Supporting information for: Understanding the molecule-surface chemical coupling in SERS

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S-1 Pyridine bond analysis

In Figure S-1 we plot the energy levels of xPy-LUMO and xPy-HOMO (where xPy is a substituted pyridine) as a function of q(xPy→Ag). We see clearly from the figure that both energy levels increase as the charge increases.

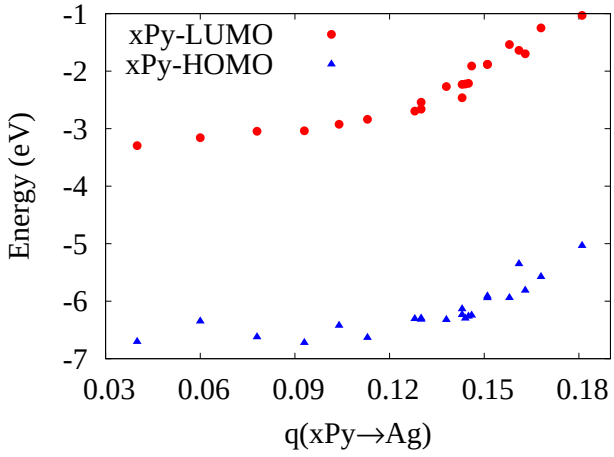


Figure S-1: Energy of xPy-LUMO (red dots) and xPy-HOMO (blue triangles) as q(xPy→Ag) changes.

To verify that the change in R_{Ag-N} is due to the concerted effects of the σ-bonding and π-back-bonding, we calculated the orbital interaction energy when all virtual orbitals except for xPy-LUMO and Ag-LUMO are removed. This was achieved by using the keyword REMOVE-FRAGORBITALS in conjunction with a fragment analysis in ADF.[1] Symmetry groups were used to remove the desired virtual orbitals. We denote the orbital interaction energy from only Ag-LUMO as ΔE^{σ}, from only xPy-LUMO as ΔE^{π}, and from both xPy-LUMO and Ag-LUMO as $\Delta E^{\sigma\pi}$. ΔE^{σ} accounts for σ-bonding only, ΔE^{π} accounts for π-back-bonding only, and $\Delta E^{\sigma\pi}$ accounts for both.

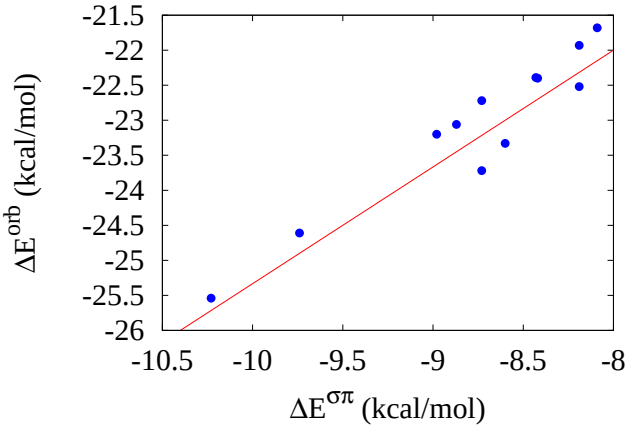
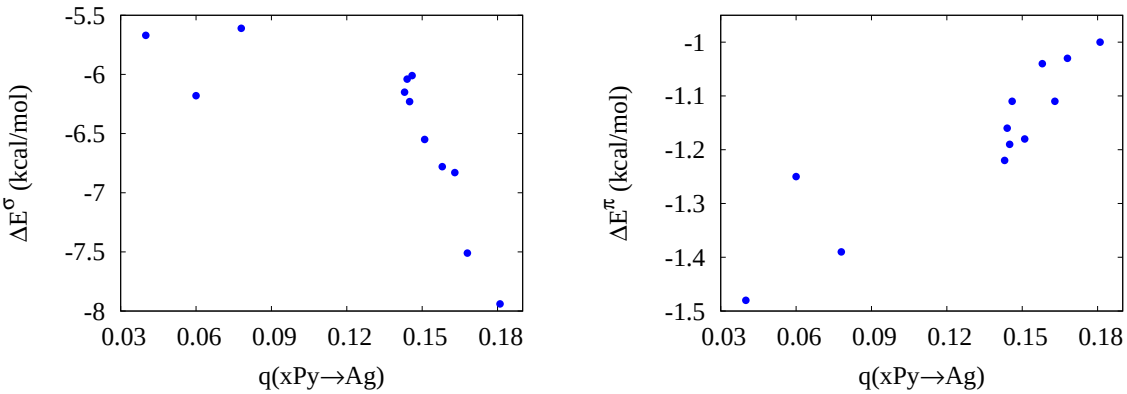


Figure S-2: The total ΔE^{orb} versus the orbital interaction energy obtained by only including the xPy-LUMO and Ag-LUMO orbitals. Line is a guide for the eye. This plot uses a reduced data set which is representative of the whole.

In Figure S-2 we plot the total orbital interaction energy, ΔE^{orb}, versus $\Delta E^{\sigma\pi}$. We see that the the orbital interaction energy due solely to xPy-LUMO and Ag-LUMO accounts for as much as 30% of the total interaction energy and that both ΔE^{orb} and $\Delta E^{\sigma\pi}$ follow the same trend. This shows that Ag-LUMO and xPy-LUMO are the major contributors to ΔE^{orb}, and therefore can be used as a model to describe the overall bonding mechanism.

In Figure Figure S-3(a) we plot ΔE^{σ}, and we see that the bonding energy increases as the functional group becomes more donating, i.e. increasing q(xPy→Ag). Conversely, in Figure Figure S-3(b) we plot ΔE^{π}, and we see that bonding energy increases as the functional group becomes



(a) Ag-LUMO (b) xPy-LUMO

Figure S-3: (a) Bond energy when only Ag-LUMO virtual orbital is included, and therefore represents only σ-bonding. (b) Bond energy when only xPy-LUMO virtual orbital is included, and therefore represents only π-back-bonding. These plots use a reduced data set which is representative of the whole.

more accepting. Additionally, from Figure Figure S-3(a) we see that the change in the σ-bonding strength is ~ 2.5 kcal mol^{-1}, but in fig. Figure S-3(b) the change in π-back-bonding strength is only ~ 0.5 kcal mol^{-1}. This explains why the change in R_{Ag-N} is slower for the accepting groups than for the donating groups. Furthermore, we also see that the magnitude of energy due to the σ-bonding is roughly 5-8 times that of the energy due to π-back-bonding, illustrated the larger contribution from σ-bonding.

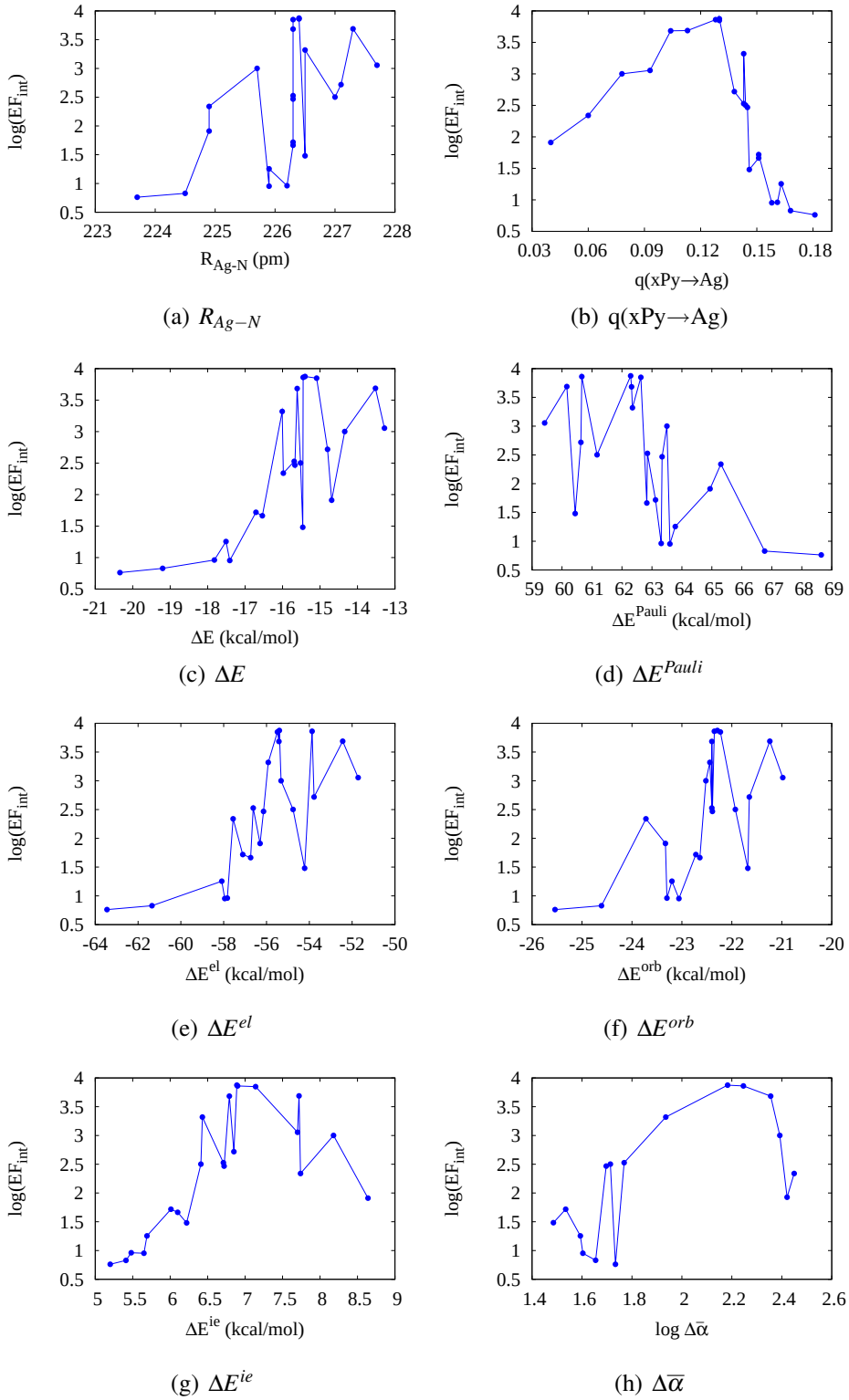
Referring to Figure 4(b) in the main text, two systems showed a different behavior in R_{Ag-N} (red triangles). This is because the bonding orbital for these two molecules is different from the other molecules. These two molecules are the pyridines with the meta-C$\equiv$N and -SO_3H functional groups. These functional groups interact more strongly with the LUMO+1 of the pyridine molecule, lowering it enough to become the LUMO in these molecules. Since this orbital is different from xPy-LUMO, they interact differently with the Ag_{20} cluster, resulting in a slightly different behavior for R_{Ag-N}.

S-2 Raman enhancements analysis for substituted pyridines

To understand the trend in the Raman enhancement, we plotted the log of the integrated enhancement EF_{int} versus the bond length R_{Ag-N}, charge transfer q(xPy→Ag), the interaction energy, ΔE, ΔE^{el}, ΔE^{Pauli}, ΔE^{orb}, ΔE^{ie} and the induced static polarizability $\Delta\overline{\alpha}$ (see Figure S-4). The different energy terms are obtained using the extended transition state method developed by Ziegler and Rauk.[2–5] ΔE is the total interaction energy. ΔE^{el} is the classical electrostatic interaction between the unperturbed charge distributions of the two fragments. ΔE^{Pauli} is the Pauli repulsion which represents the destabilization due to interaction between occupied orbitals. ΔE^{orb} is the interaction between occupied and virtual orbitals and accounts for electron pair bond formation, charge transfer and polarization. ΔE^{ie} is the sum of $\Delta E^{el} + \Delta E^{Pauli}$ and represents the steric interactions. The induced static polarizability is calculated as $\Delta\overline{\alpha} = \overline{\alpha}_{xPy-Ag} - \overline{\alpha}_{Ag} - \overline{\alpha}_{xPy}$, which is the difference between the isotropic polarizability of the cluster-molecule complex ($\overline{\alpha}_{xPy-Ag}$) and the isotropic polarizability of the free molecule ($\overline{\alpha}_{xPy}$) and cluster ($\overline{\alpha}_{Ag}$). Previously, we had related EF_{int} to $\Delta\overline{\alpha}$,[6–8] but for the extended data set used in this work we find that EF_{int} does not correlate with this quantity. From Figure S-4 it is clear that there is little correlation between the enhancements and these properties. Therefore, they not suitable quantities to explain the observed trends for the enhancements due to the variation in functional groups.

