

Supporting information for:

**Evaluation of Ultrasmall Coinage Metal  $M_{13}(\text{dppe})_6$   $M= \text{Cu}, \text{Ag}, \text{Au}$  Clusters. Bonding, Structural and Optical Properties from Relativistic DFT Calculations**

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Table S1.  $M_{\text{central}}-M_{\text{icosahedron}}$  distances for  $M=\text{Au, Ag, and Cu}$ , in  $[\text{M}_{13}(\text{dppe})_6]^{\text{q}}$ . Distances in Angstrom ( $\text{\AA}$ ).

q=	+3	+3 Exp.	+4	+5	+5 Exp.	+5 $I_h$	+6
Au							
Au1	2.743	2.690	2.793	2.802	2.702	2.838	2.752
Au2	2.754	2.691	2.794	2.807	2.702	2.838	2.755
Au3	2.758	2.697	2.795	2.807	2.702	2.866	2.755
Au4	2.759	2.698	2.901	2.827	2.703	2.866	2.838
Au5	2.759	2.711	2.904	2.827	2.703	2.866	2.841
Au6	2.759	2.712	2.905	2.829	2.923	2.866	2.841
Au7	2.773	2.891	2.917	2.912	2.923	2.866	2.916
Au8	2.997	2.904	2.919	2.914	2.924	2.866	2.924
Au9	3.001	2.937	2.919	2.916	2.924	2.866	2.926
Au10	3.037	2.947	2.920	2.922	2.924	2.866	2.964
Au11	3.052	2.971	2.922	2.929	2.925	2.866	2.970
Au12	3.071	2.973	2.925	2.930	2.925	2.866	2.974
Average	2.872	2.819	2.885	2.869	2.832	2.861	2.871
Ag	+3	+3 Exp.	+4	+5	+5 Exp.	+5 $I_h$	+6
Ag1	2.823		2.788	2.801		2.849	2.760
Ag2	2.824		2.789	2.802		2.849	2.786
Ag3	2.824		2.793	2.802		2.884	2.801
Ag4	2.893		2.867	2.869		2.884	2.821
Ag5	2.894		2.874	2.874		2.884	2.830
Ag6	2.895		2.884	2.875		2.884	2.863
Ag7	2.899		2.907	2.903		2.884	2.882
Ag8	2.902		2.909	2.906		2.884	2.911
Ag9	2.902		2.913	2.906		2.884	2.913
Ag10	2.937		2.928	2.943		2.884	2.953
Ag11	2.938		2.933	2.946		2.884	2.956
Ag12	2.939		2.934	2.949		2.884	2.983
Average	2.889		2.877	2.881		2.878	2.872
Cu	+3	+3 Exp.	+4	+5	+5 Exp.	+5 $I_h$	+6
Cu1	2.440		2.392	2.444		2.528	2.423
Cu2	2.447		2.398	2.449		2.528	2.488
cu3	2.455		2.413	2.476		2.528	2.528
Cu4	2.461		2.470	2.486		2.528	2.583
Cu5	2.463		2.494	2.488		2.528	2.618
Cu6	2.463		2.499	2.495		2.528	2.673
Cu7	2.504		2.501	2.548		2.528	2.677
cu8	2.506		2.511	2.550		2.528	2.706
Cu9	2.509		2.539	2.570		2.528	2.712
Cu10	2.513		2.567	2.608		2.528	2.723
Cu11	2.518		2.570	2.643		2.556	2.728
Cu12	2.520		2.595	2.682		2.556	2.743

Average	2.483		2.496	2.537		2.533	2.634
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Table S2.  $M_{icosahedron}-P$  distances for  $M=Au, Ag,$  and  $Cu$ , in  $[M_{13}(dppe)_6]^q$ . Distances in Angstrom ( $\text{\AA}$ ).

q=	+3	+3 Exp.	+4	+5	+5 Exp.	+5 $I_h$	+6
Au							
Au1	2.302	2.289	2.340	2.320	2.282	2.312	2.320
Au2	2.303	2.289	2.340	2.320	2.282	2.317	2.321
Au3	2.303	2.295	2.342	2.320	2.282	2.318	2.321
Au4	2.304	2.302	2.347	2.332	2.282	2.319	2.334
Au5	2.305	2.302	2.348	2.334	2.282	2.324	2.334
Au6	2.306	2.306	2.349	2.334	2.282	2.334	2.335
Au7	2.330	2.312	2.350	2.340	2.346	2.341	2.344
Au8	2.332	2.314	2.350	2.340	2.346	2.342	2.344
Au9	2.342	2.327	2.351	2.341	2.346	2.342	2.345
Au10	2.342	2.336	2.365	2.341	2.346	2.352	2.345
Au11	2.342	2.339	2.366	2.342	2.346	2.361	2.345
Au12	2.343	2.355	2.366	2.342	2.346	2.362	2.346
Average	2.321	2.314	2.351	2.334	2.314	2.335	2.336
Ag	+3	+3 Exp.	+4	+5	+5 Exp.	+5 $I_h$	+6
Ag1	2.485		2.487	2.475		2.275	2.421
Ag2	2.486		2.487	2.476		2.445	2.436
Ag3	2.486		2.490	2.477		2.450	2.442
Ag4	2.487		2.509	2.505		2.518	2.452
Ag5	2.487		2.518	2.506		2.520	2.453
Ag6	2.487		2.519	2.508		2.567	2.466
Ag7	2.515		2.519	2.510		2.619	2.466
Ag8	2.515		2.522	2.510		2.716	2.467
Ag9	2.515		2.523	2.511		2.734	2.468
Ag10	2.522		2.525	2.512		2.773	2.473
Ag11	2.522		2.527	2.515		2.939	2.473
Ag12	2.523		2.527	2.516		3.032	2.491
Average	2.503		2.513	2.502		2.632	2.459
Cu	+3	+3 Exp.	+4	+5	+5 Exp.	+5 $I_h$	+6
Cu1	2.259		2.209	2.276		2.251	2.234
Cu2	2.265		2.233	2.289		2.258	2.239
Cu3	2.267		2.243	2.294		2.268	2.247
Cu4	2.269		2.262	2.307		2.300	2.259
Cu5	2.272		2.263	2.310		2.302	2.264
Cu6	2.276		2.264	2.314		2.314	2.278
Cu7	2.278		2.273	2.314		2.323	2.287
cu8	2.279		2.285	2.316		2.333	2.289
Cu9	2.282		2.289	2.325		2.335	2.294

Cu10	2.298		2.292	2.326		2.336	2.302
Cu11	2.304		2.294	2.330		2.358	2.310
Cu12	2.304		2.321	2.339		2.365	2.313
Average	2.279		2.269	2.312		2.312	2.276

Experimental data taken from references <sup>1</sup> for  $[\text{Au}_{13}(\text{dppe})_6]^{3+}$  and <sup>2</sup> for  $[\text{Au}_{13}(\text{dppe})_6]^{5+}$ .

Table S3. Experimental  $\text{Au}_{\text{central}}\text{-Au}_{\text{icosahedron}}$  distances for  $\text{Au}_{25}(\text{PET})_{18}$  clusters. Distances in Angstrom (Å).

q=	-1	0	1
Au1	2.766	2.785	2.820
Au2	2.779	2.786	2.743
Au3	2.789	2.760	2.822
Au4	2.759	2.814	2.817
Au5	2.783	2.775	2.806
Au6	2.771	2.779	2.839
Au7	2.779	2.775	2.817
Au8	2.789	2.779	2.806
Au9	2.759	2.786	2.839
Au10	2.783	2.760	2.743
Au11	2.771	2.814	2.822
Au12	2.766	2.785	2.820
Average	2.774	2.783	2.808

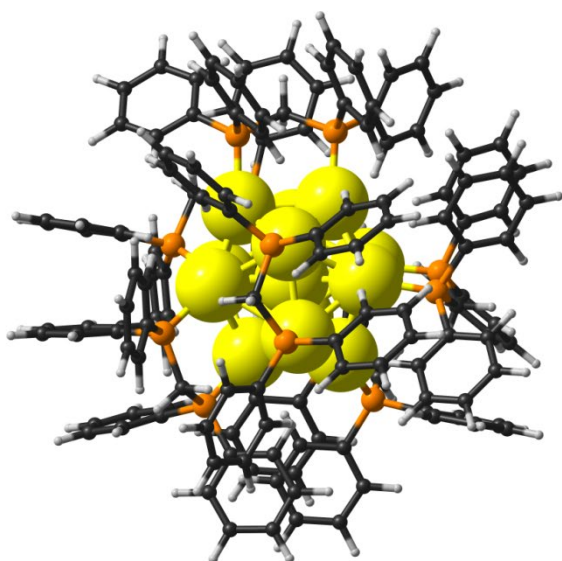
Experimental data taken from refs <sup>3,4</sup>.

## References

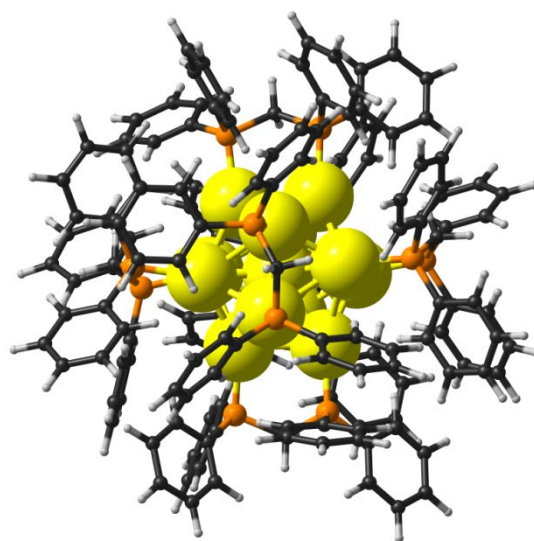
- 1 S. Jin, W. Du, S. Wang, X. Kang, M. Chen, D. Hu, S. Chen, X. Zou, G. Sun and M. Zhu, Thiol-Induced Synthesis of Phosphine-Protected Gold Nanoclusters with Atomic Precision and Controlling the Structure by Ligand/Metal Engineering, *Inorg. Chem.*, 2017, **56**, 11151–11159.
- 2 S.-S. Zhang, L. Feng, R. D. Senanayake, C. M. Aikens, X.-P. Wang, Q.-Q. Zhao, C.-H. Tung and D. Sun, Diphosphine-protected ultrasmall gold nanoclusters: opened icosahedral Au 13 and heart-shaped Au 8 clusters, *Chem. Sci.*, 2018, **9**, 1251–1258.
- 3 M. W. Heaven, A. Dass, P. S. White, K. M. Holt and R. W. Murray, Crystal structure of the gold nanoparticle  $[\text{N}(\text{C}_8\text{H}_{17})_4][\text{Au}_{25}(\text{SCH}_2\text{CH}_2\text{Ph})_{18}]$ , *J. Am. Chem. Soc.*, 2008, **130**, 3754–3755.
- 4 M. A. Tofanelli, K. Salorinne, T. W. Ni, S. Malola, B. Newell, B. Phillips, H. Häkkinen and C. J. Ackerson, Jahn-Teller effects in  $\text{Au}_{25}(\text{SR})_{18}$ , *Chem. Sci.*, 2016, **7**, 1882–1890.

