Supporting Information

Table S1. Chemical hardness (η) and electrophilicity (ω) for the optimized Ni(I)-TPA complexes.

		μ	η	ω
SOMO	**Ni(I)-F**	-0.0749	0.0809	0.0347
	Ni(I)-Cl	-0.0787	0.0876	0.0354
	Ni(I)-Br	-0.0806	0.0935	0.0347
Average	**Ni(I)-F**	-0.0854	0.1052	0.0346
	Ni(I)-Cl	-0.0882	0.1086	0.0358
	Ni(I)-Br	-0.0891	0.1116	0.0356

Table S2. Chemical potential (μ), chemical hardness (η) and electrophilicity (ε) for the optimized Ni(II)-TPA complexes.

		μ	η	ω
SOMO	**[Ni(II)-F]$^{+1}$**	-0.1373	0.1343	0.0702
	[Ni(II)-Cl]$^{+1}$	-0.1400	0.1342	0.0730
	[Ni(II)-Br]$^{+1}$	-0.1406	0.1301	0.0760
Average	**[Ni(II)-F]$^{+1}$**	-0.1309	0.1473	0.0581
	[Ni(II)-Cl]$^{+1}$	-0.1333	0.1478	0.0601
	[Ni(II)-Br]$^{+1}$	-0.1334	0.1449	0.0614

Table S3. EDA in kcal/mol of the halide dissociation for the single point and optimized Ni(I)-TPA complexes without the hydrogen bonds (in their quintet state).

	Single point			Optimized		
	Ni(I)-F	**Ni(I)-Cl'**	**Ni(I)-Br**	**Ni(I)-F**	**Ni(I)-Cl**	**Ni(I)-Br**
ΔE_{Pauli}	55.0	34.4	58.5	84.7	59.2	80.2
ΔV_{elstat}	-62.9	-52.1	-75.5	-122.2	-92.8	-109.2
ΔE_{oi}	-87.5	-59.3	-61.3	-98.0	-73.7	-73.7
ΔE_{disp}	-1.3	-6.1	-8.0	-0.4	-3.7	-5.1
ΔE_{int}	-96.8	-83.2	-86.2	-135.9	-111.1	-107.7

[a] EDA values for NI(I)-Cl are 25.6, -38.1, -55.0, -6.3, and -73.8 kcal/mol for ΔE_{Pauli}, ΔE_{elstat}, ΔE_{oi}, ΔE_{disp}, and ΔE_{int}, respectively.

Figure S1. EDA fragmentation models taken into study. Model A corresponds to the original system; model B corresponds to the system in which the 3 H atoms forming the NH···halide bonds have been removed, but the geometry kept; and model C is equivalent to model B but allowed to fully relax. In all cases the halogen has been considered as anionic (-1), whereas the Ni(TPA) fragment is +1 and doublet or +2 and triplet. All results correspond to heterolytic breaking, as only small charge transfer is observed from the halogen to the Ni(TPA) fragments.

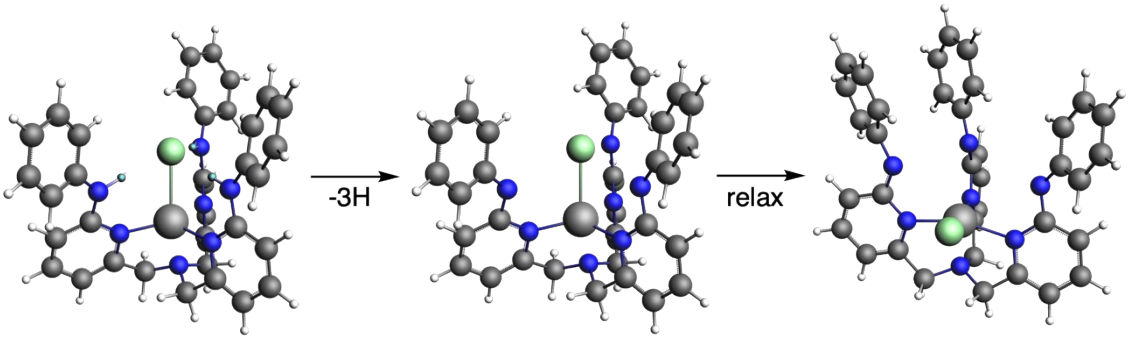
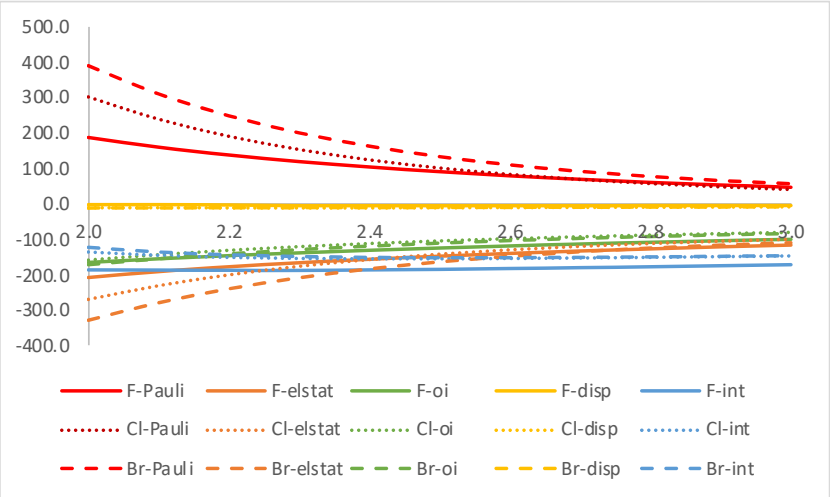


Table S4. MCI (in au), NICS(0) and HOMA aromaticity criteria for the optimized Ni(I)-TPA and Ni(II)-TPA complexes.

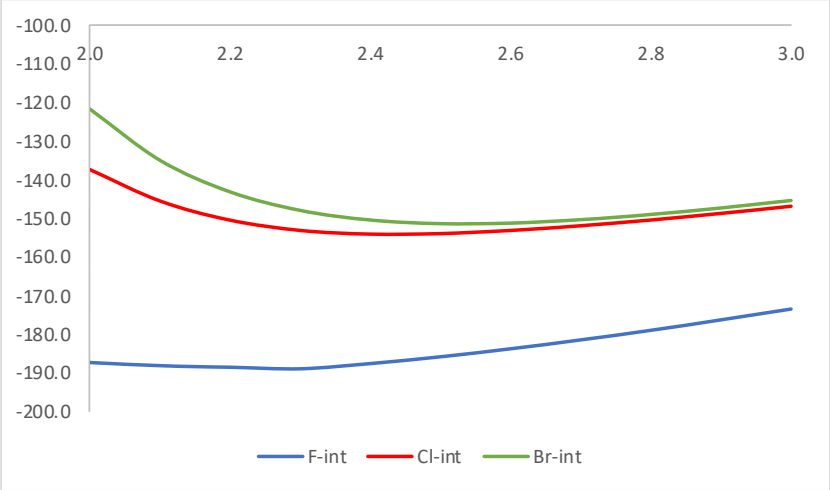
ring	**Ni(I)-F**	**[Ni(II)-F]$^{+1}$**	**Ni(I)-Cl**	**[Ni(II)-Cl]$^{+1}$**	**Ni(I)-Br**	**[Ni(II)-Br]$^{+1}$**	**[Ni(I)]$^{+1}$**	**[Ni(II)]$^{+2}$**	**ligand**
MCI									
C_6	0.059	0.061	0.060	0.061	0.059	0.062	0.058	0.062	0.059
C_5N	0.038	0.038	0.045	0.039	0.046	0.039	0.042	0.039	0.049
C_2N_2Ni	0.001	0.001	0.000	0.001	0.000	0.001	0.001	0.001	
NICS(0)									
C_6	-6.5	-6.2	-6.6	-6.4	-6.9	-6.6	-6.7	-6.5	-7.4
C_5N	-1.4	-1.9	-3.2	-1.3	-4.0	-3.0	-1.5	-2.9	-5.4
C_2N_2Ni	-1.6	5.7	-1.8	7.0	-2.6	5.5	-2.9	2.6	
HOMA									
C_6	0.952	0.962	0.962	0.964	0.955	0.965	0.940	0.970	0.957
C_5N	0.946	0.937	0.939	0.941	0.964	0.951	0.966	0.958	0.964

Figure S2. Complementary EDA analysis as a function of the Ni-X (X = F, Cl, Br) distance (in Å).

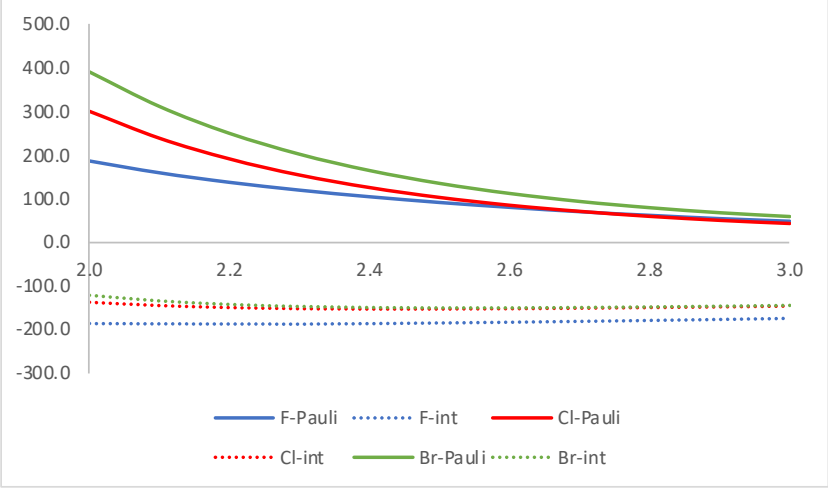
a) Complete EDA analysis.



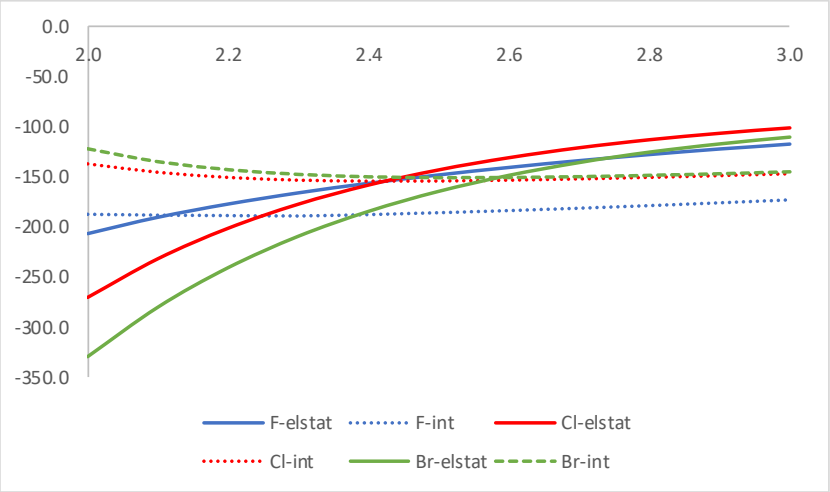
b) Interaction energies.



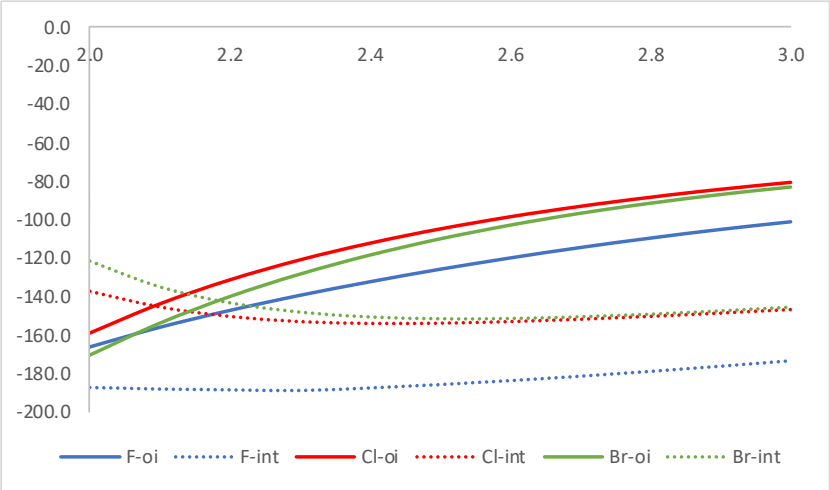
c) Pauli vs. Interaction energies.



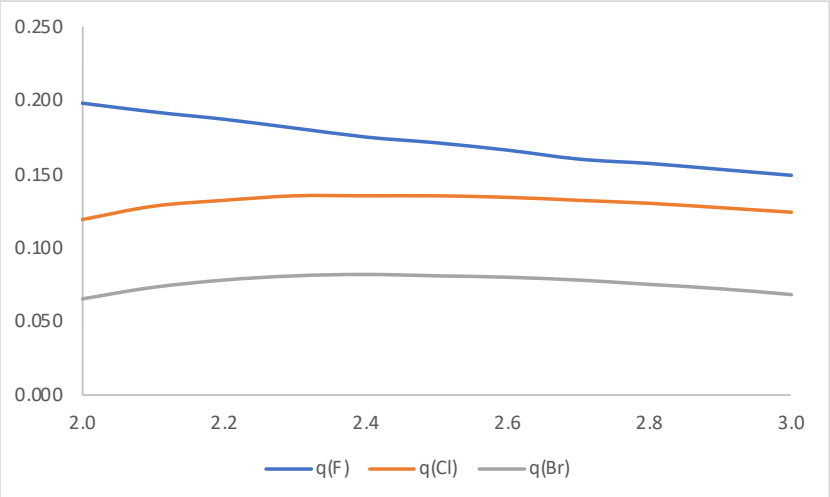
d) Electrostatic vs. Interaction energies.



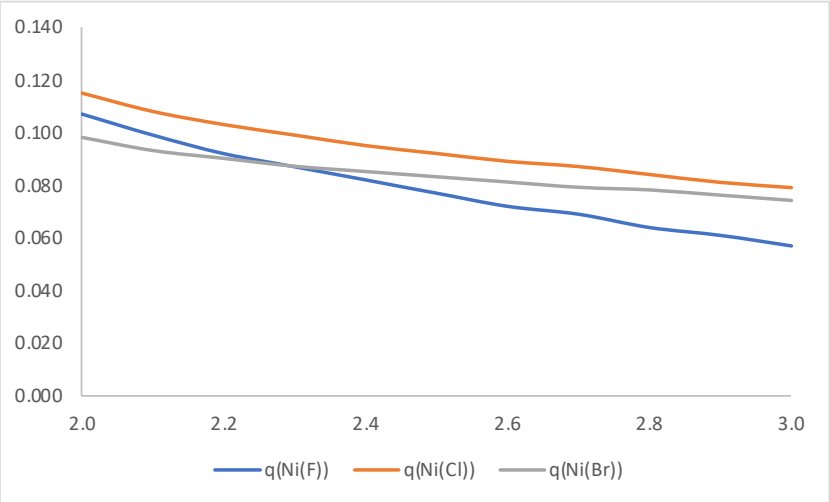
e) Orbital interactions vs. Interaction energies.



f) VDD charges of halogen.



g) VDD charges of Nickel atom.



h) Overlap between SOMO of Ni and HOMO of halogen.

