SUPPORTING INFORMATION

Quantifying electronic similarities between NHC-Gold(I) complexes and their isolobal imidazolium precursors

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Table S1. Experimentally measured([a]) and DFT calculated([b]) $\delta(^{13}C^2)$, in ppm, for the set of complexes shown at Figure 1 from the main text.([c])

Code	NHC	Solvent	$\delta(^{13}C^2)$ Exp.	$\delta(^{13}C^2)$ v–sc	$\delta(^{13}C^2)$ v+c–sc	$\delta(^{13}C^2)$ v–so	$\delta(^{13}C^2)$ v+c–so
1a	IPr	$CDCl_3$	175.5	175.9	175.5	179.9	181.2
1b	SIPr	$CDCl_3$	196.1	191.4	190.9	194.5	195.6
1c	IMes	$CDCl_3$	173.4	174.5	174.0	178.0	179.1
1d	SIMes	$CDCl_3$	195.0	191.6	191.1	194.3	195.1
1e	IPr^{Cl}	$CDCl_3$	175.1	173.5	173.1	178.3	179.8
1f	IPr*	$CDCl_3$	175.2	175.7	175.5	179.1	180.2
1g	I^{t}Bu	$CDCl_3$	168.2	170.9	170.6	175.9	176.6
1h	ICy	$CDCl_3$	168.0	171.6	171.1	175.6	176.4
1i	IAd	$CDCl_3$	166.3	168.7	168.4	173.4	174.4
2a	IPr	$CDCl_3$	171.9	178.5	178.1	178.7	179.6
2b	SIPr	CD_2Cl_2	193.5	193.1	192.7	192.9	193.6
2c	IMes	C_6D_6	172.5	176.3	175.9	175.8	176.5
2d	SIMes	C_6D_6	194.4	192.4	192.0	191.4	192.0
2e	IPr^{Cl}	C_6D_6	175.0	176.3	175.9	177.3	178.3
2f	IPr*	CD_2Cl_2	172.3	177.9	177.7	177.7	178.4
2g	I^{t}Bu	C_6D_6	168.3	173.5	173.2	174.7	175.0
2h	ICy	C_6D_6	168.6	174.3	173.8	174.5	174.8
2i	IAd	C_6D_6	166.8	171.4	171.0	172.4	173.0
3a	IPr	$CDCl_3$	193.1	181.1	180.7	194.3	197.9
3b	SIPr	$CDCl_3$	212.0	196.8	196.4	208.3	211.5
3c	IMes	$CDCl_3$	191.3	179.4	179.0	192.3	195.9
3d	SIMes	$CDCl_3$	211.6	196.5	196.1	207.6	210.8
3f	IPr*	$CDCl_3$	192.6	180.2	179.9	192.3	195.8
3i	IAd	$CDCl_3$	186.6	174.7	174.5	189.2	192.9

([a])Experimental values have been obtained from refs. 39-47.

([b])'v' and 'v+c' refer to the inclusion of valence and valence plus core electrons during the calculations, and 'sc' and 'so' refer to the inclusion of relativistic scalar and spin-orbit effects, respectively. TMS has been employed as reference with σ_{ref} = 183.3, 184.1, 183.5 and 185.0 ppm for each of these methods.

([c]) For **1**, **2** and **3** types of [Au(NHC)(X)] complexes, X = Cl^-, OH^- and $CH_3COCH_2^-$, respectively. Linear correlations between experimentally measured and DFT calculated $\delta(^{13}C^2)$ are seen, with R^2 = 0.82, 0.82, 0.99 and 0.98, respectively.

Table S2. Paramagnetic, diamagnetic and spin-orbit terms for $\sigma(^{13}C^2)$, in ppm, for a set of selected NHC molecules and their [Au(NHC)(Cl)] and [NHC(H)][Cl] complexes.

Code	Species	$\sigma(^{13}C^2)$	$\sigma_{\square}(^{13}C^2)$	$\sigma_d(^{13}C^2)$	$\sigma_{SO}(^{13}C^2)$
1a	IPr	–43.1	–296.4	252.5	0.8
1b	SIPr	–57.0	–311.0	253.0	0.9
1c	IMes	–41.8	–295.2	252.6	0.8
1d	SIMes	–61.3	–314.8	252.6	0.9
1e	IPr^{Cl}	–40.7	–292.2	250.6	0.9
1g	I^tBu	–36.2	–288.1	251.1	0.8
1h	ICy	–36.6	–289.9	252.5	0.8
1i	IAd	–33.3	–285.3	251.2	0.8

Code	Species	$\sigma(^{13}C^2)$	$\sigma_{\square}(^{13}C^2)$	$\sigma_d(^{13}C^2)$	$\sigma_{SO}(^{13}C^2)$
1a	[Au(IPr)(Cl)]	3.7	–240.4	248.6	–4.5
1b	[Au(SIPr)(Cl)]	–10.7	–254.9	247.8	–3.5
1c	[Au(IMes)(Cl)]	5.9	–237.9	247.6	–3.9
1d	[Au(SIMes)(Cl)]	–10.1	–254.1	246.8	–2.8
1e	$[Au(IPr^{Cl})(Cl)]$	5.2	–235.7	246.5	–5.6
1g	$[Au(I^tBu)(Cl)]$	8.4	–233.3	246.5	–4.8
1h	[Au(ICy)(Cl)]	8.6	–234.6	247.2	–4.1
1i	[Au(IAd)(Cl)]	10.6	–231.6	247.1	–4.9

Code	Species	$\sigma(^{13}C^2)$	$\sigma_{\square}(^{13}C^2)$	$\sigma_d(^{13}C^2)$	$\sigma_{SO}(^{13}C^2)$
1a	[IPr(H)][Cl]	33.1	–206.2	238.7	0.5
1b	[SIPr(H)][Cl]	17.8	–220.7	238.1	0.4
1c	[IMes(H)][Cl]	35.9	–202.8	238.3	0.4
1d	[SIMes(H)][Cl]	18.0	–220.4	237.9	0.4
1e	$[IPr^{Cl}(H)][Cl]$	33.6	–204.8	237.6	0.7
1g	$[I^tBu(H)][Cl]$	34.6	–203.9	238.0	0.4
1h	[ICy(H)][Cl]	38.7	–201.0	239.1	0.6
1i	[IAd(H)][Cl]	35.5	–202.9	238.0	0.4

Table S3. XX, YY and ZZ terms for $\sigma_{\square}(^{13}C^{2})$, in ppm, for a set of selected NHC molecules and their [Au(NHC)(Cl)] and [NHC(H)][Cl] complexes.

Code	Species	$\sigma_{\square}(^{13}C^{2})$	$\sigma_{\square,XX}(^{13}C^{2})$	$\sigma_{\square,YY}(^{13}C^{2})$	$\sigma_{\square,ZZ}(^{13}C^{2})$
1a	IPr	–296.4	–256.8	–523.6	–109.9
1b	SIPr	–311.0	–264.0	–562.7	–108.8
1c	IMes	–295.2	–246.0	–532.1	–106.9
1d	SIMes	–314.8	–259.3	–569.9	–107.2
1e	IPr^{Cl}	–292.2	–248.8	–513.2	–115.6
1g	I^{t}Bu	–288.1	–255.9	–518.5	–89.9
1h	ICy	–289.9	–248.7	–482.6	–138.1
1i	IAd	–285.3	–254.6	–518.3	–83.4

Code	Species	$\sigma_{\square}(^{13}C^{2})$	$\sigma_{\square,XX}(^{13}C^{2})$	$\sigma_{\square,YY}(^{13}C^{2})$	$\sigma_{\square,ZZ}(^{13}C^{2})$
1a	[Au(IPr)(Cl)]	–240.4	–248.5	–348.1	–125.3
1b	[Au(SIPr)(Cl)]	–254.9	–257.8	–378.1	–128.9
1c	[Au(IMes)(Cl)]	–237.9	–237.6	–353.3	–122.8
1d	[Au(SIMes)(Cl)]	–254.1	–253.1	–381.2	–127.0
1e	[Au(IPr^{Cl})(Cl)]	–235.7	–239.4	–345.4	–123.0
1g	[Au(I^{t}Bu)(Cl)]	–233.3	–257.2	–339.5	–103.3
1h	[Au(ICy)(Cl)]	–234.6	–242.1	–320.5	–140.8
1i	[Au(IAd)(Cl)]	–231.6	–247.2	–349.2	–98.5

Code	Species	$\sigma_{\square}(^{13}C^{2})$	$\sigma_{\square,XX}(^{13}C^{2})$	$\sigma_{\square,YY}(^{13}C^{2})$	$\sigma_{\square,ZZ}(^{13}C^{2})$
1a	[IPr(H)][Cl]	–206.2	–257.2	–281.1	–81.4
1b	[SIPr(H)][Cl]	–220.7	–270.3	–300.7	–91.0
1c	[IMes(H)][Cl]	–202.8	–248.9	–284.5	–82.4
1d	[SIMes(H)][Cl]	–220.4	–266.7	–302.9	–92.6
1e	[IPr^{Cl}(H)][Cl]	–204.8	–248.3	–285.4	–80.0
1g	[I^{t}Bu(H)][Cl]	–203.9	–256.6	–272.5	–79.6
1h	[ICy(H)][Cl]	–201.0	–249.2	–267.6	–86.0
1i	[IAd(H)][Cl]	–202.9	–256.9	–273.5	–78.5

Table S4. EDA analysis (energy values in kcal mol^{-1}) for the set of complexes shown at Figure 4 from the main text.