Table S4. Relative energies between isomers  $D_3$  and “ $O_h$ ”.

q= +3	$D_3$	“ $O_h$ ”
Au	<b>0.00</b>	5.32
Ag	<b>0.00</b>	25.18
Cu	<b>0.00</b>	29.04
q= +5	$D_3$	$O_h$
Au	<b>0.00</b>	11.46
Ag	<b>0.00</b>	10.47
Cu	<b>0.00</b>	5.60



$D_3$



“ $O_h$ ”

Table S5. Calculated TDDFT absorption energies ( $\lambda_{\text{abs}}$ ) in eV and nm, oscillator strengths  $f$  multiplied by 10 (arbitrary units), and composition in terms of the character of involved cluster orbitals, for  $q=+5$  and  $+3$  species of  $[\text{M}_{13}(\text{dppm})_6]^q$ . Ligand based orbitals are denoted as “L”.

	$\lambda_{\text{abs}}$ (eV)	$\lambda_{\text{abs}}$ (nm)	$f \times 10$	Character	
5+					
Au	1.660	747	5.80	100%	1P $\rightarrow$ 1D
	2.409	515	5.06	71%	1P $\rightarrow$ 1D
				29%	Ligand $\rightarrow$ 1D
Ag	1.703	728	4.50	100%	1P $\rightarrow$ 1D
	2.465	503	7.32	72%	1P $\rightarrow$ 1D
				28%	Ligand $\rightarrow$ 1D
Cu	1.739	713	5.72	100%	1P $\rightarrow$ 1D
	2.495	496	10.51	70%	1P $\rightarrow$ 1D
				30%	Ligand $\rightarrow$ 1D
3+					
Au	1.596	776	0.94	100%	1Dz2 $\rightarrow$ 1D
	2.194	565	3.37	100%	1P $\rightarrow$ 1D
	2.445	506	2.79	100%	1P $\rightarrow$ 1D
Ag	1.275	972	1.80	100%	1Dz2 $\rightarrow$ 1D
	1.764	702	4.37	52%	1Dz2 $\rightarrow$ L
				48%	1P $\rightarrow$ 1D
	2.249	551	2.62	100%	1P $\rightarrow$ L
Cu	1.366	907	2.53	100%	1Dz2 $\rightarrow$ 1D
	1.776	698	4.61	60%	1Dz2 $\rightarrow$ L
				40%	1P $\rightarrow$ 1D
	2.242	553	1.93	100%	1P $\rightarrow$ L

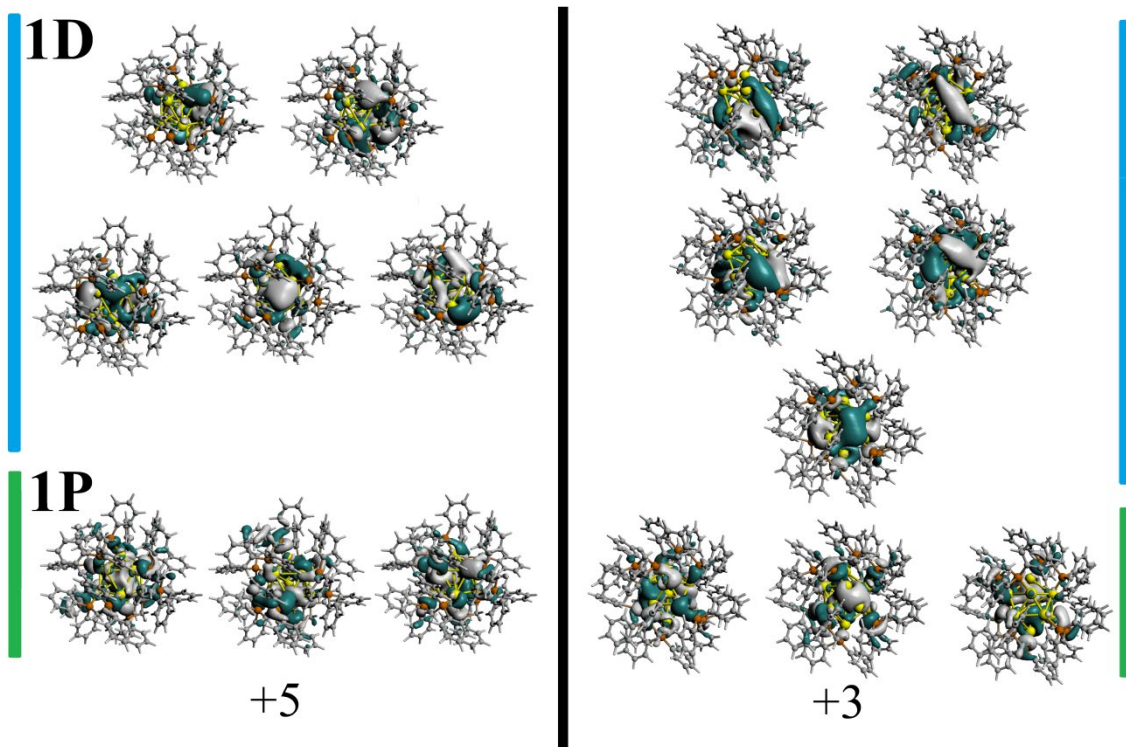


Figure S1. Isosurface at 0.01 a.u. for  $\text{Au}_{13}(\text{dppm})_6$  at +5 (left) and +3 (right) charge states.

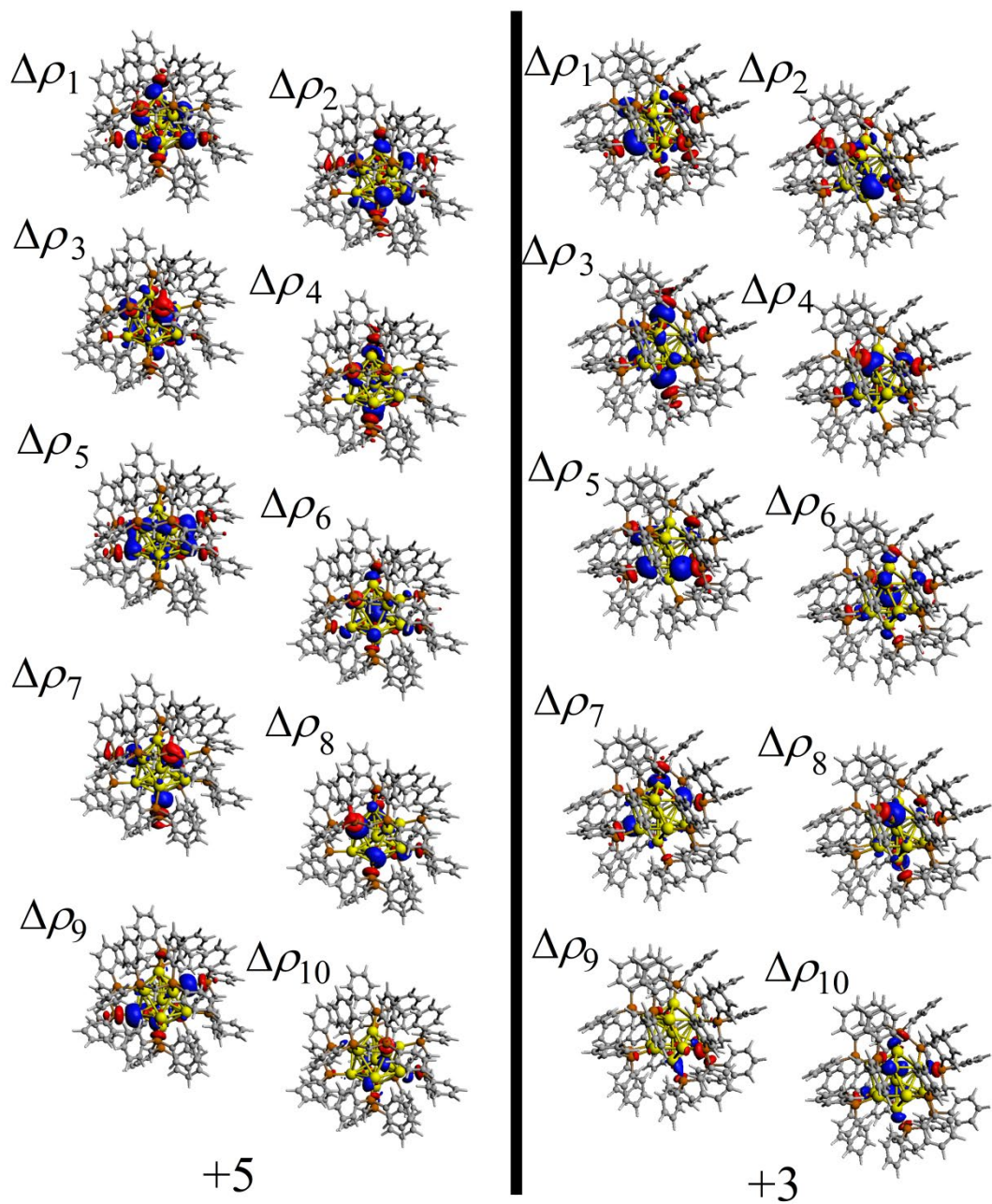


Figure S2. Deformation density channels ( $\Delta\rho$ ) for  $\text{Au}_{13}(\text{dppm})_6$  at +5 (left) and +3 (right) charge states, accounting for individual bonding patterns in the Ligand-core interaction. Isosurface set at 0.001 a.u.



