3	-72.8
$Ni(CN)_5^{3-}$	258.9	150.5	-108.4	290.3	31.4	145.6	-113.3
$Ni(CO)_3NO$	-89.0	-90.8	-1.8	-77.9	11.1	-82.8	6.2
$NiC_8N_4H_{14}O_4$ (NIMGLO10)	-37.1	4.9	42.0	-58.3	-21.2	81.4	118.5
$NiC_{10}N_2H_{12}O_8$ (Ni-EDTA)	-361.5	-374.3	-12.8	-402.2	-40.7	-520.8	-159.3
$NiC_{13}NH_{17}O_4$ (VAXSUI)	-142.3	-137.7	4.6	-94.2	48.1	-154.7	-12.4
NiF	17.5	6.5	-11.0	51.1	33.6	4.9	-12.6
NiF_2	-115.5	-89.4	26.1	-65.2	50.3	-71.9	43.6
NiF_4^{2-}	-211.5	-261.2	-49.7	-212.7	-1.2	-330.9	-119.4
$NiCH_3F$	-8.3	-35.6	-27.3	-11.5	-3.2	-4.3	4.0
$NiOF_2$	-50.8	-35.4	15.4	-47.2	3.6	-53.4	-2.6
$NiF_2.(H_2O)_2$ cis	-214.2	-213.9	0.3	-202.0	12.2	-188.1	26.1
$NiF_2.(H_2O)_2$ trans	-219.4	-220.5	-1.1	-197.4	22.0	-194.0	25.4
$NiAlH_2$	56.2	89.1	32.9	60.0	3.8	140.3	84.2
$HNiAlH_2$	121.3	106.5	-14.8	159.1	37.8	244.6	123.3
$NiSiH_3$	41.6	53.9	12.3	61.5	19.8	122.2	80.6
$HNiSiH_3$	98.6	73.7	-24.9	139.3	40.7	226.8	128.2
$HNiPH_2$	50.7	62.8	12.1	28.6	-22.1	98.7	48.0
$Ni(PF_3)_4$	-953.4	-953.4	0.0	-962.4	-9.0	-959.3	-5.9
NiS	85.4	85.4	0.0	78.6	-6.8	114.2	28.8
NiSH	20.0	35.6	15.6	47.4	27.4	79.0	59.1
$NiSH_2$	36.4	28.0	-8.4	78.0	41.6	105.7	69.3
$Ni(H_2S)_4^{2+}$	384.0	437.1	53.1	300.0	-84.0	449.3	65.3
$NiC_2N_3S_3^{2-}$ (CUSJUV)	62.9	-16.2	-79.1	39.4	-23.5	14.3	-48.6
$NiC_4S_4O4^{2-}$ (TOXNIA)	-217.9	-228.9	-11.0	-192.6	25.3	-271.2	-53.3
$NiC_8N_4S_4^{-}$ (TROPNJ)	92.8	46.2	-46.6	122.2	29.4	84.4	-8.4
$NiC_8N_2H_{14}S_2$ (BAEINI)	12.2	-20.3	-32.5	9.8	-2.4	30.8	18.6
$NiC_{10}N_2H_{20}S_6$ (ZOTVUZ)	6.4	29.8	23.4	10.4	4.0	33.9	27.5
$NiC_{11}N_2H_{21}S_2O_2^{+}$ (Square, 2S and 2N)	72.1	125.7	53.6	96.7	24.6	149.1	77.0

$Ni(N_2S_2H)_2$	95.3	62.9	-32.4	117.1	21.8	200.4	105.1
$Ni((CH_3)_2S)_2F_2$ cis	-153.5	-130.9	22.6	-135.2	18.3	-158.8	-5.3
$Ni((CH_3)_2S)_2F_2$ trans	-162.5	-131.4	31.1	-159.3	3.2	-150.2	12.3
NiCl	43.5	45.6	2.1	69.7	26.2	63.6	20.1
$NiCl_2$	-17.7	-17.2	0.5	-18.3	-0.6	19.0	36.6
$NiCl_4^{2-}$	-130.1	-133.3	-3.2	-130.6	-0.5	-116.8	13.3
$NiCH_3Cl$	37.2	2.6	-34.6	18.9	-18.3	58.4	21.2
$NiCl_2O$	-0.5	-43.8	-43.3	13.0	13.5	61.3	61.8
$NiCl_3.H_2O^-$	-188.1	-190.0	-1.9	-197.2	-9.1	-212.4	-24.3
$NiCl.(H_2O)_3^+$	-19.4	-38.3	-18.9	-20.9	-1.5	-14.4	5.0
$NiCl_2.(H_2O)_2$ cis	-150.9	-199.2	-48.3	-156.6	-5.7	-146.9	4.0
$NiCl_2.(H_2O)_2$ trans	-155.3	-199.2	-43.9	-159.0	-3.7	-165.4	-10.1
$Ni((CH_3)_2S)_2Cl_2$ cis	-89.2	-136.9	-47.7	-71.8	17.4	-55.7	33.5
$Ni((CH_3)_2S)_2Cl_2$ trans	-96.4	-131.6	-35.2	-79.7	16.7	-70.2	26.2
NiTi	211.0	172.5	-38.5	137.6	-73.4	281.0	69.9
NiV	132.9	132.8	-0.1	141.2	8.3	188.0	55.1
NiCr	105.4	99.4	-6.1	149.7	44.3	-94.1	-199.5
NiCu	137.7	137.7	0.0	122.8	-14.8	78.1	-59.5
NiZn	151.2	147.0	-4.3	-8.0	-159.3	166.1	14.8
NiBr	57.8	68.6	10.8	27.2	-30.6	63.6	5.8
$NiBr_2$	52.9	76.2	23.3	14.1	-38.8	49.5	-3.4
$NiCH_3Br$	24.6	12.1	-12.5	23.3	-1.3	45.9	21.3
$Ni((CH_3)_2S)_2Br_2$ cis	-70.8	-39.9	30.9	-57.3	13.5	-45.7	25.1
$Ni((CH_3)_2S)_2Br_2$ trans	-77.1	-53.2	23.9	-60.5	16.6	-59.7	17.4
$NiC_8N_2H_{20}S_3Br^+$ (BRUCUB)	75.1	60.9	-14.2	64.8	-10.3	124.2	49.1
NiZr	218.3	179.5	-38.8	120.5	-97.8	340.6	122.3
NiMo	296.6	296.6	0.0	227.3	-69.3	423.0	126.4
NiI	62.3	60.4	-1.9	26.1	-36.2	89.3	27.0
NiI_2	36.5	46.8	10.3	15.0	-21.5	86.6	50.1
$NiCH_3I$	37.0	42.7	5.7	29.2	-7.8	86.0	49.0
$Ni((CH_3)_2S)_2I_2$ cis	-42.3	-72.0	-29.7	-31.1	11.2	-12.8	29.5
		AM1*		**PM6**		**PM5**	
N=91							
Most positive error		53.6		79.0		267.5	
Most negative error		-108.4		-300.6		-199.5	

MSE	-6.7	-4.3	21.0
MUE	21.5	27.3	53.0
RMSD	29.9	47.0	74.2

Results for the PM6 parameterization set (*N=43*)

MSE	-12.0	1.0	7.2
MUE	26.2	16.2	47.5
RMSD	35.9	22.6	74.5

Table 6 Calculated AM1*, PM6 and PM5 Koopmans' theorem ionization potentials and dipole moments for nickel-containing compounds. The errors are color coded as follows: green up to 0.5 eV or 0.5 Debye; yellow between 0.5 and 1.0; pink larger than 1.0

		AM1*		PM6		PM5	
Compound	**Target**		**Error**		**Error**		**Error**
Koopmans' Theorem Ionization Potentials for Nickel Compounds (eV)							
Ni^+	18.17	12.59	-5.58	12.28	-5.89	13.94	-4.23
NiH	8.50	8.47	-0.03	8.38	-0.12	6.69	-1.81
NiO	9.50	10.11	0.61	7.82	-1.68	11.33	1.83
NiF_2	11.50	11.82	0.32	9.00	-2.50	13.23	1.73
NiCl	9.28	8.46	-0.82	6.61	-2.67	10.78	1.50
$NiCl_2$	11.20	11.95	0.75	10.85	-0.35	12.33	1.13
NiCO	7.30	7.30	0.00	7.88	0.58	8.52	1.22
$Ni(CO)_2$	7.79	8.13	0.34	8.12	0.33	9.02	1.23
$Ni(CO)_3$	7.69	8.89	1.20	8.14	0.45	9.69	2.00
$Ni(CO)_4$	8.72	9.41	0.69	8.06	-0.66	10.07	1.35
$Ni(Cp)_2$	6.51	9.06	2.55	7.02	0.51	8.63	2.12
		AM1*		**PM6**		**PM5**	
N=11							
MSE		0.00		-1.09		0.73	
MUE		1.17		1.43		1.83	
Dipole Moments for Nickel Compounds (Debye)							
NiH	2.40	3.16	0.76	0.33	-2.07	0.09	-2.31
NiH^+	0.83	4.24	3.41	0.77	-0.06	1.66	0.83
NiH_3	3.75	5.03	1.28	0.11	-3.64	0.32	-3.43
NiO	4.00	5.97	1.97	9.37	5.37	4.68	0.68
NiO^-	3.33	0.16	-3.17	2.15	-1.18	4.05	0.72
$Ni(OH)_2.(H_2O)_2$ cis	3.50	3.02	-0.48	1.72	-1.78	4.90	1.40
NiCO	3.35	3.95	0.60	0.81	-2.54	1.45	-1.90
NiF	4.49	2.47	-2.02	3.19	-1.30	3.22	-1.27
$NiCH_3F$	3.59	1.06	-2.54	3.04	-0.55	2.78	-0.82
$NiOF_2$	1.67	0.98	-0.69	2.58	0.91	3.46	1.79

