The nature of interfacial binding of imidazole and carbene ligands with M_{20} nanoclusters (M=Au, Ag and Cu) – A theoretical study

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Supporting Information

3.2 Geometries of IMI-M20 and n-NHC, a-NHC-M20

Cartesian coordinates and energies for IMI, n,a-NHC-M_{20} complexes at A and F positions with CAM-B3LYP/6-311G*(C,H,N)/LANL2DZ(Au, Ag, Cu) level of theory

1. IMI-Au_{20} at A- position

Atoms	Coordinates (Angstroms) X	Y	Z
Au	2.155850	0.031716	-0.001115
Au	-0.393924	-1.837783	0.093716
Au	2.044765	-2.422504	1.482864
Au	-0.439424	0.985112	1.542864
Au	-0.496528	-1.512668	2.936171
Au	2.003127	0.262100	2.856751
Au	2.045301	-2.560905	-1.227588
Au	1.899396	-2.136115	4.230743
Au	1.963518	2.539744	1.381802
Au	1.901077	-2.555875	-3.990481
Au	-2.736942	1.626786	-0.084079
Au	-2.701817	-0.957543	-1.403477
Au	-4.958548	-0.088268	0.003832
Au	-0.572685	3.280417	-0.167703
Au	-0.438351	0.822893	-1.635651
Au	1.783844	4.772804	-0.243261
Au	1.964428	2.385842	-1.632397
Au	2.004662	-0.030220	-2.867679

Au	-0.495269	-1.803968	-2.767206
Au	-2.702614	-0.809856	1.492399
N	-7.193059	-0.036212	0.000919
C	-8.055933	-1.107255	0.006651
C	-7.935064	1.047315	-0.007125
C	-9.335813	-0.652292	0.001963
H	-7.694331	-2.121907	0.013574

Zero-point correction= 0.083440 (Hartree/Particle)
Thermal correction to Energy= 0.133901
Thermal correction to Enthalpy= 0.134845
Thermal correction to Gibbs Free Energy= -0.033040
Sum of electronic and zero-point Energies= -2934.407482
Sum of electronic and thermal Energies= -2934.357021
Sum of electronic and thermal Enthalpies= -2934.356077
Sum of electronic and thermal Free Energies= -2934.523962

2. IMI-Au_{20} at F-position

Au	-2.588752	-4.351018	5.830742
Au	-0.117753	-5.052592	3.987401
Au	-2.301478	-3.403559	3.136340
Au	0.261458	-3.125263	6.476670
Au	0.477804	-2.261283	3.760525
Au	-1.945432	-1.571524	5.505411
Au	-2.763186	-6.050193	3.523987
Au	-1.682009	-0.718867	2.886986
Au	-2.088730	-2.568921	8.024363
Au	-3.084724	-8.744763	4.061977
Au	2.265627	-4.967779	7.437542
Au	1.933155	-6.723901	5.150332
Au	4.420222	-5.585711	5.743469
Au	0.164724	-4.358413	9.061768
Au	-0.284265	-6.225219	6.932352
Au	-2.126080	-3.744563	10.530482
Au	-2.605774	-5.512164	8.455442
Au	-2.923820	-7.160378	6.323326
Au	-0.494663	-7.829472	4.574095
Au	2.426522	-3.905209	4.733547
N	6.628928	-5.926207	5.791544
C	7.365204	-6.749135	4.971480
C	7.475672	-5.367645	6.625698
C	8.675130	-6.678214	5.324013
H	6.900265	-7.328983	4.191803
H	7.223553	-4.665668	7.403972
H	9.553662	-7.162292	4.933096
N	8.728026	-5.796628	6.378122
H	9.555345	-5.517596	6.879356

Zero-point correction= 0.082990 (Hartree/Particle)
Thermal correction to Energy= 0.132732
Thermal correction to Enthalpy= 0.133676
Thermal correction to Gibbs Free Energy= -0.031091
Sum of electronic and zero-point Energies= -2934.389896
Sum of electronic and thermal Energies= -2934.340155
Sum of electronic and thermal Enthalpies= -2934.339210
Sum of electronic and thermal Free Energies= -2934.503977

3. IMI-Ag_{20} at A-position

Ag	-2.232253	-0.028389	-0.016467
Ag	0.265998	0.947073	1.518260
Ag	-2.149776	0.121362	2.857377