Table S5. Coordinates for the studied species in a multiXYZ format. In Angstroms (Å).

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Au13 (dppm) 6 q= +5

Au	0.00000000	0.00000000	0.00000000
Au	0.04740000	-1.69470000	2.20009995
Au	2.53609991	-1.28330004	0.56699997
Au	-1.49129999	0.80629998	2.20009995
Au	-2.37949991	-1.55470002	0.56699997
Au	1.44389999	0.88840002	2.20009995
Au	-0.15670000	2.83800006	0.56699997
Au	0.04740000	1.69470000	-2.20009995
Au	2.53609991	1.28330004	-0.56699997
Au	-1.49129999	-0.80629998	-2.20009995
Au	-2.37949991	1.55470002	-0.56699997
Au	1.44389999	-0.88840002	-2.20009995
Au	-0.15670000	-2.83800006	-0.56699997
P	0.82599998	-3.53609991	3.36509991
P	3.49629998	-3.04959989	1.76440001
C	4.63210011	-4.05779982	0.76910001
C	5.39169979	-3.37809992	-0.19710000
H	5.30369997	-2.29609990	-0.29159999
C	6.23549986	-4.07950020	-1.05019999
H	6.80439997	-3.54419994	-1.81149995
C	6.34700012	-5.46560001	-0.92790002
H	7.01679993	-6.01949978	-1.58840001
C	5.61469984	-6.14219999	0.04690000
H	5.71869993	-7.22200012	0.15430000
C	4.75040007	-5.44710016	0.89190000
H	4.17210007	-6.00250006	1.62870002
C	4.39449978	-2.41709995	3.21309996
C	3.81649995	-1.37650001	3.95830011
H	2.86439991	-0.94250000	3.64709997
C	4.45429993	-0.89399999	5.09359980
H	4.00050020	-0.08640000	5.67049980
C	5.68410015	-1.42850006	5.47840023
H	6.19329977	-1.04200006	6.36289978
C	6.27059984	-2.45090008	4.73120022
H	7.23570013	-2.86240005	5.02899981
C	5.63049984	-2.95280004	3.59710002
H	6.09959984	-3.74729991	3.01329994
C	2.55640006	-3.85859990	5.57789993
H	3.00679994	-4.71040010	5.06659985
C	3.08319998	-3.45740008	6.80200005
H	3.92389989	-4.00209999	7.23169994
C	2.54809999	-2.35150003	7.46490002
H	2.97169995	-2.02950001	8.41670036
C	1.47449994	-1.65419996	6.91090012
H	1.07229996	-0.78839999	7.43730021
C	0.94260001	-2.04489994	5.68750000
H	0.11210000	-1.49179995	5.24459982
C	1.49049997	-3.14870000	5.01030016
C	-0.39950001	-4.87099981	3.53419995
C	-0.31970000	-5.80109978	4.57830000
H	0.49180001	-5.75500011	5.30590010
C	-1.30869997	-6.77519989	4.71019983
H	-1.24600005	-7.50000000	5.52360010
C	-2.37639999	-6.81790018	3.81279993
H	-3.15269995	-7.57609987	3.92869997
C	-2.46129990	-5.88530016	2.77819991
H	-3.31310010	-5.90210009	2.09730005
C	-1.48080003	-4.91109991	2.64129996
H	-1.57099998	-4.15549994	1.85810006
C	2.23169994	-4.26259995	2.39720011
H	2.72040009	-5.05259991	2.98979998
H	1.77649999	-4.74119997	1.51069999
P	-3.47530007	1.05270004	3.36509991
P	-4.38920021	-1.50310004	1.76440001

C	-5.83020020	-1.98259997	0.76910001
C	-5.62139988	-2.98029995	-0.19710000
H	-4.64029980	-3.44510007	-0.29159999
C	-6.65070009	-3.36039996	-1.05019999
H	-6.47160006	-4.12069988	-1.81149995
C	-7.90689993	-2.76379991	-0.92790002
H	-8.72150040	-3.06690001	-1.58840001
C	-8.12660027	-1.79139996	0.04690000
H	-9.11380005	-1.34150004	0.15430000
C	-7.09250021	-1.39040005	0.89190000
H	-7.28439999	-0.61180001	1.62870002
C	-4.29050016	-2.59719992	3.21309996
C	-3.10030007	-2.61689997	3.95830011
H	-2.24839997	-2.00939989	3.64709997
C	-3.00139999	-3.41059995	5.09359980
H	-2.07500005	-3.42129993	5.67049980
C	-4.07919979	-4.20830011	5.47840023
H	-3.99909997	-4.84250021	6.36289978
C	-5.25780010	-4.20499992	4.73120022
H	-6.09679985	-4.83510017	5.02899981
C	-5.37239981	-3.39980006	3.59710002
H	-6.29510021	-3.40879989	3.01329994
C	-4.61990023	-0.28459999	5.57789993
H	-5.58269978	-0.24879999	5.06659985
C	-4.53579998	-0.94139999	6.80200005
H	-5.42789984	-1.39709997	7.23169994
C	-3.31049991	-1.03100002	7.46490002
H	-3.24349999	-1.55879998	8.41670036
C	-2.16989994	-0.44990000	6.91090012
H	-1.21899998	-0.53439999	7.43730021
C	-2.24219990	0.20620000	5.68750000
H	-1.34800005	0.64880002	5.24459982
C	-3.47210002	0.28349999	5.01030016
C	-4.01870012	2.78150010	3.53419995
C	-4.86409998	3.17740011	4.57830000
H	-5.22989988	2.45149994	5.30590010
C	-5.21309996	4.52099991	4.71019983
H	-5.87220001	4.82910013	5.52360010
C	-4.71630001	5.46700001	3.81279993
H	-4.98470020	6.51830006	3.92869997
C	-3.86619997	5.07420015	2.77819991
H	-3.45479989	5.82030010	2.09730005
C	-3.51270008	3.73799992	2.64129996
H	-2.81320000	3.43829989	1.85810006
C	-4.80740023	0.19859999	2.39720011
H	-5.73589993	0.17030001	2.98979998
H	-4.99420023	0.83209997	1.51069999
P	2.64930010	2.48340011	3.36509991
P	0.89289999	4.55270004	1.76440001
C	1.19809997	6.04040003	0.76910001
C	0.22970000	6.35839987	-0.19710000
H	-0.66329998	5.74119997	-0.29159999
C	0.41520000	7.43989992	-1.05019999
H	-0.33289999	7.66489983	-1.81149995
C	1.55990005	8.22949982	-0.92790002
H	1.70469999	9.08650017	-1.58840001
C	2.51189995	7.93359995	0.04690000
H	3.39510012	8.56350040	0.15430000
C	2.34209991	6.83750010	0.89190000
H	3.11229992	6.61439991	1.62870002
C	-0.10400000	5.01420021	3.21309996
C	-0.71619999	3.99340010	3.95830011
H	-0.61589998	2.95190001	3.64709997
C	-1.45299995	4.30450010	5.09359980
H	-1.92540002	3.50769997	5.67049980
C	-1.60490000	5.63689995	5.47840023
H	-2.19420004	5.88460016	6.36289978
C	-1.01279998	6.65590000	4.73120022

H	-1.13900006	7.69750023	5.02899981
C	-0.25810000	6.35249996	3.59710002
H	0.19550000	7.15609980	3.01329994
C	2.06349993	4.14319992	5.57789993
H	2.57590008	4.95919991	5.06659985
C	1.45260000	4.39879990	6.80200005
H	1.50399995	5.39919996	7.23169994
C	0.76239997	3.38240004	7.46490002
H	0.27169999	3.58839989	8.41670036
C	0.69529998	2.10409999	6.91090012
H	0.14659999	1.32290006	7.43730021
C	1.29960001	1.83870006	5.68750000
H	1.23590004	0.84299999	5.24459982
C	1.98160005	2.86520004	5.01030016
C	4.41820002	2.08960009	3.53419995
C	5.18380022	2.62369990	4.57830000
H	4.73799992	3.30340004	5.30590010
C	6.52190018	2.25419998	4.71019983
H	7.11819983	2.67090011	5.52360010
C	7.09270000	1.35099995	3.81279993
H	8.13739967	1.05770004	3.92869997
C	6.32749987	0.81110001	2.77819991
H	6.76789999	0.08180000	2.09730005
C	4.99350023	1.17309999	2.64129996
H	4.38430023	0.71719998	1.85810006
C	2.57570004	4.06400013	2.39720011
H	3.01550007	4.88229990	2.98979998
H	3.21770000	3.90899992	1.51069999
P	0.82599998	3.53609991	-3.36509991
P	3.49629998	3.04959989	-1.76440001
C	4.63210011	4.05779982	-0.76910001
C	5.39169979	3.37809992	0.19710000
H	5.30369997	2.29609990	0.29159999
C	6.23549986	4.07950020	1.05019999
H	6.80439997	3.54419994	1.81149995
C	6.34700012	5.46560001	0.92790002
H	7.01679993	6.01949978	1.58840001
C	5.61469984	6.14219999	-0.04690000
H	5.71869993	7.22200012	-0.15430000
C	4.75040007	5.44710016	-0.89190000
H	4.17210007	6.00250006	-1.62870002
C	4.39449978	2.41709995	-3.21309996
C	3.81649995	1.37650001	-3.95830011
H	2.86439991	0.94250000	-3.64709997
C	4.45429993	0.89399999	-5.09359980
H	4.00050020	0.08640000	-5.67049980
C	5.68410015	1.42850006	-5.47840023
H	6.19329977	1.04200006	-6.36289978
C	6.27059984	2.45090008	-4.73120022
H	7.23570013	2.86240005	-5.02899981
C	5.63049984	2.95280004	-3.59710002
H	6.09959984	3.74729991	-3.01329994
C	2.55640006	3.85859990	-5.57789993
H	3.00679994	4.71040010	-5.06659985
C	3.08319998	3.45740008	-6.80200005
H	3.92389989	4.00209999	-7.23169994
C	2.54809999	2.35150003	-7.46490002
H	2.97169995	2.02950001	-8.41670036
C	1.47449994	1.65419996	-6.91090012
H	1.07229996	0.78839999	-7.43730021
C	0.94260001	2.04489994	-5.68750000
H	0.11210000	1.49179995	-5.24459982
C	1.49049997	3.14870000	-5.01030016
C	-0.39950001	4.87099981	-3.53419995
C	-0.31970000	5.80109978	-4.57830000
H	0.49180001	5.75500011	-5.30590010
C	-1.30869997	6.77519989	-4.71019983
H	-1.24600005	7.50000000	-5.52360010