$NiF_2.(H_2O)_2$ cis	6.48	3.22	-3.26	5.48	-1.00	8.56	2.08
NiCl	4.39	2.97	-1.42	2.95	-1.44	5.81	1.42
$NiCH_3Cl$	4.39	1.72	-2.67	3.85	-0.54	5.27	0.88
$NiCl_2O$	1.40	0.87	-0.54	0.89	-0.51	0.14	-1.26
$NiCl_2.(H_2O)_2$ cis	6.70	3.16	-3.54	3.63	-3.07	0.14	-6.56
		AM1*		**PM6**		**PM5**	
N=15							
MSE		-0.82		-0.89		-0.52	
MUE		1.89		1.73		1.82	

Table 7 Calculated AM1*, PM6 and PM5 bond lengths and angles for nickel-containing compounds. The codenames within parentheses indicate the CSD-names of the compounds. The errors are color coded as follows: green up to 0.05 Å or 0.5°; yellow between 0.05-0.1 Å or 0.5-1.0°; pink larger than 0.1 Å or 1°

Compound	Variable	Target	AM1*	Error	PM6	Error	PM5	Error
NiH	Ni-H	1.61	1.64	0.03	1.71	0.10	3.09	1.47
NiH^+	Ni-H	1.44	1.63	0.19	1.70	0.26	2.33	0.89
NiH_2	Ni-H	1.64	1.64	-0.01	1.84	0.20	3.16	1.52
	H-Ni-H	180.0	180.0	0.0	180.0	0.0	180.0	0.0
NiH_3	Ni-H	1.82	1.88	0.06	2.73	0.91	3.33	1.51
	Ni-H(2)	1.52	1.64	0.13	1.70	0.18	3.00	1.48
	H-Ni-H	167.7	168.7	0.9	171.9	4.2	173.2	5.5
	H-Ni-H	24.5	22.6	-1.9	14.1	-10.4	13.6	-10.9
$Ni(CN)_4^{2-}$	Ni-C	1.89	1.83	-0.06	1.84	-0.05	1.87	-0.02
	C#N	1.19	1.17	-0.02	1.17	-0.02	1.17	-0.02
$Ni(CN)_5^{3-}$	Ni-C(ap)	2.17	2.01	-0.16	1.92	-0.25	2.34	0.17
	Ni-C(ba)	1.87	1.84	-0.03	1.84	-0.03	2.27	0.40
NiCO	Ni-C	1.67	1.83	0.16	1.69	0.01	1.71	0.04
$Ni(CO)_2$	Ni-C	1.84	1.90	0.06	1.75	-0.09	1.77	-0.08
	C-Ni-C	180.0	180.0	0.0	180.0	0.0	180.0	0.0
$Ni(CO)_2^-$	Ni-C	1.76	1.92	0.16	1.75	-0.01	1.84	0.08
	C-Ni-C	180.0	163.6	-16.4	180.0	0.0	180.0	0.0
$Ni(CO)_3$	Ni-C	1.82	1.90	0.08	1.78	-0.04	1.79	-0.03
	C-Ni-C	120.0	120.0	0.0	120.0	0.0	120.0	0.0
$Ni(CO)_3^-$	Ni-C	1.79	1.87	0.09	1.81	0.02	1.87	0.08
	C-Ni-C	120.0	120.0	0.0	147.7	27.7	103.8	-16.2
$Ni(CO)_4$	Ni-C	1.85	1.93	0.07	1.81	-0.04	1.82	-0.04
	C-Ni-C	109.5	109.5	0.0	109.5	0.0	109.5	0.0
$Ni(NH2)_2$	Ni-N	1.81	1.96	0.15	1.83	0.02	1.83	0.03
	N-Ni-N	180.0	179.9	-0.1	180.0	0.0	168.4	-11.6
	H-N-Ni	125.5	111.9	-13.7	123.9	-1.6	126.6	1.1
$Ni(NH_3)_4^{2+}$	Ni-N	2.00	1.97	-0.03	1.96	-0.04	1.97	-0.03

$Ni(NH_3)_6^{2+}$	Ni-N	1.96	2.06	0.10	1.96	0.00	2.66	0.70
$NiC_6N_6H_{24}^{2+}$ (Ni(II)(en)$_3$)	Ni-N	2.19	2.15	-0.04	2.09	-0.10	2.50	0.31
$NiC_8N_6H_{26}^{2+}$ (AEAMNI10)	Ni-N	2.14	2.14	0.00	2.05	-0.09	2.53	0.39
	Ni-N'	2.05	2.03	-0.02	1.98	-0.07	2.35	0.30
	N-Ni-N'	81.6	84.1	2.5	85.9	4.3	101.9	20.3
$NiC_{32}N_8H_{16}$ (Nickel Phthalocyanine)	Ni-N	1.92	2.03	0.11	1.93	0.01	1.99	0.07
$Ni(CO)_3NO$	Ni-C	1.81	1.91	0.10	1.81	0.00	1.79	-0.02
	Ni-N	1.88	2.09	0.21	1.94	0.06	3.20	1.32
	C-Ni-N	108.6	106.5	-2.1	102.6	-6.0	103.2	-5.4
$NiC_{13}NH_{17}O_4$ (VAXSUI)	Ni-N	1.94	2.04	0.10	1.92	-0.02	2.44	0.50
	Ni-C	1.97	2.07	0.10	1.93	-0.04	1.98	0.01
	C-Ni-N	135.8	138.1	2.3	137.6	1.8	129.5	-6.3
	Ni-C'	1.99	2.08	0.09	1.94	-0.05	2.35	0.36
$NiC_8N_4H_{14}O_4$ (NIMGLO10)	Ni-N	1.85	2.05	0.20	1.88	0.03	2.67	0.82
	N-Ni-N	83.1	81.7	-1.4	84.6	1.5	75.4	-7.7
NiO	Ni-O	1.67	1.66	-0.01	1.62	-0.04	1.60	-0.07
NiO^-	Ni-O	1.68	1.65	-0.03	1.73	0.05	1.63	-0.05
NiO_2^-	Ni-O	1.67	1.68	0.02	1.62	-0.05	1.65	-0.02
	O-Ni-O	180.0	180.0	0.0	180.0	0.0	180.0	0.0
$Ni(OH)_2$	Ni-O	1.75	1.82	0.07	1.73	-0.02	1.79	0.04
	O-H	0.99	0.96	-0.03	0.84	-0.15	0.97	-0.02
$Ni(OH)_2.(H_2O)_2$ cis	Ni-O	2.01	2.01	0.00	1.94	-0.07	2.07	0.06
	Ni-O	1.83	1.84	0.01	1.88	0.05	1.77	-0.07
$Ni(OH)_2.(H_2O)_2$ trans	Ni-O	1.88	1.85	-0.03	1.85	-0.03	1.80	-0.08
	Ni-O	1.94	2.12	0.18	2.12	0.18	2.08	0.14
$Ni(OH).(H_2O)_3^+$	Ni-O	1.93	2.01	0.08	1.97	0.04	2.05	0.12
	Ni-O	1.80	1.82	0.02	1.83	0.03	1.76	-0.05
$Ni(H_2O)_4^{2+}$	Ni-O	1.90	2.04	0.14	2.06	0.16	2.03	0.13
$Ni(H_2O)_6^{2+}$	Ni-O	2.09	2.10	0.01	2.10	0.01	2.04	-0.05
$NiH_{12}O_6^{2+}$ (JERNID)	Ni-O	2.03	2.09	0.06	2.11	0.08	2.03	0.00
$NiC_{10}H_{18}O_6$ (AQACNI)	Ni-O	2.01	2.03	0.02	2.00	-0.01	1.87	-0.14
	O-Ni-O	91.6	95.9	4.3	90.7	-1.0	80.4	-11.2
	Ni-O(H2)	2.09	2.15	0.06	2.13	0.04	2.18	0.09
NiF	Ni-F	1.77	1.81	0.04	1.74	-0.03	1.59	-0.18
NiF_2	Ni-F	1.74	1.79	0.05	1.67	-0.07	1.59	-0.15