Ag	0.321161	-1.768214	0.074219
Ag	0.327733	-1.549158	2.936889
Ag	-2.097166	-2.492888	1.466119
Ag	-2.166091	2.488508	1.379699
Ag	-2.043755	-2.305047	4.267418
Ag	-2.063978	-2.588659	-1.322394
Ag	-2.093220	4.822133	-0.181566
Ag	2.644803	-0.843427	-1.380875
Ag	2.596212	1.710051	-0.019957
Ag	4.907376	0.070285	0.064160
Ag	0.393717	-1.745900	-2.797706
Ag	0.300832	0.843781	-1.557272
Ag	-1.945330	-2.593042	-4.128667
Ag	-2.083482	-0.075583	-2.891239
Ag	-2.133147	2.387320	-1.580117
Ag	0.293273	3.318772	-0.101802
Ag	2.613835	-0.744462	1.513741
N	7.236832	0.033017	0.021371
C	8.099573	1.035812	0.395289
C	7.985369	-0.964620	-0.383166
C	9.383474	0.628163	0.210544
H	7.738532	1.979757	0.769894
H	7.628162	-1.914716	-0.748084

Zero-point correction= 0.084725 (Hartree/Particle)
Thermal correction to Energy= 0.133945
Thermal correction to Enthalpy= 0.134889
Thermal correction to Gibbs Free Energy= -0.023040
Sum of electronic and zero-point Energies= -3140.648725
Sum of electronic and thermal Energies= -3140.599506
Sum of electronic and thermal Enthalpies= -3140.598561
Sum of electronic and thermal Free Energies= -3140.756491

4. IMI-Ag_{20} at F-position

Ag	0.825316	0.859063	-1.497577
Ag	0.825282	0.859842	1.497151
Ag	0.912570	3.329448	-0.000855
Ag	-1.999156	0.006114	-0.000034
Ag	-1.514632	2.476929	1.486558
Ag	-1.514595	2.476158	-1.487898
Ag	3.159842	1.689328	-0.000395
Ag	-1.459213	4.860321	-0.001286
Ag	-1.539246	0.064123	-2.879351
Ag	5.392714	-0.022708	0.000081
Ag	-1.540871	-2.518385	1.392965
Ag	0.880965	-1.666137	2.886970
Ag	-1.493377	-2.414290	4.202976
Ag	-1.540827	-2.519103	-1.391714
Ag	0.818555	-1.731571	0.000460
Ag	-1.493252	-2.416471	-4.201775
Ag	0.881052	-1.667635	-2.886085
Ag	3.147064	-0.867695	-1.479212
Ag	3.147025	-0.866931	1.479756
Ag	-1.539326	0.065619	2.879263
N	-4.469527	-0.017047	-0.000039
C	-5.308218	-1.103695	0.000167
C	-5.241157	1.039718	-0.000253
C	-6.604249	-0.688138	0.000074
H	-4.920330	-2.109820	0.000369
H	-4.904660	2.064929	-0.000451
H	-7.537275	-1.225928	0.000172
N	-6.546978	0.685799	-0.000196

H -7.331986 1.315145 -0.000326
Zero-point correction= 0.084307 (Hartree/Particle)
Thermal correction to Energy= 0.133722
Thermal correction to Enthalpy= 0.134666
Thermal correction to Gibbs Free Energy= -0.024035
Sum of electronic and zero-point Energies= -3140.635585
Sum of electronic and thermal Energies= -3140.586171
Sum of electronic and thermal Enthalpies= -3140.585227
Sum of electronic and thermal Free Energies= -3140.743927