C	-2.37639999	6.81790018	-3.81279993
H	-3.15269995	7.57609987	-3.92869997
C	-2.46129990	5.88530016	-2.77819991
H	-3.31310010	5.90210009	-2.09730005
C	-1.48080003	4.91109991	-2.64129996
H	-1.57099998	4.15549994	-1.85810006
C	2.23169994	4.26259995	-2.39720011
H	2.72040009	5.05259991	-2.98979998
H	1.77649999	4.74119997	-1.51069999
P	-3.47530007	-1.05270004	-3.36509991
P	-4.38920021	1.50310004	-1.76440001
C	-5.83020020	1.98259997	-0.76910001
C	-5.62139988	2.98029995	0.19710000
H	-4.64029980	3.44510007	0.29159999
C	-6.65070009	3.36039996	1.05019999
H	-6.47160006	4.12069988	1.81149995
C	-7.90689993	2.76379991	0.92790002
H	-8.72150040	3.06690001	1.58840001
C	-8.12660027	1.79139996	-0.04690000
H	-9.11380005	1.34150004	-0.15430000
C	-7.09250021	1.39040005	-0.89190000
H	-7.28439999	0.61180001	-1.62870002
C	-4.29050016	2.59719992	-3.21309996
C	-3.10030007	2.61689997	-3.95830011
H	-2.24839997	2.00939989	-3.64709997
C	-3.00139999	3.41059995	-5.09359980
H	-2.07500005	3.42129993	-5.67049980
C	-4.07919979	4.20830011	-5.47840023
H	-3.99909997	4.84250021	-6.36289978
C	-5.25780010	4.20499992	-4.73120022
H	-6.09679985	4.83510017	-5.02899981
C	-5.37239981	3.39980006	-3.59710002
H	-6.29510021	3.40879989	-3.01329994
C	-4.61990023	0.28459999	-5.57789993
H	-5.58269978	0.24879999	-5.06659985
C	-4.53579998	0.94139999	-6.80200005
H	-5.42789984	1.39709997	-7.23169994
C	-3.31049991	1.03100002	-7.46490002
H	-3.24349999	1.55879998	-8.41670036
C	-2.16989994	0.44990000	-6.91090012
H	-1.21899998	0.53439999	-7.43730021
C	-2.24219990	-0.20620000	-5.68750000
H	-1.34800005	-0.64880002	-5.24459982
C	-3.47210002	-0.28349999	-5.01030016
C	-4.01870012	-2.78150010	-3.53419995
C	-4.86409998	-3.17740011	-4.57830000
H	-5.22989988	-2.45149994	-5.30590010
C	-5.21309996	-4.52099991	-4.71019983
H	-5.87220001	-4.82910013	-5.52360010
C	-4.71630001	-5.46700001	-3.81279993
H	-4.98470020	-6.51830006	-3.92869997
C	-3.86619997	-5.07420015	-2.77819991
H	-3.45479989	-5.82030010	-2.09730005
C	-3.51270008	-3.73799992	-2.64129996
H	-2.81320000	-3.43829989	-1.85810006
C	-4.80740023	-0.19859999	-2.39720011
H	-5.73589993	-0.17030001	-2.98979998
H	-4.99420023	-0.83209997	-1.51069999
P	2.64930010	-2.48340011	-3.36509991
P	0.89289999	-4.55270004	-1.76440001
C	1.19809997	-6.04040003	-0.76910001
C	0.22970000	-6.35839987	0.19710000
H	-0.66329998	-5.74119997	0.29159999
C	0.41520000	-7.43989992	1.05019999
H	-0.33289999	-7.66489983	1.81149995
C	1.55990005	-8.22949982	0.92790002
H	1.70469999	-9.08650017	1.58840001
C	2.51189995	-7.93359995	-0.04690000

H	3.39510012	-8.56350040	-0.15430000
C	2.34209991	-6.83750010	-0.89190000
H	3.11229992	-6.61439991	-1.62870002
C	-0.10400000	-5.01420021	-3.21309996
C	-0.71619999	-3.99340010	-3.95830011
H	-0.61589998	-2.95190001	-3.64709997
C	-1.45299995	-4.30450010	-5.09359980
H	-1.92540002	-3.50769997	-5.67049980
C	-1.60490000	-5.63689995	-5.47840023
H	-2.19420004	-5.88460016	-6.36289978
C	-1.01279998	-6.65590000	-4.73120022
H	-1.13900006	-7.69750023	-5.02899981
C	-0.25810000	-6.35249996	-3.59710002
H	0.19550000	-7.15609980	-3.01329994
C	2.06349993	-4.14319992	-5.57789993
H	2.57590008	-4.95919991	-5.06659985
C	1.45260000	-4.39879990	-6.80200005
H	1.50399995	-5.39919996	-7.23169994
C	0.76239997	-3.38240004	-7.46490002
H	0.27169999	-3.58839989	-8.41670036
C	0.69529998	-2.10409999	-6.91090012
H	0.14659999	-1.32290006	-7.43730021
C	1.29960001	-1.83870006	-5.68750000
H	1.23590004	-0.84299999	-5.24459982
C	1.98160005	-2.86520004	-5.01030016
C	4.41820002	-2.08960009	-3.53419995
C	5.18380022	-2.62369990	-4.57830000
H	4.73799992	-3.30340004	-5.30590010
C	6.52190018	-2.25419998	-4.71019983
H	7.11819983	-2.67090011	-5.52360010
C	7.09270000	-1.35099995	-3.81279993
H	8.13739967	-1.05770004	-3.92869997
C	6.32749987	-0.81110001	-2.77819991
H	6.76789999	-0.08180000	-2.09730005
C	4.99350023	-1.17309999	-2.64129996
H	4.38430023	-0.71719998	-1.85810006
C	2.57570004	-4.06400013	-2.39720011
H	3.01550007	-4.88229990	-2.98979998
H	3.21770000	-3.90899992	-1.51069999

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Ag13 (dppm) 6 q= +5			
Ag	0.00000000	0.00000000	0.00000000
Ag	0.005410000	-1.71190000	2.20359993
Ag	2.53489995	-1.29639995	0.56459999
Ag	-1.50960004	0.80909997	2.20359993
Ag	-2.39010000	-1.54709995	0.56459999
Ag	1.45550001	0.90280002	2.20359993
Ag	-0.14470001	2.84340000	0.56459999
Ag	0.05410000	1.71190000	-2.20359993
Ag	2.53489995	1.29639995	-0.56459999
Ag	-1.50960004	-0.80909997	-2.20359993
Ag	-2.39010000	1.54709995	-0.56459999
Ag	1.45550001	-0.90280002	-2.20359993
Ag	-0.14470001	-2.84340000	-0.56459999
P	0.89240003	-3.66199994	3.41820002
P	3.50099993	-3.21120000	1.79770005
C	4.64440012	-4.19600010	0.78090000
C	5.37519979	-3.49830008	-0.19540000
H	5.26789999	-2.41729999	-0.28729999
C	6.22520018	-4.17600012	-1.06200004
H	6.77150011	-3.62380004	-1.82869995
C	6.36819983	-5.56050014	-0.94739997
H	7.04169989	-6.09660006	-1.61769998
C	5.66249990	-6.25570011	0.03330000
H	5.79099989	-7.33349991	0.13339999
C	4.79610014	-5.58220005	0.89420003
H	4.23990011	-6.15180016	1.63740003
C	4.44960022	-2.54760003	3.20810008

C	3.91269994	-1.46169996	3.91880012
H	2.96210003	-1.01950002	3.61170006
C	4.57859993	-0.95020002	5.02519989
H	4.15460014	-0.10970000	5.57670021
C	5.80289984	-1.49570000	5.40980005
H	6.33659983	-1.08469999	6.26789999
C	6.35400009	-2.55850005	4.69350004
H	7.31589985	-2.97819996	4.99030018
C	5.68060017	-3.09270000	3.59470010
H	6.12120008	-3.92059994	3.03570008
C	2.59470010	-3.89759994	5.67959976
H	3.00729990	-4.80760002	5.24510002
C	3.14599991	-3.41090012	6.86129999
H	3.96819997	-3.94749999	7.33440018
C	2.66050005	-2.23359990	7.42799997
H	3.10700011	-1.84599996	8.34449959
C	1.60839999	-1.54820001	6.82159996
H	1.24699998	-0.62230003	7.26819992
C	1.05289996	-2.02780008	5.64069986
H	0.23880000	-1.48249996	5.15730000
C	1.55149996	-3.20370007	5.05340004
C	-0.35080001	-4.97790003	3.61919999
C	-0.30860001	-5.89150000	4.67959976
H	0.49210000	-5.84749985	5.41970015
C	-1.31739998	-6.84490013	4.80770016
H	-1.28770006	-7.55480003	5.63590002
C	-2.36500001	-6.88910007	3.88649988
H	-3.15580010	-7.63219976	3.99970007
C	-2.41490006	-5.97359991	2.83509994
H	-3.25480008	-5.98579979	2.13980007
C	-1.41600001	-5.01630020	2.70659995
H	-1.48140001	-4.26789999	1.91320002
C	2.30830002	-4.45009995	2.50950003
H	2.82579994	-5.18359995	3.14800000
H	1.86220002	-4.99630022	1.65789998
P	-3.61759996	1.05820000	3.41820002
P	-4.53149986	-1.42639995	1.79770005
C	-5.95599985	-1.92420006	0.78090000
C	-5.71729994	-2.90590000	-0.19540000
H	-4.72739983	-3.35349989	-0.28729999
C	-6.72919989	-3.30320001	-1.06200004
H	-6.52400017	-4.05240011	-1.82869995
C	-7.99959993	-2.73469996	-0.94739997
H	-8.80070019	-3.04999995	-1.61769998
C	-8.24890041	-1.77600002	0.03330000
H	-9.24650002	-1.34840000	0.13339999
C	-7.23229980	-1.36240005	0.89420003
H	-7.44759989	-0.59590000	1.63740003
C	-4.43109989	-2.57969999	3.20810008
C	-3.22230005	-2.65759993	3.91880012
H	-2.36389995	-2.05550003	3.61170006
C	-3.11220002	-3.49009991	5.02519989
H	-2.17230010	-3.54320002	5.57670021
C	-4.19670010	-4.27759981	5.40980005
H	-4.10769987	-4.94530010	6.26789999
C	-5.39270020	-4.22349977	4.69350004
H	-6.23710012	-4.84670019	4.99030018
C	-5.51870012	-3.37319994	3.59470010
H	-6.45590019	-3.34080005	3.03570008
C	-4.67280006	-0.29820001	5.67959976
H	-5.66720009	-0.20060000	5.24510002
C	-4.52689981	-1.01900005	6.86129999
H	-5.40269995	-1.46280003	7.33440018
C	-3.26460004	-1.18719995	7.42799997
H	-3.15219998	-1.76769996	8.34449959
C	-2.14499998	-0.61879998	6.82159996
H	-1.16240001	-0.76880002	7.26819992
C	-2.28259993	0.10200000	5.64069986