	1	**2**	**3**	**4**	**5**	**6**	**7**
E_{elstat}	–212.1	–212.1	–213.6	–213.5	–212.3	–213.3	–201.2
E_{Pauli}	207.4	207.7	210.1	210.2	206.8	208.9	200.9
E_{steric}	–4.6	–4.4	–3.6	–3.4	–5.5	–4.3	–0.3
E_{int}	–74.6	–74.7	–75.7	–75.8	–73.9	–75.0	–75.7
$E(\sigma)$	–60.3	–60.3	–61.1	–61.0	–60.0	–60.9	–60.9
$E(\pi)$	–14.3	–14.4	–14.7	–14.7	–13.9	–14.2	–14.8
E_{bind}	–79.2	–79.1	–79.3	–79.1	–79.4	–79.4	–76.0
$\%(\sigma)$	81	81	81	81	81	81	80
$\%(\pi)$	19	19	19	19	19	19	20
σ_d	–45.2	–45.1	–45.2	–45.1	–45.2	–45.1	–44.3
π_{bd}	–13.4	–13.5	–13.8	–13.9	–13.0	–13.5	–13.8

	8	**9**	**10**	**11**	**12**	**13**	**14**
E_{elstat}	–211.6	–213.3	–213.6	–214.0	–216.3	–215.5	–222.9
E_{Pauli}	206.6	210.8	211.0	211.7	212.1	212.2	215.1
E_{steric}	–5.0	–2.5	–2.6	–2.3	–4.2	–3.2	–7.9
E_{int}	–73.8	–76.7	–77.2	–77.4	–76.3	–76.3	–73.7
$E(\sigma)$	–59.8	–61.4	–61.7	–61.8	–61.5	–61.4	–61.4
$E(\pi)$	–14.0	–15.4	–15.5	–15.6	–14.8	–15.0	–12.4
E_{bind}	–78.8	–79.2	–79.8	–79.7	–80.6	–79.6	–81.6
$\%(\sigma)$	81	80	80	80	81	80	83
$\%(\pi)$	19	20	20	20	19	20	17
σ_d	–45.0	–45.0	–45.2	–45.2	–45.4	–45.2	–45.8
π_{bd}	–13.1	–13.9	–14.1	–14.2	–13.7	–13.8	–11.4

	15	**16**	**17**	**18**	**19**
E_{elstat}	–218.4	–220.5	–220.8	–220.1	–221.9
E_{Pauli}	217.6	212.5	218.1	212.1	214.6
E_{steric}	–0.8	–8.0	–2.8	–8.0	–7.3
E_{int}	–76.5	–73.2	–76.9	–73.3	–74.0
$E(\sigma)$	–61.9	–60.7	–62.5	–60.8	–61.3
$E(\pi)$	–14.6	–12.5	–14.5	–12.5	–12.6
E_{bind}	–77.3	–81.3	–79.7	–81.3	–81.3
$\%(\sigma)$	81	83	81	83	83
$\%(\pi)$	19	17	19	17	17
σ_d	–44.8	–45.6	–45.5	–45.6	–45.6
π_{bd}	–13.2	–11.6	–13.1	–11.6	–11.9

Table S5. DFT calculated([a]) shielding, in ppm, for Au in the set of complexes shown at Figure 4 from the main text.

Code	σ(^{197}Au)	Code	σ(^{197}Au)	Code	σ(^{197}Au)	Code	σ(^{197}Au)
1	9088.6	**6**	9154.5	**11**	8983.5	**16**	9162.7
2	9083.0	**7**	9051.5	**12**	9049.7	**17**	8903.2
3	9069.1	**8**	9162.5	**13**	9032.3	**18**	9187.1
4	9066.5	**9**	8982.7	**14**	9170.7	**19**	9204.9
5	9177.3	**10**	8968.3	**15**	8918.8		

([a])Data including valence plus core electrons and relativistic spin-orbit effects.

XYZ Coordinates

Molecule 1

C	-0.484359	0.000027	0.000000
C	-0.899618	-2.462699	0.000000
C	-0.709077	-3.108935	1.236900
C	-0.709077	-3.108935	-1.236900
C	-0.318466	-4.452724	1.205608
C	-0.318466	-4.452724	-1.205608
C	-0.126403	-5.119583	0.000000
C	-0.899448	2.462779	0.000000
C	-0.708825	3.108992	-1.236900
C	-0.708825	3.108992	1.236900
C	-0.318081	4.452742	-1.205607
C	-0.318081	4.452742	1.205607
C	-0.125963	5.119587	0.000000
C	-0.881012	-2.402829	2.574426
C	-0.881012	-2.402829	-2.574426
C	-0.880783	2.402890	-2.574424
C	-0.880783	2.402890	2.574424
C	-2.655920	0.679583	0.000000
C	-2.655966	-0.679381	0.000000
C	-1.970028	-3.068429	3.435130
C	0.458508	-2.322807	3.329561
C	0.458763	2.322702	3.329496
C	-1.969682	3.068605	3.435187
C	-1.970028	-3.068429	-3.435130
C	0.458508	-2.322807	-3.329561
C	0.458763	2.322702	-3.329496
C	-1.969682	3.068605	-3.435187
N	-1.326402	-1.081018	0.000000
N	-1.326329	1.081129	0.000000
H	-0.153266	-4.981683	2.144042
H	-0.153266	-4.981683	-2.144042
H	-0.152811	4.981680	-2.144042
H	-0.152811	4.981680	2.144042
H	-1.204120	-1.372567	2.374968
H	-1.204120	-1.372567	-2.374968
H	-1.204020	1.372668	-2.374969
H	-1.204020	1.372668	2.374969
H	-3.469026	1.392762	0.000000
H	-3.469120	-1.392505	0.000000
H	-2.934777	-3.101050	2.911654
H	-1.697487	-4.099405	3.699093
H	-2.107762	-2.511412	4.371755
H	0.835420	-3.324527	3.577262
H	1.220651	-1.812514	2.727076
H	0.332660	-1.769954	4.270326
H	1.220816	1.812320	2.726973
H	0.835807	3.324376	3.577183
H	0.332892	1.769860	4.270265
H	-1.697008	4.099544	3.699157
H	-2.934449	3.101349	2.911753

H	-2.107441	2.511588	4.371808
H	-2.107762	-2.511412	-4.371755
H	-1.697487	-4.099405	-3.699093
H	-2.934777	-3.101050	-2.911654
H	1.220651	-1.812514	-2.727076
H	0.835420	-3.324527	-3.577262
H	0.332660	-1.769954	-4.270326
H	0.835807	3.324376	-3.577183
H	1.220816	1.812320	-2.726973
H	0.332892	1.769860	-4.270265
H	-2.934449	3.101349	-2.911753
H	-1.697008	4.099544	-3.699157
H	-2.107441	2.511588	-4.371808
H	0.183193	6.164860	0.000000
H	0.182631	-6.164893	0.000000
Cl	3.784846	-0.000086	0.000000
Au	1.501095	-0.000020	0.000000
	Molecule 2		
C	-0.422378	-0.000054	0.000000
C	-0.855814	-2.466767	0.000000
C	-0.681997	-3.120668	1.235733
C	-0.681997	-3.120668	-1.235733
C	-0.352152	-4.479229	1.208805
C	-0.352152	-4.479229	-1.208805
C	-0.199429	-5.153452	0.000000
C	-0.855938	2.466632	0.000000
C	-0.682167	3.120546	-1.235733
C	-0.682167	3.120546	1.235733
C	-0.352419	4.479130	-1.208805
C	-0.352419	4.479130	1.208805
C	-0.199742	5.153362	0.000000
C	-0.800880	-2.404251	2.573745
C	-0.800880	-2.404251	-2.573745
C	-0.801032	2.404130	-2.573748
C	-0.801032	2.404130	2.573748
C	-2.594852	0.678939	0.000000
C	-2.594813	-0.679169	0.000000
C	-0.940138	-7.398164	0.000000
C	-0.940656	7.398008	0.000000
C	-1.874799	-3.040295	3.473825
C	0.564490	-2.348225	3.284263
C	0.564314	2.348230	3.284321
C	-1.875041	3.040092	3.473780
C	-1.874799	-3.040295	-3.473825
C	0.564490	-2.348225	-3.284263
C	0.564314	2.348230	-3.284321
C	-1.875041	3.040092	-3.473780
N	-1.264944	-1.081143	0.000000
N	-1.265007	1.080989	0.000000
O	0.168944	-6.488624	0.000000
O	0.168509	6.488568	0.000000
H	-0.188770	-5.027060	2.136448
H	-0.188770	-5.027060	-2.136448
H	-0.189093	5.026977	-2.136448
H	-0.189093	5.026977	2.136448
H	-1.108559	-1.368971	2.375993
H	-1.108559	-1.368971	-2.375993
H	-1.108612	1.368821	-2.375995
H	-1.108612	1.368821	2.375995
H	-3.407225	1.392889	0.000000
H	-3.407144	-1.393166	0.000000
H	-0.513185	-8.406417	0.000000
H	-1.565157	-7.263028	0.897302
H	-1.565157	-7.263028	-0.897302
H	-0.513793	8.406300	0.000000
H	-1.565662	7.262817	-0.897302
H	-1.565662	7.262817	0.897302
H	-2.855204	-3.062082	2.979608
H	-1.612009	-4.072083	3.744427
H	-1.974627	-2.469232	4.406704
H	0.929819	-3.356927	3.520695
H	1.315850	-1.853390	2.655867
H	0.480505	-1.791241	4.227231
H	1.315750	1.853479	2.655948