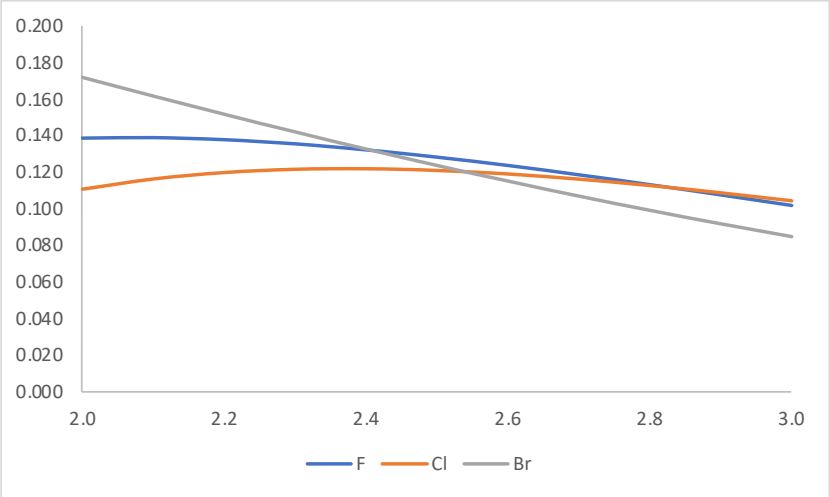
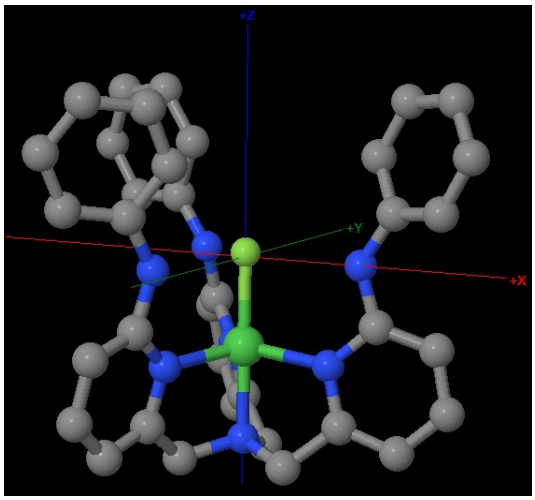


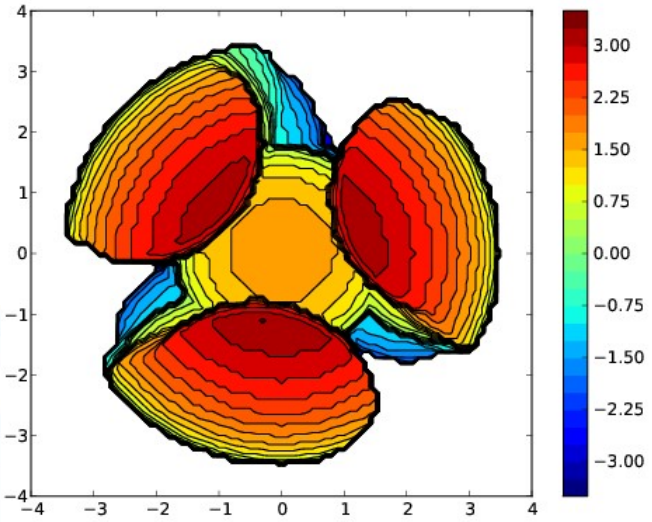
Table S5. EDA (in kcal/mol) of the halide dissociation of model Ni(I)-$(NH_3)_2$ and Ni(I)-$(NH_3)_3$ systems.

	F-Ni$(NH_3)_2$	**Cl-Ni$(NH_3)_2$**	**Br-Ni$(NH_3)_2$**	**F-Ni$(NH_3)_3$**	**Cl-Ni$(NH_3)_3$**	**Br-Ni$(NH_3)_3$**
ΔE_{Pauli}	84.4	61.5	77.7	104.6	35.6	90.7
ΔV_{elstat}	-164.3	-130.1	-138.3	-143.2	-83.9	-121.5
ΔE_{oi}	-81.5	-66.6	-68.8	-94.7	-51.8	-70.4
ΔE_{disp}	-0.7	-1.9	-2.3	-1.0	-2.4	-3.1
ΔE_{int}	-162.1	-137.1	-131.6	-134.4	-102.6	-104.4
ΔE_{int}^{desolv}	135.7	112.2	106.8	129.6	98.5	96.5
ΔE_{int}^{solv}	-26.4	-25.0	-24.7	-4.8	-4.0	-7.9

Details of the steric maps:

Ni(I)-F

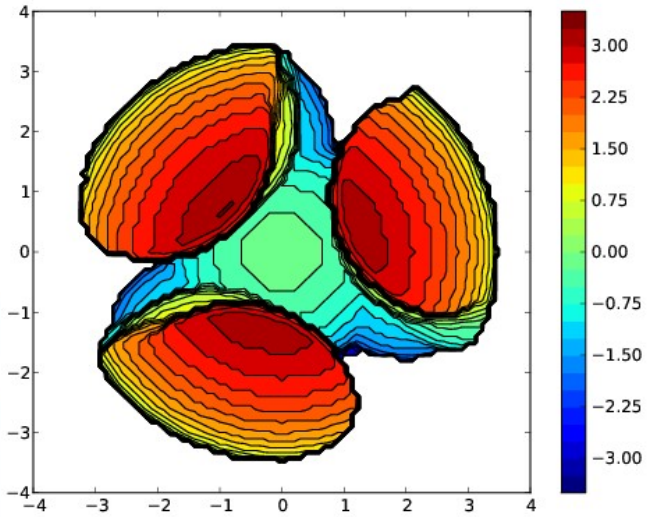




%V Free	%V Buried	% V Tot/V Ex
28.2	71.8	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	12.5	32.4	44.9	27.8	72.2
NW	6.8	38.1	44.9	15.1	84.9
NE	15.8	29.1	44.9	35.2	64.8
SE	15.5	29.3	44.9	34.6	65.4

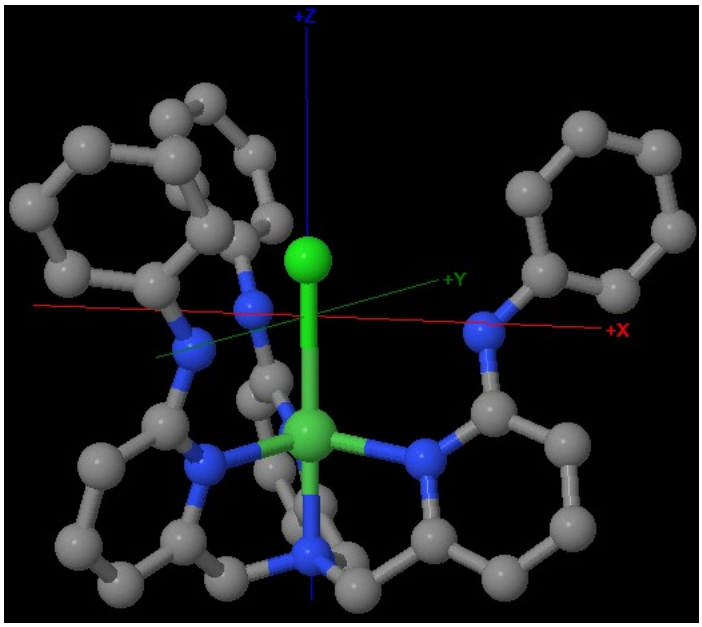
Not including the halide:

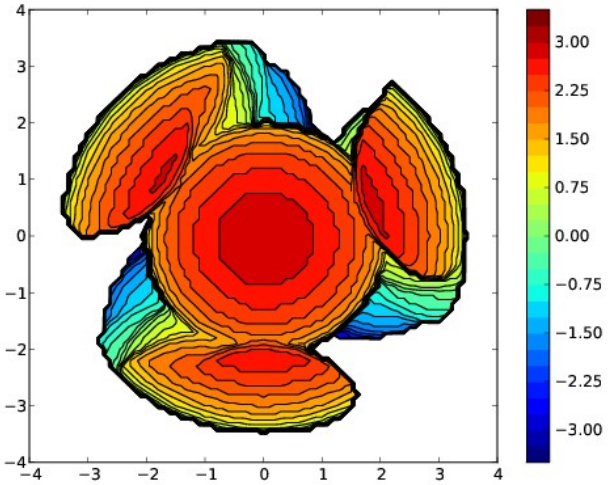


%V Free	%V Buried	% V Tot/V Ex
34.0	66.0	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	13.6	31.3	44.9	30.3	69.7
NW	8.6	36.3	44.9	19.1	80.9
NE	16.7	28.2	44.9	37.2	62.8
SE	22.2	22.7	44.9	49.4	50.6

Ni(I)-Cl

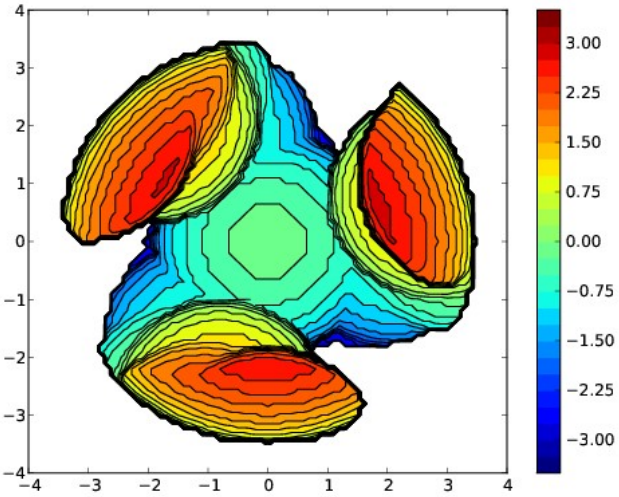




%V Free	%V Buried	% V Tot/V Ex
29.0	71.0	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	13.7	31.1	44.9	30.6	69.4
NW	8.3	36.6	44.9	18.5	81.5
NE	13.9	30.9	44.9	31.1	68.9
SE	16.2	28.7	44.9	36.0	64.0

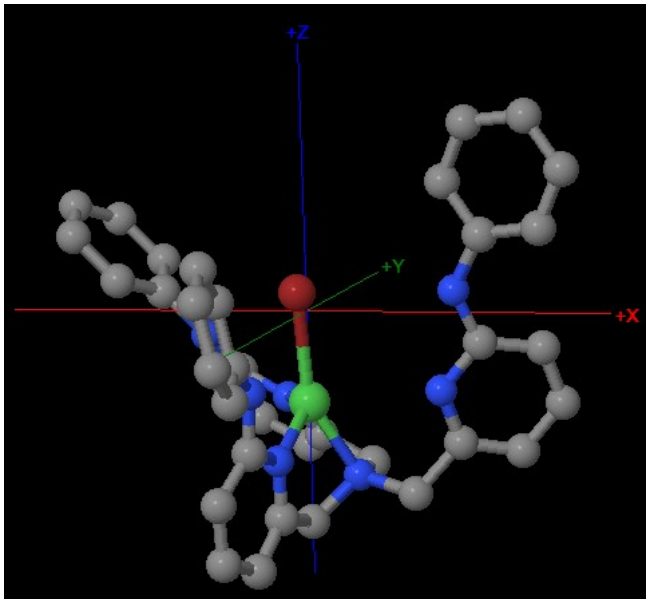
Not including the halide:

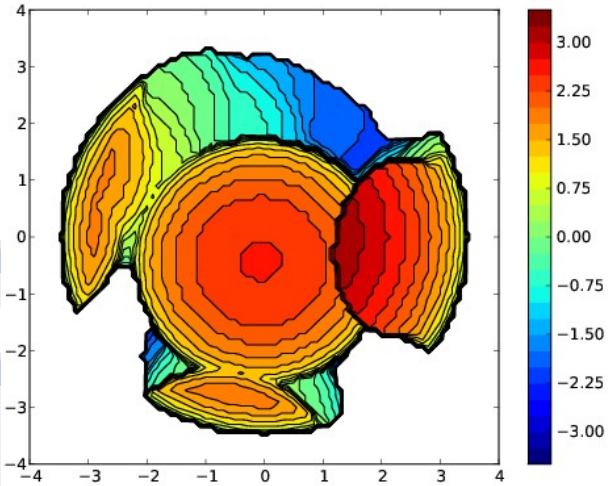


%V Free	%V Buried	% V Tot/V Ex
45.0	55.0	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	20.8	24.0	44.9	46.4	53.6
NW	14.6	30.3	44.9	32.6	67.4
NE	20.9	23.9	44.9	46.7	53.3
SE	24.4	20.5	44.9	54.3	45.7

Ni(I)-Br

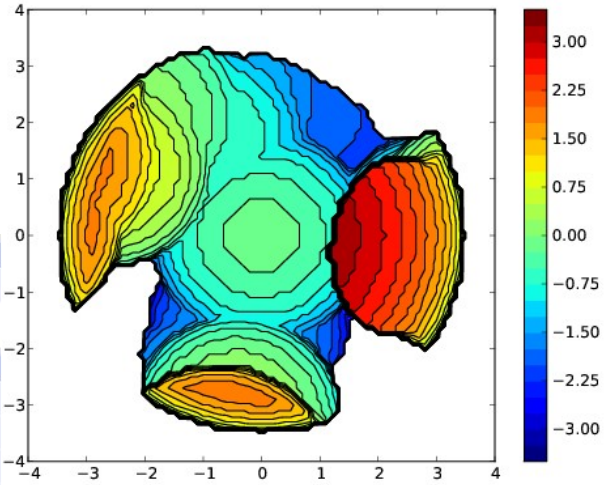




%V Free	%V Buried	% V Tot/V Ex
34.5	65.5	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	15.2	29.6	44.9	33.9	66.1
NW	14.0	30.9	44.9	31.2	68.8
NE	20.8	24.1	44.9	46.3	53.7
SE	12.0	32.9	44.9	26.6	73.4

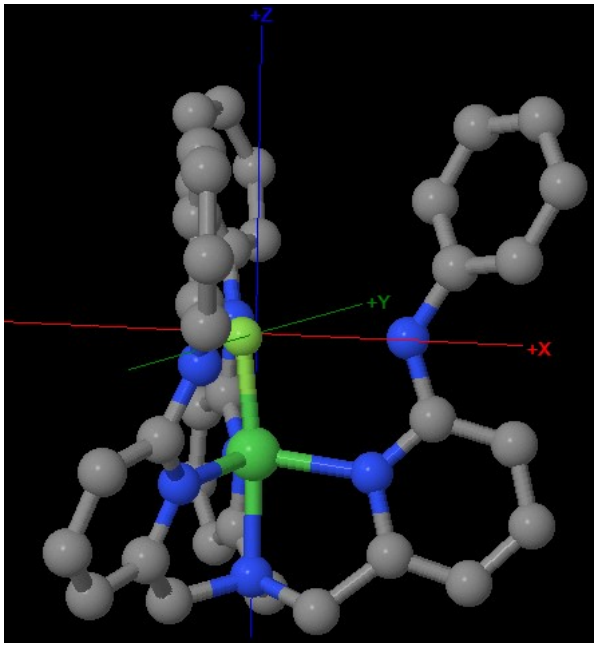
Not including the halide:

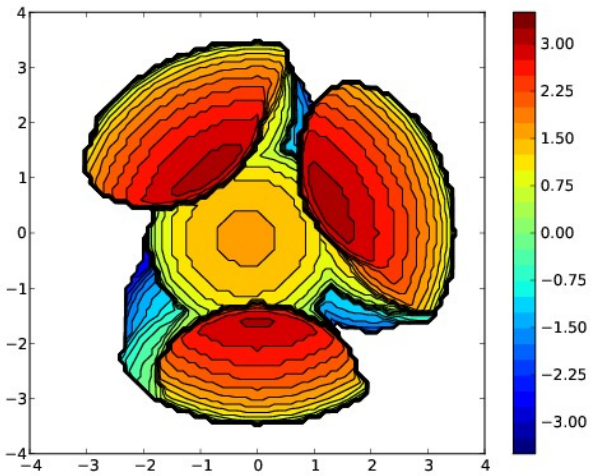


%V Free	%V Buried	% V Tot/V Ex
52.5	47.5	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	26.4	18.5	44.9	58.8	41.2
NW	19.4	25.4	44.9	43.3	56.7
NE	26.4	18.5	44.9	58.8	41.2
SE	22.0	22.9	44.9	49.0	51.0

$[Ni(II)\text{-}F]^{+1}$





%V Free	%V Buried	% V Tot/V Ex
30.5	69.5	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	19.2	25.7	44.9	42.8	57.2
NW	10.7	34.2	44.9	23.8	76.2
NE	12.2	32.7	44.9	27.1	72.9
SE	12.8	32.1	44.9	28.4	71.6