H	-1.40330005	0.53450000	5.15730000
C	-3.55019999	0.25819999	5.05340004
C	-4.13549995	2.79279995	3.61919999
C	-4.94789982	3.21300006	4.67959976
H	-5.31010008	2.49749994	5.41970015
C	-5.26919985	4.56330013	4.80770016
H	-5.89879990	4.89260006	5.63590002
C	-4.78359985	5.49270010	3.88649988
H	-5.03179979	6.54909992	3.99970007
C	-3.96589994	5.07819986	2.83509994
H	-3.55640006	5.81160021	2.13980007
C	-3.63630009	3.73440003	2.70659995
H	-2.95539999	3.41689992	1.91320002
C	-5.00799990	0.22600000	2.50950003
H	-5.90210009	0.14460000	3.14800000
H	-5.25799990	0.88550001	1.65789998
P	2.72519994	2.60380006	3.41820002
P	1.03050005	4.63759995	1.79770005
C	1.31159997	6.12020016	0.78090000
C	0.34200001	6.40420008	-0.19540000
H	-0.54049999	5.77080011	-0.28729999
C	0.50389999	7.47919989	-1.06200004
H	-0.24750000	7.67619991	-1.82869995
C	1.63150001	8.29529953	-0.94739997
H	1.75890005	9.14659977	-1.61769998
C	2.58629990	8.03180027	0.03330000
H	3.45549989	8.68190002	0.13339999
C	2.43630004	6.94460011	0.89420003
H	3.20770001	6.74779987	1.63740003
C	-0.01850000	5.12729979	3.20810008
C	-0.69040000	4.11940002	3.91880012
H	-0.59820002	3.07500005	3.61170006
C	-1.46640003	4.44029999	5.02519989
H	-1.98230004	3.65280008	5.57670021
C	-1.60609996	5.77330017	5.40980005
H	-2.22889996	6.03000021	6.26789999
C	-0.96130002	6.78200006	4.69350004
H	-1.07879996	7.82480001	4.99030018
C	-0.16200000	6.46589994	3.59470010
H	0.33480000	7.26140022	3.03570008
C	2.07809997	4.19589996	5.67959976
H	2.65989995	5.00820017	5.24510002
C	1.38100004	4.42999983	6.86129999
H	1.43449998	5.41029978	7.33440018
C	0.60409999	3.42079997	7.42799997
H	0.04520000	3.61369991	8.34449959
C	0.53659999	2.16700006	6.82159996
H	-0.08460000	1.39110005	7.26819992
C	1.22959995	1.92579997	5.64069986
H	1.16450000	0.94800001	5.15730000
C	1.99880004	2.94549990	5.05340004
C	4.48640013	2.18510008	3.61919999
C	5.25649977	2.67849994	4.67959976
H	4.81799984	3.34990001	5.41970015
C	6.58650017	2.28160000	4.80770016
H	7.18650007	2.66230011	5.63590002
C	7.14870024	1.39639997	3.88649988
H	8.18750000	1.08309996	3.99970007
C	6.38079977	0.89539999	2.83509994
H	6.81120014	0.17420000	2.13980007
C	5.05219984	1.28190005	2.70659995
H	4.43690014	0.85100001	1.91320002
C	2.69970012	4.22399998	2.50950003
H	3.07629991	5.03900003	3.14800000
H	3.39580011	4.11079979	1.65789998
P	0.89240003	3.66199994	-3.41820002
P	3.50099993	3.21120000	-1.79770005
C	4.64440012	4.19600010	-0.78090000

C	5.37519979	3.49830008	0.19540000
H	5.26789999	2.41729999	0.28729999
C	6.22520018	4.17600012	1.06200004
H	6.77150011	3.62380004	1.82869995
C	6.36819983	5.56050014	0.94739997
H	7.04169989	6.09660006	1.61769998
C	5.66249990	6.25570011	-0.03330000
H	5.79099989	7.33349991	-0.13339999
C	4.79610014	5.58220005	-0.89420003
H	4.23990011	6.15180016	-1.63740003
C	4.44960022	2.54760003	-3.20810008
C	3.91269994	1.46169996	-3.91880012
H	2.96210003	1.01950002	-3.61170006
C	4.57859993	0.95020002	-5.02519989
H	4.15460014	0.10970000	-5.57670021
C	5.80289984	1.49570000	-5.40980005
H	6.33659983	1.08469999	-6.26789999
C	6.35400009	2.55850005	-4.69350004
H	7.31589985	2.97819996	-4.99030018
C	5.68060017	3.09270000	-3.59470010
H	6.12120008	3.92059994	-3.03570008
C	2.59470010	3.89759994	-5.67959976
H	3.00729990	4.80760002	-5.24510002
C	3.14599991	3.41090012	-6.86129999
H	3.96819997	3.94749999	-7.33440018
C	2.66050005	2.23359990	-7.42799997
H	3.10700011	1.84599996	-8.34449959
C	1.60839999	1.54820001	-6.82159996
H	1.24699998	0.62230003	-7.26819992
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H	0.23880000	1.48249996	-5.15730000
C	1.55149996	3.20370007	-5.05340004
C	-0.35080001	4.97790003	-3.61919999
C	-0.30860001	5.89150000	-4.67959976
H	0.49210000	5.84749985	-5.41970015
C	-1.31739998	6.84490013	-4.80770016
H	-1.28770006	7.55480003	-5.63590002
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H	-3.15580010	7.63219976	-3.99970007
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H	-3.25480008	5.98579979	-2.13980007
C	-1.41600001	5.01630020	-2.70659995
H	-1.48140001	4.26789999	-1.91320002
C	2.30830002	4.45009995	-2.50950003
H	2.82579994	5.18359995	-3.14800000
H	1.86220002	4.99630022	-1.65789998
P	-3.61759996	-1.05820000	-3.41820002
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C	-5.95599985	1.92420006	-0.78090000
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C	-6.72919989	3.30320001	1.06200004
H	-6.52400017	4.05240011	1.82869995
C	-7.99959993	2.73469996	0.94739997
H	-8.80070019	3.04999995	1.61769998
C	-8.24890041	1.77600002	-0.03330000
H	-9.24650002	1.34840000	-0.13339999
C	-7.23229980	1.36240005	-0.89420003
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H	-4.10769987	4.94530010	-6.26789999
C	-5.39270020	4.22349977	-4.69350004
H	-6.23710012	4.84670019	-4.99030018



C	-5.51870012	3.37319994	-3.59470010
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C	-4.67280006	0.29820001	-5.67959976
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C	-4.94789982	-3.21300006	-4.67959976
H	-5.31010008	-2.49749994	-5.41970015
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C	-4.78359985	-5.49270010	-3.88649988
H	-5.03179979	-6.54909992	-3.99970007
C	-3.96589994	-5.07819986	-2.83509994
H	-3.55640006	-5.81160021	-2.13980007
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H	-2.95539999	-3.41689992	-1.91320002
C	-5.00799990	-0.22600000	-2.50950003
H	-5.90210009	-0.14460000	-3.14800000
H	-5.25799990	-0.88550001	-1.65789998
P	2.72519994	-2.60380006	-3.41820002
P	1.03050005	-4.63759995	-1.79770005
C	1.31159997	-6.12020016	-0.78090000
C	0.34200001	-6.40420008	0.19540000
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C	0.50389999	-7.47919989	1.06200004
H	-0.24750000	-7.67619991	1.82869995
C	1.63150001	-8.29529953	0.94739997
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C	2.58629990	-8.03180027	-0.03330000
H	3.45549989	-8.68190002	-0.13339999
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H	3.20770001	-6.74779987	-1.63740003
C	-0.01850000	-5.12729979	-3.20810008
C	-0.69040000	-4.11940002	-3.91880012
H	-0.59820002	-3.07500005	-3.61170006
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C	-1.60609996	-5.77330017	-5.40980005
H	-2.22889996	-6.03000021	-6.26789999
C	-0.96130002	-6.78200006	-4.69350004
H	-1.07879996	-7.82480001	-4.99030018
C	-0.16200000	-6.46589994	-3.59470010
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C	2.07809997	-4.19589996	-5.67959976
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H	1.43449998	-5.41029978	-7.33440018
C	0.60409999	-3.42079997	-7.42799997
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C	0.53659999	-2.16700006	-6.82159996
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C	1.99880004	-2.94549990	-5.05340004
C	4.48640013	-2.18510008	-3.61919999
C	5.25649977	-2.67849994	-4.67959976
H	4.81799984	-3.34990001	-5.41970015
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C	7.14870024	-1.39639997	-3.88649988