H	0.929535	3.356964	3.520785
H	0.480346	1.791224	4.227278
H	-1.612362	4.071915	3.744355
H	-2.855434	3.061766	2.979535
H	-1.974837	2.469047	4.406674
H	-1.974627	-2.469232	-4.406704
H	-1.612009	-4.072083	-3.744427
H	-2.855204	-3.062082	-2.979608
H	1.315850	-1.853390	-2.655867
H	0.929819	-3.356927	-3.520695
H	0.480505	-1.791241	-4.227231
H	0.929535	3.356964	-3.520785
H	1.315750	1.853479	-2.655948
H	0.480346	1.791224	-4.227278
H	-2.855434	3.061766	-2.979535
H	-1.612362	4.071915	-3.744355
H	-1.974837	2.469047	-4.406674
Cl	3.846078	0.000304	0.000000
Au	1.562744	0.000062	0.000000
	Molecule 3		
C	-0.511387	-0.000038	0.000000
C	-0.853622	-2.462899	0.000000
C	-0.665537	-3.120786	1.234294
C	-0.665537	-3.120786	-1.234294
C	-0.273559	-4.463905	1.204978
C	-0.273559	-4.463905	-1.204978
C	-0.080308	-5.131564	0.000000
C	-0.854113	2.462760	0.000000
C	-0.666149	3.120680	-1.234294
C	-0.666149	3.120680	1.234294
C	-0.274394	4.463863	-1.204979
C	-0.274394	4.463863	1.204979
C	-0.081254	5.131553	0.000000
C	-0.840392	-2.417406	2.572656
C	-0.840392	-2.417406	-2.572656
C	-0.840879	2.417265	-2.572654
C	-0.840879	2.417265	2.572654
C	-2.742559	0.770026	0.000000
C	-2.742407	-0.770540	0.000000
C	-1.911060	-3.098275	3.444577
C	0.502426	-2.312184	3.318871
C	0.501960	2.312277	3.318864
C	-1.911662	3.097939	3.444584
C	-1.911060	-3.098275	-3.444577
C	0.502426	-2.312184	-3.318871
C	0.501960	2.312277	-3.318864
C	-1.911662	3.097939	-3.444584
N	-1.298968	-1.095863	0.000000
N	-1.299184	1.095635	0.000000
H	-0.107870	-4.992866	2.143600
H	-0.107870	-4.992866	-2.143600
H	-0.108789	4.992851	-2.143600
H	-0.108789	4.992851	2.143600
H	-1.177654	-1.391718	2.369927
H	-1.177654	-1.391718	-2.369927
H	-1.177964	1.391519	-2.369922
H	-1.177964	1.391519	2.369922
H	-3.225777	1.197566	-0.889116
H	-3.225777	1.197566	0.889116
H	-3.225539	-1.198177	0.889116
H	-3.225539	-1.198177	-0.889116
H	-2.876852	-3.162372	2.925192
H	-1.613923	-4.119707	3.718754
H	-2.059336	-2.535608	4.376369
H	0.899441	-3.307580	3.560834
H	1.250559	-1.787724	2.710956
H	0.374232	-1.763237	4.261742
H	1.250187	1.787961	2.710941
H	0.898792	3.307744	3.560835
H	0.373871	1.763298	4.261731
H	-1.614702	4.119421	3.718770
H	-2.877467	3.161873	2.925202
H	-2.059836	2.535237	4.376371
H	-2.059336	-2.535608	-4.376369

H	-1.613923	-4.119707	-3.718754
H	-2.876852	-3.162372	-2.925192
H	1.250559	-1.787724	-2.710956
H	0.899441	-3.307580	-3.560834
H	0.374232	-1.763237	-4.261742
H	0.898792	3.307744	-3.560835
H	1.250187	1.787961	-2.710941
H	0.373871	1.763298	-4.261731
H	-2.877467	3.161873	-2.925202
H	-1.614702	4.119421	-3.718770
H	-2.059836	2.535237	-4.376371
H	0.229032	6.176542	0.000000
H	0.230143	-6.176503	0.000000
Cl	3.761411	0.000317	0.000000
Au	1.477088	0.000145	0.000000
	Molecule 4		
C	-0.449412	0.000000	0.000000
C	-0.812463	-2.467513	0.000000
C	-0.644056	-3.133483	1.233170
C	-0.644056	-3.133483	-1.233170
C	-0.318386	-4.492912	1.208199
C	-0.318386	-4.492912	-1.208199
C	-0.167960	-5.168393	0.000000
C	-0.812547	2.467500	0.000000
C	-0.644152	3.133473	-1.233170
C	-0.644152	3.133473	1.233170
C	-0.318511	4.492909	-1.208199
C	-0.318511	4.492909	1.208199
C	-0.168097	5.168393	0.000000
C	-0.762916	-2.418736	2.571730
C	-0.762916	-2.418736	-2.571730
C	-0.762999	2.418725	-2.571730
C	-0.762999	2.418725	2.571730
C	-2.681870	0.769353	0.000000
C	-2.681843	-0.769429	0.000000
C	-0.920973	-7.408679	0.000000
C	-0.921140	7.408669	0.000000
C	-1.824873	-3.062278	3.480848
C	0.605140	-2.347648	3.275585
C	0.605055	2.347676	3.275594
C	-1.824978	3.062238	3.480842
C	-1.824873	-3.062278	-3.480848
C	0.605140	-2.347648	-3.275585
C	0.605055	2.347676	-3.275594
C	-1.824978	3.062238	-3.480842
N	-1.237910	-1.095733	0.000000
N	-1.237948	1.095706	0.000000
O	0.193488	-6.506206	0.000000
O	0.193334	6.506211	0.000000
H	-0.156829	-5.041547	2.135947
H	-0.156829	-5.041547	-2.135947
H	-0.156961	5.041546	-2.135947
H	-0.156961	5.041546	2.135947
H	-1.077065	-1.385482	2.370397
H	-1.077065	-1.385482	-2.370397
H	-1.077116	1.385461	-2.370396
H	-1.077116	1.385461	2.370396
H	-3.163938	1.197968	-0.889197
H	-3.163938	1.197968	0.889197
H	-3.163897	-1.198062	0.889197
H	-3.163897	-1.198062	-0.889197
H	-0.500685	-8.419813	0.000000
H	-1.545411	-7.269691	0.897213
H	-1.545411	-7.269691	-0.897213
H	-0.500866	8.419809	0.000000
H	-1.545576	7.269672	-0.897213
H	-1.545576	7.269672	0.897213
H	-2.806488	-3.107485	2.989801
H	-1.545446	-4.087198	3.760635
H	-1.932127	-2.484897	4.409166
H	0.981694	-3.353100	3.508588
H	1.348078	-1.845823	2.642683
H	0.521605	-1.791866	4.219426
H	1.348012	1.845874	2.642695

H	0.981578	3.353136	3.508605
H	0.521530	1.791887	4.219432
H	-1.545579	4.087167	3.760627
H	-2.806592	3.107419	2.989790
H	-1.932221	2.484857	4.409161
H	-1.932127	-2.484897	-4.409166
H	-1.545446	-4.087198	-3.760635
H	-2.806488	-3.107485	-2.989801
H	1.348078	-1.845823	-2.642683
H	0.981694	-3.353100	-3.508588
H	0.521605	-1.791866	-4.219426
H	0.981578	3.353136	-3.508605
H	1.348012	1.845874	-2.642695
H	0.521530	1.791887	-4.219432
H	-2.806592	3.107419	-2.989790
H	-1.545579	4.087167	-3.760627
H	-1.932221	2.484857	-4.409161
Cl	3.821533	0.000058	0.000000
Au	1.538380	0.000036	0.000000
	Molecule 5		
C	-2.870911	-0.679378	0.000000
C	-2.870937	0.679228	0.000000
C	-0.699405	-0.000035	0.000000
C	-1.106810	-2.457891	0.000000
C	-0.905052	-3.104009	1.229618
C	-0.905052	-3.104009	-1.229618
C	-0.498488	-4.441163	1.200774
C	-0.498488	-4.441163	-1.200774
C	-0.292794	-5.127563	0.000000
C	-1.106893	2.457804	0.000000
C	-0.905137	3.103923	-1.229618
C	-0.905137	3.103923	1.229618
C	-0.498576	4.441078	-1.200774
C	-0.498576	4.441078	1.200774
C	-0.292880	5.127478	0.000000
C	-1.076795	-2.376826	2.537003
C	-1.076795	-2.376826	-2.537003
C	0.126033	-6.575929	0.000000
C	-1.076867	2.376737	-2.537003
C	-1.076867	2.376737	2.537003
C	0.125957	6.575841	0.000000
N	-1.539941	-1.081172	0.000000
N	-1.539985	1.081072	0.000000
H	-3.684331	-1.392630	0.000000
H	-3.684386	1.392447	0.000000
H	-0.325472	-4.955103	2.147838
H	-0.325472	-4.955103	-2.147838
H	-0.325562	4.955019	-2.147837
H	-0.325562	4.955019	2.147837
H	-0.335179	-1.570552	2.630774
H	-2.069951	-1.915210	2.623734
H	-0.943757	-3.062652	3.380885
H	-2.069951	-1.915210	-2.623734
H	-0.335179	-1.570552	-2.630774
H	-0.943757	-3.062652	-3.380885
H	-0.753052	-7.238148	0.000000
H	0.720391	-6.820131	-0.889102
H	0.720391	-6.820131	0.889102
H	-0.335238	1.570475	-2.630772
H	-2.070016	1.915107	-2.623737
H	-0.943837	3.062565	-3.380884
H	-2.070016	1.915107	2.623737
H	-0.335238	1.570475	2.630772
H	-0.943837	3.062565	3.380884
H	0.720318	6.820037	-0.889101
H	-0.753122	7.238068	0.000000
H	0.720318	6.820037	0.889101
Cl	3.568385	0.000271	0.000000
Au	1.284459	0.000073	0.000000
	Molecule 6		
C	-0.721501	-0.000000	0.000000
C	-1.051081	-2.457166	0.000000
C	-0.845846	-3.112403	1.226898
C	-0.845846	-3.112403	-1.226898