S-3 Functional form of ΔE^{xc}

In Figure S-3 we plot the difference in the calculated lowest excitation energy (ω_e) and the average HOMO–LUMO gap ($\overline{\omega}_{xPy-Ag}$) as a function of $\overline{\omega}_{xPy-Ag}$ to obtain a functional form for the exchange-correlation contribution, ΔE^{xc}. Note that xPy denotes substituted pyridine, and so this was fit using only the substituted pyridine data set. We fitted this difference using a function given by $e^{-b\overline{\omega}^2_{xPy-Ag}}$, where b is a fitting parameter. This functional form was found by trial and error. This function is plotted in Figure S-3 with $b = 44.72$ eV^{-2}.



(a) R_{Ag-N} (b) q(xPy→Ag)

(c) ΔE (d) ΔE^{Pauli}

(e) ΔE^{el} (f) ΔE^{orb}

(g) ΔE^{ie} (h) $\Delta\overline{\alpha}$

Figure S-4: Plots of integrated enhancement (EF_{int}) versus various quantities.

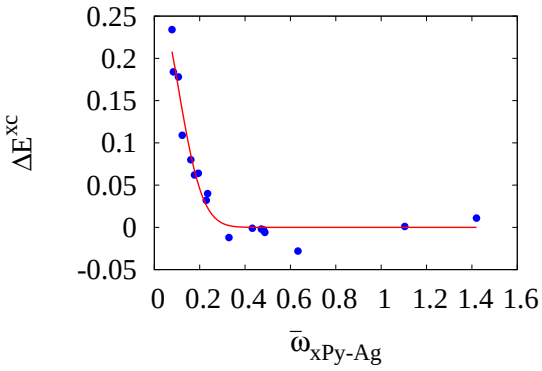
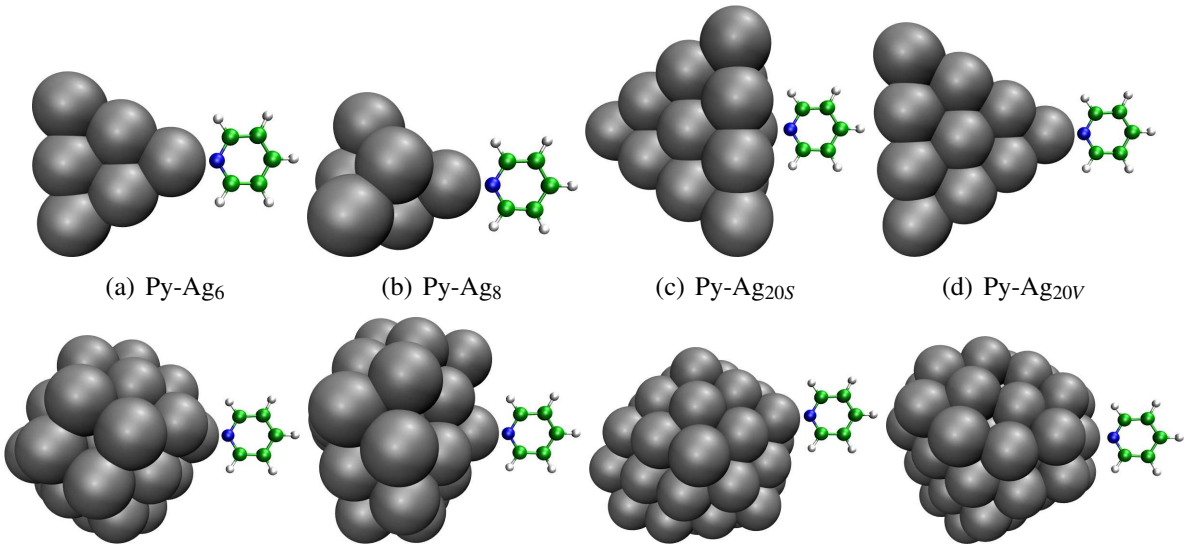


Figure S-5: (a) ΔE^{xc} as a function of $\overline{\omega}_{xPy-Ag}$. The solid line is the function $e^{-b\overline{\omega}^2_{xPy-Ag}}$ with $b = 44.72$ eV^{-2}.

S-4 Representations of the addtional data sets

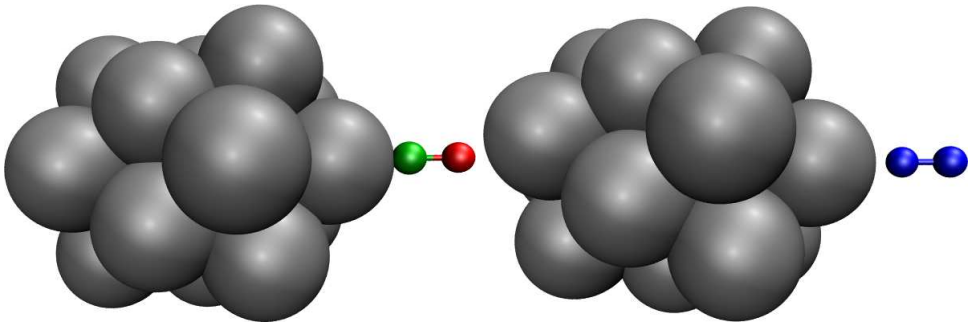
Below are representations of the three additional data sets used to verify EF^{model}_{int}. The Ag_n data set is shown in Figure S-6. The small molecules data set is shown it Figure S-7. The benzenethiol (BT) data set is shown in Figure S-8.



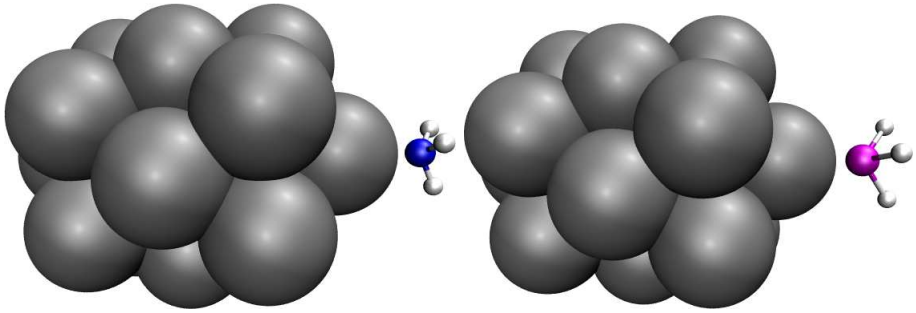
(a) Py-Ag_6 (b) Py-Ag_8 (c) Py-Ag_{20S} (d) Py-Ag_{20V}

(e) Py-Ag_{34} (f) Py-Ag_{40} (g) Py-Ag_{58} (h) Py-Ag_{68}

Figure S-6: Representations of the Ag_n data set. All images prepared with VMD.[9]



(a) C≡O-Ag_{20} (b) N_2-Ag_{20}



(c) NH_3-Ag_{20} (d) PH_3-Ag_{20}

Figure S-7: Representations of the small molecules data set. All images prepared with VMD.[9]

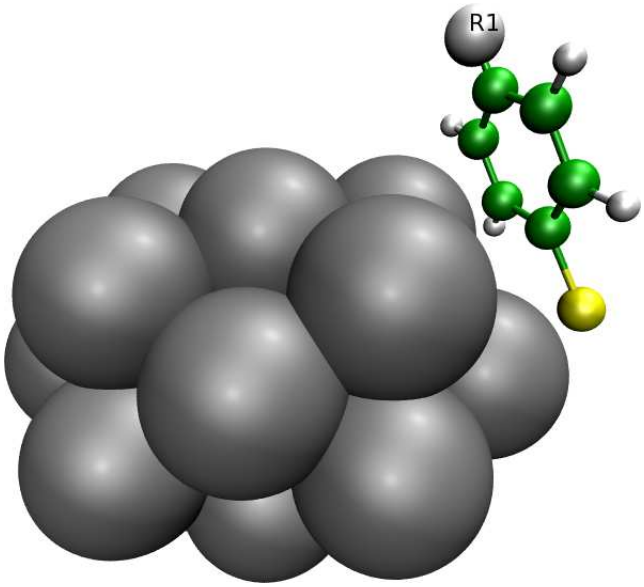


Figure S-8: Prepresentation of the benzenethiol (BT) data set. Here, R1 = OH, H, C≡N. Image was prepared with VMD.[9]

S-5 Coordinates of all systems studied

Below are the xyz coordinates in Å of all systems studied. Pyridine is denoted as "Py," and substitutions on Py are labeled with a p- or m- for para- or meta-, respectively. Like wise, thioolphenol is denoted as "BT," and the subsitutions are handled similarly to Py.

Py		-2.57325154 Hartrees	
Atom	x	y	z
C	0.000000	0.000000	0.349583
C	0.000000	1.199889	-0.365675
C	0.000000	1.144619	-1.763325
N	0.000000	0.000000	-2.468279
C	0.000000	-1.144619	-1.763325
C	0.000000	-1.199889	-0.365675
H	0.000000	2.163749	0.145937
H	0.000000	2.067685	-2.349392
H	0.000000	-2.067685	-2.349392
H	0.000000	-2.163749	0.145937
H	0.000000	0.000000	1.440883

p-C≡N-Py		-3.03152310 Hartrees	
Atom	x	y	z
C	-0.400473	0.274340	0.000000
C	0.336969	1.469846	0.000000
C	1.729481	1.384596	0.000000
N	2.412356	0.227396	0.000000
C	1.691227	-0.906338	0.000000
C	0.296650	-0.945108	0.000000
H	-0.167312	2.435337	0.000000
H	2.329416	2.297340	0.000000
H	2.260238	-1.838639	0.000000
H	-0.239419	-1.893342	0.000000
C	-1.833124	0.298368	0.000000
N	-2.998576	0.318025	0.000000

p-CO_2H -Py		-3.39717378 Hartrees	
Atom	x	y	z
C	-0.773822	-0.952945	-0.237478
C	0.546522	-1.393755	-0.396914
C	1.363379	-1.463304	0.734335
N	0.960435	-1.132490	1.972471
C	-0.309670	-0.711574	2.107623
C	-1.209433	-0.604117	1.046903
H	0.928783	-1.675538	-1.376668
H	2.397557	-1.803115	0.641422
H	-0.621825	-0.446577	3.120374
H	-2.231483	-0.258507	1.196583
C	-1.737894	-0.837489	-1.372318
O	-2.891351	-0.455905	-1.267665
O	-1.193269	-1.209451	-2.573120
H	-1.917671	-1.089097	-3.223709

p-SO_3H-Py		-3.40492381 Hartrees	
Atom	x	y	z
C	0.122688	-0.298333	-0.085313
C	1.001546	0.587934	-0.707242
C	0.815908	1.953851	-0.466397
N	-0.147846	2.451522	0.323898
C	-0.982160	1.571250	0.903171
C	-0.899593	0.186779	0.732077
H	1.789155	0.227098	-1.367380
H	1.478294	2.682926	-0.938757
H	-1.764491	1.994140	1.537429
H	-1.610889	-0.486377	1.208827
S	0.289900	-2.065683	-0.360970
O	-1.031723	-2.653403	-0.367081
O	1.261672	-2.274015	-1.423278
O	0.966731	-2.580135	1.042663
H	1.938853	-2.564625	0.907671

m-C≡N-Py		-3.03322068 Hartrees	
Atom	x	y	z
N	0.025105	0.051926	0.216593
C	-0.041649	-1.094470	0.900897
C	0.061152	1.192914	0.926370
C	-0.075212	-1.155972	2.309732
C	0.032811	1.241612	2.324085
C	-0.036695	0.047225	3.035120
H	-0.070624	-2.017456	0.318294
H	0.115564	2.115841	0.344729
H	0.064753	2.199549	2.843202
C	-0.146847	-2.419002	2.976242
H	-0.061189	0.031821	4.124214
N	-0.205284	-3.451490	3.515504

p-CCl_3-Py		-2.96963156 Hartrees	
Atom	x	y	z
C	0.041045	-0.372383	0.000000
C	0.013851	0.350524	-1.198035
C	-0.036415	1.745809	-1.140050
N	-0.063619	2.453464	0.000000
C	-0.036415	1.745809	1.140050
C	0.013851	0.350524	1.198035
H	0.038874	-0.156450	-2.161102
H	-0.051931	2.324026	-2.067113
H	-0.051931	2.324026	2.067113
H	0.038874	-0.156450	2.161102
C	0.021342	-1.893016	0.000000
Cl	0.842599	-2.581063	-1.457557
Cl	0.842599	-2.581063	1.457557
Cl	-1.708638	-2.449649	0.000000

m-SO_3H-Py		-3.40571132 Hartrees	
Atom	x	y	z
S	0.376302	0.190337	0.280054
O	-0.622382	-0.383473	-0.597654
O	1.807689	0.044146	0.062353
O	0.038128	-0.438611	1.759961
H	0.884264	-0.444958	2.257478
N	0.814630	4.149811	0.916597
C	-0.455172	4.574674	0.815424
C	1.037041	2.838284	0.751285
C	-1.541408	3.737645	0.539478
C	0.007733	1.926373	0.489014
C	-1.309386	2.375359	0.369374
H	-0.610940	5.647253	0.957509
H	2.071758	2.495637	0.812958
H	-2.548338	4.148330	0.455506
H	-2.112941	1.676305	0.138979