5. IMI-Cu_{20} at A-position

Cu 2.131524 -0.040052 -0.000048
Cu -0.060475 0.789772 -1.354983
Cu 2.030260 -0.019291 -2.521962
Cu -0.120093 -1.547635 0.004938
Cu -0.126961 -1.450175 -2.516062
Cu 1.974987 -2.236713 -1.231560
Cu 2.081322 2.128866 -1.289558
Cu 1.926536 -2.184108 -3.695192
Cu 1.975265 -2.228941 1.245255
Cu 2.078714 4.237241 -0.013521
Cu -2.133725 -0.654313 1.255237
Cu -2.084324 1.504241 -0.004443
Cu -4.167094 0.105314 0.000182
Cu -0.126414 -1.434341 2.525262
Cu -0.060199 0.798239 1.350100
Cu 1.927352 -2.160874 3.708506
Cu 2.030809 -0.003443 2.521699
Cu 2.081590 2.136935 1.275802
Cu -0.023391 2.923292 -0.009112
Cu -2.133957 -0.662171 -1.250502
N -6.198423 0.055069 0.000093
C -7.066034 1.122868 0.000182
C -6.941257 -1.027884 -0.000153
C -8.346187 0.667402 -0.000010
H -6.707827 2.139126 0.000378
H -6.575260 -2.042224 -0.000287
H -9.293735 1.178462 -0.000018
N -8.249453 -0.704707 -0.000223
H -9.017229 -1.355660 -0.000408
Zero-point correction= 0.089706 (Hartree/Particle)
Thermal correction to Energy= 0.135076
Thermal correction to Enthalpy= 0.136021
Thermal correction to Gibbs Free Energy= -0.002513
Sum of electronic and zero-point Energies= -4148.366253
Sum of electronic and thermal Energies= -4148.320883
Sum of electronic and thermal Enthalpies= -4148.319939
Sum of electronic and thermal Free Energies= -4148.458472

6. IMI-Cu_{20} at F-position

Cu 0.846370 -1.521345 0.000010
Cu 0.838573 0.732511 -1.290792
Cu 0.887886 -1.462251 -2.537207
Cu -1.798538 0.034229 -0.000003
Cu -1.212297 0.052113 -2.515304
Cu -1.211145 -2.166336 -1.232695
Cu 2.900534 -0.767949 -1.281501
Cu -1.200196 -2.113469 -3.699601
Cu -1.211144 -2.166322 1.232721

Cu	4.896899	-0.053689	-0.000002
Cu	-1.166484	2.190689	1.280185
Cu	0.943793	2.913240	-0.000020
Cu	-1.112819	4.298158	-0.000026
Cu	-1.212298	0.052140	2.515300
Cu	0.838578	0.732534	1.290792
Cu	-1.200194	-2.113426	3.699625
Cu	0.887888	-1.462218	2.537225
Cu	2.900535	-0.767934	1.281507
Cu	2.918282	1.436038	-0.000009
Cu	-1.166485	2.190673	-1.280210
N	-3.914765	0.004772	0.000002
C	-4.762845	1.085869	-0.000007
C	-4.675063	-1.062409	0.000010
C	-6.052438	0.655507	-0.000004
H	-4.381669	2.093933	-0.000014
H	-4.320332	-2.080871	0.000018
H	-6.990728	1.183738	-0.000008
N	-5.980997	-0.718817	0.000007
H	-6.759292	-1.356550	0.000012

Zero-point correction= 0.089348 (Hartree/Particle)
Thermal correction to Energy= 0.134845
Thermal correction to Enthalpy= 0.135790
Thermal correction to Gibbs Free Energy= -0.001759
Sum of electronic and zero-point Energies= -4148.348157
Sum of electronic and thermal Energies= -4148.302659
Sum of electronic and thermal Enthalpies= -4148.301715
Sum of electronic and thermal Free Energies= -4148.439263

7. n-NHC-Au_{20} at A-position

Au	-2.588265	-4.364806	5.823026
Au	-0.080623	-4.982611	3.979941
Au	-2.258437	-3.307073	3.176320
Au	0.244241	-3.148785	6.570356
Au	0.511371	-2.183278	3.890279
Au	-1.951712	-1.573967	5.621857
Au	-2.713697	-5.970011	3.447587
Au	-1.644209	-0.614738	3.046728
Au	-2.132156	-2.674868	8.096880
Au	-3.025845	-8.684414	3.869748
Au	2.256787	-5.030647	7.452006
Au	1.967437	-6.673884	5.128013
Au	4.503485	-5.578413	5.800055
Au	0.132390	-4.496727	9.091555
Au	-0.292867	-6.277307	6.890706
Au	-2.190957	-3.951721	10.548839
Au	-2.639004	-5.629667	8.397962
Au	-2.913877	-7.191745	6.194180
Au	-0.445812	-7.779884	4.460087
Au	2.447248	-3.868196	4.838721
C	8.626052	-6.837820	5.539944
H	9.331294	-7.598624	5.253597
C	6.581012	-5.902045	5.806945
N	7.260160	-6.981559	5.377408
H	6.801284	-7.787873	4.986664
N	7.549273	-5.075606	6.243456
C	8.810214	-5.622657	6.092112
H	7.350267	-4.168228	6.631411
H	9.708874	-5.108186	6.385257