H	8.18750000	-1.08309996	-3.99970007
C	6.38079977	-0.89539999	-2.83509994
H	6.81120014	-0.17420000	-2.13980007
C	5.05219984	-1.28190005	-2.70659995
H	4.43690014	-0.85100001	-1.91320002
C	2.69970012	-4.22399998	-2.50950003
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Cu13 (dppm) 6 q= +5			
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Cu	-0.01210000	-1.47790003	1.90520000
Cu	2.11899996	-1.17250001	0.52480000
Cu	-1.27380002	0.74940002	1.90520000
Cu	-2.07489991	-1.24880004	0.52480000
Cu	1.28590000	0.72839999	1.90520000
Cu	-0.04400000	2.42140007	0.52480000
Cu	-0.01210000	1.47790003	-1.90520000
Cu	2.11899996	1.17250001	-0.52480000
Cu	-1.27380002	-0.74940002	-1.90520000
Cu	-2.07489991	1.24880004	-0.52480000
Cu	1.28590000	-0.72839999	-1.90520000
Cu	-0.04400000	-2.42140007	-0.52480000
P	0.53090000	-3.33690000	3.06870008
P	3.19370008	-2.84699988	1.68910003
C	4.45069981	-3.74519992	0.73780000
C	5.30660009	-2.95799994	-0.04380000
H	5.19479990	-1.87479997	-0.03650000
C	6.26219988	-3.55170012	-0.85810000
H	6.90450001	-2.93169999	-1.48430002
C	6.38549995	-4.94280005	-0.87390000
H	7.13749981	-5.41629982	-1.50689995
C	5.56220007	-5.72870016	-0.06720000
H	5.68319988	-6.81269979	-0.06120000
C	4.59030008	-5.13649988	0.73809999
H	3.94740009	-5.76630020	1.35060000
C	4.02899981	-2.37540007	3.23469996
C	3.48449993	-1.35679996	4.02419996
H	2.58590007	-0.84009999	3.67869997
C	4.08239985	-1.00730002	5.22720003
H	3.66400003	-0.20649999	5.83820009
C	5.23519993	-1.67279994	5.64529991
H	5.71260023	-1.39359999	6.58570004
C	5.78480005	-2.68689990	4.86170006
H	6.68959999	-3.20160007	5.18739986
C	5.18839979	-3.04060006	3.65249991
H	5.63950014	-3.81929994	3.03530002
C	2.07739997	-3.90910006	5.37120008
H	2.57610011	-4.69689989	4.80989981
C	2.47519994	-3.67610002	6.68289995
H	3.26690006	-4.28270006	7.12360001
C	1.85619998	-2.67659998	7.43109989
H	2.15949988	-2.50189996	8.46380043
C	0.84090000	-1.91050005	6.86129999
H	0.33390000	-1.16159999	7.46220016
C	0.46239999	-2.10980010	5.53889990
H	-0.31150001	-1.48199999	5.09140015
C	1.07760000	-3.12050009	4.78770018
C	-0.79390001	-4.58339977	3.10859990
C	-0.85350001	-5.55350018	4.11549997
H	-0.06710000	-5.62370014	4.86870003
C	-1.95260000	-6.40649986	4.18610001
H	-2.00519991	-7.15600014	4.97749996
C	-2.99399996	-6.28919983	3.26419997
H	-3.86380005	-6.94339991	3.34060001
C	-2.93239999	-5.32880020	2.25309992
H	-3.75999999	-5.22980022	1.54970002
C	-1.83710003	-4.47730017	2.18009996

H	-1.79690003	-3.68840003	1.41859996
C	1.95589995	-4.12599993	2.19790006
H	2.40529990	-4.93209982	2.79640007
H	1.53939998	-4.57210016	1.27980006
P	-3.15529990	1.20869994	3.06870008
P	-4.06239986	-1.34230006	1.68910003
C	-5.46880007	-1.98179996	0.73780000
C	-5.21500015	-3.11669993	-0.04380000
H	-4.22100019	-3.56139994	-0.03650000
C	-6.20690012	-3.64739990	-0.85810000
H	-5.99119997	-4.51359987	-1.48430002
C	-7.47329998	-3.05870008	-0.87390000
H	-8.25940037	-3.47309995	-1.50689995
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H	-8.74160004	-1.51549995	-0.06120000
C	-6.74350023	-1.40709996	0.73809999
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C	-4.07159996	-2.30150008	3.23469996
C	-2.91729999	-2.33929992	4.02419996
H	-2.02049994	-1.81939995	3.67869997
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C	-5.22749996	-2.97300005	3.65249991
H	-6.12729979	-2.97429991	3.03530002
C	-4.42409992	0.15539999	5.37120008
H	-5.35570002	0.11750000	4.80989981
C	-4.42119980	-0.30550000	6.68289995
H	-5.34229994	-0.68790001	7.12360001
C	-3.24609995	-0.26920000	7.43109989
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H	-1.17289996	0.29159999	7.46220016
C	-2.05830002	0.65439999	5.53889990
H	-1.12769997	1.01069999	5.09140015
C	-3.24119997	0.62699997	4.78770018
C	-3.57240009	2.97919989	3.10859990
C	-4.38269997	3.51589990	4.11549997
H	-4.83669996	2.86989999	4.86870003
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C	-3.14870000	5.20389986	2.25309992
H	-2.64910007	5.87109995	1.54970002
C	-2.95889997	3.82960010	2.18009996
H	-2.29579997	3.40039992	1.41859996
C	-4.55109978	0.36910000	2.19790006
H	-5.47399998	0.38299999	2.79640007
H	-4.72930002	0.95289999	1.27980006
P	2.62439990	2.12820005	3.06870008
P	0.86870003	4.18930006	1.68910003
C	1.01810002	5.72700024	0.73780000
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H	-0.91329998	7.44530010	-1.48430002
C	1.08780003	8.00139999	-0.87390000
H	1.12189996	8.88939953	-1.50689995
C	2.18009996	7.68130016	-0.06720000
H	3.05839992	8.32810020	-0.06120000
C	2.15319991	6.54360008	0.73809999
H	3.01999998	6.30170012	1.35060000
C	0.04260000	4.67689991	3.23469996
C	-0.56730002	3.69610000	4.02419996

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C	-1.16890001	5.37020016	5.64529991
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C	-0.56550002	6.35319996	4.86170006
H	-0.57209998	7.39419985	5.18739986
C	0.03910000	6.01359987	3.65249991
H	0.48789999	6.79360008	3.03530002
C	2.34660006	3.75370002	5.37120008
H	2.77959991	4.57940006	4.80989981
C	1.94599998	3.98160005	6.68289995
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C	1.38989997	2.94580007	7.43109989
H	1.08690000	3.12109995	8.46380043
C	1.23399997	1.68350005	6.86129999
H	0.83899999	0.87000000	7.46220016
C	1.59590006	1.45529997	5.53889990
H	1.43920004	0.47130001	5.09140015
C	2.16359997	2.49349999	4.78770018
C	4.36630011	1.60420001	3.10859990
C	5.23619986	2.03760004	4.11549997
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H	7.19990015	1.84140003	4.97749996
C	6.94360018	0.55170000	3.26419997
H	7.94509983	0.12549999	3.34060001
C	6.08109999	0.12490000	2.25309992
H	6.40910006	-0.64139998	1.54970002
C	4.79600000	0.64770001	2.18009996
H	4.09270000	0.28799999	1.41859996
C	2.59520006	3.75690007	2.19790006
H	3.06859994	4.54909992	2.79640007
H	3.18989992	3.61929989	1.27980006
P	0.53090000	3.33690000	-3.06870008
P	3.19370008	2.84699988	-1.68910003
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C	5.30660009	2.95799994	0.04380000
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C	6.26219988	3.55170012	0.85810000
H	6.90450001	2.93169999	1.48430002
C	6.38549995	4.94280005	0.87390000
H	7.13749981	5.41629982	1.50689995
C	5.56220007	5.72870016	0.06720000
H	5.68319988	6.81269979	0.06120000
C	4.59030008	5.13649988	-0.73809999
H	3.94740009	5.76630020	-1.35060000
C	4.02899981	2.37540007	-3.23469996
C	3.48449993	1.35679996	-4.02419996
H	2.58590007	0.84009999	-3.67869997
C	4.08239985	1.00730002	-5.22720003
H	3.66400003	0.20649999	-5.83820009
C	5.23519993	1.67279994	-5.64529991
H	5.71260023	1.39359999	-6.58570004
C	5.78480005	2.68689990	-4.86170006
H	6.68959999	3.20160007	-5.18739986
C	5.18839979	3.04060006	-3.65249991
H	5.63950014	3.81929994	-3.03530002
C	2.07739997	3.90910006	-5.37120008
H	2.57610011	4.69689989	-4.80989981
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H	3.26690006	4.28270006	-7.12360001
C	1.85619998	2.67659998	-7.43109989
H	2.15949988	2.50189996	-8.46380043
C	0.84090000	1.91050005	-6.86129999
H	0.33390000	1.16159999	-7.46220016
C	0.46239999	2.10980010	-5.53889990
H	-0.31150001	1.48199999	-5.09140015