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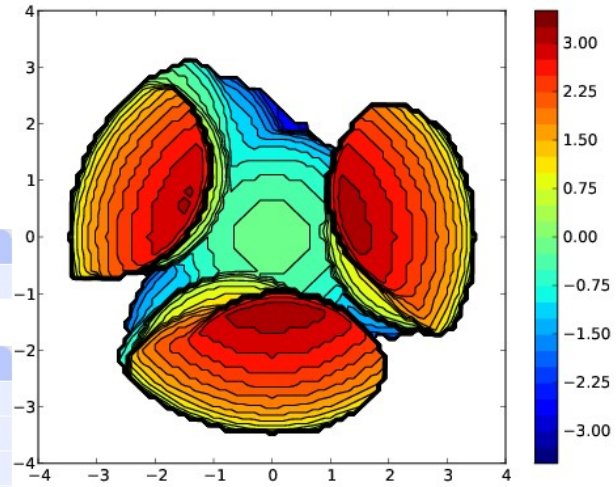
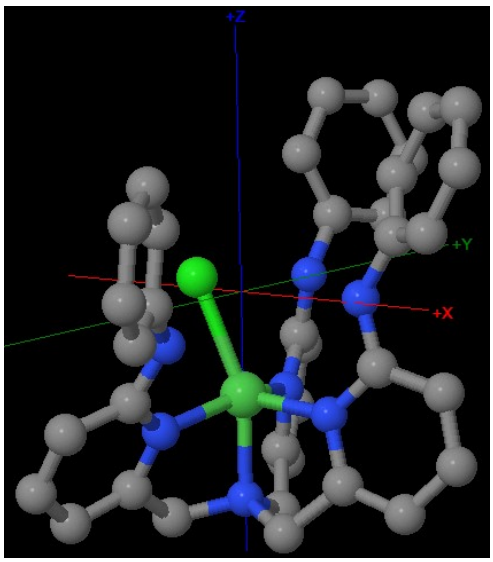
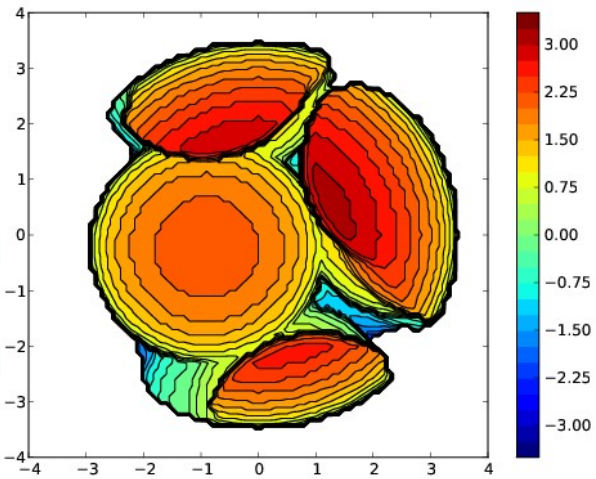


%V Free	%V Buried	% V Tot/V Ex
36.3	63.7	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	14.3	30.6	44.9	31.8	68.2
NW	15.1	29.8	44.9	33.6	66.4
NE	21.3	23.5	44.9	47.6	52.4
SE	14.4	30.5	44.9	32.0	68.0

[Ni(II)-Cl]$^{+1}$





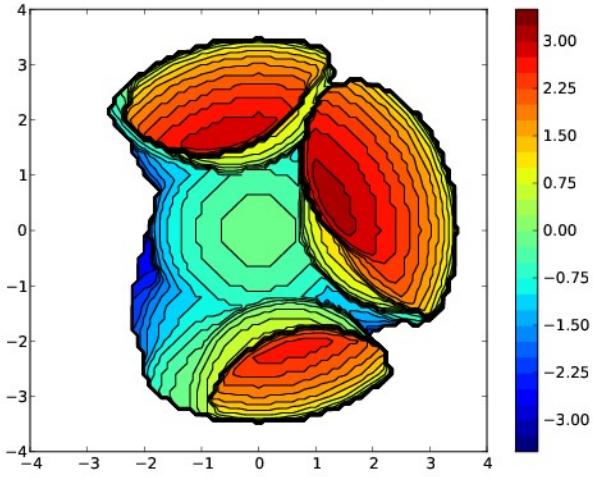
%V Free	%V Buried	% V Tot/V Ex
27.1	72.9	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	15.8	29.1	44.9	35.2	64.8
NW	12.4	32.4	44.9	27.7	72.3
NE	9.2	35.6	44.9	20.6	79.4
SE	11.2	33.7	44.9	24.9	75.1

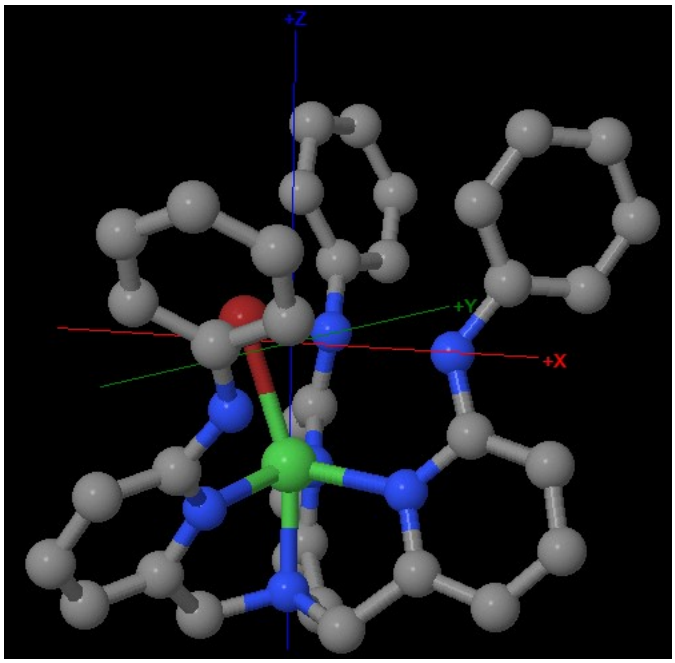
Not including the halide:

%V Free	%V Buried	% V Tot/V Ex
41.9	58.1	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	29.2	15.7	44.9	65.0	35.0
NW	21.3	23.6	44.9	47.5	52.5
NE	10.9	33.9	44.9	24.4	75.6
SE	13.8	31.1	44.9	30.7	69.3

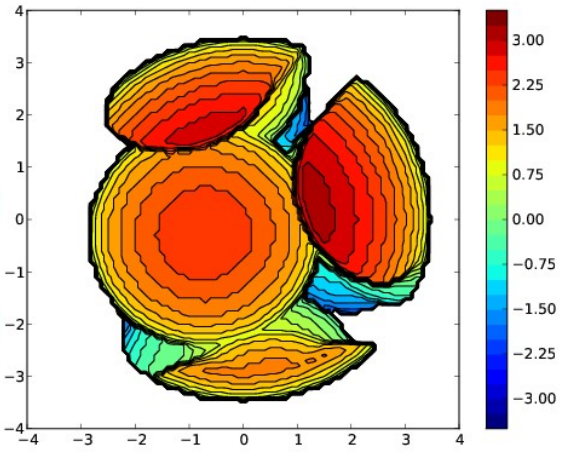


[Ni(II)-Br]$^{+1}$



%V Free	%V Buried	% V Tot/V Ex
27.3	72.7	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	14.2	30.7	44.9	31.6	68.4
NW	11.8	33.1	44.9	26.2	73.8
NE	9.6	35.2	44.9	21.4	78.6
SE	13.4	31.5	44.9	29.8	70.2



Not including the halide:

%V Free	%V Buried	% V Tot/V Ex
44.5	55.5	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	28.7	16.2	44.9	64.0	36.0
NW	21.1	23.8	44.9	46.9	53.1
NE	12.3	32.6	44.9	27.3	72.7
SE	17.8	27.1	44.9	39.7	60.3

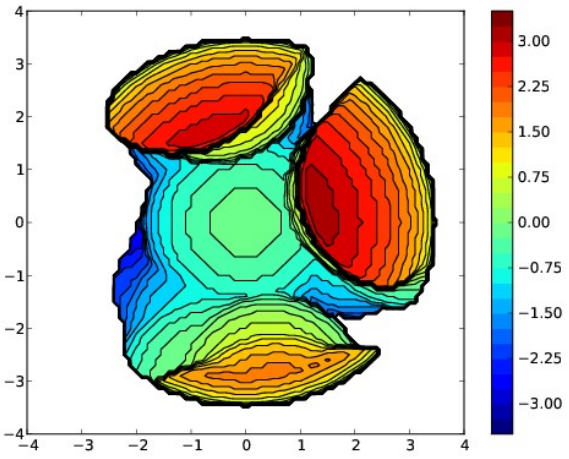


Table S5. Xyz coordinates and absolute energies (in a.u.) of all computed DFT species.

[Ni(II)-F]$^{+1}$	SCF Done: -3383.06833357 A.U.
	Ni 0.080822 -1.342830 0.011692
	F 0.125467 0.436618 -0.800071
	N 0.012181 -3.293627 0.659683
	N 2.169276 -1.736547 -0.117805
	N 2.816272 0.300525 -1.002629
	H 1.810358 0.502425 -0.965718
	N -1.654962 -1.953165 -0.993594
	N -2.542788 0.147199 -1.345754
	H -1.591751 0.455353 -1.118337
	N -0.469170 -0.933675 1.943421
	N -0.151427 1.348736 1.780830
	H 0.037625 1.130787 0.795540
	C 1.375654 -3.728224 1.034516
	H 1.480300 -4.815568 0.950002
	H 1.524276 -3.470356 2.088928
	C 2.442165 -3.018096 0.234107
	C 3.654933 -3.632279 -0.027043
	H 3.821668 -4.662679 0.266857

	C	4.643871	-2.883479	-0.678614
	H	5.599177	-3.337055	-0.927108
	C	4.403410	-1.566395	-1.016562
	H	5.151663	-0.983777	-1.536868
	C	3.146894	-0.993179	-0.709018
	C	3.637648	1.341560	-1.480888
	C	4.959042	1.540792	-1.046673
	H	5.402201	0.872520	-0.316455
	C	5.696837	2.622280	-1.530755
	H	6.718898	2.760000	-1.187593
	C	5.130144	3.531857	-2.426610
	H	5.709656	4.373645	-2.794879
	C	3.805643	3.351854	-2.835350
	H	3.346017	4.054794	-3.525149
	C	3.065039	2.265418	-2.372845
	H	2.038472	2.120369	-2.699283
	C	-0.527485	-4.047060	-0.495755
	H	-0.823452	-5.062860	-0.207575
	H	0.277577	-4.133855	-1.234546
	C	-1.696184	-3.303509	-1.106813
	C	-2.725072	-3.970872	-1.749160
	H	-2.728897	-5.054001	-1.800911
	C	-3.742978	-3.201832	-2.329442
	H	-4.552778	-3.685573	-2.868150
	C	-3.722206	-1.823992	-2.221343
	H	-4.493651	-1.220746	-2.681097
	C	-2.661197	-1.206184	-1.520901
	C	-3.462533	1.166186	-1.665036
	C	-4.845682	1.043011	-1.453377
	H	-5.255997	0.129476	-1.036541
	C	-5.694277	2.110907	-1.749856
	H	-6.762289	1.999181	-1.581957
	C	-5.183889	3.317106	-2.235301
	H	-5.850242	4.145315	-2.459078
	C	-3.804680	3.449202	-2.420404
	H	-3.389665	4.383119	-2.790187
	C	-2.949586	2.383959	-2.143995
	H	-1.878119	2.484441	-2.297456
	C	-0.903652	-3.314332	1.827548
	H	-0.746783	-4.210914	2.436795
	H	-1.930884	-3.350270	1.451245
	C	-0.739311	-2.057302	2.652591
	C	-0.908078	-2.050228	4.025679
	H	-1.118003	-2.971261	4.557933
	C	-0.782817	-0.823852	4.694594
	H	-0.876283	-0.780877	5.775991
	C	-0.528248	0.334715	3.986521
	H	-0.408116	1.280404	4.498077
	C	-0.393290	0.266228	2.579420
	C	-0.195200	2.722019	2.111178
	C	-1.143679	3.270683	2.989512
	H	-1.885312	2.635213	3.461195

	C -1.154435 4.644929 3.234651 H -1.893096 5.053988 3.918984 C -0.246003 5.491900 2.595815 H -0.263414 6.560918 2.788228 C 0.680001 4.949778 1.700199 H 1.389451 5.595465 1.189362 C 0.711461 3.576657 1.462465 H 1.439927 3.154583 0.775651
[Ni(II)-Cl]$^{+1}$	SCF Done: -3743.41471899 A.U. Ni 0.074784 -1.389732 0.129277 Cl -0.173942 0.188524 1.948235 N 0.358041 -3.202384 -0.776311 N -2.021183 -1.977031 0.032544 N -3.098605 -0.048286 0.780327 H -2.172281 0.292809 1.030701 N 2.059613 -1.851152 0.766686 N 2.915717 0.291142 0.979256 H 1.941054 0.579244 0.963438 N 0.461406 -0.639172 -1.722540 N -0.101882 1.553374 -1.240137 H -0.323693 1.184697 -0.319465 C -0.934234 -3.809840 -1.156981 H -0.882115 -4.902167 -1.099257 H -1.127384 -3.554482 -2.204677 C -2.094906 -3.277720 -0.355059 C -3.219528 -4.067690 -0.180893 H -3.210623 -5.103427 -0.501806 C -4.352991 -3.485895 0.396412 H -5.245202 -4.077491 0.580372 C -4.333165 -2.146406 0.728997 H -5.197789 -1.672040 1.174342 C -3.156252 -1.394552 0.513686 C -4.168545 0.813471 1.109571 C -5.388441 0.793123 0.413031 H -5.545352 0.081754 -0.391007 C -6.393382 1.703902 0.739935 H -7.332936 1.673019 0.194554 C -6.194089 2.660149 1.739229 H -6.979233 3.369846 1.983871 C -4.971579 2.697533 2.414426 H -4.798440 3.437583 3.191211 C -3.966817 1.779058 2.110157 H -3.023179 1.801550 2.648208 C 1.056798 -3.997550 0.262573 H 1.413986 -4.951715 -0.142745 H 0.324824 -4.222414 1.047163 C 2.208672 -3.197128 0.824473 C 3.344211 -3.812551 1.323919 H 3.422062 -4.894069 1.333573 C 4.375489 -2.995044 1.801607 H 5.269387 -3.436040 2.233160 C 4.264561 -1.619994 1.710854

	H 5.054589 -0.975029 2.072208 C 3.093424 -1.059827 1.155577 C 3.848873 1.335052 1.159982 C 5.180911 1.241618 0.724857 H 5.537509 0.337312 0.243421 C 6.044281 2.325992 0.887801 H 7.073347 2.237493 0.549623 C 5.594052 3.519633 1.456954 H 6.270831 4.361021 1.575273 C 4.261053 3.621415 1.863988 H 3.891586 4.544933 2.301854 C 3.394313 2.538750 1.723502 H 2.361312 2.617989 2.051125 C 1.202939 -2.941927 -1.971412 H 1.108971 -3.752378 -2.701172 H 2.249485 -2.910455 -1.655817 C 0.853678 -1.607349 -2.590989 C 0.998925 -1.377858 -3.947776 H 1.308804 -2.180126 -4.607898 C 0.726941 -0.090818 -4.431041 H 0.802175 0.121295 -5.493604 C 0.352283 0.913563 -3.559781 H 0.123132 1.906560 -3.922753 C 0.240545 0.620487 -2.182111 C -0.246902 2.954711 -1.379494 C 0.640595 3.734828 -2.136589 H 1.471603 3.270456 -2.656544 C 0.469633 5.118894 -2.197657 H 1.161889 5.711818 -2.789471 C -0.561157 5.742685 -1.490954 H -0.683762 6.821048 -1.537732 C -1.427772 4.966951 -0.716219 H -2.230836 5.437962 -0.155732 C -1.279245 3.581780 -0.664542 H -1.961425 2.976930 -0.073143
[Ni(II)-Br]$^{+1}$	SCF Done: -5854.93685592 A.U. Ni -0.459815 -1.238543 0.057221 Br -0.160326 0.538561 -1.604654 N -0.956885 -3.024503 0.929778 N -2.535630 -1.426603 -0.453460 N -3.218058 0.781102 -0.398793 H -2.502139 0.872910 0.310821 N -0.497191 -0.570704 1.992321 N 0.619948 1.420028 1.605754 H 0.355056 1.264473 0.633647 N 1.522715 -2.212959 -0.090038 N 2.843761 -0.524821 -0.992956 H 1.967676 -0.009137 -1.079950 C -1.797544 -3.710241 -0.077652 H -2.307901 -4.578174 0.358069 H -1.131752 -4.081888 -0.865232 C -2.806565 -2.739632 -0.652417