Zero-point correction= 0.084368 (Hartree/Particle)
Thermal correction to Energy= 0.134687

Thermal correction to Enthalpy= 0.135631
Thermal correction to Gibbs Free Energy= -0.032102
Sum of electronic and zero-point Energies= -2934.392949
Sum of electronic and thermal Energies= -2934.342630
Sum of electronic and thermal Enthalpies= -2934.341685
Sum of electronic and thermal Free Energies= -2934.509418

8. n-NHC-Au_{20} at F-position

Au	0.801232	-0.064065	-1.809563
Au	0.941114	1.459492	0.835719
Au	1.049069	2.813381	-1.667991
Au	-3.237306	0.877487	0.268388
Au	-1.412225	2.935609	0.043221
Au	-1.512369	1.390983	-2.491378
Au	3.189158	1.325493	-0.905982
Au	-1.223726	4.184218	-2.418172
Au	-1.667522	-1.263237	-2.410960
Au	5.257489	-0.290287	-0.011910
Au	-1.642454	-1.421894	2.398070
Au	0.883086	0.020953	3.287901
Au	-1.480153	0.139165	4.715051
Au	-1.668441	-2.833982	0.149623
Au	0.758570	-1.602265	0.910639
Au	-1.719489	-4.039619	-2.334640
Au	0.740963	-2.938666	-1.642916
Au	3.005236	-1.676809	-0.862797
Au	3.116830	-0.146365	1.746932
Au	-1.509390	1.572617	2.361392
C	-6.208834	-2.055413	-0.401134
H	-6.450580	-3.103744	-0.424497
N	-6.132005	0.125175	-0.467307
N	-4.948599	-1.590483	-0.085480
C	-6.964935	-0.965565	-0.643857
H	-8.000145	-0.868551	-0.921282
H	-6.396617	1.089276	-0.579941
C	-4.886034	-0.252106	-0.126397
H	-4.133644	-2.155754	0.134030

Zero-point correction= 0.084540 (Hartree/Particle)
Thermal correction to Energy= 0.134648
Thermal correction to Enthalpy= 0.135592
Thermal correction to Gibbs Free Energy= -0.030894
Sum of electronic and zero-point Energies= -2934.382270
Sum of electronic and thermal Energies= -2934.332162
Sum of electronic and thermal Enthalpies= -2934.331218
Sum of electronic and thermal Free Energies= -2934.497704

9. n-NHC-Ag_{20} at A-position

Ag	-2.244193	-0.041114	-0.000863
Ag	0.268535	0.903564	1.538739
Ag	-2.127695	0.016463	2.872444
Ag	0.320094	-1.766647	0.004342
Ag	0.365262	-1.637096	2.870928
Ag	-2.076042	-2.550879	1.400138
Ag	-2.173933	2.430372	1.472173
Ag	-1.986245	-2.451009	4.205092
Ag	-2.074743	-2.557203	-1.390228
Ag	-2.125960	4.814081	-0.011945
Ag	2.631177	-0.776139	-1.433094
Ag	2.584816	1.714214	-0.002459

Ag	4.943670	0.098641	0.002242
Ag	0.368004	-1.650253	-2.862786
Ag	0.270106	0.896502	-1.542309
Ag	-1.982159	-2.470235	-4.195524
Ag	-2.124829	0.003373	-2.874339
Ag	-2.172416	2.423596	-1.485102
Ag	0.271319	3.322336	-0.007331
Ag	2.629874	-0.769506	1.439445
C	9.397533	0.643004	-0.001188
H	10.234645	1.319632	-0.002799
C	7.201503	0.049962	0.001358
N	8.004130	-1.033202	0.002131
N	8.081361	1.071348	-0.000973
C	9.347840	-0.703023	0.000870
H	10.132989	-1.439330	0.001405
H	7.641783	-1.972051	0.003602
H	7.789534	2.034337	-0.002301

ero-point correction= 0.085533 (Hartree/Particle)
Thermal correction to Energy= 0.134669
Thermal correction to Enthalpy= 0.135613
Thermal correction to Gibbs Free Energy= -0.024010
Sum of electronic and zero-point Energies= -3140.620737
Sum of electronic and thermal Energies= -3140.571601
Sum of electronic and thermal Enthalpies= -3140.570656
Sum of electronic and thermal Free Energies= -3140.730280