	F-Ni-F	180.0	180.0	0.0	180.0	0.0	180.0	0.0
NiF_6^{2-}	Ni-F	1.70	1.79	0.09	1.71	0.01	1.70	0.00
NiF_6^{4-}	Ni-F	1.90	1.83	-0.07	1.91	0.01	1.71	-0.19
$NiCH_3F$	Ni-F	1.73	1.73	0.00	1.65	-0.08	1.56	-0.17
	Ni-C	1.86	1.93	0.07	1.94	0.08	1.87	0.01
	F-Ni-C	103.7	180.0	76.3	107.6	3.9	107.2	3.5
$NiOF_2$	Ni=O	1.61	1.69	0.08	1.52	-0.09	1.66	0.05
	Ni-F	1.73	1.72	-0.01	1.66	-0.07	1.57	-0.16
	O=Ni-F	117.7	112.1	-5.6	136.5	18.8	107.7	-10.1
$NiF_2.(H_2O)_2$ cis	Ni-O	1.97	2.04	0.07	1.97	0.00	2.09	0.12
	Ni-F	1.80	1.75	-0.05	1.68	-0.12	1.71	-0.10
$NiF_2.(H_2O)_2$ trans	Ni-O	1.93	1.87	-0.06	2.09	0.16	2.06	0.13
	Ni-F	1.81	1.75	-0.06	1.69	-0.12	1.71	-0.10
$NiC_3H_8O_2F_2$	Ni-O	2.02	2.17	0.15	1.93	-0.09	2.01	-0.01
	O-Ni-O	67.6	60.1	-7.5	74.5	6.9	67.3	-0.3
	Ni-F	1.77	1.73	-0.04	1.68	-0.09	1.59	-0.18
	F-Ni-O	95.8	95.6	-0.2	98.4	2.6	97.3	1.5
	F-Ni-O-O	174.8	173.6	-1.3	175.6	0.7	175.5	0.7
$NiAlH_2$	Ni-Al	2.33	2.33	0.00	2.25	-0.09	2.41	0.08
	Ni-Al-H	122.1	117.3	-4.9	120.0	-2.1	113.7	-8.4
$HNiAlH_2$	Ni-Al	2.52	2.36	-0.16	2.24	-0.28	2.57	0.05
	Ni-H	1.58	1.63	0.06	2.56	0.99	2.22	0.64
	H-Ni-Al	180.0	179.9	-0.1	180.0	0.0	179.9	-0.1
	Ni-Al-H	123.3	122.3	-1.0	120.1	-3.2	116.4	-6.9
$NiSiH_3$	Ni-Si	2.26	2.26	0.00	2.55	0.29	2.40	0.14
	Ni-Si-H	111.8	107.5	-4.3	109.0	-2.8	107.1	-4.7
$HNiSiH_3$	Ni-H	1.55	1.64	0.09	2.43	0.88	2.22	0.67
	Ni-Si	2.38	2.35	-0.03	2.56	0.18	2.51	0.13
	Ni-Si-H	113.3	111.3	-2.0	109.2	-4.1	108.9	-4.4
	H-Ni-Si	180.0	179.9	-0.1	179.9	-0.1	180.0	0.0
$NiSi_2C_{14}P_2H_{40}$ (DILDAD)	Ni-P	2.16	2.28	0.12	2.24	0.08	2.09	-0.08
	Ni-Si	3.19	3.20	0.01	3.21	0.02	3.08	-0.11
	Ni-C	2.07	1.99	-0.08	2.05	-0.02	1.93	-0.14
$HNiPH_2$	Ni-H	1.45	1.63	0.19	1.68	0.24	3.07	1.62
	Ni-P	2.14	2.25	0.11	2.20	0.06	2.29	0.15

	Ni-P-H	102.5	88.5	-14.0	101.4	-1.1	116.1	13.6
Ni_2PH	Ni-P	2.04	2.10	0.06	2.17	0.14	1.94	-0.10
	Ni-P-H	109.0	114.4	5.4	116.0	7.0	137.9	29.0
$Ni(PH_3)_4^{2+}$	Ni-P	2.25	2.26	0.01	2.26	0.01	2.26	0.01
NiS	Ni-S	2.00	2.10	0.10	1.92	-0.09	1.94	-0.06
NiSH	Ni-S	2.15	1.96	-0.19	2.15	0.00	2.11	-0.04
	Ni-S-H	94.0	81.4	-12.7	98.5	4.5	104.3	10.3
$NiSH_2$	Ni-S	2.08	2.08	0.00	2.12	0.04	2.39	0.30
	Ni-H	1.45	1.64	0.19	1.68	0.24	3.01	1.56
	Ni-S-H	94.9	91.2	-3.7	100.5	5.6	104.7	9.8
$Ni(H_2S)_4^{2+}$	Ni-S	2.27	2.22	-0.05	2.22	-0.05	2.22	-0.05
$NiC_6N_6H_{16}S_2$ ($Ni(II)(en)_2(NCS)_2$)	Ni-N(en)	2.10	2.16	0.06	1.97	-0.13	2.66	0.56
	Ni-N(NCS)	2.15	2.04	-0.11	2.44	0.29	3.38	1.23
	N-C	1.20	1.18	-0.02	1.17	-0.03	1.17	-0.03
	Ni-N-C	140.0	157.4	17.4	88.2	-51.8	100.1	-39.9
	C-S	1.64	1.65	0.01	1.65	0.01	1.65	0.01
$NiC_8N_2H_{14}S_2$ (BAEINI)	Ni-N	1.85	2.05	0.20	1.88	0.03	1.90	0.04
	N-Ni-N	82.9	74.3	-8.6	86.7	3.8	93.3	10.4
	Ni-S	2.17	2.19	0.02	2.14	-0.03	2.25	0.08
$NiC_{11}N_2H_{21}S_2O_2^+$ (Square, 2S and 2N)	Ni-S	2.20	2.26	0.06	2.26	0.06	2.30	0.10
	S-Ni-S	93.5	100.0	6.5	91.9	-1.6	132.2	38.7
	Ni-N	1.93	2.09	0.16	1.94	0.01	3.01	1.08
	N-Ni-S	84.7	84.0	-0.7	83.2	-1.5	42.9	-41.8
	N-Ni-S-S	-176.5	-173.3	3.2	-183.9	-7.5	-119.7	56.8
$NiC_{11}N_2H_{21}S_2O_2^+$ (Square, 2S and 2N for Ni-S-C)	C-S-Ni	106.5	99.6	-6.9	105.1	-1.3	83.0	-23.5
$Ni((CH_3)_2S)_2F_2$ cis	Ni-S	2.24	2.30	0.06	2.12	-0.12	2.35	0.11
	S-Ni-S	93.2	85.9	-7.3	94.5	1.4	75.4	-17.7
	Ni-F	1.82	1.75	-0.07	1.71	-0.11	1.61	-0.21
	F-Ni-S	87.6	93.6	6.0	87.2	-0.4	95.8	8.2
$Ni((CH_3)_2S)_2F_2$ trans	Ni-S	2.23	2.33	0.10	2.12	-0.11	2.28	0.05
	Ni-F	1.82	1.76	-0.06	1.68	-0.14	1.68	-0.14
	F-Ni-S	89.3	93.7	4.4	87.9	-1.4	92.4	3.1
$NiC_7H_{16}S_2F_2$ (Ni 2S and 2F)	Ni-S	2.24	2.36	0.12	2.15	-0.09	2.39	0.15
	S-Ni-S	91.0	94.2	3.2	88.0	-3.1	129.8	38.8

	Ni-F	1.81	1.78	-0.03	1.68	-0.13	1.65	-0.17
	F-Ni-S	88.7	105.1	16.4	92.5	3.8	100.4	11.7
	F-Ni-S-S	176.4	130.0	-46.5	173.1	-3.4	111.5	-65.0
$NiC_8P_2H_{20}S_2$ (KUSLOZ)	Ni-S	2.18	2.11	-0.07	2.24	0.06	2.18	0.00
	Ni-P	2.16	2.24	0.08	2.19	0.03	2.08	-0.08
	P-Ni-S	88.9	89.6	0.7	87.0	-1.8	96.7	7.8
$NiC_2N_3S_3^-$ (CUSJUV)	Ni-S	2.13	2.15	0.02	2.13	0.00	2.31	0.18
	Ni-S'	2.14	2.23	0.09	2.23	0.09	3.36	1.22
	S-Ni-S	95.0	97.6	2.6	95.9	0.9	91.7	-3.3
	Ni-C	1.85	1.94	0.09	1.82	-0.03	1.84	-0.01
$Ni(N_2S_2H)_2$	Ni-S	2.20	2.22	0.02	2.18	-0.02	2.24	0.04
	S-N	1.68	1.68	0.00	1.61	-0.07	1.66	-0.02
	N-S	1.59	1.61	0.02	1.63	0.04	1.58	-0.01
	Ni-N	1.66	2.11	0.45	1.70	0.04	2.51	0.85
	N-H	1.03	0.99	-0.05	1.04	0.01	1.01	-0.02
$NiC_8N_4S_4^-$ (TROPNJ)	Ni-S	2.14	2.20	0.06	2.26	0.12	2.25	0.11
	S-Ni-S	92.4	92.7	0.2	91.3	-1.1	97.7	5.3
$NiC_4S_4O_4^{2-}$ (TOXNIA)	Ni-S	2.19	2.24	0.05	2.22	0.03	2.23	0.04
	S-Ni-S	92.5	96.8	4.4	89.5	-3.0	83.7	-8.8
$NiC_{10}N_2H_{20}S_6$ (ZOTVUZ)	Ni-S	2.44	2.41	-0.03	2.33	-0.11	2.37	-0.07
	S-Ni-S	87.6	90.1	2.5	86.2	-1.4	73.5	-14.2
	Ni-N	2.02	2.14	0.12	1.93	-0.09	2.44	0.42
NiCl	Ni-Cl	2.17	2.18	0.01	2.14	-0.03	2.20	0.03
$NiCl_2$	Ni-Cl	2.11	2.15	0.04	2.06	-0.05	2.13	0.02
	Cl-Ni-Cl	180.0	180.0	0.0	180.0	0.0	180.0	0.0
$NiCl_4^{2-}$	Ni-Cl	2.29	2.14	-0.15	2.33	0.04	2.30	0.01
$NiCH_3Cl$	Ni-Cl	2.09	2.16	0.07	2.07	-0.02	2.18	0.09
	Ni-C	1.94	1.93	-0.01	1.92	-0.02	1.89	-0.05
	Cl-Ni-C	163.6	179.9	16.4	102.0	-61.5	179.1	15.6
$NiCl.(H_2O)_3^+$	Ni-O	1.93	2.00	0.07	2.06	0.13	2.05	0.12
	Ni-O	1.99	2.00	0.01	2.05	0.06	2.05	0.06
	Ni-Cl	2.13	2.17	0.04	2.12	-0.01	2.11	-0.02
$NiCl_2O$	Ni=O	1.62	1.78	0.16	1.58	-0.04	1.60	-0.02
	Ni-Cl	2.08	2.19	0.11	2.03	-0.05	2.10	0.02
	O=Ni-Cl	116.2	109.3	-6.9	114.5	-1.7	108.8	-7.4