C	-0.438601	-4.449289	1.200044
C	-0.438601	-4.449289	-1.200044
C	-0.234611	-5.137251	0.000000
C	-1.050939	2.457181	0.000000
C	-0.845677	3.112410	-1.226898
C	-0.845677	3.112410	1.226898
C	-0.438349	4.449271	-1.200043
C	-0.438349	4.449271	1.200043
C	-0.234319	5.137220	0.000000
C	-1.008240	-2.386826	2.536818
C	-1.008240	-2.386826	-2.536818
C	0.182163	-6.586254	0.000000
C	-1.008117	2.386848	-2.536819
C	-1.008117	2.386848	2.536819
C	0.182531	6.586201	0.000000
C	-2.951500	0.770740	0.000000
C	-2.951542	-0.770622	0.000000
N	-1.507733	-1.095972	0.000000
N	-1.507675	1.096013	0.000000
H	-0.262596	-4.962291	2.147315
H	-0.262596	-4.962291	-2.147315
H	-0.262301	4.962258	-2.147315
H	-0.262301	4.962258	2.147315
H	-0.291861	-1.556537	2.611722
H	-2.014234	-1.958968	2.652367
H	-0.833982	-3.065580	3.379239
H	-2.014234	-1.958968	-2.652367
H	-0.291861	-1.556537	-2.611722
H	-0.833982	-3.065580	-3.379239
H	-0.697668	-7.247594	0.000000
H	0.776266	-6.831454	-0.889081
H	0.776266	-6.831454	0.889081
H	-0.291778	1.556525	-2.611734
H	-2.014133	1.959040	-2.652362
H	-0.833832	3.065597	-3.379238
H	-2.014133	1.959040	2.652362
H	-0.291778	1.556525	2.611734
H	-0.833832	3.065597	3.379238
H	0.776648	6.831369	-0.889081
H	-0.697265	7.247590	0.000000
H	0.776648	6.831369	0.889081
H	-3.437841	1.196374	-0.888306
H	-3.437841	1.196374	0.888306
H	-3.437907	-1.196229	0.888306
H	-3.437907	-1.196229	-0.888306
Cl	3.549880	0.000032	0.000000
Au	1.265230	-0.000016	0.000000

Molecule 7

C	-0.129649	-0.000033	0.000000
C	-0.520568	-2.466080	0.000000
C	-0.318471	-3.106105	1.238005
C	-0.318471	-3.106105	-1.238005
C	0.099492	-4.441347	1.205908
C	0.099492	-4.441347	-1.205908
C	0.304437	-5.103671	0.000000
C	-0.521249	2.465901	0.000000
C	-0.319286	3.105965	-1.238006
C	-0.319286	3.105965	1.238006
C	0.098420	4.441287	-1.205909
C	0.098420	4.441287	1.205909
C	0.303230	5.103651	0.000000
C	-0.505534	-2.405190	2.575963
C	-0.505534	-2.405190	-2.575963
C	-0.506184	2.405000	-2.575962
C	-0.506184	2.405000	2.575962
C	-2.298116	0.682430	0.000000
C	-2.297930	-0.683091	0.000000
C	-1.568547	-3.104000	3.442944
C	0.835815	-2.283140	3.322506
C	0.835148	2.283455	3.322616
C	-1.569519	3.103435	3.442853
C	-1.568547	-3.104000	-3.442944
C	0.835815	-2.283140	-3.322506
C	0.835148	2.283455	-3.322616

C	-1.569519	3.103435	-3.442853
N	-0.964036	-1.088566	0.000000
N	-0.964337	1.088267	0.000000
H	0.274725	-4.967207	2.144107
H	0.274725	-4.967207	-2.144107
H	0.273578	4.967173	-2.144108
H	0.273578	4.967173	2.144108
H	-0.861801	-1.384979	2.379523
H	-0.861801	-1.384979	-2.379523
H	-0.862058	1.384656	-2.379509
H	-0.862058	1.384656	2.379509
H	-2.532593	-3.169290	2.922272
H	-1.260047	-4.123839	3.710134
H	-1.720365	-2.547999	4.377919
H	1.246010	-3.272941	3.565019
H	1.578208	-1.748042	2.716655
H	0.697874	-1.736916	4.265377
H	1.577808	1.748683	2.716807
H	1.244920	3.273408	3.565219
H	0.697342	1.737131	4.265448
H	-1.261415	4.123400	3.710021
H	-2.533558	3.168342	2.922122
H	-1.721182	2.547408	4.377839
H	-1.720365	-2.547999	-4.377919
H	-1.260047	-4.123839	-3.710134
H	-2.532593	-3.169290	-2.922272
H	1.578208	-1.748042	-2.716655
H	1.246010	-3.272941	-3.565019
H	0.697874	-1.736916	-4.265377
H	1.244920	3.273408	-3.565219
H	1.577808	1.748683	-2.716807
H	0.697342	1.737131	-4.265448
H	-2.533558	3.168342	-2.922122
H	-1.261415	4.123400	-3.710021
H	-1.721182	2.547408	-4.377839
H	0.632603	6.142694	0.000000
H	0.633992	-6.142656	0.000000
Cl	-3.619452	-1.759558	0.000000
Cl	-3.619917	1.758556	0.000000
Cl	4.135321	0.000741	0.000000
Au	1.854893	0.000298	0.000000
	Molecule 8		
C	-2.864209	-0.679422	0.000000
C	-2.864257	0.679116	0.000000
C	-0.691996	-0.000076	0.000000
C	-1.099226	-2.457968	0.000000
C	-0.902626	-3.099679	1.233871
C	-0.902626	-3.099679	-1.233871
C	-0.501620	-4.440093	1.207778
C	-0.501620	-4.440093	-1.207778
C	-0.304620	-5.104986	0.000000
C	-1.099371	2.457775	0.000000
C	-0.902799	3.099496	-1.233871
C	-0.902799	3.099496	1.233871
C	-0.501887	4.439938	-1.207778
C	-0.501887	4.439938	1.207778
C	-0.304929	5.104844	0.000000
C	-1.077581	-2.368104	2.538001
C	-1.077581	-2.368104	-2.538001
C	-1.077699	2.367907	-2.537999
C	-1.077699	2.367907	2.537999
N	-1.533029	-1.080762	0.000000
N	-1.533107	1.080546	0.000000
H	-3.677906	-1.392381	0.000000
H	-3.678004	1.392017	0.000000
H	-0.334622	-4.960251	2.151144
H	-0.334622	-4.960251	-2.151144
H	-0.334929	4.960109	-2.151145
H	-0.334929	4.960109	2.151145
H	-0.335573	-1.562171	2.631286
H	-2.070720	-1.905925	2.621324
H	-0.946667	-3.051812	3.383859
H	-2.070720	-1.905925	-2.621324
H	-0.335573	-1.562171	-2.631286

H	-0.946667	-3.051812	-3.383859
H	-0.335707	1.561953	-2.631228
H	-2.070847	1.905754	-2.621369
H	-0.946720	3.051599	-3.383860
H	-2.070847	1.905754	2.621369
H	-0.335707	1.561953	2.631228
H	-0.946720	3.051599	3.383860
H	0.012048	6.147576	0.000000
H	0.012442	-6.147693	0.000000
Cl	3.573913	0.000371	0.000000
Au	1.291368	0.000084	0.000000

Molecule 9

C	-0.393742	0.000690	0.000000
C	-0.837814	-2.475194	0.000000
C	-0.692405	-3.133009	1.240120
C	-0.692405	-3.133009	-1.240120
C	-0.383022	-4.499662	1.205662
C	-0.383022	-4.499662	-1.205662
C	-0.227205	-5.174532	0.000000
C	-0.833529	2.477262	0.000000
C	-0.685984	3.134588	-1.240121
C	-0.685984	3.134588	1.240121
C	-0.372645	4.500339	-1.205662
C	-0.372645	4.500339	1.205662
C	-0.215154	5.174819	0.000000
C	-0.847142	-2.413387	2.571565
C	-0.847142	-2.413387	-2.571565
C	-0.841740	2.415138	-2.571527
C	-0.841740	2.415138	2.571527
C	-2.564156	0.681476	0.000000
C	-2.565292	-0.676407	0.000000
C	-1.745865	-3.201962	3.551741
C	0.530573	-2.011545	3.171510
C	0.535351	2.009580	3.170458
C	-1.737906	3.205794	3.552369
C	-1.745865	-3.201962	-3.551741
C	0.530573	-2.011545	-3.171510
C	0.535351	2.009580	-3.170458
C	-1.737906	3.205794	-3.552369
C	-2.127185	-2.417311	-4.809534
C	-2.127185	-2.417311	4.809534
C	-2.120380	2.421926	-4.810305
C	-2.120380	2.421926	4.810305
C	1.449495	3.144491	-3.635215
C	1.441350	-3.149036	-3.636564
C	1.441350	-3.149036	3.636564
C	1.449495	3.144491	3.635215
N	-1.235678	-1.081153	0.000000
N	-1.233854	1.083927	0.000000
H	-0.269793	-5.044440	2.140700
H	-0.269793	-5.044440	-2.140700
H	-0.257682	5.044754	-2.140698
H	-0.257682	5.044754	2.140698
H	-1.367748	-1.464098	2.374706
H	-1.367748	-1.464098	-2.374706
H	-1.364857	1.467210	-2.374799
H	-1.364857	1.467210	2.374799
H	-3.376065	1.396113	0.000000
H	-3.378400	-1.389668	0.000000
H	-2.661177	-3.498302	3.016938
H	-1.255269	-4.140411	3.847828
H	1.062225	-1.411395	2.416788
H	0.339411	-1.332655	4.015798
H	1.064881	1.408191	2.415234
H	0.342963	1.330980	4.014696
H	-1.244860	4.143020	3.848256
H	-2.652826	3.504428	3.018168
H	-1.255269	-4.140411	-3.847828
H	-2.661177	-3.498302	-3.016938
H	1.062225	-1.411395	-2.416788
H	0.339411	-1.332655	-4.015798
H	1.064881	1.408191	-2.415234
H	0.342963	1.330980	-4.014696
H	-2.652826	3.504428	-3.018168