10. n-NHC-Ag_{20} at F-position

Ag	2.063002	-0.055134	-0.185430
Ag	-0.214750	-1.669265	0.786667
Ag	2.328328	-1.724230	2.159490
Ag	-0.477240	1.730178	1.321647
Ag	-0.053569	-0.378851	3.312241
Ag	2.226802	1.237147	2.339022
Ag	2.133449	-2.948971	-0.330790
Ag	2.428566	-0.374703	4.635219
Ag	1.949086	2.775334	0.041371
Ag	1.905761	-4.155886	-2.868346
Ag	-2.735038	1.249817	-0.562396
Ag	-2.662443	-1.708250	-0.728026
Ag	-4.838029	-0.334120	0.424021
Ag	-0.604655	2.759531	-1.471600
Ag	-0.498738	-0.074987	-1.726173
Ag	1.622182	4.243957	-2.333063
Ag	1.786926	1.444828	-2.626927
Ag	1.869767	-1.337665	-2.779375
Ag	-0.413845	-2.955962	-1.804774
Ag	-2.460222	-0.349353	1.923174
C	-2.633696	5.489081	2.510295
H	-3.315074	6.260034	2.193906
C	-1.997566	5.297510	3.682665
C	-1.386157	3.600091	2.296830
N	-2.242990	4.444531	1.691366
N	-1.248088	4.143761	3.523025
H	-0.657519	3.734619	4.227392
H	-2.011429	5.867162	4.596021
H	-2.543269	4.295197	0.739858

Zero-point correction= 0.085209 (Hartree/Particle)
Thermal correction to Energy= 0.134433
Thermal correction to Enthalpy= 0.135377
Thermal correction to Gibbs Free Energy= -0.021550
Sum of electronic and zero-point Energies= -3140.607171

Sum of electronic and thermal Energies= -3140.557946
Sum of electronic and thermal Enthalpies= -3140.557002
Sum of electronic and thermal Free Energies= -3140.713929

11. n-NHC-Cu_{20} at A-position

Ag	-2.136600	-0.030163	0.000000
Ag	0.059619	0.792168	1.355516
Ag	-2.036438	-0.002844	2.520638
Ag	0.105322	-1.553154	0.000105
Ag	0.115936	-1.445166	2.521343
Ag	-1.993424	-2.222580	1.238357
Ag	-2.075054	2.141270	1.281821
Ag	-1.943526	-2.163191	3.701056
Ag	-1.993419	-2.222748	-1.238062
Ag	-2.059464	4.244931	-0.000289
Ag	2.126389	-0.670661	-1.245231
Ag	2.087972	1.480713	-0.000097
Ag	4.201656	0.083540	0.000000
Ag	0.115944	-1.445506	-2.521148
Ag	0.059621	0.791985	-1.355619
Ag	-1.943517	-2.163689	-3.700769
Ag	-2.036432	-0.003183	-2.520641
Ag	-2.075051	2.141096	-1.282112
Ag	0.036561	2.919972	-0.000195
Ag	2.126386	-0.670493	1.245326
C	8.407098	0.638263	-0.000004
H	9.243495	1.315697	-0.000008
C	6.212643	0.042659	0.000000
N	7.091460	1.066034	-0.000006
N	7.016492	-1.040828	0.000007
H	6.654059	-1.979850	0.000012
C	8.358936	-0.708253	0.000004
H	6.797885	2.028662	-0.000011
H	9.144933	-1.443571	0.000008

Zero-point correction= 0.090388 (Hartree/Particle)
Thermal correction to Energy= 0.135706
Thermal correction to Enthalpy= 0.136650
Thermal correction to Gibbs Free Energy= -0.001983
Sum of electronic and zero-point Energies= -4148.339567
Sum of electronic and thermal Energies= -4148.294249
Sum of electronic and thermal Enthalpies= -4148.293305
Sum of electronic and thermal Free Energies= -4148.431938

12. n-NHC-Cu_{20} at F-position

Ag	0.834779	-1.528552	0.000017
Ag	0.840771	0.716772	-1.280405
Ag	0.873069	-1.465770	-2.536733
Ag	-1.842438	0.071026	-0.000005
Ag	-1.217431	0.070906	-2.509124
Ag	-1.235299	-2.141294	-1.229281
Ag	2.899423	-0.795876	-1.280826
Ag	-1.230980	-2.091928	-3.695165
Ag	-1.235304	-2.141269	1.229319
Ag	4.911163	-0.105442	0.000006
Ag	-1.136631	2.206521	1.275210
Ag	0.986515	2.903053	-0.000032
Ag	-1.066191	4.313803	-0.000045
Ag	-1.217438	0.070956	2.509118
Ag	0.840771	0.716799	1.280392
Ag	-1.230990	-2.091855	3.695203