$NiCl_2.(H_2O)_2$ cis	Ni-O	2.01	2.04	0.03	2.09	0.08	2.01	0.00
	Ni-Cl	2.16	2.16	0.00	2.18	0.02	2.16	0.00
$NiCl_2.(H_2O)_2$ trans	Ni-O	1.92	2.04	0.12	2.05	0.13	2.06	0.14
	Ni-Cl	2.20	2.17	-0.03	2.14	-0.06	2.16	-0.04
$Ni((CH_3)_2S)_2Cl_2$ cis	Ni-S	2.27	2.20	-0.07	2.14	-0.13	2.27	0.00
	S-Ni-S	87.3	100.2	12.9	87.6	0.3	89.8	2.5
	Ni-Cl	2.19	2.17	-0.02	2.16	-0.03	2.16	-0.03
	Cl-Ni-S	173.7	167.5	-6.2	177.6	3.9	135.5	-38.2
$Ni((CH_3)_2S)_2Cl_2$ trans	Ni-S	2.26	2.20	-0.06	2.15	-0.11	2.22	-0.04
	Ni-Cl	2.20	2.17	-0.03	2.16	-0.04	2.19	-0.01
	Cl-Ni-S	87.4	87.2	-0.2	85.7	-1.7	79.3	-8.1
$NiC_7H_{16}S_2Cl_2$ (Ni 2S and 2Cl)	Ni-S	2.27	2.24	-0.03	2.28	0.01	2.31	0.04
	S-Ni-S	87.7	110.1	22.4	98.0	10.3	113.4	25.6
	Ni-Cl	2.19	2.20	0.01	2.23	0.04	2.22	0.03
	Cl-Ni-S	173.8	173.6	-0.2	104.7	-69.1	102.7	-71.1
	Cl-Ni-S-S	-79.9	-97.4	-17.5	-107.7	-27.8	-110.0	-30.1
$NiCl_3.H_2O^-$	Ni-O	2.03	2.13	0.10	2.13	0.10	2.12	0.09
	Ni-Cl	2.17	2.23	0.06	2.23	0.06	2.20	0.03
	Ni-Cl	2.26	2.29	0.03	2.30	0.04	2.23	-0.03
NiTi	Ni-Ti	2.01	2.51	0.50	2.53	0.52	13.40	11.39
NiV	Ni-V	2.43	2.43	0.00	2.66	0.23	2.43	0.00
NiCr	Ni-Cr	2.13	2.21	0.08	2.67	0.54	1.40	-0.73
Ni_2	Ni-Ni	2.47	2.48	0.00	1.47	-1.00	2.45	-0.02
Ni_2^-	Ni-Ni	2.52	2.52	0.00	1.79	-0.73	1.99	-0.54
Ni_2^+	Ni-Ni	2.52	2.50	-0.02	1.65	-0.87	2.57	0.04
$Ni_2(C_5H_5)_2(CO)_2$	Ni-Ni	2.43	2.86	0.43	2.38	-0.05	2.85	0.42
$Ni_3(C_5H_5)_3(CO)_2$	Ni-Ni	2.36	3.44	1.08	2.35	-0.01	2.70	0.34
	Ni-C(Cp)	2.17	2.18	0.01	2.12	-0.05	1.90	-0.27
	Ni-C(C=O)	1.91	2.01	0.10	1.87	-0.04	2.11	0.20
NiCu	Ni-Cu	2.26	2.44	0.18	2.71	0.45	1.91	-0.35
NiZn	Ni-Zn	2.22	2.35	0.13	1.97	-0.26	2.88	0.66
NiBr	Ni-Br	2.28	2.27	0.00	2.20	-0.07	2.19	-0.08
$NiBr_2$	Ni-Br	2.22	2.35	0.13	2.18	-0.04	2.21	-0.01
$NiCH_3Br$	Ni-Br	2.19	2.36	0.17	2.22	0.03	2.18	-0.01
	Ni-C	1.85	1.93	0.08	1.91	0.06	1.87	0.02

	Br-Ni-C	107.7	179.0	71.4	103.4	-4.3	179.4	71.8
$NiBr_2O$	Ni=O	1.62	1.58	-0.05	1.73	0.11	1.60	-0.02
	Ni-Br	2.22	2.18	-0.05	2.37	0.15	2.54	0.32
	O=Ni-Br	115.1	144.0	28.9	52.1	-63.0	123.0	7.9
$NiC_3H_8Br_2O_2$ (Ni 2O and 2Br)	Ni-O	2.07	2.18	0.11	2.03	-0.04	2.02	-0.05
	O-Ni-O	65.8	59.2	-6.6	68.0	2.2	66.1	0.3
	Ni-Br	2.26	2.37	0.11	2.30	0.04	2.24	-0.02
	Br-Ni-O	164.3	148.1	-16.2	91.0	-73.3	105.0	-59.3
	Br-Ni-O-O	-16.2	-17.5	-1.3	-109.73	-93.6	-106.7	-90.6
	Br-Ni-O	98.9	90.5	-8.4	102.4	3.5	94.5	-4.3
Ni(SH)Br	Ni-Br	2.24	2.35	0.11	2.23	-0.01	2.14	-0.10
	Ni-S	2.09	2.06	-0.03	2.13	0.04	2.09	0.00
$Ni(PH_2)(NH_2)(SH)Br^{2-}$	Ni-P	2.30	2.29	-0.01	2.28	-0.02	2.25	-0.05
	Ni-Br	2.33	2.44	0.11	2.25	-0.08	2.33	0.00
	Ni-S	2.20	2.10	-0.10	2.19	-0.01	2.23	0.02
	Ni-N	1.83	2.03	0.20	1.87	0.04	2.10	0.27
$NiC_8N_2H_{20}S_3Br^+$ (BRUCUB)	Ni-Br	2.58	2.68	0.10	2.43	-0.15	2.25	-0.33
	Ni-N	2.07	2.16	0.09	2.07	0.00	2.69	0.62
	N-Ni-Br	89.9	94.1	4.2	70.2	-19.8	88.3	-1.6
	Ni-S	2.39	2.31	-0.09	2.30	-0.09	2.28	-0.11
	S-Ni-Br	89.4	62.5	-26.9	102.3	13.0	81.8	-7.6
$Ni((CH_3)_2S)_2Br_2$ cis	Ni-S	2.29	2.21	-0.08	2.16	-0.13	2.29	0.00
	S-Ni-S	86.3	95.6	9.3	82.7	-3.6	75.4	-11.0
	Ni-Br	2.33	2.38	0.05	2.31	-0.02	2.21	-0.12
	Br-Ni-S	173.8	172.4	-1.4	176.0	2.2	172.3	-1.5
$Ni((CH_3)_2S)_2Br_2$ trans	Ni-S	2.26	2.17	-0.09	2.15	-0.11	2.22	-0.04
	Ni-Br	2.35	2.38	0.03	2.35	0.00	2.25	-0.10
	Br-Ni-S	86.5	75.8	-10.7	84.3	-2.2	76.5	-10.1
$NiC_7H_{16}S_2Br_2$ (Ni 2S and 2Br)	Ni-S	2.28	2.26	-0.02	2.31	0.03	2.31	0.03
	S-Ni-S	81.9	106.5	24.6	90.4	8.5	115.0	33.1
	Ni-Br	2.33	2.38	0.05	2.33	0.00	2.26	-0.07
	Br-Ni-S	94.0	99.5	5.5	106.3	12.3	83.9	-10.1
	Br-Ni-S-S	179.8	136.1	-43.7	144.1	-35.8	118.4	-61.5
NiZr	Ni-Zr	2.21	2.73	0.52	2.43	0.23	3.49	1.28
NiMo	Ni-Mo	2.14	2.20	0.06	2.52	0.38	10.99	8.85