H	-1.244860	4.143020	-3.848256
H	0.027907	6.237529	0.000000
H	0.012881	-6.237919	0.000000
H	-2.824727	-2.993744	-5.431327
H	-2.618051	-1.467502	-4.552960
H	-1.252132	-2.182726	-5.429200
H	-2.618051	-1.467502	4.552960
H	-2.824727	-2.993744	5.431327
H	-1.252132	-2.182726	5.429200
H	-2.613766	1.473375	-4.553915
H	-2.816087	3.000006	-5.432625
H	-1.245516	2.185073	-5.429374
H	-2.816087	3.000006	5.432625
H	-2.613766	1.473375	4.553915
H	-1.245516	2.185073	5.429374
H	2.373428	2.728899	-4.057500
H	0.983472	3.764762	-4.413843
H	1.740477	3.800052	-2.804883
H	0.973166	-3.768239	-4.414744
H	2.366134	-2.736027	-4.059520
H	1.731079	-3.805172	-2.806244
H	2.366134	-2.736027	4.059520
H	0.973166	-3.768239	4.414744
H	1.731079	-3.805172	2.806244
H	0.983472	3.764762	4.413843
H	2.373428	2.728899	4.057500
H	1.740477	3.800052	2.804883
Cl	3.881514	-0.002472	0.000000
Au	1.595973	-0.000831	0.000000

Molecule 10

C	-0.368520	0.001500	0.000000
C	-0.832942	-2.475442	0.000000
C	-0.698908	-3.135935	1.240168
C	-0.698908	-3.135935	-1.240168
C	-0.423200	-4.509732	1.205408
C	-0.423200	-4.509732	-1.205408
C	-0.287393	-5.189100	0.000000
C	-0.804545	2.483070	0.000000
C	-0.661746	3.141705	-1.240144
C	-0.661746	3.141705	1.240144
C	-0.368106	4.511785	-1.205394
C	-0.368106	4.511785	1.205394
C	-0.223228	5.189298	0.000000
C	-0.824940	-2.411711	2.573078
C	-0.824940	-2.411711	-2.573078
C	-0.797020	2.419232	-2.573070
C	-0.797020	2.419232	2.573070
C	-2.535805	0.692280	0.000000
C	-2.543324	-0.665225	0.000000
C	-1.721777	-3.184962	3.566606
C	0.568404	-2.029097	3.148806
C	0.591515	2.025230	3.152751
C	-1.690421	3.200550	3.563478
C	-1.721777	-3.184962	-3.566606
C	0.568404	-2.029097	-3.148806
C	0.591515	2.025230	-3.152751
C	-1.690421	3.200550	-3.563478
C	-2.078287	-2.404340	-4.836039
C	-2.078287	-2.404340	4.836039
C	-2.053933	2.425250	-4.834187
C	-2.053933	2.425250	4.834187
C	1.511290	3.159861	-3.613249
C	1.480088	-3.171739	-3.605568
C	1.480088	-3.171739	3.605568
C	1.511290	3.159861	3.613249
C	-3.046123	-3.167745	-5.744305
C	-3.018214	3.196970	-5.739195
C	-3.046123	-3.167745	5.744305
C	-3.018214	3.196970	5.739195
C	2.811529	-2.652150	4.158233
C	2.835075	2.628626	4.173188
C	2.835075	2.628626	-4.173188
C	2.811529	-2.652150	-4.158233
N	-1.215577	-1.076567	0.000000

N	-1.203612	1.088841	0.000000
H	-0.321684	-5.056528	2.140580
H	-0.321684	-5.056528	-2.140580
H	-0.259978	5.057327	-2.140553
H	-0.259978	5.057327	2.140553
H	-1.333748	-1.455070	2.380644
H	-1.333748	-1.455070	-2.380644
H	-1.313026	1.466640	-2.379920
H	-1.313026	1.466640	2.379920
H	-3.344270	1.410781	0.000000
H	-3.359595	-1.374797	0.000000
H	-2.652700	-3.465360	3.047559
H	-1.244594	-4.133092	3.857387
H	1.098040	-1.438287	2.383413
H	0.405816	-1.343828	3.995528
H	1.118482	1.430365	2.388684
H	0.420678	1.340897	3.998621
H	-1.207663	4.146363	3.852615
H	-2.618680	3.485691	3.042226
H	-1.244594	-4.133092	-3.857387
H	-2.652700	-3.465360	-3.047559
H	1.098040	-1.438287	-2.383413
H	0.405816	-1.343828	-3.995528
H	1.118482	1.430365	-2.388684
H	0.420678	1.340897	-3.998621
H	-2.618680	3.485691	-3.042226
H	-1.207663	4.146363	-3.852615
H	0.002305	6.255881	0.000000
H	-0.076086	-6.258594	0.000000
H	-2.523406	-1.436158	-4.554157
H	-1.163491	-2.167209	-5.398916
H	-2.523406	-1.436158	4.554157
H	-1.163491	-2.167209	5.398916
H	-2.504838	1.459267	-4.553956
H	-1.141543	2.183596	-5.399050
H	-2.504838	1.459267	4.553956
H	-1.141543	2.183596	5.399050
H	1.009489	3.770584	-4.380938
H	1.723900	3.831825	-2.769191
H	0.976651	-3.777296	-4.376262
H	1.682061	-3.846252	-2.760887
H	0.976651	-3.777296	4.376262
H	1.682061	-3.846252	2.760887
H	1.009489	3.770584	4.380938
H	1.723900	3.831825	2.769191
H	-3.989986	-3.387376	-5.225308
H	-3.287667	-2.592881	-6.647982
H	-2.615356	-4.126614	-6.065730
H	-3.264324	2.625995	-6.644112
H	-3.960114	3.420957	-5.218491
H	-2.581954	4.154039	-6.058570
H	-3.287667	-2.592881	6.647982
H	-3.989986	-3.387376	5.225308
H	-2.615356	-4.126614	6.065730
H	-3.960114	3.420957	5.218491
H	-3.264324	2.625995	6.644112
H	-2.581954	4.154039	6.058570
H	3.459440	-3.478236	4.479764
H	3.354054	-2.075291	3.397469
H	2.653618	-1.994879	5.025333
H	3.376270	2.046240	3.415694
H	3.488780	3.449087	4.497387
H	2.666743	1.973524	5.039979
H	3.488780	3.449087	-4.497387
H	3.376270	2.046240	-3.415694
H	2.666743	1.973524	-5.039979
H	3.354054	-2.075291	-3.397469
H	3.459440	-3.478236	-4.479764
H	2.653618	-1.994879	-5.025333
Cl	3.910368	-0.019916	0.000000
Au	1.621608	-0.008688	0.000000

Molecule 11

C	-0.376364	-0.000875	0.000000
C	-0.806845	-2.479287	0.000000

C	-0.655377	-3.136403	1.240088
C	-0.655377	-3.136403	-1.240088
C	-0.330469	-4.499344	1.205062
C	-0.330469	-4.499344	-1.205062
C	-0.166156	-5.172474	0.000000
C	-0.823262	2.474384	0.000000
C	-0.674931	3.132139	-1.240085
C	-0.674931	3.132139	1.240085
C	-0.355314	4.496341	-1.205091
C	-0.355314	4.496341	1.205091
C	-0.193662	5.170100	0.000000
C	-0.821795	-2.423615	2.574940
C	-0.821795	-2.423615	-2.574940
C	-0.839393	2.418579	-2.574784
C	-0.839393	2.418579	2.574784
C	-2.548877	0.670766	0.000000
C	-2.544235	-0.687213	0.000000
C	-1.716419	-3.231489	3.543458
C	0.548923	-2.007683	3.180606
C	0.532304	2.006252	3.180585
C	-1.736761	3.223620	3.543169
C	-1.716419	-3.231489	-3.543458
C	0.548923	-2.007683	-3.180606
C	0.532304	2.006252	-3.180585
C	-1.736761	3.223620	-3.543169
C	-2.113374	-2.483357	-4.819661
C	-2.113374	-2.483357	4.819661
C	-2.133433	2.473675	-4.818413
C	-2.133433	2.473675	4.818413
C	1.462585	3.127712	-3.650552
C	1.482198	-3.126810	-3.650163
C	1.482198	-3.126810	3.650163
C	1.462585	3.127712	3.650552
C	-3.074217	-3.286294	-5.704385
C	-3.096639	3.274171	-5.702784
C	-3.074217	-3.286294	5.704385
C	-3.096639	3.274171	5.702784
C	2.780745	-2.581653	4.258593
C	2.762219	2.585674	4.259408
C	2.762219	2.585674	-4.259408
C	2.780745	-2.581653	-4.258593
C	-3.496822	2.540092	-6.984594
C	-3.473431	-2.554274	-6.987668
C	-3.496822	2.540092	6.984594
C	-3.473431	-2.554274	6.987668
C	3.732823	-3.683341	4.729187
C	3.711771	3.689546	4.729973
C	3.711771	3.689546	-4.729973
C	3.732823	-3.683341	-4.729187
N	-1.212978	-1.086773	0.000000
N	-1.220371	1.079309	0.000000
H	-0.211966	-5.042950	2.140002
H	-0.211966	-5.042950	-2.140002
H	-0.239200	5.040472	-2.140026
H	-0.239200	5.040472	2.140026
H	-1.352726	-1.479649	2.380122
H	-1.352726	-1.479649	-2.380122
H	-1.367613	1.473182	-2.379521
H	-1.367613	1.473182	2.379521
H	-3.364038	1.381652	0.000000
H	-3.354574	-1.403612	0.000000
H	-2.630832	-3.525960	3.003372
H	-1.220892	-4.172533	3.825795
H	1.076467	-1.398439	2.428676
H	0.349176	-1.332337	4.027263
H	1.061654	1.398668	2.428591
H	0.334242	1.330151	4.027033
H	-1.243647	4.165580	3.826652
H	-2.651355	3.516422	3.002486
H	-1.220892	-4.172533	-3.825795
H	-2.630832	-3.525960	-3.003372
H	1.076467	-1.398439	-2.428676
H	0.349176	-1.332337	-4.027263
H	1.061654	1.398668	-2.428591