Ag	0.873062	-1.465717	2.536763
Ag	2.899421	-0.795850	1.280852
Ag	2.941265	1.399537	-0.000008
Ag	-1.136631	2.206495	-1.275260
C	-6.073107	0.588274	0.000012
H	-6.917126	1.256392	0.000021
N	-4.761668	1.029681	0.000011
N	-4.664561	-1.076405	-0.000007
C	-3.873345	0.014809	0.000000
C	-6.010762	-0.758287	0.000000
H	-6.789356	-1.501525	-0.000004
H	-4.467306	1.992486	0.000018
H	-4.275581	-2.006132	-0.000015

Zero-point correction= 0.090056 (Hartree/Particle)
Thermal correction to Energy= 0.135460
Thermal correction to Enthalpy= 0.136404
Thermal correction to Gibbs Free Energy= -0.001206
Sum of electronic and zero-point Energies= -4148.324416
Sum of electronic and thermal Energies= -4148.279011
Sum of electronic and thermal Enthalpies= -4148.278067
Sum of electronic and thermal Free Energies= -4148.415677

13. a-NHC-Au_{20} at A-position

Au	-2.603012	-4.415128	5.776413
Au	-0.025116	-4.978723	4.007019
Au	-2.249197	-3.411231	3.111584
Au	0.163272	-3.078655	6.554455
Au	0.462464	-2.167982	3.857971
Au	-2.065877	-1.609653	5.516775
Au	-2.608722	-6.081147	3.441638
Au	-1.737768	-0.702363	2.927100
Au	-2.263453	-2.654523	8.014846
Au	-2.834951	-8.794503	3.927142
Au	2.233723	-4.852772	7.526693
Au	2.046281	-6.570767	5.245123
Au	4.534018	-5.362207	5.942387
Au	0.048196	-4.363550	9.108290
Au	-0.260037	-6.209344	6.950592
Au	-2.335257	-3.867445	10.497006
Au	-2.667566	-5.614550	8.382555
Au	-2.829335	-7.240787	6.215130
Au	-0.305792	-7.777986	4.551991
Au	2.440634	-3.752401	4.901550
C	7.683858	-5.153395	6.476680
C	8.476483	-6.885804	5.357488
H	7.745880	-4.278628	7.100523
H	9.143941	-7.614014	4.928926
N	8.822675	-5.858783	6.122605
H	9.768708	-5.640846	6.393883
C	6.594828	-5.758975	5.915063
N	7.154760	-6.835539	5.228151
H	6.609500	-7.496430	4.696811

Zero-point correction= 0.084380 (Hartree/Particle)
Thermal correction to Energy= 0.134635
Thermal correction to Enthalpy= 0.135579
Thermal correction to Gibbs Free Energy= -0.030951
Sum of electronic and zero-point Energies= -2934.372071
Sum of electronic and thermal Energies= -2934.321816
Sum of electronic and thermal Enthalpies= -2934.320872
Sum of electronic and thermal Free Energies= -2934.487402

14. a-NHC-Au_{20} at F-position

Au	2.199313	-0.371529	-0.295306
Au	-0.378814	-1.678876	0.706341
Au	2.178852	-2.053874	2.004541
Au	0.571203	2.836265	2.104743
Au	-0.040960	-0.310058	3.139134
Au	2.544456	0.912799	2.264132
Au	1.823957	-3.191164	-0.434835
Au	2.400083	-0.786890	4.442389
Au	2.456408	2.475611	0.071750
Au	1.401678	-4.184650	-2.993608
Au	-2.424058	1.699369	-0.696537
Au	-2.748338	-1.286752	-0.894166
Au	-4.636037	0.373460	0.302563
Au	-0.145044	2.868828	-1.399819
Au	-0.404373	0.086831	-1.849754
Au	2.285155	3.972698	-2.239231
Au	2.111083	1.245754	-2.637867
Au	1.811254	-1.440643	-2.915526
Au	-0.738372	-2.755958	-1.954432
Au	-2.317319	0.028317	1.803576
C	-1.273192	4.855639	3.687538
C	-3.119100	4.746027	2.476335
H	-0.649145	5.189912	4.497620
H	-4.120018	4.901697	2.111446
N	-2.574162	5.314057	3.547079
H	-3.044442	5.968220	4.151876
C	-1.013921	3.979741	2.673100
N	-2.199376	3.953509	1.948215
H	-2.327794	3.374977	1.117220