NiI	Ni-I	2.39	2.20	-0.19	2.27	-0.12	2.34	-0.05
NiI_2	Ni-I	2.45	2.20	-0.25	2.37	-0.07	2.36	-0.09
$NiCH_3I$	Ni-I	2.39	2.31	-0.08	2.33	-0.06	2.34	-0.05
	Ni-C	1.85	1.93	0.08	1.91	0.06	1.86	0.01
	I-Ni-C	107.5	142.9	35.4	107.5	0.0	111.5	4.0
$NiIF_3^{2-}$	Ni-F	1.88	1.76	-0.12	2.22	0.34	1.81	-0.07
NiICl	Ni-I	2.41	2.23	-0.18	2.33	-0.08	2.37	-0.04
	Ni-Cl	2.08	2.18	0.10	2.05	-0.03	2.11	0.03
	I-Ni-Cl	120.2	79.6	-40.6	113.4	-6.8	75.0	-45.2
$NiC_3H_8I_2O_2$ (Ni 2O and 2I)	Ni-O	2.10	2.10	0.00	2.02	-0.08	1.99	-0.11
	O-Ni-O	64.6	63.2	-1.4	69.4	4.8	67.7	3.2
	Ni-I	2.47	2.29	-0.18	2.58	0.11	2.69	0.22
	I-Ni-O	101.1	102.1	1.0	56.1	-45.0	110.2	9.1
	I-Ni-O-O	176.5	176.1	-0.4	237.0	60.5	150.9	-25.6
$Ni((CH_3)_2S)_2I_2$ cis	Ni-S	2.29	2.16	-0.13	2.16	-0.13	2.26	-0.03
	S-Ni-S	85.1	100.0	14.9	80.2	-4.9	82.2	-2.9
	Ni-I	2.56	2.29	-0.27	2.52	-0.04	2.46	-0.10
	I-Ni-S	167.8	121.3	-46.5	172.7	4.9	173.6	5.8
$Ni((CH_3)_2S)_2I_2$ trans	Ni-S	2.27	2.18	-0.09	2.13	-0.14	2.20	-0.07
	Ni-I	2.58	2.35	-0.23	2.53	-0.05	2.49	-0.09
	I-Ni-S	85.4	111.7	26.3	78.8	-6.6	68.9	-16.5

	AM1*	PM6	PM5
N=177			
MSE bond length	0.04	0.01	0.24
MUE bond length	0.09	0.11	0.33
N=80			
MSE bond angle	0.2	-5.1	-4.6
MUE bond angle	10.2	10.7	15.9

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AM1* Parameters for Cobalt and Nickel

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Supplementary Material

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Table S1: Sources and calculation details for the heats of formation used to parameterize.

Heat of Formation for Cobalt Containing Compounds				
Compound	**Target(kcal/mol)**	**Source**	**Reaction**	**Total Energy (a.u.)**
Co	102.0	S1		
Co^-	86.2	S2		
Co^+	281.5	S2		
Co^{2+}	677.6	S2		
Co^{3+}	1450.0	S2		
Co^{4+}	2633.0	S2		
Co^{5+}	4466.0	S2		
Co_2	183.5	S3		-290.0008295
Co_2^-	137.6	S3		-290.0969743
HCo	102.8	S3		-145.6117353
HCo^-	98.5	S1		
$C_5H_5Co^-$	114.8	S1		
$CoC_{10}H_{10}$ (bicyclopentadienyl cobalt)	73.9	S1		
$CoCp_2$ (DCYPCO)	52.0	S4		
$CoC_6N_6H_{24}^{3+}$ (COTENC01)	587.5	S4		
$CoC_6N_6H_{24}^{2+}$ (QICSOK)	280.9	S4		
$CoC_9N_6H_{15}$ (FEFRUD)	58.2	S4		
CoO^-	36.6	S1		
CoO_2^-	-34.0	S1		
$Co_2(H_2O)_4^{4+}$	1052.6	S3		-593.8648305
$Co(H_2O)_6^{2+}$	58.3	S4		
$Co(CO)_4$	-134.3	S1		
$CoH(CO)_4$	-136.0	S1		
$Co(CO)_5^+$	4.1	S4		
$CoC_6O_{12}^{3-}$ ($Co(III)(ox)_3$)	-542.2	S4		
$Co_2(CO)_8$	-283.0	S1		
$CoN_6H_{15}O_2^{2+}$ (FAMYEX)	252.3	S4		
$CoC_6N_4H_{16}O_4^+$ (AETXCO)	-93.9	S4		
$CoC_6N_4H_{16}O_4^+$ (OXENCO)	-96.0	S4		
$CoC_6N_6H_{18}O_4^+$ (NIXGEG)	27.9	S4		
$CoC_9N_4H_{19}O_5$ (AMGXCO01)	-131.7	S4		
$CoC_6N_6H_{20}O_6^+$ (NITNCO)	-39.2	S4		
CoOF	-70.8	S3		-320.1138776
CoF_2	-85.2	S1		
CoF_3	-139.6	S4		
CoF_4^-	-302.0	S1		
$CoAlH_2$	125.9	S3		-148.2359720
$HCoAlH_2$	160.3	S3		-148.7811485
$CoSiH_3$	109.6	S3		-150.7428055
CoP	131.2	S3		-151.5210650
$CoPH_2$	100.3	S3		-152.7661378
$HCoPH_2$	111.1	S3		-153.3415817
CoS	117.5	S3		-155.1464344
CoSH	82.7	S3		-155.7984653
HCoSH	87.4	S3		-156.3830504
$CoC_{10}H_{14}S_4$ (TACACO10)	-11.8	S4		
$CoC_9H_{21}S_6$ (MEDTCO10)	-65.7	S4		

$CoC_3N_3H_6S_6$ (TDTCCO)	-24.9	S4		
CoCl	46.1	S1		
CoClO	13.8	S4		
$CoCl_2$	-22.4	S1		
$CoCl_3$	-39.1	S1		
Co_2Cl_4	-83.8	S1		
$CoC_4N_5H_{19}Cl^{2+}$ (ADETCO)	254.0	S4		
$Co(NH_3)_2(H_2O)_2ClF^+$	-104.6	S4		
$CoC_2N_4H_8S_2Cl_2$ (COTUCL11)	-61.2	S4		
$CoC_6N_3H_{17}Cl_3$ (AMPRCO)	-159.2	S4		
$CoC_4N_2H_{12}SCl_3$ (CATBAA)	-128.2	S4		
CoTi	116.0	S3		-203.0453669
CoV	161.5	S3		-216.2698854
CoCr	217.7	S3		-231.2600365
CoNi	108.1	S3		-314.3285204
CoCu	143.1	S3		-341.2070649
HCoCu	150.9	S3		-341.7848971
CoZn	124.6	S3		-210.6340041
HCoZn	121.4	S3		-211.2304461
CoBr	86.4	S4		
CoBrO	19.9	S4		
$CoBr_2$	29.0	S3		-171.4941433
$CoBr_3$	15.9	S3		-184.6921504
$CoBr_4$	19.3	S3		-197.8647845
$CoBr_4^{2-}$	-99.0	S3		-198.0528852
$C_4H_8N_4O_5CoBr$ (BUKPIG)	-99.6	S4		
CoZr	209.8	S3		-191.5068270
CoMo	285.3	S3		-212.4061812
HCoMo	280.4	S3		-213.0049741
CoI	96.2	S4		
ICoO	34.0	S4		
CoI_3	19.5	S4		
CoI_4	39.0	S3		-190.7526800
$C_{10}H_{15}NS_2CoI$ (GECVEP)	-13.3	S4		
$C_4H_4N_4O_4CoI_2^-$ (FIRCOY01)	-16.8	S4		
Heats of Formation for Nickel Containing Compounds				
Ni	102.8	S1		
Ni^-	76.0	S1		
Ni^+	276.7	S2		
Ni^{2+}	697.2	S2		
Ni_2^-	128.6	S1		
Ni_2^+	428.3	S3	$Ni^+ + Ni \rightarrow Ni_2^+$	-338.2775290
NiH	85.6	S5		
NiH^+	254.5	S3		-169.5024919
NiH_2	83.5	S3		-170.3707914
NiH_3	36.1	S3		-171.0445891
$Ni(C_5H_5)_2$	79.7	S1		
$Ni2(C_5H_5)_2(CO)_2$	-27.0	S4		
NiCO	35.1	S6		
$NiCO^-$	17.2	S1		
$Ni(CO)_2$	-39.0	S6		
$Ni(CO)_2^-$	-53.0	S1		
$Ni(CO)_3$	-93.0	S1		