p-CCl_2H-Py		-3.04505376 Hartrees	
Atom	x	y	z
N	5.788408	-0.624955	-0.947663
C	6.296967	-1.864757	-0.813949
C	6.585674	0.295458	-1.508871
C	7.580388	-2.231058	-1.218532
C	7.887681	0.034157	-1.949591
C	8.401236	-1.257931	-1.801132
H	5.636974	-2.605585	-0.356484
H	6.165599	1.298695	-1.614886
H	8.484388	0.829888	-2.399631
H	7.934861	-3.253503	-1.083161
C	9.798759	-1.552547	-2.266866
Cl	10.865163	-2.074769	-0.895254
Cl	9.815452	-2.799283	-3.584769
H	10.276857	-0.669139	-2.691503

p-CFClH-Py		-3.11745991 Hartrees	
Atom	x	y	z
N	5.750609	-0.328917	-0.736879
C	6.073361	-1.595507	-1.050184
C	6.724537	0.589217	-0.852700
C	7.338294	-1.996430	-1.487497
C	8.022949	0.297123	-1.276139
C	8.338363	-1.026155	-1.604644
H	5.274968	-2.333894	-0.944130
H	6.454210	1.614217	-0.588045
H	8.769266	1.090859	-1.348434
H	7.541498	-3.040962	-1.721899
C	9.726155	-1.376425	-2.059799
F	10.058693	-2.676133	-1.711823
Cl	9.882879	-1.224898	-3.870803
H	10.490751	-0.710347	-1.647252

p-CF_2H-Py		-3.18910590 Hartrees	
Atom	x	y	z
N	5.752350	-0.643655	-1.028565
C	6.392280	-1.761854	-0.640664
C	6.403500	0.165133	-1.878455
C	7.672277	-2.117145	-1.068639
C	7.685949	-0.096386	-2.370370
C	8.335653	-1.260509	-1.953647
H	5.848058	-2.410082	0.050948
H	5.873458	1.070106	-2.186285
H	8.162723	0.598417	-3.065297
H	8.138989	-3.041051	-0.725504
C	9.726386	-1.563111	-2.440660
F	10.649281	-1.398514	-1.414247
F	9.833262	-2.882537	-2.852084
H	10.046569	-0.925082	-3.275613

m-Cl-Py		-2.51319231 Hartrees	
Atom	x	y	z
N	-0.000000	0.041006	0.217702
C	-0.000000	-1.104847	0.913403
C	-0.000000	1.191867	0.910785
C	0.000000	-1.134268	2.312107
C	0.000000	1.251672	2.307032
C	0.000000	0.059061	3.033111
H	-0.000000	-2.036915	0.344414
H	-0.000000	2.109130	0.317038
H	0.000000	2.214110	2.820754
Cl	0.000000	-2.679102	3.152034
H	0.000000	0.050350	4.122430

p-$CClH_2$-Py		-3.10853168 Hartrees	
Atom	x	y	z
N	6.008716	-0.565247	-0.848074
C	6.972375	-0.839376	0.047935
C	6.316134	-0.762606	-2.141581
C	8.241805	-1.310637	-0.292767
C	7.554635	-1.230248	-2.585476
C	8.550940	-1.515621	-1.643351
H	6.712899	-0.676490	1.097337
H	5.525972	-0.537637	-2.862787
H	7.738958	-1.369999	-3.652773
H	8.979466	-1.515120	0.486124
C	9.892766	-2.035306	-2.063744
H	10.353531	-2.654247	-1.288435
H	9.839772	-2.594145	-3.002567
Cl	11.084515	-0.672213	-2.373141

p-I-Py		-2.464329327 Hartrees	
Atom	x	y	z
C	0.000000	0.000000	0.051873
C	0.000000	1.203938	-0.648582
C	0.000000	1.140195	-2.046779
N	0.000000	0.000000	-2.753263
C	0.000000	-1.140195	-2.046779
C	0.000000	-1.203938	-0.648582
H	0.000000	2.166519	-0.138735
H	0.000000	2.068285	-2.624861
H	0.000000	-2.068285	-2.624861
H	0.000000	-2.166519	-0.138735
I	0.000000	0.000000	2.184225

p-Br-Py		-2.48897244 Hartrees	
Atom	x	y	z
C	0.000000	0.000000	0.178517
C	0.000000	1.206051	-0.517096
C	0.000000	1.141409	-1.914540
N	0.000000	0.000000	-2.620298
C	0.000000	-1.141409	-1.914540
C	0.000000	-1.206051	-0.517096
H	0.000000	2.164223	0.000884
H	0.000000	2.068773	-2.493528
H	0.000000	-2.068773	-2.493528
H	0.000000	-2.164223	0.000884
Br	0.000000	0.000000	2.103816

p-Cl-Py		2.51308502 Hartrees	
Atom	x	y	z
C	0.000000	0.000000	0.265787
C	0.000000	1.206003	-0.434329
C	0.000000	1.142131	-1.831335
N	0.000000	0.000000	-2.538130
C	0.000000	-1.142131	-1.831335
C	0.000000	-1.206003	-0.434329
H	0.000000	2.162097	0.086899
H	0.000000	2.068612	-2.410682
H	0.000000	-2.068612	-2.410682
H	0.000000	-2.162097	0.086899
Cl	0.000000	0.000000	2.021180

p-F-Py		-2.56573320 Hartrees	
Atom	x	y	z
N	-0.009297	0.144086	-0.041631
C	1.217585	0.819390	-0.039993
C	-1.207569	0.868947	-0.041952
C	1.246196	2.219553	-0.038674
C	-1.178958	2.269110	-0.040633
C	0.047924	2.944413	-0.038995
H	2.133109	0.265570	-0.039748
H	-2.144953	0.352990	-0.043202
H	-2.094482	2.822930	-0.040878
H	2.183579	2.735510	-0.037421
F	0.073870	4.214147	-0.037800

m-OH-Py		-2.81281333 Hartrees	
Atom	x	y	z
C	-0.825674	-0.925158	-0.201804
C	0.497389	-1.362894	-0.375505
N	1.374361	-1.460249	0.631062
C	0.955676	-1.119539	1.862400
C	-0.340631	-0.673431	2.132806
C	-1.253883	-0.572550	1.081683
H	0.841134	-1.640633	-1.374886
H	-0.633353	-0.408449	3.149480
H	-2.277425	-0.227706	1.252163
O	-1.633332	-0.867583	-1.315486
H	-2.513120	-0.549510	-1.042920
H	1.690136	-1.207947	2.665402

m-NH_2-Py		-3.01126588 Hartrees	
Atom	x	y	z
N	-0.112846	0.796508	0.142944
H	-0.928167	0.272533	-0.168147
H	-0.146728	1.752222	-0.204979
N	2.298812	-1.954204	-0.361751
C	3.448738	-1.262842	-0.434266
C	1.168536	-1.261362	-0.192833
C	3.500821	0.130164	-0.338286
C	1.106218	0.143221	-0.087525
C	2.318948	0.845235	-0.161043
H	4.360197	-1.847950	-0.576875
H	0.242650	-1.845598	-0.135672
H	4.458012	0.650736	-0.403620
H	2.329922	1.934903	-0.078215

p-NH_2-Py		-3.01480407 Hartrees	
Atom	x	y	z
C	-0.374747	-0.078354	-0.017071
C	0.392960	0.038160	1.155495
C	1.755278	0.305559	1.048724
N	2.416376	0.464339	-0.111815
C	1.670447	0.345188	-1.224605
C	0.303625	0.079442	-1.238803
H	-0.069337	-0.079363	2.138621
H	2.354829	0.402100	1.958464
H	2.200554	0.474138	-2.172642
H	-0.230541	-0.005066	-2.188307
N	-1.731185	-0.391791	0.028213
H	-2.266665	-0.114870	-0.790286
H	-2.203743	-0.144290	0.893538

Py-Ag_{20}		-3.99460316 Hartrees	
Atom	x	y	z
Ag	1.556647	0.674191	0.769773
Ag	3.997158	-0.019616	0.017059
Ag	1.416670	-0.975771	-1.435556
Ag	2.056445	-2.033356	1.224128
Ag	3.198200	0.303600	2.902206
Ag	3.369800	2.778150	1.044355
Ag	2.231266	2.015881	-1.544151
Ag	-0.612295	-1.353545	0.539057
Ag	0.537985	-0.756113	3.213632
Ag	1.451013	2.585854	3.089667
Ag	0.711466	3.500162	0.364713
Ag	-0.489493	1.160797	-1.151323
Ag	-0.839397	1.359485	1.651917
Ag	-3.229887	2.046272	2.597363
Ag	1.714779	0.797005	5.255261
Ag	-2.244993	-0.765446	2.795193
Ag	-2.920103	0.301943	0.156003
Ag	-0.891433	1.474405	4.375003
Ag	-0.952679	3.976128	2.625412
Ag	-2.121497	3.219989	0.048590
N	6.067288	-0.595017	-0.692248
C	6.543468	-1.844358	-0.507282
C	6.867377	0.304612	-1.302617
C	7.816006	-2.235535	-0.918328
C	8.152323	-0.005265	-1.743525
C	8.638097	-1.299597	-1.548825
H	5.871734	-2.545783	-0.011587
H	6.451604	1.303780	-1.436515
H	8.756244	0.760327	-2.230700
H	8.150234	-3.258299	-0.743743
H	9.639853	-1.574196	-1.882718

p-OH-Py		-2.81674435 Hartrees	
Atom	x	y	z
C	-0.410156	0.128687	-0.125373
C	0.268883	1.156567	-0.789384
C	1.658955	1.196915	-0.687702
N	2.402251	0.315089	0.006185
C	1.726144	-0.661409	0.634098
C	0.337316	-0.804097	0.604978
H	-0.282563	1.898699	-1.366407
H	2.210410	1.990488	-1.197802
H	2.327710	-1.378594	1.198156
H	-0.148695	-1.624030	1.139870
O	-1.777801	0.084762	-0.222422
H	-2.097420	-0.680846	0.289604

p-CH_3-Py		-3.17522995 Hartrees	
Atom	x	y	z
C	0.010985	-0.433406	0.000000
C	0.008031	0.304607	-1.192812
C	-0.002403	1.700628	-1.140479
N	-0.008479	2.412010	0.000000
C	-0.002403	1.700628	1.140479
C	0.008031	0.304607	1.192812
H	0.017530	-0.202487	-2.160669
H	-0.003066	2.280913	-2.067081
H	-0.003066	2.280913	2.067081
H	0.017530	-0.202487	2.160669
C	-0.008433	-1.942171	0.000000
H	0.486297	-2.350012	-0.890838
H	0.486297	-2.350012	0.890838
H	-1.044860	-2.314023	0.000000

p-$N(CH_3)_2$-Py		-4.18808394 Hartrees	
Atom	x	y	z
C	-0.192160	-0.117344	-0.272352
C	0.495937	0.921502	0.403039
C	1.885926	0.973983	0.344648
N	2.667544	0.106209	-0.324269
C	2.005776	-0.867097	-0.977176
C	0.622669	-1.024494	-0.994808
H	-0.037602	1.685439	0.966181
H	2.407005	1.777885	0.871873
H	2.625328	-1.575111	-1.534545
H	0.192372	-1.843753	-1.568490
N	-1.568962	-0.245019	-0.218928
C	-2.237970	-1.180761	-1.112690
C	-2.366949	0.831373	0.352319
H	-2.136216	-0.901931	-2.177547
H	-3.304260	-1.209445	-0.862917
H	-1.839669	-2.196168	-0.982426
H	-2.047986	1.048106	1.380973
H	-3.414868	0.514309	0.390851
H	-2.306579	1.766504	-0.234071

p-C≡N-Py-Ag_{20}		-4.44967341 Hartrees	
Atom	x	y	z
Ag	1.285179	0.618044	0.966895
Ag	3.716718	-0.060056	0.175208
Ag	1.149853	-1.013464	-1.256294
Ag	1.815642	-2.084335	1.399463
Ag	2.965629	0.247303	3.071448
Ag	3.099421	2.718451	1.231916
Ag	1.928873	1.961543	-1.354338
Ag	-0.864165	-1.418872	0.737040
Ag	0.300205	-0.850741	3.420724
Ag	1.207069	2.530836	3.299906
Ag	0.422014	3.429282	0.580815
Ag	-0.783842	1.089127	-0.940194
Ag	-1.106138	1.276308	1.869095
Ag	-3.485357	1.990054	2.812601
Ag	1.505117	0.719243	5.437300
Ag	-2.486224	-0.856285	3.019185
Ag	-3.193411	0.205564	0.381119
Ag	-1.126922	1.376274	4.589515
Ag	-1.218924	3.887729	2.856695
Ag	-2.415291	3.137879	0.278032
N	5.778576	-0.544621	-0.582491
C	6.310667	-1.783642	-0.466379
C	6.544303	0.419313	-1.146553
C	7.590304	-2.104633	-0.895718
C	7.834410	0.194136	-1.603797
C	8.382075	-1.097648	-1.481652
H	5.673772	-2.539581	-0.007715
H	6.090704	1.406901	-1.230252
H	8.410093	1.003658	-2.050020
H	7.971777	-3.117658	-0.779739
C	9.704756	-1.377874	-1.941521
N	10.785897	-1.604628	-2.315938