	C	-3.939474	-3.182336	-1.314315
	H	-4.113288	-4.243619	-1.455335
	C	-4.852190	-2.220911	-1.765328
	H	-5.756559	-2.526674	-2.283495
	C	-4.635043	-0.880263	-1.502856
	H	-5.371835	-0.136204	-1.774949
	C	-3.465028	-0.501569	-0.809559
	C	-3.814053	1.988214	-0.816672
	C	-4.243133	2.208084	-2.134956
	H	-4.125193	1.433832	-2.885438
	C	-4.795669	3.439812	-2.489558
	H	-5.124608	3.595663	-3.513650
	C	-4.906441	4.470393	-1.553258
	H	-5.332120	5.428106	-1.838894
	C	-4.453826	4.259005	-0.247729
	H	-4.525083	5.052767	0.491218
	C	-3.917404	3.027218	0.122844
	H	-3.574926	2.859304	1.140987
	C	-1.707239	-2.673860	2.163372
	H	-1.739978	-3.524277	2.852869
	H	-2.737592	-2.435589	1.887736
	C	-1.084718	-1.467094	2.827042
	C	-1.145439	-1.283131	4.197325
	H	-1.606332	-2.034248	4.828941
	C	-0.610127	-0.102780	4.728628
	H	-0.666107	0.091718	5.795711
	C	-0.013944	0.824387	3.895514
	H	0.381433	1.750680	4.290019
	C	0.051484	0.561608	2.509545
	C	1.418921	2.561923	1.832180
	C	2.368931	2.637974	2.862945
	H	2.512559	1.802765	3.539734
	C	3.155513	3.782952	2.999479
	H	3.885517	3.829100	3.803329
	C	3.028631	4.849255	2.106330
	H	3.648825	5.734264	2.216270
	C	2.101128	4.761137	1.064667
	H	1.994281	5.578070	0.355996
	C	1.296222	3.631465	0.929623
	H	0.567433	3.570991	0.125655
	C	0.258918	-3.795933	1.257863
	H	0.041987	-4.868569	1.300101
	H	0.583287	-3.489667	2.258742
	C	1.397337	-3.504378	0.315517
	C	2.315868	-4.496122	0.016384
	H	2.152386	-5.511100	0.361314
	C	3.450066	-4.144455	-0.724758
	H	4.177663	-4.898168	-1.011604
	C	3.643134	-2.827003	-1.086056
	H	4.514449	-2.529074	-1.654177
	C	2.675475	-1.860382	-0.727452
	C	3.958386	0.111167	-1.585219

	C 5.273882 -0.123332 -1.154362 H 5.466484 -0.831251 -0.354810 C 6.332331 0.573179 -1.739173 H 7.346347 0.378771 -1.399769 C 6.096878 1.525617 -2.734069 H 6.925194 2.068022 -3.181066 C 4.784507 1.779622 -3.141591 H 4.584218 2.522966 -3.908710 C 3.721106 1.075978 -2.577838 H 2.700922 1.268641 -2.898238
Ni(II)-F_2	SCF Done: -3483.05994152 A.U. C 3.207533 -2.915004 -0.506152 H 3.082329 -3.147635 -1.565931 H 3.893278 -3.649635 -0.066016 C 3.780104 -1.518090 -0.402643 C 5.141525 -1.294177 -0.249504 H 5.825855 -2.126200 -0.123447 C 5.594178 0.030622 -0.287771 H 6.654946 0.249005 -0.199206 C 4.694873 1.069397 -0.452878 H 5.039293 2.092730 -0.519664 C 3.318413 0.766206 -0.566662 C 2.430999 3.104892 -0.774481 C 1.628334 3.808131 -1.691451 H 1.003329 3.249551 -2.383428 C 1.641253 5.201844 -1.719037 H 1.015163 5.725902 -2.436534 C 2.460912 5.920488 -0.843792 H 2.478018 7.006341 -0.872625 C 3.250656 5.225200 0.074889 H 3.878133 5.769776 0.775803 C 3.231458 3.830210 0.124460 H 3.815738 3.311519 0.876903 C 1.955052 -2.891897 1.590469 H 2.989808 -2.653071 1.859268 H 1.741875 -3.868525 2.039919 C 1.069804 -1.841790 2.231755 C 0.928461 -1.857805 3.616554 H 1.382293 -2.650363 4.202535 C 0.227521 -0.811598 4.218501 H 0.131066 -0.763899 5.299840 C -0.340086 0.177021 3.433683 H -0.860644 1.010605 3.885629 C -0.212565 0.092698 2.029923 C -1.704926 2.018115 1.423141 C -2.737984 1.904718 2.370579 H -2.842704 1.002541 2.962549 C -3.659545 2.941055 2.530889 H -4.449267 2.834275 3.270304 C -3.589412 4.091891 1.742893 H -4.312552 4.892369 1.871701

	C -2.581187 4.194916 0.780082 H -2.514041 5.078914 0.150997 C -1.646336 3.173758 0.622714 H -0.857574 3.264090 -0.118907 C 1.081006 -4.138700 -0.351494 H 1.322058 -5.041563 0.222882 H 1.364869 -4.325992 -1.391173 C -0.412129 -3.883489 -0.334720 C -1.314402 -4.924034 -0.151651 H -0.963483 -5.920239 0.095640 C -2.674165 -4.648808 -0.334525 H -3.411033 -5.441302 -0.235426 C -3.089012 -3.368572 -0.659735 H -4.133602 -3.159420 -0.844723 C -2.117723 -2.348420 -0.777230 C -3.630715 -0.388593 -1.248421 C -4.781539 -0.694165 -0.501138 H -4.756806 -1.470917 0.254265 C -5.957475 0.032501 -0.699242 H -6.837542 -0.220638 -0.113446 C -6.006117 1.084198 -1.616163 H -6.924620 1.645723 -1.761810 C -4.852944 1.411558 -2.336240 H -4.867073 2.233832 -3.047090 C -3.678746 0.683927 -2.159049 H -2.785214 0.934660 -2.725017 N 1.864339 -2.974859 0.114566 N 2.885093 -0.516591 -0.536469 N 2.332784 1.701667 -0.760612 H 1.434230 1.308118 -1.067399 N 0.515368 -0.900330 1.444767 N -0.763036 1.003556 1.167215 H -0.473878 0.890417 0.184595 N -0.799665 -2.623329 -0.616509 N -2.395800 -1.042096 -1.093391 H -1.567261 -0.473647 -1.305498 Ni 0.891999 -1.302703 -0.693760 F 1.264752 -1.843744 -2.488030 F -0.028638 0.390747 -1.350468
Ni(II)-Cl_2	SCF Done: -4203.78463763 A.U. C 2.615340 -3.441318 -0.062580 H 2.456769 -3.843052 -1.065839 H 3.118941 -4.203316 0.544475 C 3.461769 -2.197421 -0.156539 C 4.838389 -2.267873 -0.000349 H 5.313940 -3.218190 0.216691 C 5.579121 -1.089300 -0.136082 H 6.662235 -1.105806 -0.053275 C 4.924368 0.103267 -0.376334 H 5.477005 1.025655 -0.499216 C 3.515295 0.106474 -0.483688 C 3.256337 2.591788 -0.623907

C	2.789374	3.510539	-1.579544
H	2.140618	3.163829	-2.379174
C	3.161171	4.853219	-1.506746
H	2.789184	5.549335	-2.253975
C	4.014754	5.298753	-0.494225
H	4.310811	6.342792	-0.444502
C	4.478345	4.386841	0.457790
H	5.130527	4.721279	1.260468
C	4.096284	3.045942	0.407079
H	4.434531	2.358485	1.175588
C	1.410768	-2.767866	1.939072
H	2.467680	-2.577638	2.151856
H	1.123908	-3.628220	2.553053
C	0.643783	-1.545021	2.383194
C	0.410881	-1.387628	3.743517
H	0.685303	-2.176505	4.435588
C	-0.135970	-0.181528	4.186787
H	-0.292576	-0.001951	5.246793
C	-0.465749	0.793206	3.266176
H	-0.862657	1.747250	3.586108
C	-0.269915	0.537942	1.890021
C	-1.382242	2.631048	1.072156
C	-2.529220	2.703937	1.880136
H	-2.855650	1.836190	2.443062
C	-3.267699	3.886536	1.940757
H	-4.151193	3.926840	2.572541
C	-2.895376	5.000500	1.184402
H	-3.477977	5.916210	1.232002
C	-1.769235	4.921096	0.361011
H	-1.468346	5.776823	-0.237724
C	-1.012556	3.750979	0.309081
H	-0.126883	3.698845	-0.317648
C	0.306997	-4.184593	0.253671
H	0.430081	-4.999466	0.976258
H	0.510170	-4.581531	-0.745052
C	-1.112522	-3.676246	0.260547
C	-2.146224	-4.499141	0.683978
H	-1.929076	-5.476829	1.100243
C	-3.458678	-4.040776	0.528529
H	-4.298657	-4.665747	0.818775
C	-3.687134	-2.790610	-0.012757
H	-4.695141	-2.431210	-0.171473
C	-2.582840	-1.987972	-0.381426
C	-3.912699	0.017223	-1.080486
C	-4.871663	0.139258	-0.061261
H	-4.724346	-0.368093	0.886546
C	-6.004123	0.930519	-0.258602
H	-6.739365	1.011519	0.537844
C	-6.186125	1.629987	-1.454306
H	-7.067061	2.248941	-1.599644
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H	-5.344346	2.070833	-3.393114

	C -4.095001 0.725000 -2.279873 H -3.352386 0.636000 -3.068111 N 1.285621 -3.103219 0.498050 N 2.795023 -1.042274 -0.399352 N 2.798586 1.259806 -0.691741 H 1.884605 1.124750 -1.126334 N 0.305745 -0.620340 1.454288 N -0.616335 1.451110 0.931671 H -0.296053 1.249756 -0.016489 N -1.307231 -2.434697 -0.243913 N -2.729001 -0.735707 -0.920386 H -1.899570 -0.358246 -1.380243 Ni 0.625100 -1.452628 -0.555796 Cl 0.858163 -2.685111 -2.741825 Cl -0.009550 0.582959 -2.073834
Ni(II)-Br_2	SCF Done: -8426.82811228 A.U. C 2.831135 -3.101374 0.471939 H 2.710788 -3.619910 -0.482092 H 3.358039 -3.766512 1.168028 C 3.630938 -1.842465 0.245184 C 5.019464 -1.879703 0.287950 H 5.533673 -2.808439 0.511647 C 5.717766 -0.697996 0.028645 H 6.804163 -0.691102 0.012580 C 5.017536 0.473734 -0.198547 H 5.537956 1.399667 -0.404978 C 3.607199 0.443514 -0.173009 C 3.220491 2.919858 -0.390324 C 2.500565 3.765288 -1.255037 H 1.708342 3.342189 -1.866952 C 2.794784 5.126075 -1.317855 H 2.227065 5.761616 -1.992592 C 3.815906 5.668702 -0.532378 H 4.050588 6.727851 -0.589193 C 4.524163 4.832936 0.334509 H 5.307919 5.242489 0.966675 C 4.227839 3.471615 0.419574 H 4.760896 2.848416 1.129441 C 1.574380 -2.275380 2.369649 H 2.563759 -1.824195 2.493215 H 1.520427 -3.113235 3.073836 C 0.565329 -1.218774 2.741467 C 0.182875 -1.115947 4.072312 H 0.514789 -1.855749 4.792594 C -0.593747 -0.018328 4.454219 H -0.881613 0.121360 5.492580 C -0.982384 0.899757 3.500656 H -1.557186 1.774360 3.774617 C -0.611882 0.694830 2.149756 C -1.936243 2.620020 1.239684 C -3.165250 2.505230 1.909830 H -3.423425 1.582381 2.418231

	C -4.066805 3.570491 1.904512 H -5.012439 3.466878 2.430280 C -3.773935 4.749334 1.214195 H -4.483285 5.572259 1.208416 C -2.562083 4.856116 0.526837 H -2.320975 5.765099 -0.018061 C -1.645583 3.805048 0.543956 H -0.694511 3.898291 0.027136 C 0.573937 -3.935086 0.857966 H 0.728579 -4.638165 1.685018 H 0.830627 -4.450551 -0.072434 C -0.879924 -3.547784 0.754548 C -1.857806 -4.423325 1.209305 H -1.576968 -5.323305 1.745703 C -3.192534 -4.127114 0.919524 H -3.986739 -4.801992 1.226507 C -3.500647 -2.975811 0.219434 H -4.523193 -2.752110 -0.052579 C -2.456015 -2.104020 -0.163508 C -3.887313 -0.299956 -1.182401 C -4.995816 -0.248561 -0.320172 H -4.952766 -0.719207 0.655773 C -6.148540 0.438875 -0.704300 H -6.997571 0.465292 -0.026118 C -6.210899 1.103373 -1.931087 H -7.110112 1.639732 -2.220716 C -5.097601 1.079069 -2.776166 H -5.124136 1.598507 -3.730543 C -3.948201 0.380720 -2.411586 H -3.086626 0.356885 -3.073189 N 1.477114 -2.770884 0.975096 N 2.923557 -0.717500 -0.001089 N 2.830946 1.570523 -0.320341 H 1.901358 1.372296 -0.692515 N 0.173542 -0.354424 1.775567 N -0.997917 1.564451 1.166391 H -0.602313 1.400862 0.237741 N -1.156823 -2.393415 0.108438 N -2.676623 -0.938795 -0.852352 H -1.840438 -0.513902 -1.254152 Ni 0.722837 -1.275819 -0.255817 Br 1.094229 -2.610151 -2.346643 Br 0.051850 0.695505 -1.810176
[Ni(II)-F(CH_3CN)]$^{+1}$	SCF Done: -3515.83985981 A.U. C 1.729164 -3.857253 0.291804 H 1.686737 -4.181151 -0.752650 H 1.994712 -4.730133 0.899127 C 2.777825 -2.774053 0.421001 C 4.062844 -3.056168 0.855441 H 4.330142 -4.060871 1.163758 C 4.986323 -2.002295 0.896119 H 5.993851 -2.171226 1.265736