$Ni(CO)_3^-$	-118.8	S1		
$Ni(CO)_4$	-144.0	S1		
NiO	75.0	S7		
NiO^-	41.1	S1		
NiO_2^-	-28.3	S1		
$Ni(OH)_2.(H_2O)_2$ cis	-180.9	S4		
$Ni(OH)_2.(H_2O)_2$ trans	-177.6	S4		
$Ni(OH).(H_2O)_3^+$	-36.3	S4		
$Ni(H_2O)_4$	221.9	S4		
$Ni(H_2O)_6$	55.7	S4		
$NiH_{12}O_6^{2+}$ (JERNID)	54.4	S4		
$Ni(NH_2)_2$	39.4	S3		-281.2357903
$Ni(NH_3)_4^{2+}$	319.5	S4		
$Ni(NH_3)_6^{2+}$	271.4	S4		
$Ni(CN)_4^{2-}$	99.1	S4		
$Ni(CN)_5^{3-}$	258.9	S4		
$Ni(CO)_3NO$	-89.0	S4		
$NiC_8N_4H_{14}O_4$ (NIMGLO10)	-37.1	S4		
$NiC_{10}N_2H_{12}O_8$ (Ni-EDTA)	-361.5	S4		
$NiC_{13}NH_{17}O_4$ (VAXSUI)	-142.3	S4		
NiF	17.5	S5		
NiF_2	-115.5	S3		-369.0729517
NiF_4^{2-}	-211.5	S4		
$NiCH_3F$	-8.3	S4		
$NiOF_2$	-50.8	S4		
$NiF_2.(H_2O)_2$ cis	-214.2	S4		
$NiF_2.(H_2O)_2$ trans	-219.4	S4		
$NiAlH_2$	56.2	S3		-172.4784624
$HNiAlH_2$	121.3	S3		-172.9677957
$NiSiH_3$	41.6	S3		-174.9826293
$HNiSiH_3$	98.6	S3		-175.4857194
$HNiPH_2$	50.7	S3		-177.5719902
$Ni(PF_3)_4$	-953.4	S1		
NiS	85.4	S1		
NiSH	20.0	S3		-108. 0291688
$NiSH_2$	36.4	S3		-180.5989403
$Ni(H_2S)_4^{2+}$	384.0	S4		
$NiC_2N_3S_3^{2-}$ (CUSJUV)	62.9	S4		
$NiC_4S_4O4^{2-}$ (TOXNIA)	-217.9	S4		
$NiC_8N_4S_4^-$ (TROPNJ)	92.8	S4		
$NiC_8N_2H_{14}S_2$ (BAEINI)	12.2	S4		
$NiC_{10}N_2H_{20}S_6$ (ZOTVUZ)	6.4	S4		
$NiC_{11}N_2H_{21}S_2O_2^+$ (Square, 2S and 2N)	72.1	S4		
$Ni(N_2S_2H)_2$	95.3	S4		
$Ni((CH_3)_2S)_2F_2$ cis	-153.5	S4		
$Ni((CH_3)_2S)_2F_2$ trans	-162.5	S4		
NiCl	43.5	S1		
$NiCl_2$	-17.7	S1		
$NiCl_4^{2-}$	-130.1	S4		
$NiCH_3Cl$	37.2	S4		
$NiCl_2O$	-0.5	S4		
$NiCl_3.H_2O^-$	-188.1	S4		
$NiCl.(H_2O)_3^+$	-19.4	S4		

$NiCl_2.(H_2O)_2$ cis	-150.9	S4		
$NiCl_2.(H_2O)_2$ trans	-155.3	S4		
$Ni((CH_3)_2S)_2Cl_2$ cis	-89.2	S4		
$Ni((CH_3)_2S)_2Cl_2$ trans	-96.4	S4		
NiTi	211.0	S3		-227.2232292
NiCu	137.7	S3		-365.4450882
NiZn	151.2	S3		-234.821028
NiBr	57.8	S3		-182.4989681
$NiBr_2$	52.9	S3		-195.6842375
$NiCH_3Br$	24.6	S4		
$Ni((CH_3)_2S)_2Br_2$ cis	-70.8	S4		
$Ni((CH_3)_2S)_2Br_2$ trans	-77.1	S4		
$NiC_8N_2H_{20}S_3Br^+$ (BRUCUB)	75.1	S4		
NiZr	218.3	S3		-215.7227516
NiMo	296.6	S3		-236.6177257
NiI	62.3	S3		-180.7185192
NiI_2	36.5	S3		-192.1710311
$NiCH_3I$	37.0	S4		
$Ni((CH_3)_2S)_2I_2$ cis	-42.3	S4		

Table S2: Sources and calculation details for the ionization potentials and dipole moments used to parameterize.

Koopmans' Theorem Ionization Potentials for Cobalt Containing Compounds		
Compound	**Target(eV)**	**Source**
$CoCH_3$	7.00	S1
$CoC_{10}H_{10}$	5.55	S1
$Co(CO)_4$	8.30	S1
$Co_2(CO)_8$	8.30	S1
CoCl	8.90	S1
$CoCl_2$	10.70	S1
$CoBr_2$	9.90	S1
Koopmans' Theorem Ionization Potentials for Nickel Containing Compounds		
Ni^+	18.17	S7
NiH	8.50	S1
NiO	9.50	S1
NiF_2	11.50	S1
NiCl	9.28	S8
$NiCl_2$	11.20	S1
NiCO	7.30	S6
$Ni(CO)_2$	7.79	S6
$Ni(CO)_3$	7.69	S6
$Ni(CO)_4$	8.72	S1
$Ni(Cp)_2$	6.51	S1

Dipole Moments for Cobalt Containing Compounds		
Compound	**Target(Debye)**	**Source**
$CoC_5H_5^-$	1.61	S3

CoO^-	1.07	S3
$Co(CO)_4$	0.25	S3
$CoH(CO)_4$	0.42	S3
$Co_2(CO)_8$	1.23	S3
CoOF	0.16	S4
CoClO	0.93	S4
CoBr	3.65	S4
CoBrO	1.81	S4
CoI	2.32	S4
CoIO	2.40	S4
Dipole Moments for Nickel Containing Compounds		
NiH	2.40	S9
NiH^+	0.83	S3
NiH_3	3.75	S3
NiO	4.00	S4
NiO^-	3.33	S3
$Ni(OH)_2.(H_2O)_2$ cis	3.50	S4
NiCO	3.35	S3
NiF	4.49	S4
$NiCH_3F$	3.59	S4
$NiOF_2$	1.67	S4
$NiF_2.(H_2O)_2$ cis	6.48	S4
NiCl	4.39	S4
$NiCH_3Cl$	4.39	S4
$NiCl_2O$	1.40	S4
$NiCl_2.(H_2O)_2$ cis	6.70	S4

Table S3: Sources and calculation details for the geometrical variables used to parameterize.

Geometrical Variables for Cobalt Containing Compounds			
Compound	**Variable**	**Target**	**Source**
Co_2	Co-Co	2.30	S3
Co_2^-	Co-Co	2.63	S3
HCo	Co-H	1.55	S3
HCo^-	Co-H	1.66	S3
$CoC_5H_5^-$	Co-C	1.93	S3
$CoCp_2$ (DCYPCO)	Co-C	2.08	S10
$Co(CN)_4^+$	Co-C	1.81	S4
	C-N	1.20	S4
$Co(CN)_6^{3-}$	Co-C	1.97	S4
$CoC_6N_6H_{24}$ ($Co(II)(en)_3$)	Co-N	2.06	S4
$CoC_6N_6H_{24}^{3+}$ (COTENC01)	Co-N	2.00	S10
	N-Co-N	90.2	S10
$CoC_6N_6H_{24}^{2+}$ (QICSOK)	Co-N	2.20	S10
	N-Co-N	78.7	S10
$CoC_9N_6H_{15}$ (FEFRUD)	Co-N	2.01	S10

	N-Co-N	90.3	S10
	Co-C	1.89	S10
CoO^-	Co=O	1.65	S3
CoO_2^-	Co=O	1.68	S3
$Co(H_2O)_4^{2+}$	Co-O	1.94	S3
$Co(H_2O)_6^{3+}$	Co-O	2.03	S3
$Co_2(H_2O)_4^{4+}$	Co-O	2.17	S3
$Co(H_2O)_6^{2+}$ (NAZVOZ)	Co-O	2.06	S10
	Co-O'	2.12	S10
$Co(H_2O)_6^{2+}$	Co-O	2.12	S4
	Co-O'	1.96	S4
$Co(CO)_4$	Co-C	1.85	S3
$Co(CO)_4^-$ (FUBYOQ)	Co-C	1.75	S10
$CoH(CO)_4$	Co-H	1.55	S3
	Co-C	1.81	S3
$Co(CO)_5^+$	Co-C(eq)	1.83	S4
	Co-C(ax)	1.89	S4
$CoC_6O_{12}^{3-}$ (Co(iii)(ox)$_3$)	Co-O	1.95	S4
$Co_2(CO)_8$	Co-Co	2.47	S4
$Co(CO)_3NO$	Co-C	1.81	S4
	C-Co-C	103.2	S4
	Co-N	1.67	S4
$Co(NO_3)_3$	Co-O	1.89	S4
	O-Co-O	68.0	S4
	O-Co-O'	93.0	S4
$CoN_6H_{15}O_2^{2+}$ (FAMYEX)	Co-N(O2)	1.95	S10
	Co-N(H3)	1.96	S10
	N-Co-N	90.0	S10
$CoC_6N_4H_{16}O_4^+$ (OXENCO)	Co-N	1.98	S10
	N-Co-N	86.0	S10
	Co-O	1.94	S10
$CoC_6N_4H_{16}O_4^+$ (AETXCO)	Co-O	1.92	S10
	O-Co-O	84.8	S10
	Co-N(H2C)	1.98	S10
	Co-N(H3)	1.95	S10
	C-N(HC2)	1.92	S10
$CoC_6N_6H_{18}O_4^+$ (NIXGEG)	Co-N(C3)	1.96	S10
	Co-N(CH2)	1.96	S10
	N-Co-N	86.8	S10
	Co-N(O2)	1.99	S10
	Co-N(O2)	1.93	S10
$CoC_9N_4H_{19}O_5$ (AMGXCO01)	Co-N	1.89	S10
	N-Co-N	82.0	S10
	Co-C	1.98	S10
	Co-O	2.06	S10
$CoC_{15}H_{21}O_6^-$ (Co(II)(Acac)$_3$(-) IKEYAY)	Co-O	2.06	S10
	O-Co-O	88.0	S10
$CoC_6N_6H_{20}O_6^+$ (NITNCO)	Co-N	2.00	S10
	N-Co-N	87.7	S10
	Co-O	1.90	S10
CoF	Co-F	1.91	S4
CoOF	Co=O	1.59	S4