H	0.334242	1.330151	-4.027033
H	-2.651355	3.516422	-3.002486
H	-1.243647	4.165580	-3.826652
H	0.055760	6.231333	0.000000
H	0.087673	-6.232660	0.000000
H	-2.583185	-1.521462	-4.551929
H	-1.215340	-2.231375	-5.405024
H	-2.583185	-1.521462	4.551929
H	-1.215340	-2.231375	5.405024
H	-2.601245	1.511155	-4.549405
H	-1.235523	2.222846	-5.404449
H	-2.601245	1.511155	4.549405
H	-1.235523	2.222846	5.404449
H	0.955575	3.762351	-4.396861
H	1.716775	3.783814	-2.804066
H	0.977024	-3.762737	-4.396626
H	1.737719	-3.782268	-2.803582
H	0.977024	-3.762737	4.396626
H	1.737719	-3.782268	2.803582
H	0.955575	3.762351	4.396861
H	1.716775	3.783814	2.804066
H	-3.978096	-3.534737	-5.125019
H	-2.605531	-4.249793	-5.961713
H	-4.000005	3.522092	-5.122397
H	-2.629638	4.237994	-5.961948
H	-3.978096	-3.534737	5.125019
H	-2.605531	-4.249793	5.961713
H	-4.000005	3.522092	5.122397
H	-2.629638	4.237994	5.961948
H	3.286803	-1.949196	3.513582
H	2.534572	-1.920790	5.105563
H	3.269865	1.954190	3.514644
H	2.517332	1.924447	5.106472
H	3.269865	1.954190	-3.514644
H	2.517332	1.924447	-5.106472
H	3.286803	-1.949196	-3.513582
H	2.534572	-1.920790	-5.105563
H	-3.996899	1.587971	-6.757622
H	-4.185663	3.140554	-7.593338
H	-2.617394	2.312096	-7.603264
H	-3.974875	-1.602424	-6.762601
H	-2.593345	-2.326039	-7.605314
H	-4.160696	-3.156271	-7.596674
H	-4.185663	3.140554	7.593338
H	-3.996899	1.587971	6.757622
H	-2.617394	2.312096	7.603264
H	-3.974875	-1.602424	6.762601
H	-4.160696	-3.156271	7.596674
H	-2.593345	-2.326039	7.605314
H	4.650659	-3.262239	5.160387
H	3.263842	-4.316911	5.496160
H	4.027508	-4.334968	3.894509
H	3.241238	4.322259	5.496698
H	4.630421	3.270528	5.161469
H	4.005221	4.341613	3.895208
H	4.630421	3.270528	-5.161469
H	3.241238	4.322259	-5.496698
H	4.005221	4.341613	-3.895208
H	3.263842	-4.316911	-5.496160
H	4.650659	-3.262239	-5.160387
H	4.027508	-4.334968	-3.894509
Cl	3.902027	0.013636	0.000000
Au	1.614033	0.005938	0.000000

Molecule 12

C	0.077197	0.026336	0.000000
C	-0.185737	-2.435821	0.000000
C	0.095101	-3.062528	1.228098
C	0.095101	-3.062528	-1.228098
C	0.744305	-4.300165	1.198970
C	0.744305	-4.300165	-1.198970
C	1.091228	-4.927893	0.000000
C	-0.428854	2.474128	0.000000
C	-0.252562	3.141157	-1.228546
C	-0.252562	3.141157	1.228546

C	0.064930	4.502039	-1.196894
C	0.064930	4.502039	1.196894
C	0.212536	5.205023	0.000000
C	-0.343657	-2.450240	2.556425
C	-0.343657	-2.450240	-2.556425
C	-0.368692	2.428454	-2.575813
C	-0.368692	2.428454	2.575813
C	-2.117601	0.616800	0.000000
C	-2.064317	-0.740808	0.000000
C	-1.763212	-2.892942	2.922768
C	-2.194284	-4.219217	2.782461
C	-2.666817	-1.953250	3.436172
C	-3.485308	-4.595887	3.156134
C	-3.959860	-2.324876	3.806828
C	-4.373792	-3.650435	3.670834
C	0.684005	-2.667816	3.674084
C	0.389739	-3.352760	4.857362
C	1.970439	-2.128660	3.511622
C	1.358966	-3.499614	5.855119
C	2.935230	-2.272457	4.505465
C	2.632752	-2.961059	5.683758
C	-1.763212	-2.892942	-2.922768
C	-2.666817	-1.953250	-3.436172
C	-2.194284	-4.219217	-2.782461
C	-3.959860	-2.324876	-3.806828
C	-3.485308	-4.595887	-3.156134
C	-4.373792	-3.650435	-3.670834
C	0.684005	-2.667816	-3.674084
C	1.970439	-2.128660	-3.511622
C	0.389739	-3.352760	-4.857362
C	2.935230	-2.272457	-4.505465
C	1.358966	-3.499614	-5.855119
C	2.632752	-2.961059	-5.683758
C	-1.760056	2.519563	3.207054
C	-2.768346	3.361706	2.726428
C	-2.037395	1.727531	4.333539
C	-4.019721	3.411121	3.349548
C	-3.281771	1.776019	4.957824
C	-4.281918	2.619684	4.466015
C	0.749938	2.881140	3.524534
C	2.054913	2.422198	3.295256
C	0.525726	3.764394	4.587239
C	3.109222	2.835922	4.107117
C	1.582204	4.180403	5.401859
C	2.876464	3.718013	5.165030
C	-1.760056	2.519563	-3.207054
C	-2.768346	3.361706	-2.726428
C	-2.037395	1.727531	-4.333539
C	-4.019721	3.411121	-3.349548
C	-3.281771	1.776019	-4.957824
C	-4.281918	2.619684	-4.466015
C	0.749938	2.881140	-3.524534
C	0.525726	3.764394	-4.587239
C	2.054913	2.422198	-3.295256
C	1.582204	4.180403	-5.401859
C	3.109222	2.835922	-4.107117
C	2.876464	3.718013	-5.165030
C	0.534426	6.677420	0.000000
C	1.805393	-6.255434	0.000000
N	-0.719394	-1.090572	0.000000
N	-0.803550	1.075541	0.000000
H	1.013656	-4.767917	2.146496
H	1.013656	-4.767917	-2.146496
H	0.231189	5.017325	-2.143063
H	0.231189	5.017325	2.143063
H	-0.394800	-1.361230	2.410171
H	-0.394800	-1.361230	-2.410171
H	-0.183687	1.359629	-2.388484
H	-0.183687	1.359629	2.388484
H	-2.958713	1.295613	0.000000
H	-2.849122	-1.484373	0.000000
H	-1.517663	-4.966725	2.369762
H	-2.358067	-0.912818	3.543692
H	-3.799008	-5.633382	3.039667

H	-4.645006	-1.572886	4.198330
H	-5.383441	-3.944028	3.957788
H	-0.604153	-3.771589	5.008978
H	2.219404	-1.592542	2.592848
H	1.110558	-4.036031	6.771235
H	3.925959	-1.843301	4.357828
H	3.386376	-3.072838	6.463267
H	-2.358067	-0.912818	-3.543692
H	-1.517663	-4.966725	-2.369762
H	-4.645006	-1.572886	-4.198330
H	-3.799008	-5.633382	-3.039667
H	-5.383441	-3.944028	-3.957788
H	2.219404	-1.592542	-2.592848
H	-0.604153	-3.771589	-5.008978
H	3.925959	-1.843301	-4.357828
H	1.110558	-4.036031	-6.771235
H	3.386376	-3.072838	-6.463267
H	-2.575687	3.992906	1.859591
H	-1.256563	1.080322	4.735860
H	-4.789969	4.076232	2.958377
H	-3.470474	1.155652	5.834144
H	-5.255603	2.660686	4.953849
H	2.250334	1.740538	2.463931
H	-0.482666	4.124841	4.788897
H	4.115165	2.466461	3.909556
H	1.388840	4.867221	6.226174
H	3.699995	4.040697	5.801978
H	-2.575687	3.992906	-1.859591
H	-1.256563	1.080322	-4.735860
H	-4.789969	4.076232	-2.958377
H	-3.470474	1.155652	-5.834144
H	-5.255603	2.660686	-4.953849
H	-0.482666	4.124841	-4.788897
H	2.250334	1.740538	-2.463931
H	1.388840	4.867221	-6.226174
H	4.115165	2.466461	-3.909556
H	3.699995	4.040697	-5.801978
H	1.110291	6.959845	-0.889765
H	-0.386857	7.279619	0.000000
H	1.110291	6.959845	0.889765
H	1.087152	-7.089455	0.000000
H	2.437731	-6.367169	-0.889310
H	2.437731	-6.367169	0.889310
Cl	4.352567	0.165331	0.000000
Au	2.066231	0.095016	0.000000

Molecule 13

C	0.081133	0.015634	0.000000
C	-0.227203	-2.447121	0.000000
C	0.030843	-3.080593	1.231369
C	0.030843	-3.080593	-1.231369
C	0.605408	-4.354606	1.208952
C	0.605408	-4.354606	-1.208952
C	0.895153	-4.983046	0.000000
C	-0.403959	2.471440	0.000000
C	-0.231105	3.137018	-1.231568
C	-0.231105	3.137018	1.231568
C	0.079133	4.499457	-1.207062
C	0.079133	4.499457	1.207062
C	0.215403	5.179116	0.000000
C	-0.343459	-2.432407	2.563032
C	-0.343459	-2.432407	-2.563032
C	-0.354395	2.427025	-2.579632
C	-0.354395	2.427025	2.579632
C	-2.107468	0.632788	0.000000
C	-2.070770	-0.724662	0.000000
C	0.646276	-7.336369	0.000000
C	-0.547789	7.416795	0.000000
C	-1.779033	-2.783318	2.963208
C	-2.293917	-4.081392	2.841355
C	-2.611798	-1.787567	3.490267
C	-3.597140	-4.376553	3.244478
C	-3.917044	-2.077152	3.890139
C	-4.414744	-3.375445	3.771286
C	0.695565	-2.711921	3.656790