	C	4.616284	-0.740130	0.473380
	H	5.314207	0.085455	0.519354
	C	3.296305	-0.531516	0.006478
	C	3.572208	1.818825	-0.832469
	C	2.946922	3.067728	-0.675235
	H	1.955641	3.112425	-0.233069
	C	3.590296	4.236928	-1.076779
	H	3.087680	5.191790	-0.946322
	C	4.872528	4.185754	-1.630776
	H	5.377937	5.098173	-1.934466
	C	5.493102	2.945619	-1.796151
	H	6.482391	2.886267	-2.242524
	C	4.850299	1.766643	-1.414081
	H	5.336094	0.813294	-1.590111
	C	0.289810	-3.170265	2.132877
	H	1.306762	-3.163601	2.539920
	H	-0.220104	-4.033578	2.572849
	C	-0.364942	-1.883885	2.576711
	C	-0.984189	-1.816103	3.816630
	H	-1.093562	-2.708151	4.423780
	C	-1.451525	-0.570674	4.250259
	H	-1.966822	-0.478107	5.202233
	C	-1.263503	0.547949	3.460757
	H	-1.636529	1.514336	3.772603
	C	-0.615281	0.407489	2.212167
	C	-0.520880	2.835361	1.593782
	C	-0.903526	3.653097	0.514540
	H	-1.139027	3.193155	-0.441154
	C	-0.987726	5.035758	0.669315
	H	-1.287270	5.647899	-0.177447
	C	-0.702858	5.630628	1.901727
	H	-0.777935	6.707424	2.024009
	C	-0.310712	4.822796	2.971627
	H	-0.065397	5.270908	3.931081
	C	-0.206115	3.438776	2.824016
	H	0.144063	2.836366	3.654940
	C	-0.712868	-4.136044	0.098857
	H	-0.915203	-5.016500	0.719386
	H	-0.393767	-4.496699	-0.884545
	C	-1.972657	-3.322441	-0.097524
	C	-3.223718	-3.915905	-0.023407
	H	-3.322388	-4.953651	0.275716
	C	-4.336741	-3.142309	-0.375973
	H	-5.332260	-3.577053	-0.360063
	C	-4.172827	-1.824657	-0.761193
	H	-5.022129	-1.228206	-1.066597
	C	-2.871367	-1.271031	-0.769579
	C	-3.485157	1.068661	-1.438430
	C	-3.133182	1.948441	-2.476975
	H	-2.223451	1.763602	-3.042560
	C	-3.945590	3.039343	-2.783808
	H	-3.657475	3.707986	-3.590747

	C -5.127040 3.264235 -2.071660 H -5.764391 4.108867 -2.317649 C -5.474509 2.395914 -1.034126 H -6.380389 2.569368 -0.459054 C -4.658362 1.312095 -0.705514 H -4.921725 0.675647 0.132449 C 0.689456 -2.346016 -3.344569 C 0.860197 -2.602255 -4.764465 H 0.478276 -1.752973 -5.339581 H 0.309187 -3.505276 -5.045408 H 1.922275 -2.742047 -4.988894 N 0.393948 -3.325405 0.657353 N 2.385941 -1.537642 0.031263 N 2.838402 0.671750 -0.458645 H 1.833136 0.699809 -0.661464 N -0.202758 -0.812212 1.770157 N -0.395987 1.454447 1.355879 H -0.183675 1.172527 0.390071 N -1.792717 -2.027483 -0.441920 N -2.592854 0.018577 -1.136919 H -1.596199 0.226046 -1.259993 N 0.553560 -2.148026 -2.212628 F 0.152082 0.369747 -1.054503 Ni 0.264835 -1.450790 -0.249379
[Ni(II)-Cl(CH_3CN)]$^{+1}$	SCF Done: -3876.18776719 A.U. C 1.458968 -3.914654 0.539291 H 1.411782 -4.322275 -0.474350 H 1.629991 -4.751798 1.225202 C 2.589227 -2.919855 0.618836 C 3.824772 -3.298201 1.117005 H 3.976026 -4.303958 1.492795 C 4.849918 -2.343913 1.132342 H 5.825549 -2.590192 1.541678 C 4.610396 -1.078083 0.639767 H 5.379677 -0.317343 0.666267 C 3.329111 -0.766103 0.123936 C 3.923035 1.502035 -0.765071 C 3.519759 2.830073 -0.556545 H 2.573106 3.026103 -0.061050 C 4.328746 3.885243 -0.977002 H 4.001200 4.907884 -0.809394 C 5.555651 3.632575 -1.596342 H 6.189649 4.455448 -1.914513 C 5.956050 2.311041 -1.808410 H 6.899565 2.100012 -2.304974 C 5.144032 1.248155 -1.409759 H 5.449577 0.227855 -1.616676 C 0.056966 -2.925654 2.271382 H 1.052660 -3.023189 2.716512 H -0.580554 -3.660630 2.772363 C -0.425938 -1.527033 2.576145 C -0.937675 -1.271805 3.839852

	H	-1.078098	-2.085431	4.543233
	C	-1.250286	0.048661	4.174452
	H	-1.674466	0.286522	5.145850
	C	-1.023335	1.054259	3.256709
	H	-1.271048	2.082185	3.486139
	C	-0.496786	0.726787	1.986748
	C	-0.264272	3.091038	1.209501
	C	-0.853619	3.886983	0.214105
	H	-1.339480	3.411449	-0.632932
	C	-0.821582	5.277820	0.316296
	H	-1.281961	5.879294	-0.463114
	C	-0.217806	5.894273	1.415093
	H	-0.203168	6.977429	1.497496
	C	0.373536	5.103535	2.403921
	H	0.861042	5.569607	3.256170
	C	0.366171	3.712094	2.300787
	H	0.859562	3.109879	3.057030
	C	-0.974577	-4.059544	0.347270
	H	-1.171208	-4.894712	1.028585
	H	-0.697464	-4.485086	-0.621814
	C	-2.212394	-3.219993	0.165229
	C	-3.464722	-3.760514	0.411088
	H	-3.556488	-4.768187	0.801148
	C	-4.588048	-2.977844	0.121485
	H	-5.588832	-3.373525	0.269629
	C	-4.420167	-1.697528	-0.366572
	H	-5.274908	-1.085206	-0.621609
	C	-3.111134	-1.195141	-0.553328
	C	-3.793791	1.118010	-1.237010
	C	-3.638802	1.914748	-2.384065
	H	-2.858258	1.671710	-3.099724
	C	-4.483072	3.002615	-2.606046
	H	-4.347480	3.607866	-3.498528
	C	-5.502985	3.303780	-1.699699
	H	-6.166473	4.145083	-1.878956
	C	-5.655360	2.515386	-0.556334
	H	-6.433553	2.747497	0.166026
	C	-4.802542	1.437827	-0.313143
	H	-4.909948	0.861542	0.599826
	C	0.518314	-2.959942	-3.106418
	C	0.674070	-3.494703	-4.447451
	H	0.177744	-2.834568	-5.165811
	H	0.226255	-4.491793	-4.502447
	H	1.738283	-3.561536	-4.694427
	N	0.167287	-3.246181	0.823820
	N	2.320188	-1.678065	0.139910
	N	3.032981	0.471285	-0.376467
	H	2.060047	0.613785	-0.640161
	N	-0.227413	-0.564964	1.641745
	N	-0.257232	1.686743	1.038976
	H	-0.165250	1.357499	0.077752
	N	-2.017178	-1.960271	-0.296889

	N -2.871720 0.069510 -1.024977 H -1.934091 0.226580 -1.396023 N 0.395034 -2.534587 -2.038001 Cl 0.188873 0.518111 -1.915087 Ni 0.156342 -1.490948 -0.269136
[Ni(II)-Br(CH_3CN)]$^{+1}$	SCF Done: -5987.71133132 A.U. C 1.438403 -3.930044 0.647059 H 1.428623 -4.337744 -0.367407 H 1.573689 -4.766870 1.341334 C 2.569131 -2.941859 0.778582 C 3.762217 -3.317434 1.372790 H 3.879993 -4.319062 1.770960 C 4.783398 -2.363213 1.463238 H 5.722355 -2.605119 1.953015 C 4.584368 -1.102723 0.940910 H 5.350116 -0.342060 1.019191 C 3.351077 -0.797929 0.314271 C 4.035741 1.454370 -0.547641 C 3.632663 2.786825 -0.372822 H 2.655485 2.994961 0.053736 C 4.480530 3.832060 -0.738794 H 4.152798 4.858851 -0.599859 C 5.746336 3.563123 -1.265782 H 6.410236 4.377949 -1.540728 C 6.148436 2.236712 -1.441395 H 7.124299 2.013863 -1.864787 C 5.298176 1.184394 -1.098256 H 5.607734 0.159516 -1.274553 C -0.006667 -2.908868 2.319184 H 0.988481 -2.935306 2.775472 H -0.607062 -3.669277 2.828250 C -0.568208 -1.533226 2.583777 C -1.235856 -1.306992 3.778086 H -1.439740 -2.132521 4.451117 C -1.628370 0.000123 4.079831 H -2.185411 0.214280 4.987529 C -1.306364 1.023633 3.211185 H -1.613824 2.040243 3.415173 C -0.605503 0.725996 2.020842 C -0.286875 3.102832 1.259500 C -0.549784 3.854165 0.099577 H -0.737562 3.334293 -0.835638 C -0.552507 5.246768 0.147309 H -0.758443 5.808918 -0.759798 C -0.302500 5.915893 1.348697 H -0.314898 7.001465 1.386738 C -0.023611 5.171598 2.497184 H 0.195377 5.677115 3.434150 C -0.000463 3.776476 2.459140 H 0.260744 3.220153 3.352398 C -0.986840 -4.071314 0.387777 H -1.183426 -4.909108 1.066046

	H -0.694772 -4.491853 -0.578879 C -2.230151 -3.242511 0.195149 C -3.479596 -3.795009 0.432661 H -3.564407 -4.805354 0.817340 C -4.608065 -3.020383 0.143426 H -5.606178 -3.425829 0.282838 C -4.448331 -1.733099 -0.329915 H -5.306647 -1.124929 -0.583072 C -3.142747 -1.219295 -0.505000 C -3.811829 1.123907 -1.130335 C -3.596220 1.987746 -2.218336 H -2.782943 1.781154 -2.908827 C -4.415806 3.099040 -2.409636 H -4.232356 3.755876 -3.255860 C -5.470422 3.360938 -1.530848 H -6.114492 4.221771 -1.686357 C -5.681255 2.507681 -0.444996 H -6.485790 2.708536 0.257633 C -4.854917 1.403182 -0.231918 H -5.007992 0.777323 0.640670 C 0.560901 -3.104203 -3.015743 C 0.722062 -3.702620 -4.328957 H 0.047411 -3.215330 -5.039981 H 0.486260 -4.770367 -4.280168 H 1.755451 -3.575410 -4.666489 N 0.142385 -3.249906 0.880042 N 2.338394 -1.705372 0.265787 N 3.103182 0.435501 -0.221408 H 2.182573 0.548693 -0.643405 N -0.284749 -0.556620 1.687243 N -0.239376 1.700067 1.127203 H -0.051780 1.370285 0.180340 N -2.042010 -1.979957 -0.259765 N -2.909234 0.055247 -0.952685 H -1.968212 0.218124 -1.309527 N 0.432697 -2.627540 -1.969676 Br 0.238004 0.472873 -1.890602 Ni 0.171136 -1.511006 -0.241555
Ni(I)-F	SCF Done: -3383.15387357 A.U. Ni -1.251331 0.340639 0.179839 F 0.641219 -0.309544 -0.381123 N -3.147163 0.992783 0.695438 N -2.226670 -1.475140 -0.074387 N -0.481736 -2.627383 -1.038679 H 0.009920 -1.738716 -0.850968 N -1.421310 1.862223 -1.227889 N 0.809446 1.962414 -1.778014 H 0.819145 1.057168 -1.282204 N -0.800934 0.944626 2.123635 N 1.308105 0.045796 2.195932 H 1.086243 -0.145953 1.205952 C -3.875567 -0.199671 1.160691

	H	-4.961735	-0.036898	1.180939
	H	-3.557634	-0.393772	2.192051
	C	-3.525713	-1.405347	0.316951
	C	-4.469942	-2.377205	0.020485
	H	-5.495979	-2.258928	0.353404
	C	-4.063290	-3.491907	-0.722682
	H	-4.778438	-4.258476	-1.007411
	C	-2.735658	-3.608965	-1.102295
	H	-2.405186	-4.449982	-1.697826
	C	-1.821447	-2.599405	-0.733940
	C	0.321730	-3.685215	-1.486632
	C	0.076103	-5.042697	-1.207512
	H	-0.781938	-5.334580	-0.613280
	C	0.959045	-6.024102	-1.662346
	H	0.748461	-7.066238	-1.434999
	C	2.106536	-5.683426	-2.381451
	H	2.788125	-6.454007	-2.730438
	C	2.368496	-4.333762	-2.638043
	H	3.259895	-4.045411	-3.189536
	C	1.488226	-3.346705	-2.202029
	H	1.689243	-2.299715	-2.413304
	C	-3.727157	1.562156	-0.533158
	H	-4.598286	2.197380	-0.320897
	H	-4.083663	0.722058	-1.141689
	C	-2.691345	2.324873	-1.330573
	C	-3.054374	3.389046	-2.144547
	H	-4.084305	3.729965	-2.169433
	C	-2.067523	3.977577	-2.943322
	H	-2.317862	4.784282	-3.626548
	C	-0.760937	3.519812	-2.862878
	H	0.010044	3.941855	-3.494065
	C	-0.452333	2.478169	-1.964168
	C	2.061695	2.466072	-2.150340
	C	2.346746	3.830732	-2.344078
	H	1.575073	4.579141	-2.207595
	C	3.640630	4.236775	-2.677469
	H	3.837191	5.296241	-2.822689
	C	4.676539	3.309709	-2.807648
	H	5.679815	3.635413	-3.067471
	C	4.403444	1.955671	-2.587174
	H	5.196941	1.217150	-2.670612
	C	3.115528	1.536518	-2.266024
	H	2.907568	0.483888	-2.092881
	C	-2.949536	1.992294	1.761222
	H	-3.881708	2.207940	2.300838
	H	-2.628196	2.922370	1.277599
	C	-1.861606	1.546407	2.715735
	C	-1.943348	1.774308	4.081757
	H	-2.819774	2.253403	4.505708
	C	-0.875663	1.354587	4.885499
	H	-0.913999	1.482121	5.963732
	C	0.233830	0.763453	4.300741

	H 1.053000 0.408907 4.912157 C 0.263626 0.597623 2.899614 C 2.614383 -0.270804 2.591454 C 3.315286 0.379606 3.623887 H 2.854179 1.188975 4.177389 C 4.631457 0.015227 3.916025 H 5.153229 0.531052 4.718370 C 5.282983 -0.979660 3.184779 H 6.307182 -1.255630 3.419416 C 4.599256 -1.607887 2.138414 H 5.090886 -2.377828 1.548977 C 3.282734 -1.263324 1.845418 H 2.753686 -1.755591 1.033488
Ni(I)-Cl	SCF Done: -3743.50709270 A.U. Ni -0.200337 -0.876134 -0.753608 Cl 0.041270 1.238792 1.251653 N -0.382864 -2.375065 -2.119318 N -2.326168 -0.966863 -0.832890 N -2.877558 0.088918 1.149329 H -1.864673 0.220323 1.209528 N 0.835520 -2.396803 0.305329 N 2.085358 -1.116736 1.777754 H 1.410591 -0.378401 1.557507 N 0.841638 0.049173 -2.353868 N 0.799567 2.250701 -1.653966 H 0.358351 1.840177 -0.827319 C -1.608941 -2.073897 -2.872165 H -1.920348 -2.914376 -3.507415 H -1.389262 -1.228249 -3.533909 C -2.714648 -1.686363 -1.921747 C -4.025081 -2.054744 -2.182861 H -4.258126 -2.635543 -3.068957 C -5.017116 -1.675879 -1.271545 H -6.053319 -1.962401 -1.427537 C -4.659033 -0.952055 -0.150125 H -5.397935 -0.679735 0.592162 C -3.304972 -0.596344 0.042841 C -3.635985 0.797944 2.104143 C -4.790619 1.531372 1.781779 H -5.146116 1.565653 0.757591 C -5.469052 2.241651 2.773675 H -6.361831 2.801471 2.506767 C -5.000348 2.256614 4.089532 H -5.530750 2.815370 4.855586 C -3.837294 1.549237 4.407255 H -3.455697 1.554097 5.425005 C -3.163962 0.820265 3.428277 H -2.268901 0.258113 3.679419 C -0.479235 -3.617662 -1.340439 H -0.348662 -4.509045 -1.969416 H -1.489687 -3.665188 -0.918941 C 0.526831 -3.615680 -0.213717