C	1.07760000	3.12050009	-4.78770018
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C	-2.93239999	5.32880020	-2.25309992
H	-3.75999999	5.22980022	-1.54970002
C	-1.83710003	4.47730017	-2.18009996
H	-1.79690003	3.68840003	-1.41859996
C	1.95589995	4.12599993	-2.19790006
H	2.40529990	4.93209982	-2.79640007
H	1.53939998	4.57210016	-1.27980006
P	-3.15529990	-1.20869994	-3.06870008
P	-4.06239986	1.34230006	-1.68910003
C	-5.46880007	1.98179996	-0.73780000
C	-5.21500015	3.11669993	0.04380000
H	-4.22100019	3.56139994	0.03650000
C	-6.20690012	3.64739990	0.85810000
H	-5.99119997	4.51359987	1.48430002
C	-7.47329998	3.05870008	0.87390000
H	-8.25940037	3.47309995	1.50689995
C	-7.74219990	1.95260000	0.06720000
H	-8.74160004	1.51549995	0.06120000
C	-6.74350023	1.40709996	-0.73809999
H	-6.96750021	0.53539997	-1.35060000
C	-4.07159996	2.30150008	-3.23469996
C	-2.91729999	2.33929992	-4.02419996
H	-2.02049994	1.81939995	-3.67869997
C	-2.91359997	3.03180003	-5.22720003
H	-2.01079988	3.06979990	-5.83820009
C	-4.06629992	3.69740009	-5.64529991
H	-4.06320000	4.25040007	-6.58570004
C	-5.21929979	3.66630006	-4.86170006
H	-6.11749983	4.19259977	-5.18739986
C	-5.22749996	2.97300005	-3.65249991
H	-6.12729979	2.97429991	-3.03530002
C	-4.42409992	-0.15539999	-5.37120008
H	-5.35570002	-0.11750000	-4.80989981
C	-4.42119980	0.30550000	-6.68289995
H	-5.34229994	0.68790001	-7.12360001
C	-3.24609995	0.26920000	-7.43109989
H	-3.24640012	0.61919999	-8.46380043
C	-2.07500005	-0.22700000	-6.86129999
H	-1.17289996	-0.29159999	-7.46220016
C	-2.05830002	-0.65439999	-5.53889990
H	-1.12769997	-1.01069999	-5.09140015
C	-3.24119997	-0.62699997	-4.78770018
C	-3.57240009	-2.97919989	-3.10859990
C	-4.38269997	-3.51589990	-4.11549997
H	-4.83669996	-2.86989999	-4.86870003
C	-4.57189989	-4.89429998	-4.18610001
H	-5.19469976	-5.31459999	-4.97749996
C	-3.94959998	-5.73750019	-3.26419997
H	-4.08129978	-6.81790018	-3.34060001
C	-3.14870000	-5.20389986	-2.25309992
H	-2.64910007	-5.87109995	-1.54970002
C	-2.95889997	-3.82960010	-2.18009996
H	-2.29579997	-3.40039992	-1.41859996
C	-4.55109978	-0.36910000	-2.19790006
H	-5.47399998	-0.38299999	-2.79640007
H	-4.72930002	-0.95289999	-1.27980006
P	2.62439990	-2.12820005	-3.06870008
P	0.86870003	-4.18930006	-1.68910003
C	1.01810002	-5.72700024	-0.73780000
C	-0.09160000	-6.07460022	0.04380000

H	-0.97380000	-5.43620014	0.03650000
C	-0.05530000	-7.19899988	0.85810000
H	-0.91329998	-7.44530010	1.48430002
C	1.08780003	-8.00139999	0.87390000
H	1.12189996	-8.88939953	1.50689995
C	2.18009996	-7.68130016	0.06720000
H	3.05839992	-8.32810020	0.06120000
C	2.15319991	-6.54360008	-0.73809999
H	3.01999998	-6.30170012	-1.35060000
C	0.04260000	-4.67689991	-3.23469996
C	-0.56730002	-3.69610000	-4.02419996
H	-0.56540000	-2.65949988	-3.67869997
C	-1.16880000	-4.03910017	-5.22720003
H	-1.65310001	-3.27640009	-5.83820009
C	-1.16890001	-5.37020016	-5.64529991
H	-1.64940000	-5.64400005	-6.58570004
C	-0.56550002	-6.35319996	-4.86170006
H	-0.57209998	-7.39419985	-5.18739986
C	0.03910000	-6.01359987	-3.65249991
H	0.48789999	-6.79360008	-3.03530002
C	2.34660006	-3.75370002	-5.37120008
H	2.77959991	-4.57940006	-4.80989981
C	1.94599998	-3.98160005	-6.68289995
H	2.07540011	-4.97049999	-7.12360001
C	1.38989997	-2.94580007	-7.43109989
H	1.08690000	-3.12109995	-8.46380043
C	1.23399997	-1.68350005	-6.86129999
H	0.83899999	-0.87000000	-7.46220016
C	1.59590006	-1.45529997	-5.53889990
H	1.43920004	-0.47130001	-5.09140015
C	2.16359997	-2.49349999	-4.78770018
C	4.36630011	-1.60420001	-3.10859990
C	5.23619986	-2.03760004	-4.11549997
H	4.90380001	-2.75379992	-4.86870003
C	6.52449989	-1.51220000	-4.18610001
H	7.19990015	-1.84140003	-4.97749996
C	6.94360018	-0.55170000	-3.26419997
H	7.94509983	-0.12549999	-3.34060001
C	6.08109999	-0.12490000	-2.25309992
H	6.40910006	0.64139998	-1.54970002
C	4.79600000	-0.64770001	-2.18009996
H	4.09270000	-0.28799999	-1.41859996
C	2.59520006	-3.75690007	-2.19790006
H	3.06859994	-4.54909992	-2.79640007
H	3.18989992	-3.61929989	-1.27980006
307			
Au13 (dppm) 6 q= +3			
Au	0.00000000	0.00000000	0.00000000
Au	0.01180000	-1.63900006	2.22210002
Au	2.71059990	-1.22800004	0.52620000
Au	-1.42530000	0.80919999	2.22210002
Au	-2.41880012	-1.73339999	0.52620000
Au	1.41349995	0.82969999	2.22210002
Au	-0.29179999	2.96140003	0.52620000
Au	0.01180000	1.63900006	-2.22210002
Au	2.71059990	1.22800004	-0.52620000
Au	-1.42530000	-0.80919999	-2.22210002
Au	-2.41880012	1.73339999	-0.52620000
Au	1.41349995	-0.82969999	-2.22210002
Au	-0.29179999	-2.96140003	-0.52620000
P	0.77359998	-3.53449988	3.29169989
P	3.44899988	-3.08369994	1.73959994
C	4.62580013	-4.10169983	0.78810000
C	5.41989994	-3.41989994	-0.14920001
H	5.33339977	-2.33730006	-0.24150001
C	6.28149986	-4.11740017	-0.98640001
H	6.86689997	-3.57579994	-1.73099995
C	6.37820005	-5.50640011	-0.87760001

H	7.05639982	-6.05919981	-1.52890003
C	5.61420012	-6.18550014	0.06960000
H	5.70079994	-7.26779985	0.16450000
C	4.73320007	-5.49149990	0.89829999
H	4.12410021	-6.04850006	1.60880005
C	4.35949993	-2.47620010	3.20280004
C	3.80669999	-1.41470003	3.93580008
H	2.86050010	-0.96910000	3.62249994
C	4.46420002	-0.91890001	5.05490017
H	4.02650023	-0.09250000	5.61759996
C	5.69280005	-1.45799994	5.43419981
H	6.22009993	-1.05569994	6.30009985
C	6.25600004	-2.50099993	4.69880009
H	7.22219992	-2.91599989	4.98929977
C	5.59310007	-3.01780009	3.58500004
H	6.04549980	-3.82719994	3.00900006
C	2.48950005	-3.90179992	5.53020000
H	2.91249990	-4.77050018	5.02699995
C	3.04010010	-3.49780011	6.74319983
H	3.87249994	-4.05569983	7.17259979
C	2.54649997	-2.36750007	7.39109993
H	2.99359989	-2.03810000	8.32960033
C	1.49119997	-1.64870000	6.83209991
H	1.12769997	-0.75610000	7.33769989
C	0.93760002	-2.04430008	5.61920023
H	0.13880000	-1.46210003	5.15600014
C	1.44130003	-3.17260003	4.95380020
C	-0.42680001	-4.89909983	3.47729993
C	-0.31880000	-5.83960009	4.50850010
H	0.50190002	-5.78739977	5.22469997
C	-1.29180002	-6.82810020	4.64690018
H	-1.21010005	-7.55530024	5.45520020
C	-2.37430000	-6.87739992	3.76799989
H	-3.14140010	-7.64279985	3.89319992
C	-2.48729992	-5.93660021	2.74530005
H	-3.35080004	-5.95069981	2.07940006
C	-1.52079999	-4.94780016	2.60220003
H	-1.63059998	-4.18650007	1.82850003
C	2.19120002	-4.29769993	2.36999989
H	2.66319990	-5.07889986	2.98600006
H	1.74450004	-4.78410006	1.48409998
P	-3.44779992	1.09730005	3.29169989
P	-4.39499998	-1.44509995	1.73959994
C	-5.86509991	-1.95519996	0.78810000
C	-5.67170000	-2.98379993	-0.14920001
H	-4.69089985	-3.45020008	-0.24150001
C	-6.70660019	-3.38129997	-0.98640001
H	-6.53020000	-4.15899992	-1.73099995
C	-7.95769978	-2.77049994	-0.87760001
H	-8.77569962	-3.08139992	-1.52890003
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H	-9.14449978	-1.30320001	0.16450000
C	-7.12239981	-1.35339999	0.89829999
H	-7.30019999	-0.54740000	1.60880005
C	-4.32420015	-2.53740001	3.20280004
C	-3.12849998	-2.58940005	3.93580008
H	-2.26950002	-1.99269998	3.62249994
C	-3.02780008	-3.40669990	5.05490017
H	-2.09330010	-3.44079995	5.61759996
C	-4.10909986	-4.20109987	5.43419981
H	-4.02430010	-4.85900021	6.30009985
C	-5.29390001	-4.16739988	4.69880009
H	-6.13640022	-4.79670000	4.98929977
C	-5.41009998	-3.33489990	3.58500004
H	-6.33720016	-3.32200003	3.00900006
C	-4.62379980	-0.20500000	5.53020000
H	-5.58769989	-0.13710000	5.02699995
C	-4.54920006	-0.88389999	6.74319983