p-CO_2H-Py-Ag_{20}	-4.81691297 Hartrees		
Atom	x	y	z
Ag	1.201569	0.791991	0.920121
Ag	3.625274	0.068907	0.140619
Ag	1.321605	0.758267	-1.834581
Ag	1.201540	-1.726757	-0.280501
Ag	2.262707	-1.099048	2.558334
Ag	3.187299	1.858543	2.565486
Ag	2.553243	2.986114	-0.062962
Ag	-1.126538	-0.152681	-0.677154
Ag	-0.524003	-1.461814	1.921782
Ag	0.856101	1.028029	3.899621
Ag	0.873997	3.459976	2.198819
Ag	-0.280225	2.754641	-0.518838
Ag	-1.212693	1.427696	1.800978
Ag	-3.629579	2.021668	2.737570
Ag	0.380004	-1.666045	4.587260
Ag	-3.118705	-0.554613	1.316704
Ag	-3.036768	1.935799	-0.219260
Ag	-1.846122	0.000370	4.039459
Ag	-1.165134	2.974655	4.126697
Ag	-1.830484	4.108996	1.508151
N	5.686359	-0.488979	-0.565790
C	5.947314	-1.696980	-1.118467
C	6.714597	0.379532	-0.431986
C	7.212403	-2.071277	-1.549402
C	8.011765	0.086074	-0.835757
C	8.274979	-1.166282	-1.410844
H	5.099926	-2.375714	-1.211897
H	6.473386	1.343470	0.015878
H	8.803836	0.821126	-0.706114
H	7.391372	-3.050388	-1.991463
C	9.626442	-1.579876	-1.880971
O	9.882648	-2.662419	-2.381619
O	10.570655	-0.605509	-1.691440
H	11.403864	-0.993596	-2.035459

p-SO_3H-Py-Ag_{20}	-4.82010816 Hartrees		
Atom	x	y	z
Ag	1.558204	0.674868	0.766776
Ag	4.001941	-0.018821	0.022711
Ag	1.423788	-0.975692	-1.435319
Ag	2.061319	-2.031789	1.227210
Ag	3.201301	0.304352	2.903794
Ag	3.371593	2.778693	1.047868
Ag	2.235792	2.015269	-1.544068
Ag	-0.607923	-1.351499	0.539629
Ag	0.540789	-0.755851	3.213938
Ag	1.452277	2.585513	3.090680
Ag	0.712927	3.498383	0.365496
Ag	-0.485775	1.159647	-1.153477
Ag	-0.838400	1.359005	1.650439
Ag	-3.229750	2.044624	2.594118
Ag	1.715182	0.797023	5.255536
Ag	-2.242966	-0.764221	2.794022
Ag	-2.917777	0.300737	0.152591
Ag	-0.891614	1.473836	4.373957
Ag	-0.953606	3.972330	2.624666
Ag	-2.120409	3.217539	0.045031
N	6.069564	-0.592689	-0.676415
C	6.541875	-1.848213	-0.505645
C	6.869736	0.311060	-1.284042
C	7.805799	-2.247514	-0.926275
C	8.152286	0.007862	-1.732617
C	8.620225	-1.294252	-1.544363
H	5.870179	-2.554034	-0.017337
H	6.455589	1.310529	-1.416689
H	8.763562	0.757139	-2.233752
H	8.140522	-3.274894	-0.789437
S	10.253528	-1.755805	-2.134259
O	10.761328	-0.670831	-2.960611
O	10.194130	-3.136093	-2.564344
O	11.131692	-1.779822	-0.746519
H	11.592827	-0.914221	-0.695907

m-C≡N-Py-Ag_{20}	-4.44892848 Hartrees		
Atom	x	y	z
Ag	1.545534	0.654883	0.770490
Ag	3.976830	-0.057872	0.018190
Ag	1.398651	-0.997341	-1.432552
Ag	2.031284	-2.053687	1.231146
Ag	3.192701	0.275869	2.900948
Ag	3.380850	2.742598	1.038188
Ag	2.234442	1.982749	-1.548372
Ag	-0.635419	-1.349379	0.547577
Ag	0.521468	-0.760172	3.220156
Ag	1.462858	2.573602	3.086683
Ag	0.727007	3.484488	0.358053
Ag	-0.495551	1.154467	-1.152913
Ag	-0.842187	1.365807	1.651721
Ag	-3.223906	2.077995	2.597085
Ag	1.715995	0.786814	5.254251
Ag	-2.263147	-0.741222	2.803651
Ag	-2.933382	0.323548	0.159382
Ag	-0.887624	1.487214	4.375896
Ag	-0.930371	3.984032	2.618404
Ag	-2.109884	3.233164	0.042119
N	6.082726	-0.554751	-0.689757
C	6.603396	-1.782720	-0.535217
C	6.856192	0.403826	-1.249609
C	7.912072	-2.104412	-0.931682
C	8.164022	0.169217	-1.668139
C	8.710347	-1.101207	-1.512314
H	5.963247	-2.539710	-0.082049
H	6.396000	1.385922	-1.359103
H	8.743986	0.977196	-2.112780
C	8.410077	-3.431056	-0.742996
H	9.728446	-1.327238	-1.827994
N	8.820423	-4.511236	-0.591463

p-CCl_3-Py-Ag_{20}	-4.38647785 Hartrees		
Atom	x	y	z
Ag	1.557898	0.679627	0.768188
Ag	4.005035	-0.006405	0.014931
Ag	1.427159	-0.974044	-1.432093
Ag	2.073247	-2.021302	1.230206
Ag	3.205793	0.322774	2.898833
Ag	3.360135	2.792119	1.037048
Ag	2.223460	2.016557	-1.549313
Ag	-0.600983	-1.353625	0.547524
Ag	0.549005	-0.748585	3.219232
Ag	1.445773	2.597918	3.085882
Ag	0.696771	3.498173	0.358164
Ag	-0.494343	1.151650	-1.151527
Ag	-0.842709	1.356837	1.652287
Ag	-3.235574	2.034916	2.600054
Ag	1.723023	0.814712	5.252455
Ag	-2.235577	-0.769474	2.804121
Ag	-2.921123	0.286357	0.162167
Ag	-0.890283	1.478005	4.375870
Ag	-0.966780	3.972428	2.619476
Ag	-2.137005	3.205955	0.045152
N	6.078532	-0.582174	-0.685247
C	6.498038	-1.865427	-0.664657
C	6.943946	0.345177	-1.146840
C	7.757851	-2.262242	-1.098198
C	8.222272	0.036487	-1.600044
C	8.648439	-1.297602	-1.588526
H	5.786546	-2.600280	-0.288149
H	6.588719	1.375592	-1.155639
H	8.871482	0.829752	-1.965592
H	8.035029	-3.314080	-1.060863
C	10.053893	-1.679922	-2.016098
Cl	11.126383	-1.638116	-0.543358
Cl	10.110731	-3.343285	-2.722479
Cl	10.722884	-0.538132	-3.246377

m-SO_3H-Py-Ag_{20}		-4.81979691 Hartrees	
Atom	x	y	z
Ag	1.536783	0.670100	0.729130
Ag	3.958293	-0.007852	-0.077983
Ag	1.356602	-1.088315	-1.387617
Ag	2.117487	-2.000747	1.293642
Ag	3.270371	0.436419	2.812124
Ag	3.315135	2.820593	0.833297
Ag	2.099461	1.908727	-1.672296
Ag	-0.591004	-1.407229	0.680623
Ag	0.646886	-0.660720	3.280180
Ag	1.481707	2.688479	2.961121
Ag	0.617426	3.452795	0.221449
Ag	-0.588443	1.020023	-1.134528
Ag	-0.836307	1.346991	1.671246
Ag	-3.202418	2.028863	2.677178
Ag	1.870749	1.010833	5.196337
Ag	-2.150503	-0.748043	2.970401
Ag	-2.948967	0.176784	0.307975
Ag	-0.784261	1.591635	4.388076
Ag	-0.968739	4.002488	2.521399
Ag	-2.220162	3.099220	0.028588
N	6.037406	-0.588755	-0.788020
C	6.478205	-1.862419	-0.696600
C	6.880418	0.342031	-1.278681
C	7.754091	-2.256041	-1.096343
C	8.174364	0.019980	-1.684592
C	8.629531	-1.299548	-1.608409
H	5.768516	-2.584909	-0.292595
H	6.505804	1.362028	-1.363165
S	9.240492	1.304680	-2.346514
H	8.052048	-3.300691	-1.012091
H	9.629748	-1.560702	-1.952929
O	10.117029	0.685942	-3.316799
O	8.424378	2.476603	-2.622880
O	10.200367	1.653818	-1.061869
H	9.817720	2.453398	-0.639308

p-CCl_2H-Py-Ag_{20}		-4.46272923 Hartrees	
Atom	x	y	z
Ag	1.266154	0.597923	0.457669
Ag	3.711182	-0.112027	-0.264264
Ag	1.144953	-1.079309	-1.726984
Ag	1.758264	-2.102454	0.952642
Ag	2.891054	0.252525	2.607003
Ag	3.082211	2.702603	0.718927
Ag	1.965017	1.906504	-1.868364
Ag	-0.904231	-1.423687	0.236517
Ag	0.223786	-0.796470	2.912456
Ag	1.147957	2.542874	2.751164
Ag	0.432797	3.420178	0.006333
Ag	-0.761464	1.063888	-1.488251
Ag	-1.135111	1.303884	1.308845
Ag	-3.530532	2.012550	2.224153
Ag	1.389245	0.781070	4.940417
Ag	-2.555648	-0.799541	2.469632
Ag	-3.206336	0.231950	-0.189934
Ag	-1.208461	1.455463	4.029644
Ag	-1.247364	3.933225	2.245328
Ag	-2.398208	3.145374	-0.331714
N	5.802435	-0.635033	-0.955674
C	6.308616	-1.881883	-0.814140
C	6.591937	0.302318	-1.515724
C	7.590604	-2.230086	-1.219255
C	7.889728	0.037894	-1.948370
C	8.407480	-1.252546	-1.802251
H	5.648343	-2.618962	-0.357350
H	6.161665	1.298674	-1.618782
H	8.482536	0.837385	-2.394810
H	7.949276	-3.250476	-1.083328
C	9.804051	-1.549055	-2.269017
Cl	10.857377	-2.073268	-0.889788
Cl	9.802499	-2.797851	-3.583568
H	10.284942	-0.667567	-2.694508

p-CFClH-Py-Ag_{20}		-4.53522149 Hartrees	
Atom	x	y	z
Ag	1.240290	0.998528	0.608506
Ag	3.682145	0.247098	-0.078111
Ag	1.126015	-0.716009	-1.547366
Ag	1.702323	-1.699867	1.155694
Ag	2.840088	0.675653	2.781729
Ag	3.073451	3.088252	0.856262
Ag	1.974669	2.262119	-1.730387
Ag	-0.944664	-1.008436	0.401476
Ag	0.163242	-0.345487	3.078748
Ag	1.116337	2.982587	2.871457
Ag	0.437043	3.820324	0.104756
Ag	-0.763689	1.450352	-1.363912
Ag	-1.162341	1.738855	1.426156
Ag	-3.561902	2.475827	2.308183
Ag	1.320931	1.255145	5.092598
Ag	-2.611563	-0.334408	2.608794
Ag	-3.226041	0.659817	-0.076949
Ag	-1.261405	1.935919	4.144490
Ag	-1.262623	4.382414	2.317725
Ag	-2.393879	3.564717	-0.257541
N	5.764578	-0.332147	-0.752335
C	6.080121	-1.609986	-1.052410
C	6.733132	0.600146	-0.870005
C	7.346910	-1.999940	-1.475781
C	8.025855	0.297622	-1.283592
C	8.344514	-1.027891	-1.598018
H	5.278760	-2.340919	-0.946212
H	6.451805	1.622370	-0.617909
H	8.768998	1.092412	-1.361184
H	7.552844	-3.045498	-1.700321
C	9.731127	-1.382022	-2.054154
F	10.048722	-2.684782	-1.714156
Cl	9.869039	-1.213680	-3.861962
H	10.499857	-0.724355	-1.636481