	C 1.065116 -4.810085 0.240754 H 0.789160 -5.744868 -0.235881 C 1.949433 -4.771590 1.323785 H 2.363002 -5.687544 1.736229 C 2.296281 -3.547557 1.865696 H 2.971152 -3.486509 2.709829 C 1.750713 -2.367195 1.315316 C 3.126768 -0.758468 2.654792 C 4.409372 -1.330788 2.582168 H 4.622326 -2.093618 1.840644 C 5.418638 -0.902628 3.445101 H 6.402974 -1.358561 3.374890 C 5.181350 0.112681 4.375447 H 5.973371 0.445293 5.040588 C 3.914260 0.699431 4.433486 H 3.712729 1.494224 5.147235 C 2.892595 0.266106 3.589298 H 1.906342 0.717352 3.644260 C 0.829681 -2.304572 -2.947882 H 0.750586 -2.929752 -3.847523 H 1.660549 -2.695209 -2.349534 C 1.118939 -0.870021 -3.318520 C 1.640277 -0.553279 -4.563100 H 1.828084 -1.338105 -5.288076 C 1.892798 0.792098 -4.855032 H 2.277167 1.086016 -5.827656 C 1.624931 1.752359 -3.897302 H 1.776370 2.802811 -4.109165 C 1.114046 1.353770 -2.641724 C 1.149852 3.611957 -1.541861 C 2.382755 4.129278 -1.975254 H 3.119601 3.475783 -2.429474 C 2.676570 5.482187 -1.796763 H 3.634186 5.864833 -2.140672 C 1.767377 6.334245 -1.165496 H 2.004894 7.385137 -1.025545 C 0.551500 5.816455 -0.709923 H -0.165694 6.463685 -0.211620 C 0.239675 4.471445 -0.901591 H -0.711882 4.074050 -0.560050
Ni(I)-Cl'	78 SERGI-ClnoD3-NiI+0delBr SCF Done: -3743.50717955 A.U. Ni -0.260235 -0.987004 0.462178 Cl 0.188090 1.120990 -0.999293 N 0.511460 -2.619678 1.459574 N 2.783546 -0.929798 0.662019 N 3.513365 0.701478 -0.771654 H 2.511037 0.885058 -0.844252 N -0.923602 -2.313590 -0.838400 N -2.229544 -0.826822 -2.022596 H -1.523969 -0.157309 -1.711031 N -0.923159 -0.430505 2.243994

	N	-1.282560	1.809194	1.832911
	H	-0.768468	1.599355	0.974780
	C	1.784922	-2.501821	2.210817
	H	2.017944	-3.457293	2.701154
	H	1.621072	-1.760227	2.999971
	C	2.958654	-2.057404	1.367483
	C	4.159089	-2.765801	1.383511
	H	4.258763	-3.674263	1.968304
	C	5.220219	-2.269441	0.617521
	H	6.167771	-2.800626	0.584204
	C	5.060054	-1.106388	-0.118555
	H	5.862228	-0.731939	-0.741574
	C	3.810249	-0.447280	-0.065698
	C	4.362156	1.587200	-1.452004
	C	5.676052	1.868727	-1.035683
	H	6.083730	1.391695	-0.151304
	C	6.452162	2.791043	-1.739610
	H	7.465755	2.992982	-1.402293
	C	5.936550	3.465336	-2.848773
	H	6.545701	4.185043	-3.388329
	C	4.622070	3.206703	-3.249002
	H	4.199369	3.725579	-4.105696
	C	3.843580	2.274955	-2.565760
	H	2.826515	2.068693	-2.888316
	C	0.575049	-3.709101	0.463102
	H	0.554116	-4.697953	0.941309
	H	1.536212	-3.618443	-0.055601
	C	-0.536625	-3.585762	-0.550989
	C	-1.091886	-4.705842	-1.152669
	H	-0.761575	-5.697564	-0.861711
	C	-2.063185	-4.518080	-2.141016
	H	-2.498792	-5.368538	-2.657483
	C	-2.464490	-3.230691	-2.465526
	H	-3.193383	-3.058332	-3.246780
	C	-1.892295	-2.141091	-1.784197
	C	-3.307333	-0.297892	-2.751940
	C	-4.578565	-0.898280	-2.789533
	H	-4.764706	-1.820121	-2.249668
	C	-5.617617	-0.292400	-3.497556
	H	-6.592792	-0.772487	-3.515734
	C	-5.422857	0.922036	-4.159641
	H	-6.238118	1.388946	-4.705039
	C	-4.166178	1.532031	-4.103487
	H	-3.995830	2.480112	-4.607313
	C	-3.116219	0.929106	-3.413991
	H	-2.138409	1.402018	-3.381914
	C	-0.603079	-2.814507	2.418975
	H	-0.368148	-3.585011	3.165544
	H	-1.471403	-3.164598	1.847896
	C	-0.953456	-1.504483	3.081046
	C	-1.330027	-1.425473	4.412048
	H	-1.332959	-2.316428	5.030811

	C -1.693449 -0.173859 4.923394 H -1.968911 -0.063409 5.968286 C -1.687388 0.932978 4.090474 H -1.936511 1.914170 4.473058 C -1.314668 0.776985 2.739653 C -1.784593 3.118125 1.947312 C -2.974105 3.428092 2.629942 H -3.550386 2.643970 3.108523 C -3.436382 4.744597 2.667650 H -4.356814 4.965123 3.202390 C -2.744558 5.766341 2.013155 H -3.113169 6.787780 2.043509 C -1.575679 5.455426 1.312108 H -1.026963 6.235935 0.791258 C -1.094048 4.148126 1.282882 H -0.179151 3.912166 0.746459
Ni(I)-Br	SCF Done: -5855.03362192 A.U. Ni -0.390998 -0.998598 0.515328 Br 0.168242 0.927754 -1.030799 N 0.335840 -2.686177 1.498738 N 2.779504 -1.144675 0.702257 N 3.584052 0.497817 -0.655772 H 2.600027 0.767241 -0.632583 N -1.290897 -2.333366 -0.657234 N -2.642671 -0.781758 -1.679662 H -1.874512 -0.170827 -1.400802 N -0.843402 -0.367644 2.364697 N -1.060274 1.880289 1.943331 H -0.693306 1.579887 1.038258 C 1.662961 -2.697304 2.174103 H 1.826553 -3.676468 2.645413 H 1.619766 -1.949377 2.971775 C 2.820410 -2.360869 1.261945 C 3.874588 -3.252051 1.058962 H 3.877019 -4.227174 1.534819 C 4.919509 -2.845534 0.221363 H 5.754176 -3.513050 0.024057 C 4.885875 -1.595529 -0.379819 H 5.671221 -1.288184 -1.058214 C 3.780498 -0.758441 -0.110689 C 4.411756 1.280963 -1.469583 C 5.812141 1.317598 -1.344005 H 6.310763 0.719332 -0.589700 C 6.565899 2.157063 -2.166483 H 7.647296 2.170012 -2.055233 C 5.949427 2.985964 -3.106339 H 6.543871 3.638634 -3.739428 C 4.554886 2.971230 -3.212858 H 4.054882 3.615599 -3.931640 C 3.791820 2.126884 -2.410307 H 2.707952 2.111815 -2.495931 C 0.235222 -3.799130 0.531862

	H 0.167071 -4.770544 1.041599 H 1.162817 -3.805565 -0.051899 C -0.930651 -3.617590 -0.410721 C -1.551402 -4.710823 -1.001250 H -1.235108 -5.717446 -0.748344 C -2.567580 -4.474815 -1.930624 H -3.053810 -5.301694 -2.440225 C -2.956583 -3.170303 -2.202180 H -3.727429 -2.964699 -2.932734 C -2.318997 -2.114226 -1.528681 C -3.621396 -0.168767 -2.479725 C -4.917040 -0.683996 -2.656062 H -5.212141 -1.606949 -2.169875 C -5.845429 0.015056 -3.430270 H -6.842467 -0.398822 -3.557827 C -5.514768 1.237356 -4.019337 H -6.244984 1.775635 -4.616973 C -4.234861 1.764399 -3.819730 H -3.961396 2.719239 -4.261436 C -3.294347 1.070250 -3.062866 H -2.298051 1.476940 -2.907366 C -0.725315 -2.764801 2.534766 H -0.523336 -3.561075 3.263772 H -1.665429 -3.009927 2.026930 C -0.878497 -1.427680 3.215171 C -1.077524 -1.306142 4.581778 H -1.092332 -2.189511 5.211088 C -1.238681 -0.021419 5.112379 H -1.361590 0.122664 6.181976 C -1.228634 1.076407 4.266469 H -1.316839 2.077432 4.665686 C -1.059074 0.875958 2.881496 C -1.334199 3.252600 2.044130 C -2.220132 3.819376 2.977379 H -2.756958 3.195454 3.681606 C -2.448635 5.197442 2.974586 H -3.135249 5.616600 3.705815 C -1.826597 6.029303 2.042112 H -2.012149 7.099640 2.047937 C -0.973110 5.461321 1.090369 H -0.491354 6.088195 0.344246 C -0.725396 4.091784 1.089358 H -0.077420 3.645714 0.339326
$[Ni(I)\text{-}F_2]^{-1}$	SCF Done: -3483.10909419 A.U. C 3.320827 -2.828494 -0.638031 H 3.186302 -3.046199 -1.701909 H 4.011751 -3.575204 -0.222684 C 3.903668 -1.438027 -0.498790 C 5.276565 -1.226828 -0.414506 H 5.960518 -2.068577 -0.382087 C 5.737518 0.092839 -0.393875 H 6.803781 0.300250 -0.359322

	C	4.836186	1.147082	-0.424996
	H	5.184345	2.171155	-0.439888
	C	3.455139	0.855319	-0.467891
	C	2.545985	3.198616	-0.385268
	C	1.628409	3.972724	-1.122371
	H	0.927877	3.469397	-1.783554
	C	1.620617	5.361686	-1.010358
	H	0.904388	5.937884	-1.590636
	C	2.531574	6.011388	-0.171703
	H	2.531506	7.094840	-0.092092
	C	3.435422	5.246903	0.569471
	H	4.137122	5.734031	1.241962
	C	3.442102	3.853722	0.478267
	H	4.122176	3.280881	1.098629
	C	2.077276	-2.819198	1.464669
	H	2.970444	-2.220740	1.692351
	H	2.240012	-3.817165	1.894078
	C	0.879826	-2.156680	2.078839
	C	0.393530	-2.552123	3.325442
	H	0.777980	-3.455567	3.791068
	C	-0.544431	-1.747274	3.965884
	H	-0.922182	-2.005813	4.951317
	C	-0.997545	-0.578496	3.324596
	H	-1.680036	0.090348	3.830433
	C	-0.516397	-0.274478	2.042714
	C	-1.937134	1.752914	1.527370
	C	-3.123565	1.475310	2.233541
	H	-3.296229	0.488835	2.645605
	C	-4.110352	2.454754	2.368004
	H	-5.016827	2.214279	2.918479
	C	-3.956707	3.717501	1.792981
	H	-4.729780	4.473017	1.902754
	C	-2.793908	3.989447	1.064334
	H	-2.655569	4.962187	0.598531
	C	-1.797387	3.025872	0.935798
	H	-0.889972	3.250142	0.381419
	C	1.152142	-4.020905	-0.472505
	H	1.415826	-4.951909	0.048872
	H	1.389768	-4.160638	-1.536093
	C	-0.314571	-3.720581	-0.324955
	C	-1.244285	-4.712845	-0.012569
	H	-0.897516	-5.688799	0.318104
	C	-2.600685	-4.444816	-0.178289
	H	-3.349852	-5.203010	0.032301
	C	-3.002562	-3.167949	-0.641366
	H	-4.045122	-2.968014	-0.843501
	C	-2.024214	-2.196686	-0.878522
	C	-3.470454	-0.217170	-1.547128
	C	-4.690527	-0.485722	-0.896431
	H	-4.750449	-1.258812	-0.141174
	C	-5.824329	0.279099	-1.181735
	H	-6.753790	0.050293	-0.665602

	C -5.774138 1.333804 -2.094359 H -6.662038 1.921594 -2.310084 C -4.556499 1.626969 -2.718762 H -4.488787 2.450666 -3.425373 C -3.423181 0.864537 -2.453015 H -2.482280 1.090927 -2.948731 N 1.987952 -2.888339 -0.011968 N 3.011577 -0.423527 -0.516598 N 2.459186 1.803603 -0.506095 H 1.543020 1.432951 -0.799992 N 0.432351 -1.037640 1.424463 N -0.899388 0.835552 1.311622 H -0.451164 0.890272 0.386755 N -0.693545 -2.460097 -0.737615 N -2.274309 -0.906041 -1.324983 H -1.426530 -0.347053 -1.455048 Ni 0.986085 -1.178457 -0.715102 F 1.379328 -1.500823 -2.569928 F 0.110745 0.607766 -1.202373
Ni(I)-F(CH_3CN)	SCF Done: -3515.90374616 A.U. C -1.318731 -3.836281 0.073134 H -1.295566 -4.024015 1.154327 H -1.224170 -4.807739 -0.432685 C -2.632704 -3.186807 -0.280823 C -3.662988 -3.898628 -0.880719 H -3.529866 -4.944313 -1.137302 C -4.857959 -3.221658 -1.152268 H -5.680000 -3.731270 -1.647223 C -4.987575 -1.887651 -0.799206 H -5.893793 -1.344720 -1.033143 C -3.906310 -1.234609 -0.166757 C -4.981139 0.972848 0.385824 C -4.675955 2.348550 0.338421 H -3.649743 2.652299 0.150489 C -5.668150 3.305909 0.531113 H -5.405193 4.359928 0.487449 C -6.991476 2.920679 0.770149 H -7.767414 3.668026 0.910388 C -7.296887 1.559923 0.835924 H -8.315105 1.240135 1.043831 C -6.308149 0.589972 0.657053 H -6.568020 -0.456689 0.761833 C -0.030966 -2.719908 -1.682120 H -1.037025 -2.743475 -2.115352 H 0.546744 -3.511862 -2.174763 C 0.556104 -1.358061 -1.975526 C 1.436522 -1.162106 -3.031857 H 1.764593 -2.002893 -3.633724 C 1.903496 0.135472 -3.266918 H 2.631667 0.326448 -4.050515 C 1.435123 1.183816 -2.491085 H 1.808418 2.187503 -2.642375

	C	0.486448	0.917776	-1.478699
	C	-0.122631	3.266706	-0.787309
	C	-0.434991	3.979884	0.390384
	H	-0.606281	3.423794	1.308076
	C	-0.529090	5.368517	0.381156
	H	-0.768475	5.890835	1.304193
	C	-0.310099	6.088766	-0.798036
	H	-0.373785	7.173260	-0.803288
	C	-0.019823	5.388902	-1.970377
	H	0.130491	5.927770	-2.902776
	C	0.066231	3.994805	-1.977661
	H	0.243893	3.483310	-2.915606
	C	1.047707	-3.615886	0.348479
	H	1.054477	-4.667791	0.029876
	H	0.927503	-3.593054	1.435115
	C	2.393996	-3.016508	-0.011762
	C	3.257465	-3.700824	-0.871161
	H	2.956354	-4.639207	-1.324595
	C	4.522735	-3.154407	-1.108518
	H	5.232041	-3.671912	-1.748981
	C	4.885403	-1.955683	-0.512503
	H	5.875231	-1.542297	-0.657312
	C	3.940950	-1.320107	0.322392
	C	5.210341	0.803757	0.879626
	C	5.538585	1.563132	2.018557
	H	5.011737	1.373392	2.950713
	C	6.524825	2.544644	1.955442
	H	6.759992	3.119847	2.847368
	C	7.214590	2.783386	0.762657
	H	7.989969	3.542893	0.716883
	C	6.885209	2.037913	-0.371283
	H	7.396718	2.223203	-1.312468
	C	5.886420	1.063475	-0.325708
	H	5.615720	0.533043	-1.231478
	C	0.224015	-1.303744	3.432186
	C	0.684667	-1.342697	4.812337
	H	0.848547	-0.324626	5.181730
	H	1.628116	-1.895316	4.878351
	H	-0.056603	-1.833131	5.453472
	N	-0.163568	-2.955547	-0.227116
	N	-2.725961	-1.879338	0.054730
	N	-3.912090	0.080821	0.226687
	H	-2.984477	0.429549	0.545207
	N	0.105935	-0.357754	-1.184790
	N	-0.097364	1.871334	-0.683828
	H	-0.671357	1.469392	0.087274
	N	2.733737	-1.857447	0.573439
	N	4.174138	-0.134015	0.996886
	H	3.497121	0.043746	1.730838
	N	-0.142039	-1.279845	2.326134
	F	-1.562297	0.775903	1.185168
	Ni	-0.858305	-1.076937	0.564908