C	0.387589	-3.375833	4.848453
C	2.010628	-2.261855	3.457897
C	1.372542	-3.591404	5.817921
C	2.991417	-2.475545	4.422983
C	2.675682	-3.144404	5.608992
C	-1.779033	-2.783318	-2.963208
C	-2.611798	-1.787567	-3.490267
C	-2.293917	-4.081392	-2.841355
C	-3.917044	-2.077152	-3.890139
C	-3.597140	-4.376553	-3.244478
C	-4.414744	-3.375445	-3.771286
C	0.695565	-2.711921	-3.656790
C	2.010628	-2.261855	-3.457897
C	0.387589	-3.375833	-4.848453
C	2.991417	-2.475545	-4.422983
C	1.372542	-3.591404	-5.817921
C	2.675682	-3.144404	-5.608992
C	-1.735365	2.569808	3.226329
C	-2.751734	3.370601	2.694685
C	-2.000455	1.862914	4.411323
C	-3.996716	3.465672	3.325002
C	-3.238304	1.957981	5.043538
C	-4.245306	2.761624	4.501312
C	0.794178	2.839320	3.510498
C	2.068267	2.299088	3.287044
C	0.628968	3.763144	4.549615
C	3.149922	2.668856	4.083830
C	1.712834	4.135205	5.349058
C	2.975593	3.589116	5.119846
C	-1.735365	2.569808	-3.226329
C	-2.751734	3.370601	-2.694685
C	-2.000455	1.862914	-4.411323
C	-3.996716	3.465672	-3.325002
C	-3.238304	1.957981	-5.043538
C	-4.245306	2.761624	-4.501312
C	0.794178	2.839320	-3.510498
C	0.628968	3.763144	-4.549615
C	2.068267	2.299088	-3.287044
C	1.712834	4.135205	-5.349058
C	3.149922	2.668856	-4.083830
C	2.975593	3.589116	-5.119846
N	-0.730182	-1.090857	0.000000
N	-0.787591	1.075801	0.000000
O	1.533151	-6.210119	0.000000
O	0.568359	6.515992	0.000000
H	0.871827	-4.848328	2.142600
H	0.871827	-4.848328	-2.142600
H	0.254933	5.033744	-2.139675
H	0.254933	5.033744	2.139675
H	-0.327085	-1.343539	2.408892
H	-0.327085	-1.343539	-2.408892
H	-0.211364	1.352472	-2.389330
H	-0.211364	1.352472	2.389330
H	-2.940579	1.321308	0.000000
H	-2.864658	-1.458442	0.000000
H	1.280498	-8.228623	0.000000
H	0.007574	-7.339834	0.897831
H	0.007574	-7.339834	-0.897831
H	-0.128130	8.427929	0.000000
H	-1.170605	7.277509	-0.898209
H	-1.170605	7.277509	0.898209
H	-1.672783	-4.871328	2.420799
H	-2.238379	-0.767365	3.586115
H	-3.975492	-5.393857	3.142456
H	-4.545651	-1.282083	4.291042
H	-5.434021	-3.604750	4.081650
H	-0.628336	-3.724649	5.028525
H	2.270194	-1.742210	2.532719
H	1.113902	-4.110869	6.740932
H	4.005604	-2.118369	4.246189
H	3.442610	-3.312641	6.364944
H	-2.238379	-0.767365	-3.586115
H	-1.672783	-4.871328	-2.420799
H	-4.545651	-1.282083	-4.291042

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H             -3.975492   -5.393857   -3.142456
H             -5.434021   -3.604750   -4.081650
H              2.270194   -1.742210   -2.532719
H             -0.628336   -3.724649   -5.028525
H              4.005604   -2.118369   -4.246189
H              1.113902   -4.110869   -6.740932
H              3.442610   -3.312641   -6.364944
H             -2.570049    3.935665    1.781230
H             -1.215363    1.247905    4.853278
H             -4.771849    4.099052    2.892993
H             -3.416178    1.406336    5.966886
H             -5.213092    2.839564    4.996256
H              2.218982    1.588045    2.470951
H             -0.354946    4.188254    4.747160
H              4.130799    2.235364    3.890664
H              1.565698    4.853575    6.155784
H              3.820247    3.878266    5.745052
H             -2.570049    3.935665   -1.781230
H             -1.215363    1.247905   -4.853278
H             -4.771849    4.099052   -2.892993
H             -3.416178    1.406336   -5.966886
H             -5.213092    2.839564   -4.996256
H             -0.354946    4.188254   -4.747160
H              2.218982    1.588045   -2.470951
H              1.565698    4.853575   -6.155784
H              4.130799    2.235364   -3.890664
H              3.820247    3.878266   -5.745052
Cl             4.356964    0.059771    0.000000
Au             2.070586    0.046491    0.000000
                 Molecule 14
C             -2.699771   -0.686522    0.000000
C             -2.699948    0.685775    0.000000
C             -0.533712   -0.000098    0.000000
C             -0.807087    2.463563    0.000000
C             -0.806449   -2.463814    0.000000
C             -1.148844    3.227461   -1.280991
C             -1.148844    3.227461    1.280991
C             -1.148007   -3.227835   -1.280979
C             -1.148007   -3.227835    1.280979
C             -3.868963    1.612737    0.000000
C             -3.868538   -1.613798    0.000000
N             -1.360018   -1.086685    0.000000
N             -1.360296    1.086282    0.000000
H             -2.208553    3.505368   -1.337054
H             -0.563433    4.155190   -1.310504
H             -0.890636    2.635965   -2.167608
H             -0.563433    4.155190    1.310504
H             -2.208553    3.505368    1.337054
H             -0.890636    2.635965    2.167608
H             -0.561901   -4.155117   -1.310764
H             -2.207526   -3.506540   -1.336727
H             -0.890515   -2.636069   -2.167623
H             -2.207526   -3.506540    1.336727
H             -0.561901   -4.155117    1.310764
H             -0.890515   -2.636069    2.167623
H              0.278097   -2.275382    0.000000
H              0.277511    2.275414    0.000000
H             -3.886347    2.260269    0.886365
H             -3.886347    2.260269   -0.886365
H             -4.799653    1.035454    0.000000
H             -3.885737   -2.261330   -0.886368
H             -3.885737   -2.261330    0.886368
H             -4.799389   -1.036774    0.000000
Cl             3.752177    0.000583    0.000000
Au             1.466455    0.000189    0.000000
                 Molecule 15
C             -3.029153   -0.682632    0.000000
C             -3.031203    0.673467    0.000000
C             -0.877942   -0.001325    0.000000
C             -1.235946    2.537874    0.000000
C             -1.228248   -2.541572    0.000000
C             -0.398852    2.768048    1.268581
C             -0.398852    2.768048   -1.268581
C             -0.390456   -2.769228    1.268583
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C	-0.390456	-2.769228	-1.268583
C	-2.417423	-3.542196	0.000000
C	-2.428113	3.534948	0.000000
N	-1.709238	-1.097067	0.000000
N	-1.712548	1.091909	0.000000
H	-3.876994	-1.347757	0.000000
H	-3.881051	1.336019	0.000000
H	0.473509	2.102507	1.298550
H	-0.044162	3.806514	1.279755
H	-1.006338	2.598835	2.167593
H	-0.044162	3.806514	-1.279755
H	0.473509	2.102507	-1.298550
H	-1.006338	2.598835	-2.167593
H	-0.032662	-3.806630	1.279759
H	0.479917	-2.101082	1.298559
H	-0.998452	-2.601834	2.167592
H	0.479917	-2.101082	-1.298559
H	-0.032662	-3.806630	-1.279759
H	-0.998452	-2.601834	-2.167592
H	-3.407584	-3.083746	0.000000
H	-2.369556	-4.186404	-0.885118
H	-2.369556	-4.186404	0.885118
H	-3.416895	3.073543	0.000000
H	-2.382189	4.179296	0.885117
H	-2.382189	4.179296	-0.885117
Cl	3.423930	0.005092	0.000000
Au	1.135596	0.001680	0.000000

Molecule 16

C	0.676880	2.757529	0.000000
C	-0.683723	2.755831	0.000000
C	-0.000771	0.597043	0.000000
C	-2.480555	0.956452	0.000000
C	2.478150	0.962628	0.000000
C	-3.223424	1.387879	-1.271743
C	-3.223424	1.387879	1.271743
C	3.219683	1.396137	-1.271691
C	3.219683	1.396137	1.271691
C	-4.659653	0.844199	1.267229
C	-4.659653	0.844199	-1.267229
C	4.657563	0.857191	-1.267149
C	4.657563	0.857191	1.267149
C	-5.417965	1.260599	0.000000
C	5.414666	1.276207	0.000000
N	1.081174	1.432771	0.000000
N	-1.084765	1.430086	0.000000
H	1.374726	3.583711	0.000000
H	-1.383612	3.580289	0.000000
H	-2.383984	-0.141047	0.000000
H	2.384239	-0.135145	0.000000
H	-3.248536	2.488998	-1.327895
H	-2.674179	1.031078	-2.154166
H	-3.248536	2.488998	1.327895
H	-2.674179	1.031078	2.154166
H	3.241262	2.497368	-1.327871
H	2.671699	1.037462	-2.154141
H	3.241262	2.497368	1.327871
H	2.671699	1.037462	2.154141
H	-5.189050	1.192306	2.165184
H	-4.627794	-0.255470	1.329851
H	-5.189050	1.192306	-2.165184
H	-4.627794	-0.255470	-1.329851
H	5.185726	1.206739	-2.165266
H	4.629459	-0.242625	-1.329472
H	5.185726	1.206739	2.165266
H	4.629459	-0.242625	1.329472
H	-5.554597	2.355219	0.000000
H	-6.424910	0.819901	0.000000
H	6.423087	0.838914	0.000000
H	5.547657	2.371287	0.000000
Cl	0.004205	-3.681553	0.000000
Au	0.001600	-1.396670	0.000000