p-CF_2H-Py-Ag_{20}		-4.61007307 Hartrees	
Atom	x	y	z
Ag	1.256891	0.595670	0.447046
Ag	3.691193	-0.127812	-0.288990
Ag	1.119167	-1.062392	-1.752540
Ag	1.737926	-2.113585	0.916023
Ag	2.893233	0.220808	2.583363
Ag	3.091420	2.683904	0.714316
Ag	1.957382	1.917267	-1.871866
Ag	-0.922840	-1.410476	0.216796
Ag	0.221869	-0.814791	2.893445
Ag	1.166992	2.521186	2.755553
Ag	0.442817	3.425163	0.023084
Ag	-0.773695	1.090217	-1.486412
Ag	-1.134067	1.308474	1.314204
Ag	-3.519067	2.020048	2.249019
Ag	1.409356	0.739088	4.927691
Ag	-2.559074	-0.797935	2.462181
Ag	-3.217117	0.261415	-0.184843
Ag	-1.188091	1.434900	4.035617
Ag	-1.223304	3.928571	2.274971
Ag	-2.390844	3.170932	-0.304196
N	5.763678	-0.649684	-1.032632
C	6.396279	-1.777961	-0.641265
C	6.408296	0.176548	-1.880794
C	7.672993	-2.119179	-1.074560
C	7.688075	-0.088717	-2.363571
C	8.335544	-1.257228	-1.955817
H	5.847306	-2.423191	0.044738
H	5.871300	1.077509	-2.178624
H	8.164219	0.613182	-3.050409
H	8.139378	-3.043888	-0.734848
C	9.727422	-1.565950	-2.444846
F	10.642668	-1.389204	-1.418142
F	9.823670	-2.887980	-2.839646
H	10.046062	-0.936928	-3.286905

m-Cl-Py-Ag_{20}		-3.93074813 Hartrees	
Atom	x	y	z
Ag	1.555657	0.666913	0.775234
Ag	3.994514	-0.034163	0.028840
Ag	1.416950	-0.987251	-1.427607
Ag	2.047769	-2.041744	1.236016
Ag	3.193105	0.295600	2.911674
Ag	3.375030	2.766510	1.048958
Ag	2.239178	2.001990	-1.540702
Ag	-0.618344	-1.355119	0.544138
Ag	0.528375	-0.755702	3.220249
Ag	1.451747	2.583820	3.091229
Ag	0.719891	3.494779	0.362291
Ag	-0.485081	1.155281	-1.151506
Ag	-0.839822	1.361332	1.650950
Ag	-3.229765	2.058745	2.589866
Ag	1.706381	0.798358	5.261090
Ag	-2.254458	-0.757048	2.796002
Ag	-2.921250	0.306811	0.152966
Ag	-0.896829	1.482088	4.374067
Ag	-0.946890	3.981139	2.618847
Ag	-2.113528	3.222663	0.040596
N	6.075120	-0.585463	-0.696471
C	6.558220	-1.831133	-0.533720
C	6.855148	0.337089	-1.298028
C	7.835513	-2.188064	-0.969576
C	8.138529	0.048305	-1.755440
C	8.647654	-1.240317	-1.592515
H	5.912788	-2.560662	-0.045375
H	6.424713	1.331994	-1.409226
H	8.734095	0.824592	-2.235193
Cl	8.397981	-3.825926	-0.726218
H	9.645863	-1.509981	-1.936531

p-$CClH_2$-Py-Ag_{20}		-4.53098151 Hartrees	
Atom	x	y	z
Ag	1.474522	0.694257	0.490127
Ag	3.952311	0.090455	-0.215998
Ag	2.045345	-1.903044	1.222787
Ag	3.141074	0.377153	2.706832
Ag	3.150615	2.810192	0.794673
Ag	2.162684	1.817672	-1.969758
Ag	1.435104	-1.005584	-1.682399
Ag	0.437812	-0.412909	3.052913
Ag	1.249575	2.443281	2.928983
Ag	0.569366	3.444815	-0.320699
Ag	-0.551773	1.046701	-1.661076
Ag	-0.608322	-1.243502	0.331191
Ag	-0.957953	1.419832	1.227329
Ag	-3.385068	2.209084	1.980788
Ag	1.646539	4.989681	1.779750
Ag	-1.242986	1.681962	3.992853
Ag	-2.373580	-0.581634	2.522733
Ag	-1.004130	4.021761	2.039254
Ag	-2.211073	3.108409	-0.611851
Ag	-2.966429	0.293863	-0.313963
N	6.023430	-0.567762	-0.852655
C	6.983422	-0.837930	0.056841
C	6.320235	-0.760961	-2.155242
C	8.245158	-1.308345	-0.293264
C	7.557974	-1.227389	-2.587051
C	8.552483	-1.517543	-1.644010
H	6.717247	-0.673479	1.101061
H	5.526678	-0.536061	-2.868068
H	7.740546	-1.365140	-3.653923
H	8.980796	-1.511934	0.486416
C	9.893240	-2.041525	-2.064149
H	10.350885	-2.661379	-1.288022
H	9.837361	-2.601104	-3.002145
Cl	11.070353	-0.671199	-2.368553

p-I-Py-Ag_{20}		-3.88599934 Hartrees	
Atom	x	y	z
Ag	1.556647	0.674191	0.769773
Ag	3.997158	-0.019616	0.017059
Ag	1.416670	-0.975771	-1.435556
Ag	2.056445	-2.033356	1.224128
Ag	3.198200	0.303600	2.902206
Ag	3.369800	2.778150	1.044355
Ag	2.231266	2.015881	-1.544151
Ag	-0.612295	-1.353545	0.539057
Ag	0.537985	-0.756113	3.213632
Ag	1.451013	2.585854	3.089667
Ag	0.711466	3.500162	0.364713
Ag	-0.489493	1.160797	-1.151323
Ag	-0.839397	1.359485	1.651917
Ag	-3.229887	2.046272	2.597363
Ag	1.714779	0.797005	5.255261
Ag	-2.244993	-0.765446	2.795193
Ag	-2.920103	0.301943	0.156003
Ag	-0.891433	1.474405	4.375003
Ag	-0.952679	3.976128	2.625412
Ag	-2.121497	3.219989	0.048590
N	6.067288	-0.595017	-0.692248
C	6.543468	-1.844358	-0.507282
C	6.867377	0.304612	-1.302617
C	7.816006	-2.235535	-0.918328
C	8.152323	-0.005265	-1.743525
C	8.638097	-1.299597	-1.548825
H	5.871734	-2.545783	-0.011587
H	6.451604	1.303780	-1.436515
H	8.756244	0.760327	-2.230700
H	8.150234	-3.258299	-0.743743
I	10.595598	-1.836182	-2.201275

p-Br-Py-Ag_{20}		-3.90884745 Hartrees	
Atom	x	y	z
Ag	1.556973	0.673946	0.769946
Ag	3.997662	-0.020079	0.017683
Ag	1.417238	-0.976210	-1.435297
Ag	2.056509	-2.033692	1.224543
Ag	3.198188	0.303418	2.902604
Ag	3.370269	2.777801	1.044656
Ag	2.232058	2.015384	-1.543908
Ag	-0.612140	-1.353692	0.539104
Ag	0.537849	-0.756180	3.213840
Ag	1.451167	2.585819	3.089798
Ag	0.712012	3.499991	0.364668
Ag	-0.488953	1.160573	-1.151418
Ag	-0.839373	1.359533	1.651596
Ag	-3.229677	2.046525	2.596724
Ag	1.714524	0.797046	5.255481
Ag	-2.245075	-0.765367	2.795007
Ag	-2.919876	0.301950	0.155578
Ag	-0.891582	1.474592	4.374832
Ag	-0.952369	3.976240	2.625137
Ag	-2.120984	3.220033	0.048054
N	6.074383	-0.597323	-0.693613
C	6.554064	-1.844883	-0.510828
C	6.876234	0.300014	-1.303528
C	7.824891	-2.243442	-0.919303
C	8.161915	-0.000802	-1.747904
C	8.634544	-1.297593	-1.547917
H	5.888152	-2.552085	-0.015899
H	6.466427	1.301021	-1.440062
H	8.769633	0.759914	-2.234944
H	8.165056	-3.263380	-0.748388
Br	10.391833	-1.779265	-2.136559

p-Cl-Py-Ag_{20}		-3.93282117 Hartrees	
Atom	x	y	z
Ag	1.556647	0.674191	0.769773
Ag	3.997158	-0.019616	0.017059
Ag	1.416670	-0.975771	-1.435556
Ag	2.056445	-2.033356	1.224128
Ag	3.198200	0.303600	2.902206
Ag	3.369800	2.778150	1.044355
Ag	2.231266	2.015881	-1.544151
Ag	-0.612295	-1.353545	0.539057
Ag	0.537985	-0.756113	3.213632
Ag	1.451013	2.585854	3.089667
Ag	0.711466	3.500162	0.364713
Ag	-0.489493	1.160797	-1.151323
Ag	-0.839397	1.359485	1.651917
Ag	-3.229887	2.046272	2.597363
Ag	1.714779	0.797005	5.255261
Ag	-2.244993	-0.765446	2.795193
Ag	-2.920103	0.301943	0.156003
Ag	-0.891433	1.474405	4.375003
Ag	-0.952679	3.976128	2.625412
Ag	-2.121497	3.219989	0.048590
N	6.067288	-0.595017	-0.692248
C	6.543468	-1.844358	-0.507282
C	6.867377	0.304612	-1.302617
C	7.816006	-2.235535	-0.918328
C	8.152323	-0.005265	-1.743525
C	8.638097	-1.299597	-1.548825
H	5.871734	-2.545783	-0.011587
H	6.451604	1.303780	-1.436515
H	8.756244	0.760327	-2.230700
H	8.150234	-3.258299	-0.743743
Cl	10.249454	-1.741298	-2.085903

p-F-Py-Ag_{20}		-4.00255664 Hartrees	
Atom	x	y	z
Ag	1.556647	0.674191	0.769773
Ag	3.997158	-0.019616	0.017059
Ag	1.416670	-0.975771	-1.435556
Ag	2.056445	-2.033356	1.224128
Ag	3.198200	0.303600	2.902206
Ag	3.369800	2.778150	1.044355
Ag	2.231266	2.015881	-1.544151
Ag	-0.612295	-1.353545	0.539057
Ag	0.537985	-0.756113	3.213632
Ag	1.451013	2.585854	3.089667
Ag	0.711466	3.500162	0.364713
Ag	-0.489493	1.160797	-1.151323
Ag	-0.839397	1.359485	1.651917
Ag	-3.229887	2.046272	2.597363
Ag	1.714779	0.797005	5.255261
Ag	-2.244993	-0.765446	2.795193
Ag	-2.920103	0.301943	0.156003
Ag	-0.891433	1.474405	4.375003
Ag	-0.952679	3.976128	2.625412
Ag	-2.121497	3.219989	0.048590
N	6.067288	-0.595017	-0.692248
C	6.543468	-1.844358	-0.507282
C	6.867377	0.304612	-1.302617
C	7.816006	-2.235535	-0.918328
C	8.152323	-0.005265	-1.743525
C	8.638097	-1.299597	-1.548825
H	5.871734	-2.545783	-0.011587
H	6.451604	1.303780	-1.436515
H	8.756244	0.760327	-2.230700
H	8.150234	-3.258299	-0.743743
F	9.822513	-1.624266	-1.943600

m-OH-Py-Ag_{20}	-4.23377322 Hartrees		
Atom	x	y	z
Ag	1.554963	0.668005	0.770185
Ag	3.993267	-0.030314	0.018343
Ag	1.411653	-0.983387	-1.434051
Ag	2.049132	-2.040347	1.226402
Ag	3.196416	0.295089	2.902482
Ag	3.373298	2.768309	1.042893
Ag	2.232734	2.006139	-1.545114
Ag	-0.618388	-1.354795	0.541190
Ag	0.533502	-0.757939	3.214947
Ag	1.455013	2.582082	3.088361
Ag	0.717307	3.495960	0.362328
Ag	-0.489692	1.157798	-1.151391
Ag	-0.838533	1.360408	1.651641
Ag	-3.226578	2.055362	2.596259
Ag	1.714710	0.793947	5.254952
Ag	-2.249387	-0.759656	2.796948
Ag	-2.922046	0.306786	0.157096
Ag	-0.889882	1.477792	4.374433
Ag	-0.944582	3.978732	2.622651
Ag	-2.115934	3.222925	0.046562
N	6.073194	-0.570032	-0.692312
C	6.557228	-1.811030	-0.514875
C	6.851775	0.356323	-1.290834
C	7.843887	-2.177618	-0.929887
C	8.141326	0.065777	-1.729148
C	8.652489	-1.219196	-1.549565
H	5.911323	-2.543278	-0.029983
H	6.418054	1.347807	-1.414306
H	8.740075	0.840410	-2.207482
O	8.228677	-3.471102	-0.697028
H	9.661169	-1.474625	-1.884318
H	9.136178	-3.595691	-1.031073