Zero-point correction= 0.084447 (Hartree/Particle)
Thermal correction to Energy= 0.134518
Thermal correction to Enthalpy= 0.135463
Thermal correction to Gibbs Free Energy= -0.030714
Sum of electronic and zero-point Energies= -2934.364256
Sum of electronic and thermal Energies= -2934.314184
Sum of electronic and thermal Enthalpies= -2934.313240
Sum of electronic and thermal Free Energies= -2934.479416

15. a-NHC-Ag_{20} at A-position

Ag	-2.247570	0.048648	0.000035
Ag	0.323813	0.828743	1.539819
Ag	-2.125166	0.101626	2.874533
Ag	0.207339	-1.835406	0.006084
Ag	0.262800	-1.708154	2.872331
Ag	-2.235151	-2.462164	1.403741
Ag	-2.017830	2.509892	1.471260
Ag	-2.140198	-2.367415	4.207274
Ag	-2.235893	-2.472182	-1.385702
Ag	-1.821526	4.882048	-0.017279
Ag	2.581175	-1.000247	-1.429980
Ag	2.680972	1.487803	-0.006554
Ag	4.949100	-0.261079	-0.000694
Ag	0.261308	-1.728696	-2.861008
Ag	0.322930	0.817704	-1.546678
Ag	-2.142402	-2.397436	-4.189931
Ag	-2.126727	0.081036	-2.874782
Ag	-2.018642	2.499350	-1.488886
Ag	0.477103	3.240194	-0.012098
Ag	2.581865	-0.989990	1.434803

C	8.177963	-1.100306	-0.010787
C	9.222720	0.844646	0.008007
H	8.116817	-2.175386	-0.021632
H	9.991097	1.599206	0.015007
N	9.413844	-0.467836	-0.005337
H	10.317529	-0.914109	-0.010507
C	7.183810	-0.160237	-0.000596
N	7.906244	1.034700	0.010883
H	7.470964	1.943734	0.020299

Zero-point correction= 0.085434 (Hartree/Particle)
Thermal correction to Energy= 0.134505
Thermal correction to Enthalpy= 0.135449
Thermal correction to Gibbs Free Energy= -0.021432
Sum of electronic and zero-point Energies= -3140.597242
Sum of electronic and thermal Energies= -3140.548172
Sum of electronic and thermal Enthalpies= -3140.547228
Sum of electronic and thermal Free Energies= -3140.704109

16. a-NHC-Ag_{20} at F-position

Ag	-0.926324	0.759491	1.474149
Ag	-0.926327	0.759442	-1.474161
Ag	-1.358574	3.205890	-0.000045
Ag	2.294204	0.417936	-0.000014
Ag	1.159512	2.687898	-1.474539
Ag	1.159519	2.687943	1.474456
Ag	-3.366098	1.281053	-0.000008
Ag	0.763372	5.053461	-0.000077
Ag	1.518283	0.303148	2.841440
Ag	-5.372233	-0.706523	0.000027
Ag	1.808961	-2.251449	-1.375170
Ag	-0.676745	-1.732299	-2.885698
Ag	1.788537	-2.153436	-4.184421
Ag	1.808974	-2.251415	1.375217
Ag	-0.654327	-1.849659	0.000029
Ag	1.788569	-2.153317	4.184466
Ag	-0.676722	-1.732215	2.885748
Ag	-3.037295	-1.234701	1.485919
Ag	-3.037305	-1.234741	-1.485862
Ag	1.518267	0.303067	-2.841462
C	5.654242	0.974527	0.000010
C	6.417484	-1.098281	0.000007
H	5.743095	2.047723	0.000015
H	7.072418	-1.953165	0.000009
N	6.791696	0.175996	0.000015
H	7.748929	0.490975	0.000024
C	4.541325	0.178661	-0.000002
N	5.089126	-1.102017	-0.000003
H	4.507921	-1.932889	-0.000009