Molecule 17

C	-2.852989	-0.679058	0.000000
C	-2.853124	0.678465	0.000000

C	-0.695573	-0.000091	0.000000
C	-1.087559	2.525808	0.000000
C	-1.087403	-2.526190	0.000000
C	-0.252386	2.815219	-1.266719
C	-0.252386	2.815219	1.266719
C	-0.252357	-2.815869	-1.266748
C	-0.252357	-2.815869	1.266748
C	-2.315584	-3.460475	0.000000
C	-2.315463	3.460471	0.000000
C	-1.852545	4.934166	0.000000
C	-1.853123	-4.934315	0.000000
C	-1.010011	-5.213132	-1.258074
C	-1.010011	-5.213132	1.258074
C	-1.009347	5.212716	1.258077
C	-1.009347	5.212716	-1.258077
C	0.216812	-4.283315	1.258723
C	0.216812	-4.283315	-1.258723
C	0.217199	4.282534	-1.258718
C	0.217199	4.282534	1.258718
C	1.067998	4.542264	0.000000
C	1.067536	-4.543277	0.000000
N	-1.529752	-1.089518	0.000000
N	-1.529956	1.089154	0.000000
H	-3.685483	-1.365365	0.000000
H	-3.685753	1.364600	0.000000
H	0.612589	2.135463	-1.292529
H	-0.864039	2.607367	-2.158852
H	0.612589	2.135463	1.292529
H	-0.864039	2.607367	2.158852
H	0.612814	-2.136364	-1.292607
H	-0.863981	-2.607870	-2.158868
H	0.612814	-2.136364	1.292607
H	-0.863981	-2.607870	2.158868
H	-2.935330	-3.272860	0.890663
H	-2.935330	-3.272860	-0.890663
H	-2.935265	3.273057	-0.890665
H	-2.935265	3.273057	0.890665
H	-2.745929	5.576549	0.000000
H	-2.746707	-5.576418	0.000000
H	-0.690795	-6.266603	-1.268622
H	-1.612948	-5.049144	-2.165274
H	-1.612948	-5.049144	2.165274
H	-0.690795	-6.266603	1.268622
H	-0.689812	6.266090	1.268633
H	-1.612330	5.048903	2.165277
H	-1.612330	5.048903	-2.165277
H	-0.689812	6.266090	-1.268633
H	0.822614	-4.463394	2.158851
H	0.822614	-4.463394	-2.158851
H	0.823057	4.462425	-2.158845
H	0.823057	4.462425	2.158845
H	1.952125	3.888005	0.000000
H	1.430807	5.581695	0.000000
H	1.951848	-3.889267	0.000000
H	1.430053	-5.582812	0.000000
Cl	3.605729	0.000801	0.000000
Au	1.314178	0.000311	0.000000

Molecule 18

C	-2.337811	-0.680436	0.000000
C	-2.337704	0.680615	0.000000
C	-0.547288	-2.487622	0.000000
C	-0.990452	-3.151204	1.325499
C	-0.990452	-3.151204	-1.325499
C	-0.232871	-4.444328	1.722656
C	-0.232871	-4.444328	-1.722656
C	-0.546881	2.487512	0.000000
C	-0.989921	3.151184	-1.325494
C	-0.989921	3.151184	1.325494
C	-0.232033	4.444123	-1.722667
C	-0.232033	4.444123	1.722667
C	-1.116997	-5.699203	-1.766917
C	-1.116997	-5.699203	1.766917
C	-1.115851	5.699213	1.766922
C	-1.115851	5.699213	-1.766922

C	-1.186817	-8.252896	1.326927
C	-1.186817	-8.252896	-1.326927
C	-1.185053	8.252916	-1.326926
C	-1.185053	8.252916	1.326926
C	-0.805284	-8.944391	0.000000
C	-0.803347	8.944316	0.000000
C	-0.178129	-0.000082	0.000000
C	-0.335698	7.022267	-1.742933
C	-0.335698	7.022267	1.742933
C	-0.337164	-7.022449	-1.742929
C	-0.337164	-7.022449	1.742929
N	-1.012905	-1.082199	0.000000
N	-1.012736	1.082167	0.000000
H	-3.162223	-1.380367	0.000000
H	-3.162007	1.380675	0.000000
H	0.550071	-2.393824	0.000000
H	-2.072535	-3.356385	1.280788
H	-0.856370	-2.394411	2.109897
H	-2.072535	-3.356385	-1.280788
H	-0.856370	-2.394411	-2.109897
H	0.245727	-4.297165	2.701224
H	0.596923	-4.617896	1.023526
H	0.245727	-4.297165	-2.701224
H	0.596923	-4.617896	-1.023526
H	0.550461	2.393521	0.000000
H	-2.071954	3.356628	-1.280762
H	-0.856037	2.394356	-2.109892
H	-2.071954	3.356628	1.280762
H	-0.856037	2.394356	2.109892
H	0.246521	4.296841	-2.701239
H	0.597811	4.617491	-1.023545
H	0.246521	4.296841	2.701239
H	0.597811	4.617491	1.023545
H	-1.768759	-5.664875	-2.654963
H	-1.800038	-5.679150	-0.906552
H	-1.768759	-5.664875	2.654963
H	-1.800038	-5.679150	0.906552
H	-1.767625	5.665047	2.654965
H	-1.798894	5.679323	0.906554
H	-1.767625	5.665047	-2.654965
H	-1.798894	5.679323	-0.906554
H	-1.124611	-9.014877	2.117255
H	-2.250372	-7.964739	1.282844
H	-1.124611	-9.014877	-2.117255
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H	-1.122667	9.014883	-2.117253
H	-2.248676	7.965013	-1.282839
H	-1.122667	9.014883	2.117253
H	-2.248676	7.965013	1.282839
H	0.278563	-9.149657	0.000000
H	-1.293211	-9.931613	0.000000
H	0.280551	9.149308	0.000000
H	-1.291027	9.931660	0.000000
H	0.113727	7.195140	-2.732061
H	0.515696	6.917645	-1.054445
H	0.113727	7.195140	2.732061
H	0.515696	6.917645	1.054445
H	0.112219	-7.195428	-2.732058
H	0.514255	-6.918034	-1.054440
H	0.112219	-7.195428	2.732058
H	0.514255	-6.918034	1.054440
Cl	4.101222	-0.000339	0.000000
Au	1.815668	-0.000205	0.000000

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C	-0.579810	-2.486772	0.000000
C	-1.003776	-3.176114	1.321784
C	-1.003776	-3.176114	-1.321784
C	-0.198279	-4.440079	1.721347
C	-0.198279	-4.440079	-1.721347
C	-0.579366	2.486562	0.000000
C	-1.003196	3.176040	-1.321749
C	-1.003196	3.176040	1.321749
C	-0.197384	4.439827	-1.721235
C	-0.197384	4.439827	1.721235

C	-1.034465	-5.727508	-1.767236
C	-1.034465	-5.727508	1.767236
C	-1.033209	5.727499	1.766983
C	-1.033209	5.727499	-1.766983
C	-1.011060	-8.281793	1.326962
C	-1.011060	-8.281793	-1.326962
C	-1.009048	8.281823	-1.326926
C	-1.009048	8.281823	1.326926
C	-0.604555	-8.958459	0.000000
C	-0.602329	8.958412	0.000000
C	-0.289755	-0.000133	0.000000
C	-0.205335	7.020903	-1.743079
C	-0.205335	7.020903	1.743079
C	-0.206963	-7.021147	-1.743205
C	-0.206963	-7.021147	1.743205
C	-2.506610	0.771448	0.000000
C	-2.506751	-0.771321	0.000000
N	-1.070558	-1.098067	0.000000
N	-1.070363	1.097938	0.000000
H	0.516475	-2.377830	0.000000
H	-2.075354	-3.430035	1.272184
H	-0.902968	-2.417791	2.110600
H	-2.075354	-3.430035	-1.272184
H	-0.902968	-2.417791	-2.110600
H	0.274558	-4.274825	2.699980
H	0.637478	-4.583174	1.022468
H	0.274558	-4.274825	-2.699980
H	0.637478	-4.583174	-1.022468
H	0.516901	2.377437	0.000000
H	-2.074710	3.430224	-1.272132
H	-0.902575	2.417721	-2.110592
H	-2.074710	3.430224	1.272132
H	-0.902575	2.417721	2.110592
H	0.275346	4.274516	-2.699909
H	0.638458	4.582634	-1.022394
H	0.275346	4.274516	2.699909
H	0.638458	4.582634	1.022394
H	-1.686528	-5.717450	-2.655869
H	-1.718699	-5.733383	-0.907586
H	-1.686528	-5.717450	2.655869
H	-1.718699	-5.733383	0.907586
H	-1.685363	5.717630	2.655550
H	-1.717355	5.733566	0.907256
H	-1.685363	5.717630	-2.655550
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H	-0.920773	-9.041309	2.117038
H	-2.084496	-8.032644	1.283194
H	-0.920773	-9.041309	-2.117038
H	-2.084496	-8.032644	-1.283194
H	-0.918528	9.041274	-2.117038
H	-2.082560	8.033002	-1.283142
H	-0.918528	9.041274	2.117038
H	-2.082560	8.033002	1.283142
H	0.486220	-9.122893	0.000000
H	-1.055308	-9.963322	0.000000
H	0.488497	9.122509	0.000000
H	-1.052781	9.963410	0.000000
H	0.249851	7.177455	-2.732332
H	0.641837	6.885472	-1.054747
H	0.249851	7.177455	2.732332
H	0.641837	6.885472	1.054747
H	0.248224	-7.177901	-2.732425
H	0.640216	-6.885910	-1.054843
H	0.248224	-7.177901	2.732425
H	0.640216	-6.885910	1.054843
H	-2.999204	1.188879	-0.888901
H	-2.999204	1.188879	0.888901
H	-2.999421	-1.188663	0.888900
H	-2.999421	-1.188663	-0.888900
Cl	3.996361	-0.000216	0.000000
Au	1.709897	-0.000239	0.000000