p-OH-Py-Ag_{20}	-4.23929032 Hartrees		
Atom	x	y	z
Ag	1.354473	1.003056	0.815007
Ag	3.772435	0.218066	0.080115
Ag	1.166022	-0.668865	-1.370556
Ag	1.761083	-1.714312	1.304612
Ag	2.975956	0.603716	2.958039
Ag	3.237057	3.047931	1.070295
Ag	2.081669	2.292313	-1.513019
Ag	-0.881164	-0.953319	0.601280
Ag	0.280085	-0.361692	3.272814
Ag	1.306055	2.946068	3.110957
Ag	0.606609	3.850873	0.371940
Ag	-0.667919	1.534450	-1.119700
Ag	-1.020052	1.779743	1.679873
Ag	-3.389231	2.558730	2.607894
Ag	1.502294	1.176247	5.299539
Ag	-2.500540	-0.282322	2.844246
Ag	-3.130667	0.774412	0.189359
Ag	-1.077037	1.930335	4.401382
Ag	-1.047991	4.410941	2.620711
Ag	-2.233397	3.662528	0.048835
N	5.821248	-0.434400	-0.613606
C	6.263287	-1.693861	-0.415031
C	6.659675	0.426882	-1.233324
C	7.519153	-2.134820	-0.813395
C	7.931084	0.081647	-1.667478
C	8.376433	-1.229636	-1.455134
H	5.574482	-2.374325	0.085853
H	6.283134	1.438725	-1.383658
H	8.573858	0.807980	-2.162996
H	7.821260	-3.167127	-0.625465
O	9.626740	-1.557037	-1.886708
H	9.801258	-2.493375	-1.674375

m-NH_2-Py-Ag_{20}	-4.43369916 Hartrees		
Atom	x	y	z
Ag	8.947567	3.491934	3.139160
Ag	8.344498	1.629188	1.358323
Ag	7.004563	1.822843	4.160413
Ag	9.799859	0.961902	3.949678
Ag	11.137594	2.681784	1.751856
Ag	8.942406	4.500088	0.537174
Ag	6.474602	4.024419	2.040298
Ag	8.979183	2.724627	6.016261
Ag	11.556245	3.063190	4.575805
Ag	10.961631	5.520757	2.204660
Ag	8.121073	6.295606	2.574376
Ag	6.942953	4.623445	4.816468
Ag	9.680700	5.343653	4.877327
Ag	10.476114	7.202525	6.606312
Ag	13.368415	4.134208	2.696410
Ag	11.098083	4.316940	7.052907
Ag	8.321190	5.206103	7.289069
Ag	12.356323	5.838897	4.719875
Ag	10.260364	7.806012	3.691258
Ag	7.802661	7.351346	5.217465
N	7.760545	0.051504	-0.154235
C	8.182159	-1.216910	-0.020806
C	7.002826	0.380863	-1.220856
C	7.876424	-2.232570	-0.946144
C	6.649133	-0.562738	-2.184248
C	7.084057	-1.877620	-2.052625
H	8.790011	-1.438166	0.859131
H	6.683864	1.419641	-1.291470
H	6.036307	-0.264209	-3.034560
N	8.294962	-3.541896	-0.728716
H	6.814468	-2.630418	-2.796591
H	9.106099	-3.648508	-0.125373
H	8.362280	-4.121023	-1.560571

p-CH_3-Py-Ag_{20}	-4.59807603 Hartrees		
Atom	x	y	z
Ag	1.556687	0.674347	0.770295
Ag	3.997365	-0.019243	0.018529
Ag	1.417415	-0.975963	-1.435226
Ag	2.056640	-2.033447	1.224928
Ag	3.198024	0.303861	2.903324
Ag	3.369967	2.778554	1.045253
Ag	2.231878	2.016060	-1.543762
Ag	-0.612192	-1.353789	0.539063
Ag	0.537533	-0.756070	3.214187
Ag	1.450462	2.586288	3.090309
Ag	0.711389	3.500497	0.364833
Ag	-0.489176	1.160750	-1.151536
Ag	-0.839781	1.359588	1.651914
Ag	-3.230783	2.046356	2.596810
Ag	1.713892	0.797235	5.256178
Ag	-2.245624	-0.765642	2.795054
Ag	-2.920276	0.301724	0.155473
Ag	-0.892459	1.474623	4.375232
Ag	-0.953504	3.976555	2.625396
Ag	-2.121789	3.220089	0.048065
N	6.064479	-0.593566	-0.688429
C	6.546615	-1.841604	-0.510080
C	6.868395	0.300019	-1.302594
C	7.814111	-2.231409	-0.930137
C	8.147514	-0.014154	-1.750637
C	8.655743	-1.309110	-1.570046
H	5.880495	-2.548379	-0.014621
H	6.458604	1.301142	-1.439076
H	8.743973	0.754647	-2.245156
H	8.140578	-3.258965	-0.760132
C	10.042886	-1.685515	-2.020820
H	10.766823	-1.515057	-1.208695
H	10.100670	-2.746495	-2.294664
H	10.363178	-1.082222	-2.879365

p-NH_2-Py-Ag_{20}		-4.43998599 Hartrees	
Atom	x	y	z
Ag	1.555149	0.673433	0.768180
Ag	3.995733	-0.021793	0.009051
Ag	1.408345	-0.976371	-1.437988
Ag	2.052659	-2.033660	1.221966
Ag	3.198910	0.301944	2.899147
Ag	3.370022	2.775984	1.040944
Ag	2.225236	2.016727	-1.546784
Ag	-0.615595	-1.354547	0.539707
Ag	0.538531	-0.757407	3.213427
Ag	1.454089	2.584986	3.088530
Ag	0.711952	3.500558	0.364147
Ag	-0.494169	1.161364	-1.154042
Ag	-0.838554	1.359483	1.652086
Ag	-3.227059	2.047084	2.595979
Ag	1.719045	0.795115	5.256843
Ag	-2.244292	-0.764832	2.796273
Ag	-2.920053	0.303364	0.158761
Ag	-0.887286	1.474147	4.377825
Ag	-0.948561	3.976096	2.625020
Ag	-2.119759	3.219747	0.050522
N	6.048155	-0.593403	-0.699040
C	6.544047	-1.836538	-0.506235
C	6.864669	0.302698	-1.299146
C	7.820325	-2.221354	-0.882151
C	8.155068	0.011135	-1.709454
C	8.673341	-1.283658	-1.500347
H	5.876338	-2.550156	-0.022916
H	6.453068	1.300866	-1.450418
H	8.757731	0.784079	-2.189236
H	8.153833	-3.243626	-0.696458
N	9.936185	-1.630878	-1.925894
H	10.354504	-2.460064	-1.518634
H	10.592463	-0.878705	-2.104717

p-$N(CH_3)_2$-Py-Ag_{20}		-5.61436567 Hartrees	
Atom	x	y	z
Ag	1.369400	-0.636457	1.019531
Ag	3.867918	-0.944477	0.192824
Ag	1.407949	-2.171181	-1.269197
Ag	2.246125	-3.266567	1.319820
Ag	3.091886	-0.883341	3.104008
Ag	2.881318	1.681777	1.381221
Ag	1.799573	0.903697	-1.226721
Ag	-0.504719	-2.930378	0.711381
Ag	0.611710	-2.316548	3.397052
Ag	1.052233	1.121158	3.439761
Ag	0.134139	2.063468	0.780187
Ag	-0.766752	-0.338364	-0.842254
Ag	-1.078233	-0.336510	1.973421
Ag	-3.520045	-0.033866	2.989560
Ag	1.607332	-0.722394	5.501671
Ag	-2.151882	-2.689387	3.021265
Ag	-3.024859	-1.590941	0.454636
Ag	-1.085244	-0.368175	4.698145
Ag	-1.527999	2.186446	3.088900
Ag	-2.638104	1.408976	0.493498
N	5.960110	-1.195784	-0.557287
C	6.591793	-2.388772	-0.465759
C	6.653421	-0.193484	-1.145181
C	7.874815	-2.624048	-0.926236
C	7.940172	-0.326703	-1.637411
C	8.613192	-1.572722	-1.531281
H	6.026019	-3.195579	0.000870
H	6.137221	0.763543	-1.225271
H	8.410128	0.535821	-2.104997
H	8.291946	-3.622574	-0.816394
N	9.895301	-1.750911	-1.980125
C	10.568907	-0.684786	-2.714423
C	10.489449	-3.084037	-1.978020
H	10.100516	-0.492630	-3.694841
H	11.611950	-0.972213	-2.879280
H	10.566111	0.249468	-2.136277
H	10.464352	-3.522081	-0.970471
H	11.537514	-3.005975	-2.282756
H	9.974488	-3.770231	-2.671703

Py-Ag_6		-2.93743901 Hartrees	
Atom	x	y	z
Ag	0.000000	1.365698	-0.769207
Ag	0.000000	2.687380	1.600029
Ag	0.000000	0.000000	1.702340
Ag	0.000000	-1.365698	-0.769207
Ag	0.000000	0.000000	-3.113186
Ag	0.000000	-2.687380	1.600029
N	0.000000	0.000000	-5.414159
C	0.000000	0.000000	-8.215184
C	0.000000	1.201005	-7.502694
C	0.000000	-1.201005	-7.502694
C	0.000000	1.155575	-6.109209
C	0.000000	-1.155575	-6.109209
H	0.000000	2.071656	-5.517309
H	0.000000	-2.071656	-5.517309
H	0.000000	2.163773	-8.013775
H	0.000000	-2.163773	-8.013775
H	0.000000	0.000000	-9.305993

Py-Ag_8		-3.08401278 Hartrees	
Atom	x	y	z
Ag	1.447700	-0.959868	0.000000
Ag	-0.015374	-1.619980	-2.272110
Ag	0.034211	1.022063	-1.407432
Ag	-2.294944	1.588335	0.000000
Ag	0.034211	1.022063	1.407432
Ag	2.357230	1.685458	0.000000
Ag	-1.466118	-1.043068	0.000000
Ag	-0.015374	-1.619980	2.272110
N	4.212636	3.058488	0.000000
C	4.081200	4.400607	0.000000
C	5.459746	2.545694	0.000000
C	6.605339	3.340339	0.000000
C	5.172487	5.268276	0.000000
C	6.460797	4.729318	0.000000
H	3.059503	4.782344	0.000000
H	5.008363	6.345861	0.000000
H	7.336154	5.379892	0.000000
H	7.589824	2.872437	0.000000
H	5.530667	1.457400	0.000000

Py-Ag_{20S}		-4.00177487 Hartrees	
Atom	x	y	z
Ag	0.402826	-0.003156	0.000000
Ag	2.605681	1.681712	0.000000
Ag	2.608350	-0.837403	1.450590
Ag	2.608350	-0.837403	-1.450590
Ag	4.907641	-1.705004	0.000000
Ag	4.894310	0.859240	1.484383
Ag	4.894310	0.859240	-1.484383
Ag	4.855093	3.280681	0.000000
Ag	4.846424	-1.644207	2.841592
Ag	4.846424	-1.644207	-2.841592
Ag	7.745516	-0.004280	0.000000
Ag	7.235021	2.422911	-1.455691
Ag	7.235021	2.422911	1.455691
Ag	7.218588	0.041306	-2.837595
Ag	7.218588	0.041306	2.837595
Ag	7.233221	-2.473951	-1.378549
Ag	7.233221	-2.473951	1.378549
Ag	7.183135	4.774719	0.000000
Ag	7.172418	-2.394989	-4.143328
Ag	7.172418	-2.394989	4.143328
N	10.203808	0.047583	0.000000
C	13.005715	0.031151	0.000000
C	12.292668	0.035800	-1.200959
C	12.292668	0.035800	1.200959
C	10.898192	0.044225	-1.152745
C	10.898192	0.044225	1.152745
H	10.301774	0.050029	-2.067876
H	10.301774	0.050029	2.067876
H	12.803896	0.033465	-2.164089
H	12.803896	0.033465	2.164089
H	14.096750	0.024794	0.000000