Zero-point correction= 0.085062 (Hartree/Particle)
Thermal correction to Energy= 0.134191
Thermal correction to Enthalpy= 0.135135
Thermal correction to Gibbs Free Energy= -0.020992
Sum of electronic and zero-point Energies= -3140.582430
Sum of electronic and thermal Energies= -3140.533301
Sum of electronic and thermal Enthalpies= -3140.532357
Sum of electronic and thermal Free Energies= -3140.688484

17. a-NHC-Cu_{20} at A-position

Cu	2.136447	0.103431	-0.000215
Cu	-0.121586	0.736466	-1.362505

Cu	2.034500	0.108290	-2.520352
Cu	0.020537	-1.590196	0.008212
Cu	0.003289	-1.501617	-2.514118
Cu	2.167827	-2.098906	-1.226137
Cu	1.900351	2.254121	-1.293888
Cu	2.119168	-2.057477	-3.687865
Cu	2.167349	-2.085978	1.248637
Cu	1.719112	4.356158	-0.022472
Cu	-2.069693	-0.875262	1.247340
Cu	-2.190797	1.268868	-0.007182
Cu	-4.198671	-0.277789	0.000531
Cu	0.002331	-1.475261	2.529480
Cu	-0.122160	0.750676	1.354530
Cu	2.117797	-2.018881	3.709762
Cu	2.033496	0.134611	2.519702
Cu	1.899826	2.267494	1.270814
Cu	-0.264545	2.867413	-0.015140
Cu	-2.069229	-0.888243	-1.239152
C	-7.199617	-1.137691	0.000608
C	-8.237568	0.811344	-0.000471
H	-7.140623	-2.212913	0.001113
H	-9.003769	1.568057	-0.000949
N	-8.432474	-0.501018	0.000122
H	-9.337274	-0.944918	0.000195
C	-6.201932	-0.199931	0.000307
N	-6.921338	0.998441	-0.000365
H	-6.482023	1.905812	-0.000734

Zero-point correction= 0.090269 (Hartree/Particle)
Thermal correction to Energy= 0.135550
Thermal correction to Enthalpy= 0.136494
Thermal correction to Gibbs Free Energy= -0.001034
Sum of electronic and zero-point Energies= -4148.316297
Sum of electronic and thermal Energies= -4148.271016
Sum of electronic and thermal Enthalpies= -4148.270072
Sum of electronic and thermal Free Energies= -4148.407600

18. a-NHC-Cu_{20} at F-position

Cu	0.932962	-1.472262	0.007415
Cu	0.803853	0.727549	-1.308487
Cu	1.024118	-1.479950	-2.516150
Cu	-1.872182	-0.254002	0.002175
Cu	-1.187481	-0.167434	-2.497586
Cu	-1.027873	-2.372040	-1.218359
Cu	2.971861	-0.607416	-1.270069
Cu	-0.991916	-2.319861	-3.687119
Cu	-1.026241	-2.357716	1.246155
Cu	4.910595	0.305563	-0.005601
Cu	-1.325595	1.980157	1.264456
Cu	0.704768	2.906780	-0.017920
Cu	-1.525935	4.063167	-0.023143
Cu	-1.184135	-0.138377	2.499853
Cu	0.805652	0.742734	1.297863
Cu	-0.986984	-2.276821	3.714088
Cu	1.027495	-1.450610	2.530759
Cu	2.973575	-0.592649	1.272002
Cu	2.810335	1.608543	-0.011775
Cu	-1.327346	1.965321	-1.286701
C	-4.930383	-1.073320	0.009157
C	-5.889147	0.917133	-0.001676
H	-4.913150	-2.149852	0.015383
H	-6.623933	1.704322	-0.005700

N	-6.138319	-0.387322	0.006065
H	-7.060355	-0.793456	0.009093
C	-3.897696	-0.174489	0.003193
N	-4.567875	1.050192	-0.003414
H	-4.073708	1.933285	-0.008890

Zero-point correction= 0.089924 (Hartree/Particle)
Thermal correction to Energy= 0.135294
Thermal correction to Enthalpy= 0.136238
Thermal correction to Gibbs Free Energy= -0.000881
Sum of electronic and zero-point Energies= -4148.298837
Sum of electronic and thermal Energies= -4148.253467
Sum of electronic and thermal Enthalpies= -4148.252523
Sum of electronic and thermal Free Energies= -4148.389642