	Co-F	1.72	S4
CoF_2	Co-F	1.72	S3
CoF_3	Co-F	1.72	S4
	F-Co-F	108.5	S4
CoF_4^-	Co-F	1.79	S3
$CoAlH_2$	Co-Al	2.40	S3
$HCoAlH_2$	Co-Al	2.53	S3
$CoSiH_3$	Co-Si	2.33	S3
$CoSiC_4O_4F_3$ (FUZMAO)	Co-Si	2.23	S10
	Si-F	1.50	S10
	F-Si-Co	114.8	S10
	Co-C	1.79	S10
	C-O	1.11	S10
CoP	Co≡P	2.16	S3
$CoPH_2$	Co-P	2.26	S3
$HCoPH_2$	Co-P	2.32	S3
CoS	Co=S	2.01	S3
CoSH	Co-S	2.16	S3
HCoSH	Co-S	2.23	S3
$CoC_{10}H_{14}S_4$ (TACACO10)	Co-S	2.17	S10
	S-Co-S	96.9	S10
$CoC_9H_{21}S_6$ (MEDTCO10)	Co-S	2.30	S10
	S-Co-S	89.8	S10
$CoC_3N_3H_6S_6$ (TDTCCO)	Co-S	2.29	S10
	S-Co-S	76.3	S10
CoCl	Co-Cl	2.07	S4
CoClO	Co=O	1.61	S4
	Co-Cl	2.07	S4
$CoCl_2$	Co-Cl	2.11	S3
$CoCl_3$	Co-Cl	2.13	S3
$CoCl_4^{2-}$ (DMDPCO)	Co-Cl	2.25	S10
Co_2Cl_4	Co-Cl	2.12	S3
	Co-Cl'	2.21	S3
$CoCH_3ClOH$	Co-O	1.73	S4
	Co-C	1.91	S4
	Co-Cl	2.10	S4
$CoC_4N_5H_{19}Cl^{2+}$ (ADETCO)	Co-Cl	2.28	S10
	Co-N(H3)	1.97	S10
	N-Co-Cl	87.7	S10
	Co-N(C2H)	1.94	S10
	N-Co-N	94.3	S10
	Co-N(H2C)	1.99	S10
$Co(NH_3)_2(H_2O)_2ClF^+$	Co-Cl	2.23	S4
	Co-N	1.97	S4
	Co-F	1.85	S4
	Co-O	1.97	S4
$CoC_9P_3H_{27}Cl$ (BUTDEZ)	Co-Cl	2.22	S10
	Co-P	2.24	S10
	Cl-Co-P	113.8	S10
$CoC_2N_4H_8S_2Cl_2$ (COTUCL11)	Co-Cl	2.26	S10
	Co-Cl'	2.27	S10
	Cl-Co-Cl	107.7	S10
	Co-S	2.30	S10

	Co-C	3.31	S10
$CoC_6N_3H_{17}Cl_3$ (AMPRCO)	Co-Cl	2.24	S10
	Co-Cl'	2.31	S10
	Cl-Co-Cl	91.2	S10
	Co-N	1.97	S10
$CoC_4N_2H_{12}SCl_3$ (CATBAA)	Co-Cl	2.28	S10
	Cl-Co-Cl	91.7	S10
	Co-N	1.93	S10
	Co-S	2.22	S10
CoTi	Co-Ti	2.35	S3
CoV	Co-V	2.34	S3
CoCr	Co-Cr	2.35	S3
CoNi	Co-Ni	2.38	S3
CoCu	Co-Cu	2.29	S3
HCoCu	Co-Cu	2.35	S3
CoZn	Co-Zn	2.54	S3
HCoZn	Co-Zn	2.49	S3
CoBr	Co-Br	2.21	S4
BrCoO	Co=O	1.60	S4
	Co-Br	2.19	S4
$CoBr_2$	Co-Br	2.27	S3
$CoBr_3$	Co-Br	2.28	S3
$CoBr_4$	Co-Br	2.43	S3
$CoBr_4^{2-}$	Co-Br	2.40	S3
$C_4H_8N_4O_5CoBr$ (BUKPIG)	Co-Br	2.36	S10
	Co-O	1.96	S10
	Co-N	1.91	S10
CoZr	Co-Zr	2.16	S3
CoMo	Co-Mo	2.33	S3
CoI_2	Co-I	2.57	S3
CoI_4	Co-I	2.61	S3
CoI	Co-I	2.39	S4
ICoO	Co=O	1.60	S4
	Co-I	2.40	S4
$C_{10}H_{15}NS_2CoI$ (GECVEP)	Co-I	2.60	S10
	Co-S	2.25	S10
	I-Co-S	95.6	S10
	S-Co-S	76.5	S10
$C_4H_4N_4O_4CoI_2^-$ (FIRCOY01)	Co-I	2.58	S10
	Co-N	1.88	S10
CoI_3	Co-I	2.42	S4
$CoCH_3ICl$	Co-I	2.47	S4
	Co-C	1.95	S4
	Co-Cl	2.14	S4
	C-Co-I	101.5	S4
	C-Co-Cl	97.1	S4
Geometrical Variables for Nickel Containing Compounds			
NiH	Ni-H	1.61	S3
NiH^+	Ni-H	1.44	S3
NiH_2	Ni-H	1.64	S3
	H-Ni-H	180.0	S3
NiH_3	Ni-H	1.82	S3
	Ni-H(2)	1.52	S3

	H-Ni-H	167.7	S3
	H-Ni-H	24.5	S3
$Ni(CN)_4^{2-}$	Ni-C	1.89	S4
	C#N	1.19	S4
$Ni(CN)_5^{3-}$	Ni-C(ap)	2.17	S11
	Ni-C(ba)	1.87	S11
NiCO	Ni-C	1.67	S3
$Ni(CO)_2$	Ni-C	1.84	S3
	C-Ni-C	180.0	S3
$Ni(CO)_2^-$	Ni-C	1.76	S3
	C-Ni-C	180.0	S3
$Ni(CO)_3$	Ni-C	1.82	S3
	C-Ni-C	120.0	S3
$Ni(CO)_3^-$	Ni-C	1.79	S3
	C-Ni-C	120.0	S3
$Ni(CO)_4$	Ni-C	1.85	S3
	C-Ni-C	109.5	S3
$Ni(NH2)_2$	Ni-N	1.81	S3
	N-Ni-N	180.0	S3
	H-N-Ni	125.5	S3
$Ni(NH_3)_4^{2+}$	Ni-N	2.00	S4
$Ni(NH_3)_6^{2+}$	Ni-N	1.96	S4
$NiC_6N_6H_{24}^{2+}$ ($Ni(II)(en)_3$)	Ni-N	2.19	S4
$NiC_8N_6H_{26}^{2+}$ (AEAMNI10)	Ni-N	2.14	S10
	Ni-N'	2.05	S10
	N-Ni-N'	81.6	S10
$NiC_{32}N_8H_{16}$ (Nickel Phthalocyanine)	Ni-N	1.92	S4
$Ni(CO)_3NO$	Ni-C	1.81	S4
	Ni-N	1.88	S4
	C-Ni-N	108.6	S4
$NiC_{13}NH_{17}O_4$ (VAXSUI)	Ni-N	1.94	S10
	Ni-C	1.97	S10
	C-Ni-N	135.8	S10
	Ni-C'	1.99	S10
$NiC_8N_4H_{14}O_4$ (NIMGLO10)	Ni-N	1.85	S10
	N-Ni-N	83.1	S10
NiO	Ni-O	1.67	S3
NiO^-	Ni-O	1.68	S3
NiO_2^-	Ni-O	1.67	S3
	O-Ni-O	180.0	S3
$Ni(OH)_2$	Ni-O	1.75	S4
	O-H	0.99	S4
$Ni(OH)_2.(H_2O)_2$ cis	Ni-O	2.01	S4
	Ni-O	1.83	S4
$Ni(OH)_2.(H_2O)_2$ trans	Ni-O	1.88	S4
	Ni-O	1.94	S4
$Ni(OH).(H_2O)_3^+$	Ni-O	1.93	S4
	Ni-O	1.80	S4
$Ni(H_2O)_4^{2+}$	Ni-O	1.90	S4
$Ni(H2O)_6^{2+}$	Ni-O	2.09	S4
$NiH_{12}O_6^{2+}$ (JERNID)	Ni-O	2.03	S10
$NiC_{10}H_{18}O_6$ (AQACNI)	Ni-O	2.01	S10
	O-Ni-O	91.6	S10