Py-Ag_{20V}		-4.01638388 Hartrees	
Atom	x	y	z
Ag	-0.337207	-0.000721	0.000000
Ag	-2.582483	1.648470	0.000000
Ag	-2.584132	-0.827413	1.428016
Ag	-2.584132	-0.827413	-1.428016
Ag	-4.860742	-1.767082	0.000000
Ag	-4.857786	0.882462	1.529085
Ag	-4.857786	0.882462	-1.529085
Ag	-4.833347	3.268800	0.000000
Ag	-4.835707	-1.635326	2.830963
Ag	-4.835707	-1.635326	-2.830963
Ag	-7.360939	-0.000047	0.000000
Ag	-7.233654	2.432964	-1.453069
Ag	-7.233654	2.432964	1.453069
Ag	-7.235014	0.042958	-2.832921
Ag	-7.235014	0.042958	2.832921
Ag	-7.237259	-2.475346	-1.380000
Ag	-7.237259	-2.475346	1.380000
Ag	-7.156887	4.779780	0.000000
Ag	-7.160051	-2.388452	-4.139027
Ag	-7.160051	-2.388452	4.139027
N	1.961723	0.004195	0.000000
C	4.761708	0.015139	0.000000
C	4.049523	0.012361	-1.201277
C	4.049523	0.012361	1.201277
C	2.656275	0.006858	-1.156263
C	2.656275	0.006858	1.156263
H	2.064507	0.004215	-2.072314
H	2.064507	0.004215	2.072314
H	4.560494	0.014236	-2.164080
H	4.560494	0.014236	2.164080
H	5.852612	0.019210	0.000000

Py-Ag_{34}		-5.13320437 Hartrees	
Atom	x	y	z
Ag	1.441363	1.467854	-0.248836
Ag	4.211142	1.360407	-0.234460
Ag	2.821563	3.835254	0.290763
Ag	-2.780833	3.777663	0.406886
Ag	-1.387081	1.408161	-0.199922
Ag	-4.199920	1.398561	-0.166365
Ag	0.004656	3.882504	0.378351
Ag	-1.411607	-1.422314	-0.193873
Ag	-4.214711	-1.385018	-0.147175
Ag	-2.794196	-3.772249	0.419419
Ag	2.765823	-3.786933	0.404035
Ag	1.397202	-1.405398	-0.201141
Ag	4.203957	-1.424732	-0.199797
Ag	-0.008893	-3.896773	0.460937
Ag	0.017149	0.016975	2.595689
Ag	2.814405	0.012416	1.892455
Ag	-2.790904	0.018311	1.940874
Ag	1.441020	2.436581	2.410286
Ag	-1.381772	2.436829	2.479071
Ag	-1.406272	-2.403339	2.500419
Ag	1.420580	-2.396194	2.482927
Ag	-0.000609	-0.017206	-2.228583
Ag	3.149758	-0.061790	-2.499025
Ag	-3.154615	-0.003497	-2.435112
Ag	0.034619	3.068871	-2.351120
Ag	-0.033520	-3.116003	-2.287873
Ag	2.869111	2.758294	-2.363657
Ag	-2.812725	2.827550	-2.260473
Ag	-2.872391	-2.837508	-2.245515
Ag	2.803609	-2.874961	-2.266338
Ag	1.387218	1.354820	-4.262471
Ag	-1.415807	1.402981	-4.208385
Ag	-1.432186	-1.449699	-4.196166
Ag	1.368541	-1.489734	-4.214394
N	4.107514	5.734755	0.487404
C	5.451770	5.650101	0.562588
C	3.554995	6.962364	0.400024
C	6.282269	6.769113	0.549505
C	4.312099	8.132452	0.379602
C	5.703013	8.036011	0.453685
H	5.865099	4.642888	0.629964
H	2.466372	6.994806	0.340705
H	3.813808	9.099104	0.303489
H	7.363307	6.642319	0.609662
H	6.325044	8.932253	0.434896

Py-Ag_{40}		-5.62758194 Hartrees	
Atom	x	y	z
Ag	0.015541	0.203433	0.000000
Ag	0.062314	2.898351	0.000000
Ag	0.811921	1.316910	2.443111
Ag	-2.063012	1.401935	1.506628
Ag	-2.063012	1.401935	-1.506628
Ag	0.811921	1.316910	-2.443111
Ag	2.602582	1.324915	0.000000
Ag	-0.799324	-1.110698	2.361743
Ag	-2.463888	-1.184351	0.000000
Ag	-0.799324	-1.110698	-2.361743
Ag	2.053354	-1.153498	-1.455648
Ag	2.053354	-1.153498	1.455648
Ag	0.029110	-2.614931	0.000000
Ag	-4.249561	2.330756	0.000000
Ag	2.774153	-0.157954	3.967493
Ag	0.086767	-0.152646	4.827289
Ag	-2.925625	-0.111688	3.841270
Ag	-4.548509	-0.069794	1.533511
Ag	-4.548509	-0.069794	-1.533511
Ag	-2.925625	-0.111688	-3.841270
Ag	0.086767	-0.152646	-4.827289
Ag	2.774153	-0.157954	-3.967493
Ag	4.665170	-0.109305	-1.413096
Ag	4.665170	-0.109305	1.413096
Ag	1.264146	-2.604206	3.904907
Ag	-1.550278	-2.479306	4.664242
Ag	-3.363599	-2.573022	2.404495
Ag	-4.921084	-2.480566	0.000000
Ag	-3.363599	-2.573022	-2.404495
Ag	-1.550278	-2.479306	-4.664242
Ag	1.264146	-2.604206	-3.904907
Ag	4.005636	-2.484604	-2.899981
Ag	4.136861	-2.561204	0.000000
Ag	4.005636	-2.484604	2.899981
Ag	-0.810529	-4.001201	2.366317
Ag	-2.553743	-4.084402	0.000000
Ag	-0.810529	-4.001201	-2.366317
Ag	2.045027	-4.022397	-1.482770
Ag	2.045027	-4.022397	1.482770
Ag	0.035757	-5.403942	0.000000
N	0.028759	5.178116	0.000000
C	1.160410	5.913735	0.000000
C	-1.152620	5.831084	0.000000
C	1.155060	7.307176	0.000000
C	-1.245582	7.221539	0.000000
C	-0.070843	7.976051	0.000000
H	2.096574	5.354641	0.000000
H	-2.045490	5.202971	0.000000
H	-2.226124	7.698079	0.000000
H	2.098992	7.852632	0.000000
H	-0.109700	9.066409	0.000000

Py-Ag_{58}		-7.20281483 Hartrees	
Atom	x	y	z
Ag	-0.849713	-1.479324	1.437757
Ag	1.369458	-2.384958	-0.273952
Ag	0.002716	0.000829	-0.803714
Ag	-1.379221	-2.373591	-1.367770
Ag	0.385143	-4.130697	1.782911
Ag	1.188411	-2.069361	3.541202
Ag	1.695402	-0.003802	1.444121
Ag	-2.749751	-0.001297	-0.282990
Ag	-2.308506	-3.987755	0.775552
Ag	-1.781806	-3.072521	3.434823
Ag	-2.380465	0.001028	3.530426
Ag	-0.851103	1.466797	1.438200
Ag	-3.763984	-1.718315	1.772148
Ag	-1.682890	-0.003689	-3.048203
Ag	0.010703	4.857842	-0.973265
Ag	2.718955	-4.726578	0.153349
Ag	3.365971	-2.403659	1.779361
Ag	0.392954	4.111551	1.765733
Ag	4.210315	-2.442689	-0.953121
Ag	0.848031	1.475192	-3.082531
Ag	-4.223016	-2.426706	-0.963869
Ag	1.680510	-2.921040	-5.237040
Ag	-2.703300	4.702078	-2.002710
Ag	-3.348260	-0.004200	-5.250322
Ag	2.246337	-3.897123	-2.579716
Ag	3.369123	2.390811	1.772587
Ag	2.736625	-0.010540	-1.363353
Ag	1.706171	2.912397	-5.316426
Ag	3.634800	1.471061	-3.655930
Ag	-0.002200	-4.862798	-0.957247
Ag	5.434210	-0.011546	-1.977480
Ag	3.551464	-0.010472	3.433067
Ag	-1.779825	3.082354	3.421298
Ag	-0.870746	1.498484	-5.369917
Ag	-4.485241	0.002124	-2.591574
Ag	-0.526629	-3.910341	-3.666226
Ag	-0.869684	-1.527315	-5.362685
Ag	-5.448565	0.002554	0.144440
Ag	-2.299361	3.989267	0.759772
Ag	-4.206776	2.430717	-0.969896
Ag	-3.760658	1.724228	1.771148
Ag	2.728679	4.711383	0.132581
Ag	3.646267	-1.503949	-3.668437
Ag	-3.114315	-2.410613	-3.676896
Ag	2.245017	3.868012	-2.609329
Ag	4.607988	-0.004045	0.777785
Ag	-0.508195	3.884132	-3.693851
Ag	-1.366047	2.367654	-1.376097
Ag	1.375477	2.372172	-0.287305
Ag	1.183505	2.056023	3.530704
Ag	-2.724783	-4.706562	-1.981145
Ag	0.839196	-1.471575	-3.038325
Ag	-3.107308	2.405320	-3.682941
Ag	1.742768	-0.028201	-5.349383
Ag	4.210915	2.430585	-0.964036
Ag	1.604371	-0.000528	5.397973
Ag	-0.812679	1.398481	5.393792
Ag	-0.812771	-1.391097	5.407294
N	2.820203	3.366574	-7.322741
C	4.039880	2.810889	-7.472489
C	2.259378	3.955232	-8.397984
C	4.733086	2.814860	-8.680783
C	2.881732	4.002641	-9.645275
C	4.141906	3.419065	-9.791996
H	4.458825	2.337997	-6.581642
H	1.273771	4.397239	-8.245671
H	2.381254	4.486690	-10.484264
H	5.715099	2.345185	-8.743499
H	4.653729	3.433414	-10.755237

Py-Ag_{68}		-7.97732599 Hartrees	
Atom	x	y	z
Ag	-0.844335	1.462430	-1.229200
Ag	0.829978	1.437565	-3.654249
Ag	-0.889140	4.451347	-1.270120
Ag	-2.526180	1.419422	1.138968
Ag	-3.315312	2.849174	3.482378
Ag	-3.315312	-2.849174	3.482378
Ag	-2.484108	4.302601	1.131499
Ag	-2.526180	-1.419422	1.138968
Ag	-3.453400	0.000000	3.528831
Ag	-2.484108	-4.302601	1.131499
Ag	-0.844335	-1.462430	-1.229200
Ag	0.829978	-1.437565	-3.654249
Ag	-0.889140	-4.451347	-1.270120
Ag	0.000000	0.000000	1.188688
Ag	1.688669	0.000000	-1.229200
Ag	0.033835	2.897447	1.138968
Ag	0.033835	-2.897447	1.138968
Ag	1.680098	2.910015	-1.228488
Ag	-0.826765	1.431999	3.536161
Ag	-0.826765	-1.431999	3.536161
Ag	-0.809801	-4.295732	3.482378
Ag	-0.809801	4.295732	3.482378
Ag	1.680098	-2.910015	-1.228488
Ag	-3.360196	0.000000	-1.228488
Ag	-1.659957	0.000000	-3.654249
Ag	-5.132372	0.000000	1.163148
Ag	-3.410410	2.995691	-1.270120
Ag	-3.410410	-2.995691	-1.270120
Ag	-1.642892	2.845572	-3.543578
Ag	-4.951271	2.829126	1.115757
Ag	-4.951271	-2.829126	1.115757
Ag	-1.642892	-2.845572	-3.543578
Ag	2.492346	1.478025	1.138968
Ag	1.726700	-2.990732	3.528831
Ag	1.653530	0.000000	3.536161
Ag	2.492346	-1.478025	1.138968
Ag	-4.179740	1.429865	-3.524406
Ag	-5.862367	1.428970	-1.216285
Ag	-5.862367	-1.428970	-1.216285
Ag	-4.179740	-1.429865	-3.524406
Ag	4.299549	1.455656	-1.270120
Ag	4.299549	-1.455656	-1.270120
Ag	2.566186	4.444765	1.163148
Ag	1.726700	2.990732	3.528831
Ag	3.285783	0.000000	-3.543578
Ag	0.025540	5.702490	1.115757
Ag	4.125113	1.446557	3.482378
Ag	4.968216	0.000000	1.131499
Ag	4.925731	2.873363	1.115757
Ag	3.328169	2.904829	-3.524406
Ag	0.851571	4.334693	-3.524406
Ag	1.693659	5.791444	-1.216285
Ag	4.168708	4.362474	-1.216285
Ag	4.125113	-1.446557	3.482378
Ag	4.925731	-2.873363	1.115757
Ag	2.566186	-4.444765	1.163148
Ag	0.025540	-5.702490	1.115757
Ag	4.168708	-4.362474	-1.216285
Ag	0.851571	-4.334693	-3.524406
Ag	1.693659	-5.791444	-1.216285
Ag	3.328169	-2.904829	-3.524406
Ag	2.442847	1.419374	5.851302
Ag	2.442847	-1.419374	5.851302
Ag	0.000000	0.000000	6.334960
Ag	0.007790	-2.825254	5.851302
Ag	0.007790	2.825254	5.851302
Ag	-2.450637	1.405881	5.851302
Ag	-2.450637	-1.405881	5.851302
N	-0.028022	-0.145938	8.900657
C	1.115942	-0.236482	9.600535
C	-1.185788	-0.207328	9.580746
C	1.152029	-0.391819	10.986933
C	-1.249606	-0.361823	10.966286
C	-0.055924	-0.457051	11.684679
H	2.037563	-0.184398	9.014810
H	-2.095326	-0.131798	8.978705
H	-2.217539	-0.407536	11.466980
H	2.109701	-0.461450	11.504278
H	-0.066888	-0.580610	12.768841