Ni(I)-Cl(CH_3CN)	SCF Done: -3876.26881552 A.U.
	C 1.395524 -3.843433 -0.182938
	H 1.331921 -3.999602 -1.266954
	H 1.341290 -4.829737 0.297810
	C 2.701585 -3.173194 0.156564
	C 3.749994 -3.883292 0.722028
	H 3.645131 -4.943278 0.926645
	C 4.921907 -3.185578 1.039478
	H 5.759189 -3.696851 1.506196
	C 5.003284 -1.830829 0.775530
	H 5.887881 -1.268816 1.044373
	C 3.902848 -1.176768 0.174014
	C 4.956396 1.089715 -0.051123
	C 4.662442 2.399861 0.364363
	H 3.647776 2.643161 0.666825
	C 5.659239 3.374117 0.389077
	H 5.411746 4.382082 0.711937
	C 6.968348 3.057420 0.014645
	H 7.746910 3.814711 0.044589
	C 7.262569 1.758572 -0.406207
	H 8.271647 1.501618 -0.718267
	C 6.266316 0.781540 -0.454520
	H 6.503813 -0.209955 -0.825029
	C 0.190416 -2.730933 1.648254
	H 1.218197 -2.746545 2.025464
	H -0.355834 -3.512522 2.189309
	C -0.389715 -1.366431 1.944863
	C -1.128180 -1.143840 3.097345
	H -1.344119 -1.964864 3.772551
	C -1.591486 0.152899 3.347516
	H -2.194632 0.363973 4.226228
	C -1.289180 1.168168 2.458382
	H -1.661636 2.172059 2.615787
	C -0.510140 0.874679 1.316386
	C -0.267341 3.225107 0.489922
	C -0.589925 3.957570 -0.665515
	H -0.796777 3.423968 -1.587970
	C -0.640868 5.350248 -0.627835
	H -0.890617 5.898977 -1.532400
	C -0.385940 6.037629 0.562350
	H -0.436136 7.122565 0.592392
	C -0.060000 5.313330 1.711485
	H 0.156779 5.833828 2.640938
	C 0.013258 3.919723 1.679163
	H 0.303456 3.375087 2.571445
	C -0.993463 -3.696532 -0.294985
	H -0.948882 -4.741149 0.041848
	H -0.944965 -3.691583 -1.387372
	C -2.326308 -3.122759 0.145485
	C -3.110899 -3.808860 1.075607
	H -2.756477 -4.730258 1.525259
	C -4.369977 -3.286875 1.388385

	H -5.021963 -3.807782 2.084519 C -4.800679 -2.108728 0.797180 H -5.788931 -1.717568 1.001259 C -3.930235 -1.466058 -0.110022 C -5.275070 0.627029 -0.618273 C -5.659972 1.384090 -1.741353 H -5.168992 1.202987 -2.694539 C -6.656504 2.351161 -1.636479 H -6.935541 2.924118 -2.517113 C -7.300366 2.578960 -0.416101 H -8.083997 3.327145 -0.337493 C -6.913717 1.837452 0.702018 H -7.388395 2.014704 1.663804 C -5.903979 0.877057 0.614367 H -5.588336 0.352347 1.508585 C -0.233408 -1.524017 -3.466091 C -0.730888 -1.682821 -4.823720 H -0.581765 -0.752402 -5.382332 H -1.800719 -1.918049 -4.811283 H -0.196779 -2.490232 -5.336519 N 0.235492 -2.995638 0.191150 N 2.753344 -1.845322 -0.114766 N 3.889680 0.164510 -0.104077 H 3.034643 0.515601 -0.550833 N -0.082804 -0.389639 1.053237 N -0.174845 1.821030 0.382325 H 0.298394 1.474790 -0.460704 N -2.731539 -1.982986 -0.435637 N -4.232587 -0.296122 -0.784584 H -3.603861 -0.114118 -1.559417 N 0.163088 -1.385022 -2.380956 Cl 1.782032 1.465364 -2.140620 Ni 0.832925 -1.152411 -0.630761
Ni(I)-Br(CH_3CN)	SCF Done: -5987.78824392 A.U. C 2.281994 -3.473319 0.836638 H 2.415684 -3.888078 -0.169746 H 2.445809 -4.286370 1.557543 C 3.284132 -2.367501 1.040863 C 4.450748 -2.548972 1.768708 H 4.645537 -3.498160 2.256665 C 5.344250 -1.476672 1.861545 H 6.254107 -1.563657 2.448407 C 5.054409 -0.288067 1.208605 H 5.713153 0.564567 1.303753 C 3.865626 -0.185333 0.459344 C 4.198702 2.078575 -0.625211 C 3.441683 3.222423 -0.951416 H 2.358475 3.169459 -0.883966 C 4.068015 4.388016 -1.382448 H 3.461747 5.256679 -1.626911 C 5.461008 4.447512 -1.497251

	H	5.949570	5.360830	-1.824773
	C	6.211823	3.309527	-1.198189
	H	7.293561	3.327083	-1.305468
	C	5.596388	2.129063	-0.775228
	H	6.204494	1.250848	-0.596253
	C	0.621411	-2.598749	2.343877
	H	1.539839	-2.160466	2.744504
	H	0.434493	-3.527284	2.900084
	C	-0.489040	-1.606420	2.607341
	C	-1.590113	-1.935246	3.399751
	H	-1.712270	-2.939950	3.791137
	C	-2.524561	-0.929877	3.669274
	H	-3.401419	-1.145758	4.274255
	C	-2.349152	0.344769	3.146895
	H	-3.086314	1.119211	3.317338
	C	-1.206548	0.582666	2.353810
	C	-1.572906	3.010886	1.769554
	C	-1.627372	3.794574	0.599993
	H	-1.212294	3.390159	-0.319958
	C	-2.205934	5.061186	0.624377
	H	-2.237624	5.647918	-0.290333
	C	-2.751326	5.572522	1.806512
	H	-3.209708	6.557311	1.821486
	C	-2.691354	4.801004	2.969543
	H	-3.094836	5.189257	3.901508
	C	-2.100120	3.536390	2.963233
	H	-2.025362	2.973257	3.887217
	C	-0.036907	-3.985252	0.431383
	H	-0.056989	-4.827413	1.138257
	H	0.373618	-4.368544	-0.508874
	C	-1.455659	-3.528717	0.151311
	C	-2.517094	-4.427710	0.294241
	H	-2.355183	-5.419508	0.704472
	C	-3.778545	-4.014099	-0.139213
	H	-4.625958	-4.692582	-0.083034
	C	-3.960753	-2.735365	-0.652488
	H	-4.929072	-2.428541	-1.023493
	C	-2.841600	-1.876769	-0.700352
	C	-3.878797	0.290355	-1.544221
	C	-3.525817	1.375044	-2.374932
	H	-2.488283	1.484062	-2.680768
	C	-4.482675	2.299359	-2.782790
	H	-4.183467	3.125171	-3.423473
	C	-5.816564	2.167778	-2.381458
	H	-6.565116	2.883661	-2.708907
	C	-6.166431	1.108444	-1.542919
	H	-7.192490	1.002228	-1.199329
	C	-5.213917	0.180649	-1.114522
	H	-5.509625	-0.597265	-0.422031
	C	0.794237	-2.754934	-3.218875
	C	0.711742	-3.299120	-4.565777
	H	-0.073438	-2.787451	-5.132753

	H 0.476115 -4.367952 -4.524884 H 1.666168 -3.168685 -5.087706 N 0.894742 -2.938156 0.910799 N 2.965114 -1.209169 0.406629 N 3.482696 0.939491 -0.231962 H 2.506235 0.914791 -0.532923 N -0.295062 -0.376397 2.116870 N -0.923098 1.773659 1.699364 H -0.390263 1.603101 0.843356 N -1.615378 -2.292733 -0.325644 N -2.846403 -0.574258 -1.164375 H -1.903832 -0.185609 -1.232794 N 0.855347 -2.320369 -2.140647 Br 0.344633 0.880801 -1.389748 Ni 1.186042 -1.386448 -0.525882

Table S6. Xyz coordinates and absolute energies (in a.u.) of all computed DFT species, including dispersion corrections by the D3 model.

Ni(I)-F	78 SERGI-F-NiI+0arreglat SCF Done: -3383.25640891 A.U. Ni -0.960925 1.007287 0.029429 F -0.095039 -0.759363 -0.774217 N -1.756707 2.806868 0.655685 N -2.869110 0.357672 0.136005 N -2.516281 -1.768361 -0.657448 H -1.551073 -1.411561 -0.703916 N -0.064473 2.252044 -1.373927 N 1.699857 0.858324 -1.859065 H 1.049971 0.157515 -1.474393 N 0.207777 1.220970 1.726270 N 1.183164 -0.848643 1.563392 H 0.627174 -0.870681 0.694513 C -3.028395 2.466532 1.309708 H -3.692387 3.336890 1.397708 H -2.781725 2.134152 2.325544 C -3.712861 1.319297 0.604700 C -5.094070 1.234404 0.526641 H -5.708127 2.045009 0.905621 C -5.661214 0.090773 -0.049293 H -6.737364 0.002455 -0.166169 C -4.828259 -0.938538 -0.468499 H -5.238403 -1.826240 -0.931922 C -3.435127 -0.802680 -0.322825 C -2.628812 -3.146705 -0.833748 C -3.717971 -3.936157 -0.419265 H -4.565602 -3.487407 0.083442 C -3.694019 -5.319267 -0.615543 H -4.546620 -5.908913 -0.287223 C -2.597361 -5.948477 -1.207674 H -2.591346 -7.024541 -1.356248 C -1.501477 -5.169209 -1.597691 H -0.630329 -5.637396 -2.049365 C -1.514188 -3.790077 -1.418096 H -0.661141 -3.185556 -1.715387 C -1.938203 3.551953 -0.605692 H -2.219191 4.599274 -0.431464 H -2.762271 3.067805 -1.142956 C -0.677853 3.458571 -1.434610 C -0.177929 4.530992 -2.158438 H -0.699981 5.482054 -2.155304 C 1.004339 4.343924 -2.886620 H 1.408989 5.146345 -3.496806 C 1.662102 3.124638 -2.820577 H 2.567836 2.948070 -3.387689 C 1.121503 2.097899 -2.020687 C 3.047245 0.488976 -1.809924 C 4.128401 1.388244 -1.772097

	H 3.956289 2.457746 -1.790641 C 5.435565 0.906573 -1.667781 H 6.255451 1.620165 -1.637213 C 5.697666 -0.462496 -1.585148 H 6.717908 -0.825495 -1.499106 C 4.622364 -1.358205 -1.604110 H 4.797967 -2.427328 -1.519194 C 3.316439 -0.893482 -1.721405 H 2.483848 -1.591389 -1.720524 C -0.790451 3.429041 1.579277 H -1.273009 4.156194 2.244473 H -0.061501 3.980116 0.975776 C -0.030416 2.383244 2.375305 C 0.449561 2.644225 3.651240 H 0.227690 3.588328 4.137900 C 1.216929 1.656675 4.283306 H 1.587336 1.812169 5.292734 C 1.496520 0.470186 3.622851 H 2.065031 -0.315231 4.104931 C 0.992425 0.283668 2.318654 C 2.209258 -1.801601 1.609750 C 3.470332 -1.583811 2.191702 H 3.699488 -0.635924 2.664849 C 4.453905 -2.572286 2.119533 H 5.424358 -2.382707 2.571472 C 4.213682 -3.780487 1.460918 H 4.986435 -4.542161 1.407257 C 2.964955 -3.992106 0.865506 H 2.759744 -4.922053 0.341114 C 1.971104 -3.020029 0.941928 H 1.002087 -3.186818 0.477959
Ni(I)-Cl	78 symmetry c1 Ni 0.616527000 -0.822276000 0.278373000 Cl 0.122532000 0.986566000 -0.327532000 N 1.107154000 -2.764234000 0.716379000 N 2.762346000 -0.662601000 0.525488000 N 3.268648000 1.157010000 -0.822717000 H 2.281493000 1.004179000 -1.023776000 N -0.137030000 -1.941623000 -1.484685000 N -1.856157000 -0.563886000 -2.096739000 H -1.348867000 0.038766000 -1.449645000 N -0.866433000 -1.266719000 1.877525000 N -1.583013000 0.847168000 2.336071000 H -1.000831000 0.981364000 1.509057000 C 2.168853000 -2.683382000 1.731175000 H 2.614076000 -3.665879000 1.940667000 H 1.708591000 -2.314349000 2.654880000 C 3.218480000 -1.712606000 1.266653000 C 4.548052000 -1.917835000 1.604820000 H 4.826993000 -2.781447000 2.199857000 C 5.505343000 -1.026114000 1.124827000

	H	6.560668000	-1.178844000	1.332517000
	C	5.092034000	0.027886000	0.329540000
	H	5.819541000	0.679519000	-0.134006000
	C	3.716586000	0.203675000	0.063729000
	C	3.657338000	2.488375000	-0.986860000
	C	4.476173000	3.215972000	-0.100503000
	H	4.832047000	2.762311000	0.815675000
	C	4.790192000	4.547910000	-0.371789000
	H	5.422069000	5.089889000	0.327533000
	C	4.294162000	5.191585000	-1.508168000
	H	4.547965000	6.228071000	-1.711358000
	C	3.458277000	4.480230000	-2.374802000
	H	3.052685000	4.961119000	-3.261379000
	C	3.143750000	3.147377000	-2.122092000
	H	2.514630000	2.591782000	-2.813816000
	C	1.576824000	-3.358274000	-0.545404000
	H	1.773210000	-4.433564000	-0.440236000
	H	2.520136000	-2.866510000	-0.803123000
	C	0.565038000	-3.091002000	-1.631649000
	C	0.379554000	-3.977466000	-2.684133000
	H	0.960619000	-4.892256000	-2.735120000
	C	-0.567875000	-3.652759000	-3.659127000
	H	-0.714330000	-4.297824000	-4.521592000
	C	-1.332541000	-2.506703000	-3.518676000
	H	-2.065312000	-2.238002000	-4.267523000
	C	-1.126707000	-1.687895000	-2.387209000
	C	-2.970866000	0.014231000	-2.708463000
	C	-3.994996000	-0.719609000	-3.332421000
	H	-3.945170000	-1.801995000	-3.369161000
	C	-5.103517000	-0.057431000	-3.861392000
	H	-5.883620000	-0.640970000	-4.343687000
	C	-5.229172000	1.330545000	-3.760122000
	H	-6.096279000	1.836411000	-4.175145000
	C	-4.228599000	2.057171000	-3.106160000
	H	-4.315185000	3.135896000	-3.003030000
	C	-3.109393000	1.411138000	-2.587070000
	H	-2.327935000	1.979301000	-2.085515000
	C	-0.087824000	-3.452008000	1.232984000
	H	0.154911000	-4.412217000	1.704620000
	H	-0.748881000	-3.635956000	0.380221000
	C	-0.821403000	-2.580043000	2.212855000
	C	-1.451896000	-3.134588000	3.316165000
	H	-1.377855000	-4.200881000	3.505216000
	C	-2.180032000	-2.293174000	4.163532000
	H	-2.667451000	-2.684647000	5.051915000
	C	-2.255746000	-0.948042000	3.855524000
	H	-2.758563000	-0.252363000	4.515814000
	C	-1.616730000	-0.474977000	2.689205000
	C	-2.500420000	1.882618000	2.559514000
	C	-3.822844000	1.703340000	3.002394000
	H	-4.201421000	0.709561000	3.211317000
	C	-4.663913000	2.806969000	3.155229000