	Ni-O(H2)	2.09	S10
NiF	Ni-F	1.77	S3
NiF_2	Ni-F	1.74	S3
	F-Ni-F	180.0	S3
NiF_6^{2-}	Ni-F	1.70	S12
NiF_6^{4-}	Ni-F	1.90	S4
$NiCH_3F$	Ni-F	1.73	S4
	Ni-C	1.86	S4
	F-Ni-C	103.7	S4
$NiOF_2$	Ni=O	1.61	S4
	Ni-F	1.73	S4
	O=Ni-F	117.7	S4
$NiF_2.(H_2O)_2$ cis	Ni-O	1.97	S4
	Ni-F	1.80	S4
$NiF_2.(H_2O)_2$ trans	Ni-O	1.93	S4
	Ni-F	1.81	S4
$NiC_3H_8O_2F_2$	Ni-O	2.02	S4
	O-Ni-O	67.6	S4
	Ni-F	1.77	S4
	F-Ni-O	95.8	S4
	F-Ni-O-O	174.8	S4
$NiAlH_2$	Ni-Al	2.33	S3
	Ni-Al-H	122.1	S3
$HNiAlH_2$	Ni-Al	2.52	S3
	Ni-H	1.58	S3
	H-Ni-Al	180.0	S3
	Ni-Al-H	123.3	S3
$NiSiH_3$	Ni-Si	2.26	S3
	Ni-Si-H	111.8	S3
$HNiSiH_3$	Ni-H	1.55	S3
	Ni-Si	2.38	S3
	Ni-Si-H	113.3	S3
	H-Ni-Si	180.0	S3
$NiSi_2C_{14}P_2H_{40}$ (DILDAD)	Ni-P	2.16	S10
	Ni-Si	3.19	S10
	Ni-C	2.07	S10
$HNiPH_2$	Ni-H	1.45	S3
	Ni-P	2.14	S3
	Ni-P-H	102.5	S3
Ni_2PH	Ni-P	2.04	S3
	Ni-P-H	109.0	S3
$Ni(PH_3)_4^{2+}$	Ni-P	2.25	S4
NiS	Ni-S	2.00	S3
NiSH	Ni-S	2.15	S3
	Ni-S-H	94.0	S3
$NiSH_2$	Ni-S	2.08	S3
	Ni-H	1.45	S3
	Ni-S-H	94.9	S3
$Ni(H_2S)_4^{2+}$	Ni-S	2.27	S4
$NiC_6N_6H_{16}S_2$ $(Ni(II)(en)_2(NCS)_2)$	Ni-N(en)	2.10	S12
	Ni-N(NCS)	2.15	S12
	N-C	1.20	S12
	Ni-N-C	140.0	S12

	C-S	1.64	S12
$NiC_8N_2H_{14}S_2$ (BAEINI)	Ni-N	1.85	S10
	N-Ni-N	82.9	S10
	Ni-S	2.17	S10
$NiC_{11}N_2H_{21}S_2O_2^+$ (Square, 2S and 2N)	Ni-S	2.20	S4
	S-Ni-S	93.5	S4
	Ni-N	1.93	S4
	N-Ni-S	84.7	S4
	N-Ni-S-S	-176.5	S4
$NiC_{11}N_2H_{21}S_2O_2^+$ (Square, 2S and 2N for Ni-S-C)	C-S-Ni	106.5	S4
$Ni((CH_3)_2S)_2F_2$ cis	Ni-S	2.24	S4
	S-Ni-S	93.2	S4
	Ni-F	1.82	S4
	F-Ni-S	87.6	S4
$Ni((CH_3)_2S)_2F_2$ trans	Ni-S	2.23	S4
	Ni-F	1.82	S4
	F-Ni-S	89.3	S4
$NiC_7H_{16}S_2F_2$ (Ni 2S and 2F)	Ni-S	2.24	S4
	S-Ni-S	91.0	S4
	Ni-F	1.81	S4
	F-Ni-S	88.7	S4
	F-Ni-S-S	176.4	S4
$NiC_8P_2H_{20}S_2$ (KUSLOZ)	Ni-S	2.18	S10
	Ni-P	2.16	S10
	P-Ni-S	88.9	S10
$NiC_2N_3S_3^-$ (CUSJUV)	Ni-S	2.13	S10
	Ni-S'	2.14	S10
	S-Ni-S	95.0	S10
	Ni-C	1.85	S10
$Ni(N_2S_2H)_2$	Ni-S	2.20	S4
	S-N	1.68	S4
	N-S	1.59	S4
	Ni-N	1.66	S4
	N-H	1.03	S4
$NiC_8N_4S_4^-$ (TROPNJ)	Ni-S	2.14	S10
	S-Ni-S	92.4	S10
$NiC_4S_4O_4^{2-}$ (TOXNIA)	Ni-S	2.19	S10
	S-Ni-S	92.5	S10
$NiC_{10}N_2H_{20}S_6$ (ZOTVUZ)	Ni-S	2.44	S10
	S-Ni-S	87.6	S10
	Ni-N	2.02	S10
NiCl	Ni-Cl	2.17	S4
$NiCl_2$	Ni-Cl	2.11	S3
	Cl-Ni-Cl	180.0	S3
$NiCl_4^{2-}$	Ni-Cl	2.29	S4
$NiCH_3Cl$	Ni-Cl	2.09	S4
	Ni-C	1.94	S4
	Cl-Ni-C	163.6	S4
$NiCl.(H_2O)_3^+$	Ni-O	1.93	S4
	Ni-O	1.99	S4
	Ni-Cl	2.13	S4
$NiCl_2O$	Ni=O	1.62	S4

	Ni-Cl	2.08	S4
	O=Ni-Cl	116.2	S4
$NiCl_2.(H_2O)_2$ cis	Ni-O	2.01	S4
	Ni-Cl	2.16	S4
$NiCl_2.(H_2O)_2$ trans	Ni-O	1.92	S4
	Ni-Cl	2.20	S4
$Ni((CH_3)_2S)_2Cl_2$ cis	Ni-S	2.27	S4
	S-Ni-S	87.3	S4
	Ni-Cl	2.19	S4
	Cl-Ni-S	173.7	S4
$Ni((CH_3)_2S)_2Cl_2$ trans	Ni-S	2.26	S4
	Ni-Cl	2.20	S4
	Cl-Ni-S	87.4	S4
$NiC_7H_{16}S_2Cl_2$ (Ni 2S and 2Cl)	Ni-S	2.27	S4
	S-Ni-S	87.7	S4
	Ni-Cl	2.19	S4
	Cl-Ni-S	173.8	S4
	Cl-Ni-S-S	-79.9	S4
$NiCl_3.H_2O^-$	Ni-O	2.03	S4
	Ni-Cl	2.17	S4
	Ni-Cl	2.26	S4
NiTi	Ni-Ti	2.01	S3
Ni_2	Ni-Ni	2.47	S3
Ni_2^-	Ni-Ni	2.52	S3
Ni_2^+	Ni-Ni	2.52	S3
$Ni_2(C_5H_5)_2(CO)_2$	Ni-Ni	2.43	S4
$Ni_3(C_5H_5)_3(CO)_2$	Ni-Ni	2.36	S4
	Ni-C(Cp)	2.17	S4
	Ni-C(C=O)	1.91	S4
NiCu	Ni-Cu	2.26	S3
NiZn	Ni-Zn	2.22	S3
NiBr	Ni-Br	2.28	S3
$NiBr_2$	Ni-Br	2.22	S3
$NiCH_3Br$	Ni-Br	2.19	S4
	Ni-C	1.85	S4
	Br-Ni-C	107.7	S4
$NiBr_2O$	Ni=O	1.62	S4
	Ni-Br	2.22	S4
	O=Ni-Br	115.1	S4
$NiC_3H_8Br_2O_2$ (Ni 2O and 2Br)	Ni-O	2.07	S4
	O-Ni-O	65.8	S4
	Ni-Br	2.26	S4
	Br-Ni-O	164.3	S4
	Br-Ni-O-O	-16.2	S4
	Br-Ni-O	98.9	S4
Ni(SH)Br	Ni-Br	2.24	S4
	Ni-S	2.09	S4
$Ni(PH_2)(NH_2)(SH)Br^{2-}$	Ni-P	2.30	S4
	Ni-Br	2.33	S4
	Ni-S	2.20	S4
	Ni-N	1.83	S4
$NiC_8N_2H_{20}S_3Br^+$ (BRUCUB)	Ni-Br	2.58	S10
	Ni-N	2.07	S10

	N-Ni-Br	89.9	S10
	Ni-S	2.39	S10
	S-Ni-Br	89.4	S10
$Ni((CH_3)_2S)_2Br_2$ cis	Ni-S	2.29	S4
	S-Ni-S	86.3	S4
	Ni-Br	2.33	S4
	Br-Ni-S	173.8	S4
$Ni((CH_3)_2S)_2Br_2$ trans	Ni-S	2.26	S4
	Ni-Br	2.35	S4
	Br-Ni-S	86.5	S4
$NiC_7H_{16}S_2Br_2$ (Ni 2S and 2Br)	Ni-S	2.28	S4
	S-Ni-S	81.9	S4
	Ni-Br	2.33	S4
	Br-Ni-S	94.0	S4
	Br-Ni-S-S	179.8	S4
NiZr	Ni-Zr	2.21	S3
NiMo	Ni-Mo	2.14	S3
NiI	Ni-I	2.39	S4
NiI_2	Ni-I	2.45	S3
$NiCH_3I$	Ni-I	2.39	S4
	Ni-C	1.85	S4
	I-Ni-C	107.5	S4
$NiIF_3^{2-}$	Ni-F	1.88	S4
NiICl	Ni-I	2.41	S4
	Ni-Cl	2.08	S4
	I-Ni-Cl	120.2	S4
$NiC_3H_8I_2O_2$ (Ni 2O and 2I)	Ni-O	2.10	S4
	O-Ni-O	64.6	S4
	Ni-I	2.47	S4
	I-Ni-O	101.1	S4
	I-Ni-O-O	176.5	S4
$Ni((CH_3)_2S)_2I_2$ cis	Ni-S	2.29	S4
	S-Ni-S	85.1	S4
	Ni-I	2.56	S4
	I-Ni-S	167.8	S4
$Ni((CH_3)_2S)_2I_2$ trans	Ni-S	2.27	S4
	Ni-I	2.58	S4
	I-Ni-S	85.4	S4

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