C≡O		-0.53984680 Hartrees	
Atom	x	y	z
C	0.000000	0.000000	3.491231
O	0.000000	0.000000	4.631605

N_2		-0.60643759 Hartrees	
Atom	x	y	z
N	0.000000	0.000000	-0.553034
N	0.000000	0.000000	0.553034

NH_3		-0.70841607 Hartrees	
Atom	x	y	z
N	0.000000	0.000000	-5.959181
H	0.471008	-0.815810	-6.359854
H	-0.942016	0.000000	-6.359854
H	0.471008	0.815810	-6.359854

PH_3		-0.56171946 Hartrees	
Atom	x	y	z
P	6.210253	-0.630648	-0.744715
H	7.077171	-1.518803	-0.024757
H	6.482033	-1.287840	-1.990859
H	7.266133	0.318421	-0.952737

C≡O-Ag_{20}		-1.95829885 Hartrees	
Atom	x	y	z
Ag	1.554681	0.676462	0.766749
Ag	3.991924	-0.016617	0.013299
Ag	1.420251	-0.978376	-1.438645
Ag	2.051852	-2.036727	1.220717
Ag	3.198183	0.301872	2.897116
Ag	3.367870	2.786161	1.043965
Ag	2.236500	2.018615	-1.546945
Ag	-0.614774	-1.354389	0.537410
Ag	0.536943	-0.759181	3.216785
Ag	1.451370	2.588580	3.090730
Ag	0.709490	3.503676	0.362438
Ag	-0.488143	1.159876	-1.154306
Ag	-0.840576	1.359120	1.652392
Ag	-3.229429	2.044126	2.602502
Ag	1.724467	0.794420	5.254272
Ag	-2.245825	-0.768905	2.798136
Ag	-2.920830	0.301187	0.154489
Ag	-0.885432	1.475592	4.377319
Ag	-0.952396	3.977097	2.627233
Ag	-2.122420	3.219757	0.046912
C	5.894824	-0.548394	-0.638807
O	6.956582	-0.829093	-0.960783

N_2-Ag_{20}		-2.00813416 Hartrees	
Atom	x	y	z
Ag	1.552147	0.692283	0.766508
Ag	3.973308	-0.015413	0.016121
Ag	1.414683	-0.978250	-1.435573
Ag	2.053027	-2.036642	1.220549
Ag	3.194468	0.301569	2.892916
Ag	3.367055	2.788047	1.043582
Ag	2.230471	2.020552	-1.546558
Ag	-0.616525	-1.352108	0.538809
Ag	0.536939	-0.762190	3.219849
Ag	1.450472	2.590024	3.093353
Ag	0.706073	3.503483	0.363263
Ag	-0.495092	1.162425	-1.151672
Ag	-0.847262	1.337245	1.655404
Ag	-3.223041	2.057644	2.594727
Ag	1.725068	0.792183	5.252161
Ag	-2.243421	-0.770182	2.800119
Ag	-2.927668	0.300528	0.152543
Ag	-0.886953	1.477930	4.381629
Ag	-0.953849	3.975151	2.629717
Ag	-2.122064	3.221812	0.044542
N	6.116297	-0.612742	-0.705860
N	7.161677	-0.869675	-0.965651

NH_3-Ag_{20}		-2.13127952 Hartrees	
Atom	x	y	z
Ag	1.553563	0.676829	0.767465
Ag	3.991869	-0.015730	0.015430
Ag	1.417677	-0.977363	-1.438767
Ag	2.047793	-2.035785	1.221601
Ag	3.193115	0.303729	2.898585
Ag	3.364498	2.788294	1.045095
Ag	2.234711	2.020006	-1.546864
Ag	-0.616623	-1.355519	0.537668
Ag	0.534734	-0.758786	3.216850
Ag	1.449378	2.589327	3.090311
Ag	0.708662	3.505400	0.362998
Ag	-0.488159	1.159750	-1.155118
Ag	-0.840730	1.359501	1.652528
Ag	-3.228442	2.042757	2.603965
Ag	1.719902	0.796564	5.255802
Ag	-2.247070	-0.769811	2.799336
Ag	-2.919711	0.300010	0.154877
Ag	-0.887043	1.476074	4.379299
Ag	-0.952839	3.977843	2.628653
Ag	-2.120642	3.219496	0.047601
N	6.097928	-0.604127	-0.703447
H	6.556466	-1.248607	-0.053699
H	6.079096	-1.063975	-1.618283
H	6.706810	0.214818	-0.793051

PH_3-Ag_{20}		-1.98267900 Hartrees	
Atom	x	y	z
Ag	1.544878	0.664058	0.767876
Ag	3.995935	-0.004059	0.014178
Ag	1.410917	-0.978437	-1.432948
Ag	2.045628	-2.034370	1.229557
Ag	3.191929	0.304593	2.899254
Ag	3.363777	2.791685	1.043675
Ag	2.231532	2.021740	-1.546443
Ag	-0.617361	-1.353539	0.534140
Ag	0.537101	-0.763651	3.215872
Ag	1.444199	2.589768	3.098030
Ag	0.702494	3.507586	0.369073
Ag	-0.491525	1.162613	-1.152258
Ag	-0.849300	1.341325	1.654409
Ag	-3.229692	2.066300	2.597279
Ag	1.724833	0.796655	5.256993
Ag	-2.250694	-0.768778	2.800681
Ag	-2.924267	0.302052	0.153216
Ag	-0.885873	1.476170	4.377227
Ag	-0.953691	3.973894	2.628181
Ag	-2.122703	3.218345	0.046023
P	6.215620	-0.631739	-0.746430
H	7.027316	-1.523535	0.014477
H	6.418902	-1.288286	-1.997827
H	7.214146	0.357144	-0.932291

BT		-2.87318879 Hartrees	
Atom	x	y	z
C	0.286697	-0.054135	-0.441957
C	-0.949261	-0.699348	-0.268060
C	-0.990359	-2.029924	0.152870
C	0.192909	-2.730653	0.410892
C	1.422244	-2.086810	0.234527
C	1.474583	-0.756575	-0.187673
H	-1.877070	-0.160276	-0.462217
H	-1.956521	-2.519051	0.279755
H	0.157575	-3.767373	0.745134
H	2.353272	-2.620791	0.426632
H	2.439692	-0.266218	-0.318813
S	0.264203	1.645558	-0.984745
H	1.606796	1.812356	-1.002723

p-OH-BT		-3.11187545 Hartrees	
Atom	x	y	z
C	0.292939	-0.059643	-0.440662
C	-0.930557	-0.729161	-0.273598
C	-0.965504	-2.055874	0.151352
C	0.228581	-2.736441	0.416966
C	1.452653	-2.077494	0.253322
C	1.483857	-0.747891	-0.172703
H	-1.867914	-0.210888	-0.476973
H	-1.915085	-2.573908	0.280501
H	2.389478	-2.601241	0.458436
H	2.446661	-0.251570	-0.294356
S	0.248596	1.640530	-0.988734
H	1.588397	1.827471	-0.996157
O	0.138122	-4.050725	0.835741
H	1.041417	-4.385516	0.978818

p-C≡N-BT		-3.33581924 Hartrees	
Atom	x	y	z
C	0.051825	-0.560171	-1.416176
C	-1.277354	-0.997987	-1.275163
C	-1.548623	-2.281725	-0.817374
C	-0.494378	-3.156674	-0.490217
C	0.835485	-2.716639	-0.632019
C	1.104695	-1.432011	-1.090153
H	-2.101702	-0.330358	-1.525043
H	-2.579407	-2.616496	-0.709726
H	1.654696	-3.388963	-0.380515
H	2.139761	-1.107347	-1.194118
S	0.313738	1.092718	-2.006675
C	-0.770486	-4.477152	-0.019290
N	-0.996099	-5.555452	0.365266
H	1.666011	1.047616	-1.973947

BT-Ag_{19}		-4.09472037 Hartrees	
Atom	x	y	z
Ag	-4.826466	3.420341	9.654344
Ag	-4.272892	4.402291	12.090642
Ag	-2.242789	2.835046	10.393955
Ag	-4.618777	1.508644	11.619529
Ag	-6.930358	3.359269	11.428776
Ag	-5.985051	5.880485	10.091375
Ag	-3.098967	5.538840	9.497915
Ag	-3.693783	0.817049	8.988833
Ag	-6.627402	1.167240	9.601436
Ag	-7.521758	3.934537	8.689245
Ag	-5.069124	5.292370	7.435109
Ag	-2.734481	3.404455	7.630139
Ag	-5.417597	2.438832	7.187555
Ag	-6.265302	1.346532	4.833632
Ag	-5.731397	-0.282262	7.306048
Ag	-3.304794	1.024065	6.182661
Ag	-8.044115	1.580697	7.166829
Ag	-7.140077	4.108728	5.873916
Ag	-4.132584	3.815400	5.161202
C	-4.328632	2.270714	2.498778
C	-3.093936	1.610908	2.332792
C	-1.886907	2.316876	2.335980
C	-1.865702	3.704740	2.512773
C	-3.077919	4.387499	2.672892
C	-4.300650	3.682404	2.667868
H	-3.098048	0.529450	2.189978
H	-0.950506	1.773525	2.198222
H	-0.922054	4.250175	2.514639
H	-3.089189	5.475707	2.753766
H	-5.247512	4.225278	2.667221
S	-5.865609	1.370166	2.443821

p-OH-BT-Ag_{19}		-4.33501348 Hartrees	
Atom	x	y	z
Ag	-4.832735	3.417214	9.608200
Ag	-4.273190	4.360658	12.063122
Ag	-2.228677	2.898590	10.320210
Ag	-4.491515	1.433244	11.489581
Ag	-6.880549	3.235868	11.443624
Ag	-6.026010	5.834180	10.210310
Ag	-3.167163	5.608810	9.512604
Ag	-3.616693	0.907399	8.787333
Ag	-6.539870	1.099101	9.548833
Ag	-7.519615	3.925505	8.728678
Ag	-5.177111	5.382312	7.498181
Ag	-2.761553	3.546322	7.587347
Ag	-5.424928	2.477036	7.095315
Ag	-6.587786	1.415980	4.823367
Ag	-5.673838	-0.230823	7.169660
Ag	-3.223763	1.231866	5.990777
Ag	-8.068393	1.603401	7.231969
Ag	-7.199431	4.171774	5.901126
Ag	-4.208491	4.068490	5.193251
C	-4.207369	1.768627	2.862795
C	-3.179811	0.897297	3.298668
C	-1.873781	1.354131	3.544852
C	-1.553824	2.707425	3.354910
C	-2.555459	3.596211	2.938933
C	-3.863672	3.130726	2.699148
H	-3.400327	-0.168528	3.373182
H	-1.079810	0.657059	3.815058
O	-0.253529	3.093039	3.587636
H	-2.308676	4.642563	2.740862
H	-4.614203	3.814308	2.299166
S	-5.849272	1.176065	2.528219
H	-0.184416	4.053082	3.435434

p-C≡N-BT-Ag_{19}		-4.55788553 Hartrees	
Atom	x	y	z
Ag	-4.829507	3.419389	9.665315
Ag	-4.311708	4.369032	12.121908
Ag	-2.263345	2.823802	10.446691
Ag	-4.665564	1.497644	11.635017
Ag	-6.963914	3.367063	11.408666
Ag	-5.971107	5.885845	10.100059
Ag	-3.091009	5.531516	9.546550
Ag	-3.708345	0.812036	9.021895
Ag	-6.642328	1.176544	9.590851
Ag	-7.505674	3.959352	8.666827
Ag	-5.026327	5.296699	7.440976
Ag	-2.710271	3.400982	7.670591
Ag	-5.399118	2.439374	7.191392
Ag	-6.236503	1.362767	4.834050
Ag	-5.724075	-0.277429	7.310021
Ag	-3.265975	1.017421	6.230630
Ag	-8.031839	1.609035	7.150933
Ag	-7.087564	4.131056	5.863353
Ag	-4.074810	3.783017	5.174905
C	-4.346754	2.201792	2.393065
C	-3.088836	1.648978	2.066816
C	-1.945135	2.435936	1.985774
C	-2.006447	3.823640	2.230767
C	-3.253089	4.404167	2.544431
C	-4.402458	3.605420	2.625370
H	-3.025143	0.577799	1.873827
H	-0.987157	1.982085	1.732047
H	-3.328987	5.484407	2.670261
H	-5.379360	4.074915	2.747048
S	-5.790582	1.181589	2.450685
C	-0.833047	4.630516	2.147635
N	0.127379	5.290348	2.081565

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