	H -5.679527000 2.647623000 3.508422000 C -4.227593000 4.096163000 2.840677000 H -4.890741000 4.948148000 2.960643000 C -2.924563000 4.272503000 2.363061000 H -2.566176000 5.265538000 2.103897000 C -2.068373000 3.183553000 2.226766000 H -1.049809000 3.330524000 1.874551000
Ni(I)-Br	78 SERGI-Br-NiI+0arreglat SCF Done: -5855.13969438 A.U. Ni -0.377892 -1.064621 0.446026 Br 0.220737 0.900916 -1.008620 N 0.224098 -2.851065 1.298956 N 2.688790 -1.285284 0.656599 N 3.526305 0.499501 -0.488855 H 2.552879 0.794522 -0.413774 N -1.417293 -2.239158 -0.772015 N -2.716695 -0.534018 -1.589771 H -1.903768 0.001084 -1.288228 N -0.761604 -0.531858 2.333493 N -0.823301 1.739476 2.045079 H -0.512434 1.458575 1.114499 C 1.558859 -2.975014 1.941765 H 1.700414 -4.001337 2.306891 H 1.557473 -2.306000 2.807116 C 2.688111 -2.573945 1.025340 C 3.660179 -3.483415 0.611959 H 3.623157 -4.518240 0.935798 C 4.672138 -3.015381 -0.234936 H 5.442720 -3.692263 -0.594194 C 4.684601 -1.687207 -0.635233 H 5.443900 -1.320548 -1.314041 C 3.660120 -0.838866 -0.159909 C 4.321801 1.278570 -1.344513 C 5.725740 1.276126 -1.278458 H 6.232992 0.649062 -0.552730 C 6.466639 2.103361 -2.123883 H 7.551872 2.086709 -2.062696 C 5.829015 2.960612 -3.024657 H 6.411889 3.606503 -3.675327 C 4.431467 2.983184 -3.071634 H 3.918975 3.647958 -3.762466 C 3.680684 2.147112 -2.247220 H 2.594717 2.151818 -2.292770 C 0.049829 -3.872928 0.247151 H -0.042693 -4.880919 0.674529 H 0.958150 -3.857879 -0.365646 C -1.132651 -3.557970 -0.635680 C -1.842758 -4.562093 -1.279423 H -1.582787 -5.602445 -1.114535 C -2.873169 -4.191600 -2.148192 H -3.427853 -4.944575 -2.700590 C -3.189896 -2.848498 -2.302241

	H	-3.972416	-2.540203	-2.982500
	C	-2.466110	-1.889760	-1.572713
	C	-3.658564	0.212703	-2.314055
	C	-4.987927	-0.195427	-2.513513
	H	-5.337964	-1.138044	-2.108033
	C	-5.873754	0.634372	-3.203941
	H	-6.898567	0.303871	-3.352817
	C	-5.464622	1.881540	-3.681939
	H	-6.162139	2.522224	-4.214048
	C	-4.149017	2.300122	-3.455860
	H	-3.815573	3.271958	-3.810809
	C	-3.250607	1.475982	-2.783199
	H	-2.226357	1.795681	-2.606398
	C	-0.826294	-2.934597	2.343216
	H	-0.671849	-3.793419	3.009477
	H	-1.787380	-3.072904	1.834882
	C	-0.869485	-1.638750	3.114165
	C	-1.034319	-1.589403	4.489168
	H	-1.107331	-2.507458	5.062010
	C	-1.083159	-0.331482	5.101645
	H	-1.172975	-0.246931	6.180798
	C	-1.005321	0.815152	4.325828
	H	-1.005978	1.792677	4.788387
	C	-0.877998	0.689512	2.927677
	C	-1.021633	3.116759	2.201808
	C	-1.827960	3.696670	3.196416
	H	-2.361876	3.076220	3.905689
	C	-1.980507	5.084310	3.247701
	H	-2.605415	5.515102	4.025976
	C	-1.360993	5.912543	2.309980
	H	-1.486262	6.990500	2.358569
	C	-0.590215	5.331962	1.296402
	H	-0.115203	5.957011	0.544450
	C	-0.418467	3.952399	1.239602
	H	0.158185	3.495943	0.439371

Table S6. Most intense bands (in nm) of the UV/Vis spectra for **Ni(I)-X** species, in THF.

Ni(I)-F

Excited State 1: 2.914-A 1.0399 eV 1192.32 nm f=0.0270 <S**2>=1.873
166B ->169B 0.25874
166B ->170B 0.62340
167B ->168B -0.21330
167B ->169B 0.61429
167B ->170B -0.34979
167B ->180B 0.13944
166B <-170B 0.15318
167B <-169B 0.15320
Excited State 2: 2.974-A 1.0574 eV 1172.57 nm f=0.0780 <S**2>=1.961
166B ->168B 0.11885
166B ->169B -0.55433
166B ->170B 0.22323
167B ->169B 0.38404
167B ->170B 0.69744
166B <-169B -0.15981
167B <-170B 0.13985
Excited State 4: 2.632-A 1.2869 eV 963.47 nm f=0.0283 <S**2>=1.482
165B ->180B -0.10723
166B ->168B -0.25704
166B ->170B 0.17421
166B ->180B 0.14929
167B ->168B 0.73999
167B ->169B 0.18749
167B ->180B -0.49727
167B ->183B -0.12255
Excited State 5: 2.668-A 1.3489 eV 919.12 nm f=0.0331 <S**2>=1.530
164B ->180B 0.14373
166B ->168B 0.68109
166B ->169B 0.31499
166B ->170B -0.15924
166B ->180B -0.48166
166B ->183B -0.12008
167B ->168B 0.31296
167B ->169B 0.14195
Excited State 6: 2.412-A 1.4301 eV 866.93 nm f=0.0102 <S**2>=1.205
165B ->180B 0.49148
165B ->183B 0.12258
166B ->168B -0.32770
166B ->180B -0.16552
167B ->168B 0.43988
167B ->180B 0.58764
167B ->183B 0.13080
Excited State 7: 2.278-A 1.4657 eV 845.90 nm f=0.0101 <S**2>=1.047
164B ->170B 0.10112
164B ->180B -0.77690
164B ->183B -0.18893
164B ->190B -0.11209
166B ->168B 0.33530

166B ->180B 0.32467
167B ->168B 0.17449
167B ->180B 0.13817
Excited State 11: 2.900-A 2.0990 eV 590.68 nm f=0.0123 <S**2>=1.853
166B ->172B 0.14070
167B ->171B 0.92829
167B ->172B 0.26384
167B ->173B -0.10745
Excited State 12: 2.908-A 2.1461 eV 577.73 nm f=0.0105 <S**2>=1.864
166B ->171B 0.82469
166B ->172B -0.16727
167B ->172B 0.44039
167B ->173B 0.23924
Excited State 13: 2.900-A 2.1902 eV 566.09 nm f=0.0168 <S**2>=1.852
166B ->171B -0.37685
166B ->173B -0.41464
167B ->171B -0.18906
167B ->172B 0.76799
167B ->173B -0.16953
Excited State 19: 2.800-A 2.6114 eV 474.79 nm f=0.0220 <S**2>=1.710
168A ->169A 0.96951
Excited State 24: 2.761-A 2.7053 eV 458.29 nm f=0.0310 <S**2>=1.656
166A ->169A -0.17882
166A ->170A -0.11331
167A ->169A 0.76568
168A ->171A -0.42539
164B ->170B 0.23866
165B ->168B 0.25586
165B ->169B -0.11373
Excited State 25: 2.729-A 2.7113 eV 457.28 nm f=0.0117 <S**2>=1.612
166A ->169A 0.47565
166A ->170A -0.14798
167A ->169A 0.50354
167A ->170A -0.21960
168A ->170A 0.31055
168A ->171A 0.46413
164B ->169B 0.15710
164B ->170B -0.15114
165B ->168B -0.16400
Excited State 30: 2.723-A 2.7689 eV 447.78 nm f=0.0543 <S**2>=1.604
166A ->170A -0.13015
167A ->171A -0.55728
168A ->170A 0.61016
168A ->171A -0.16967
164B ->168B 0.27803
164B ->169B -0.14275
164B ->170B 0.18122
165B ->168B -0.14625
165B ->169B -0.14389
165B ->170B -0.12421
Excited State 31: 2.519-A 2.7781 eV 446.29 nm f=0.0394 <S**2>=1.337
166A ->169A 0.63659

166A ->170A -0.15987
167A ->169A -0.21122
167A ->170A -0.35320
167A ->171A 0.12854
168A ->170A -0.11413
168A ->171A -0.48144
164B ->170B 0.20059
165B ->168B -0.12062
165B ->169B -0.17276
Excited State 34: 2.661-A 2.8509 eV 434.89 nm f=0.0295 <S**2>=1.521
166A ->169A 0.48135
167A ->170A 0.81901
167A ->171A -0.12228
168A ->171A -0.12917

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Excited State 5: 2.921-A 1.3382 eV 926.48 nm f=0.0323 <S**2>=1.883
168B ->184B 0.20333
170B ->173B 0.56569
170B ->174B 0.29272
171B ->173B -0.15748
171B ->174B 0.70129
170B <-173B 0.10283
Excited State 6: 2.941-A 1.3427 eV 923.42 nm f=0.0544 <S**2>=1.912
169B ->184B 0.23156
170B ->173B -0.25302
170B ->174B 0.63481
171B ->173B -0.62597
171B ->174B -0.22158
Excited State 8: 2.901-A 1.5201 eV 815.65 nm f=0.0266 <S**2>=1.853
170B ->172B 0.21568
171B ->172B 0.94708
171B ->173B 0.16272
171B ->184B 0.11519
Excited State 9: 2.917-A 1.5471 eV 801.42 nm f=0.0400 <S**2>=1.877
170B ->172B 0.94682
170B ->173B 0.14216
170B ->184B 0.11831
171B ->172B -0.19351
Excited State 11: 2.884-A 2.2855 eV 542.48 nm f=0.0133 <S**2>=1.830
170B ->177B 0.11848
171B ->175B 0.96023
171B ->176B -0.14289
171B ->181B 0.12901
Excited State 12: 2.890-A 2.3032 eV 538.32 nm f=0.0119 <S**2>=1.838
170B ->175B 0.94137
170B ->176B 0.21025
170B ->181B 0.11162
171B ->176B -0.11312
171B ->177B 0.15212
Excited State 13: 2.895-A 2.3807 eV 520.79 nm f=0.0139 <S**2>=1.846
170B ->176B -0.57868

170B ->177B -0.10575
171B ->176B -0.13500
171B ->177B 0.77148
171B ->183B -0.12220
Excited State 17: 2.785-A 2.6275 eV 471.88 nm f=0.0299 <S**2>=1.689
172A ->173A 0.98616
Excited State 18: 2.794-A 2.6675 eV 464.79 nm f=0.0186 <S**2>=1.702
171A ->173A 0.96979
171A ->174A -0.13344
172A ->175A 0.13736
Excited State 19: 2.745-A 2.7117 eV 457.23 nm f=0.0294 <S**2>=1.633
171A ->173A -0.13516
172A ->174A 0.18757
172A ->175A 0.93834
169B ->173B 0.13781
Excited State 20: 2.695-A 2.7311 eV 453.98 nm f=0.0553 <S**2>=1.566
171A ->175A 0.64236
172A ->174A 0.69504
169B ->174B -0.17901
Excited State 21: 2.882-A 2.7557 eV 449.92 nm f=0.0106 <S**2>=1.826
171A ->174A 0.46161
171A ->175A -0.12823
172A ->174A 0.14506
168B ->173B -0.47732
168B ->174B 0.12980
169B ->174B 0.67316
Excited State 22: 2.808-A 2.7629 eV 448.75 nm f=0.0200 <S**2>=1.721
171A ->174A 0.74897
171A ->175A -0.11940
168B ->173B 0.28422
168B ->174B 0.31160
169B ->173B 0.18765
169B ->174B -0.39161
Excited State 25: 2.962-A 2.8919 eV 428.73 nm f=0.0105 <S**2>=1.944
171A ->174A -0.10815
171A ->175A -0.10040
172A ->174A -0.11185
168B ->172B 0.36206
168B ->173B -0.42205
168B ->174B 0.43078
169B ->172B 0.44977
169B ->173B -0.31464
169B ->174B -0.36140

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Excited State 5: 2.984-A 1.3803 eV 898.22 nm f=0.0276 <S**2>=1.976
171A ->174A 0.12563
168B ->184B -0.10263
170B ->172B -0.27706
170B ->173B -0.25099
170B ->184B 0.17071
171B ->172B -0.25678

171B ->173B 0.77119
171B ->174B -0.28866
Excited State 6: 2.989-A 1.4141 eV 876.79 nm f=0.0654 <S**2>=1.984
172A ->173A -0.10552
170B ->172B -0.18912
170B ->173B 0.49566
170B ->174B -0.23240
171B ->172B 0.61509
171B ->173B 0.31347
171B ->174B 0.19381
171B ->181B -0.13457
171B ->184B -0.27313
171B ->185B -0.11712
Excited State 12: 2.883-A 2.3615 eV 525.02 nm f=0.0107 <S**2>=1.828
170B ->174B 0.11925
170B ->176B -0.10025
171B ->174B 0.20050
171B ->175B 0.88768
171B ->176B -0.23597
171B ->177B -0.23586
171B ->182B 0.11104
Excited State 19: 2.766-A 2.6578 eV 466.49 nm f=0.0521 <S**2>=1.662
171A ->174A 0.37349
172A ->173A -0.29863
172A ->174A -0.38005
170B ->175B -0.35836
170B ->176B 0.64576
171B ->177B -0.11110
Excited State 20: 2.759-A 2.6711 eV 464.17 nm f=0.0824 <S**2>=1.653
171A ->173A 0.11298
171A ->174A -0.36255
172A ->173A 0.26554
172A ->174A 0.43406
170B ->175B 0.14214
170B ->176B 0.69578
171B ->177B -0.14800
Excited State 26: 2.743-A 3.0443 eV 407.26 nm f=0.0162 <S**2>=1.631
170A ->174A 0.10966
171A ->173A -0.17579
171A ->174A 0.36548
171A ->175A 0.12496
172A ->173A 0.43516
172A ->174A 0.11602
172A ->175A -0.29897
168B ->172B -0.35236
168B ->173B -0.27721
169B ->172B 0.12617
169B ->174B -0.34692
170B ->172B -0.10561
170B ->173B -0.12408
171B ->173B -0.10407
171B ->174B 0.10646

171B ->179B 0.11586

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Excited State 6: 3.031-A 1.4524 eV 853.63 nm f=0.0773 <S**2>=2.047
181A ->183A -0.13150
179B ->181B 0.35284
179B ->182B 0.30355
179B ->183B 0.18881
180B ->181B -0.46853
180B ->182B 0.58789
180B ->190B 0.15157
180B ->193B 0.27637
180B ->194B 0.11632

Excited State 18: 2.615-A 2.6113 eV 474.80 nm f=0.0812 <S**2>=1.459
180A ->182A 0.70051
180A ->183A 0.36339
180A ->184A 0.18118
181A ->182A 0.34752
181A ->183A -0.11013
179B ->184B 0.31116
179B ->185B -0.16956
180B ->185B 0.10872

Excited State 19: 2.861-A 2.6351 eV 470.52 nm f=0.0114 <S**2>=1.796
180A ->182A 0.12352
181A ->183A -0.12646
179B ->185B 0.86976
179B ->186B -0.17576
180B ->184B 0.19696
180B ->186B 0.32752

Excited State 22: 2.826-A 2.9140 eV 425.47 nm f=0.0171 <S**2>=1.746
180A ->183A -0.31093
181A ->182A 0.18378
181A ->183A 0.15858
177B ->181B 0.78142
177B ->183B 0.26109
177B ->193B -0.12825
178B ->183B -0.16515
179B ->182B 0.11330