H	-5.44859982	-1.32579994	7.17259979
C	-3.32360005	-1.02160001	7.39109993
H	-3.26180005	-1.57340002	8.32960033
C	-2.17339993	-0.46709999	6.83209991
H	-1.21870005	-0.59859997	7.33769989
C	-2.23920012	0.21020000	5.61920023
H	-1.33560002	0.61080003	5.15600014
C	-3.46819997	0.33809999	4.95380020
C	-4.02930021	2.81920004	3.47729993
C	-4.89779997	3.19589996	4.50850010
H	-5.26300001	2.45910001	5.22469997
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H	-5.04820013	6.54190016	3.89319992
C	-3.89759994	5.12239981	2.74530005
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C	-3.52449989	3.79099989	2.60220003
H	-2.81030011	3.50539994	1.82850003
C	-4.81759977	0.25119999	2.36999989
H	-5.73000002	0.23310000	2.98600006
H	-5.01539993	0.88129997	1.48409998
P	2.67420006	2.43720007	3.29169989
P	0.94610000	4.52869987	1.73959994
C	1.23930001	6.05690002	0.78810000
C	0.25180000	6.40369987	-0.14920001
H	-0.64260000	5.78749990	-0.24150001
C	0.42500001	7.49870014	-0.98640001
H	-0.33669999	7.73479986	-1.73099995
C	1.57959998	8.27680016	-0.87760001
H	1.71930003	9.14060020	-1.52890003
C	2.54970002	7.95480013	0.06960000
H	3.44370008	8.57100010	0.16450000
C	2.38910007	6.84480000	0.89829999
H	3.17610002	6.59579992	1.60880005
C	-0.03530000	5.01350021	3.20280004
C	-0.67820001	4.00400019	3.93580008
H	-0.59100002	2.96180010	3.62249994
C	-1.43630004	4.32550001	5.05490017
H	-1.93320000	3.53329992	5.61759996
C	-1.58369994	5.65910006	5.43419981
H	-2.19580007	5.91459990	6.30009985
C	-0.96210003	6.66830015	4.69880009
H	-1.08580005	7.71260023	4.98929977
C	-0.18310000	6.35270023	3.58500004
H	0.29170001	7.14919996	3.00900006
C	2.13439989	4.10690022	5.53020000
H	2.67510009	4.90759993	5.02699995
C	1.50919998	4.38170004	6.74319983
H	1.57609999	5.38149977	7.17259979
C	0.77710003	3.38910007	7.39109993
H	0.26830000	3.61150002	8.32960033
C	0.68220001	2.11579990	6.83209991
H	0.09100000	1.35469997	7.33769989
C	1.30170000	1.83410001	5.61920023
H	1.19679999	0.85130000	5.15600014
C	2.02690005	2.83450007	4.95380020
C	4.45620012	2.07990003	3.47729993
C	5.21659994	2.64369988	4.50850010
H	4.76109982	3.32830000	5.22469997
C	6.55919981	2.29530001	4.64690018
H	7.14809990	2.72970009	5.45520020
C	7.14319992	1.38250005	3.76799989
H	8.18959999	1.10090005	3.89319992
C	6.38490009	0.81419998	2.74530005
H	6.82889986	0.07350000	2.07940006
C	5.04540014	1.15680003	2.60220003
H	4.44099998	0.68110001	1.82850003



C	2.62639999	4.04650021	2.36999989
H	3.06680012	4.84579992	2.98600006
H	3.27090001	3.90289998	1.48409998
P	0.77359998	3.53449988	-3.29169989
P	3.44899988	3.08369994	-1.73959994
C	4.62580013	4.10169983	-0.78810000
C	5.41989994	3.41989994	0.14920001
H	5.33339977	2.33730006	0.24150001
C	6.28149986	4.11740017	0.98640001
H	6.86689997	3.57579994	1.73099995
C	6.37820005	5.50640011	0.87760001
H	7.05639982	6.05919981	1.52890003
C	5.61420012	6.18550014	-0.06960000
H	5.70079994	7.26779985	-0.16450000
C	4.73320007	5.49149990	-0.89829999
H	4.12410021	6.04850006	-1.60880005
C	4.35949993	2.47620010	-3.20280004
C	3.80669999	1.41470003	-3.93580008
H	2.86050010	0.96910000	-3.62249994
C	4.46420002	0.91890001	-5.05490017
H	4.02650023	0.09250000	-5.61759996
C	5.69280005	1.45799994	-5.43419981
H	6.22009993	1.05569994	-6.30009985
C	6.25600004	2.50099993	-4.69880009
H	7.22219992	2.91599989	-4.98929977
C	5.59310007	3.01780009	-3.58500004
H	6.04549980	3.82719994	-3.00900006
C	2.48950005	3.90179992	-5.53020000
H	2.91249990	4.77050018	-5.02699995
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H	3.87249994	4.05569983	-7.17259979
C	2.54649997	2.36750007	-7.39109993
H	2.99359989	2.03810000	-8.32960033
C	1.49119997	1.64870000	-6.83209991
H	1.12769997	0.75610000	-7.33769989
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H	0.13880000	1.46210003	-5.15600014
C	1.44130003	3.17260003	-4.95380020
C	-0.42680001	4.89909983	-3.47729993
C	-0.31880000	5.83960009	-4.50850010
H	0.50190002	5.78739977	-5.22469997
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C	-2.48729992	5.93660021	-2.74530005
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C	2.19120002	4.29769993	-2.36999989
H	2.66319990	5.07889986	-2.98600006
H	1.74450004	4.78410006	-1.48409998
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P	-4.39499998	1.44509995	-1.73959994
C	-5.86509991	1.95519996	-0.78810000
C	-5.67170000	2.98379993	0.14920001
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H	-6.53020000	4.15899992	1.73099995
C	-7.95769978	2.77049994	0.87760001
H	-8.77569962	3.08139992	1.52890003
C	-8.16390038	1.76929998	-0.06960000
H	-9.14449978	1.30320001	-0.16450000
C	-7.12239981	1.35339999	-0.89829999
H	-7.30019999	0.54740000	-1.60880005
C	-4.32420015	2.53740001	-3.20280004
C	-3.12849998	2.58940005	-3.93580008
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H	-2.09330010	3.44079995	-5.61759996
C	-4.10909986	4.20109987	-5.43419981
H	-4.02430010	4.85900021	-6.30009985
C	-5.29390001	4.16739988	-4.69880009
H	-6.13640022	4.79670000	-4.98929977
C	-5.41009998	3.33489990	-3.58500004
H	-6.33720016	3.32200003	-3.00900006
C	-4.62379980	0.20500000	-5.53020000
H	-5.58769989	0.13710000	-5.02699995
C	-4.54920006	0.88389999	-6.74319983
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C	-3.32360005	1.02160001	-7.39109993
H	-3.26180005	1.57340002	-8.32960033
C	-2.17339993	0.46709999	-6.83209991
H	-1.21870005	0.59859997	-7.33769989
C	-2.23920012	-0.21020000	-5.61920023
H	-1.33560002	-0.61080003	-5.15600014
C	-3.46819997	-0.33809999	-4.95380020
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C	-4.89779997	-3.19589996	-4.50850010
H	-5.26300001	-2.45910001	-5.22469997
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C	-4.76879978	-5.49490023	-3.76799989
H	-5.04820013	-6.54190016	-3.89319992
C	-3.89759994	-5.12239981	-2.74530005
H	-3.47810006	-5.87729979	-2.07940006
C	-3.52449989	-3.79099989	-2.60220003
H	-2.81030011	-3.50539994	-1.82850003
C	-4.81759977	-0.25119999	-2.36999989
H	-5.73000002	-0.23310000	-2.98600006
H	-5.01539993	-0.88129997	-1.48409998
P	2.67420006	-2.43720007	-3.29169989
P	0.94610000	-4.52869987	-1.73959994
C	1.23930001	-6.05690002	-0.78810000
C	0.25180000	-6.40369987	0.14920001
H	-0.64260000	-5.78749990	0.24150001
C	0.42500001	-7.49870014	0.98640001
H	-0.33669999	-7.73479986	1.73099995
C	1.57959998	-8.27680016	0.87760001
H	1.71930003	-9.14060020	1.52890003
C	2.54970002	-7.95480013	-0.06960000
H	3.44370008	-8.57100010	-0.16450000
C	2.38910007	-6.84480000	-0.89829999
H	3.17610002	-6.59579992	-1.60880005
C	-0.03530000	-5.01350021	-3.20280004
C	-0.67820001	-4.00400019	-3.93580008
H	-0.59100002	-2.96180010	-3.62249994
C	-1.43630004	-4.32550001	-5.05490017
H	-1.93320000	-3.53329992	-5.61759996
C	-1.58369994	-5.65910006	-5.43419981
H	-2.19580007	-5.91459990	-6.30009985
C	-0.96210003	-6.66830015	-4.69880009
H	-1.08580005	-7.71260023	-4.98929977
C	-0.18310000	-6.35270023	-3.58500004
H	0.29170001	-7.14919996	-3.00900006
C	2.13439989	-4.10690022	-5.53020000
H	2.67510009	-4.90759993	-5.02699995
C	1.50919998	-4.38170004	-6.74319983
H	1.57609999	-5.38149977	-7.17259979
C	0.77710003	-3.38910007	-7.39109993
H	0.26830000	-3.61150002	-8.32960033
C	0.68220001	-2.11579990	-6.83209991
H	0.09100000	-1.35469997	-7.33769989
C	1.30170000	-1.83410001	-5.61920023
H	1.19679999	-0.85130000	-5.15600014
C	2.02690005	-2.83450007	-4.95380020

C	4.45620012	-2.07990003	-3.47729993
C	5.21659994	-2.64369988	-4.50850010
H	4.76109982	-3.32830000	-5.22469997
C	6.55919981	-2.29530001	-4.64690018
H	7.14809990	-2.72970009	-5.45520020
C	7.14319992	-1.38250005	-3.76799989
H	8.18959999	-1.10090005	-3.89319992
C	6.38490009	-0.81419998	-2.74530005
H	6.82889986	-0.07350000	-2.07940006
C	5.04540014	-1.15680003	-2.60220003
H	4.44099998	-0.68110001	-1.82850003
C	2.62639999	-4.04650021	-2.36999989
H	3.06680012	-4.84579992	-2.98600006
H	3.27090001	-3.90289998	-1.48409998

307

Ag13 (dppm) 6 q= +3			
Ag	0.00000000	0.00000000	0.00000000
Ag	0.00120000	-1.61960006	2.28719997
Ag	2.57680011	-1.26400006	0.48740000
Ag	-1.40320003	0.80870003	2.28719997
Ag	-2.38299990	-1.59959996	0.48740000
Ag	1.40199995	0.81080002	2.28719997
Ag	-0.19380000	2.86360002	0.48740000
Ag	0.00120000	1.61960006	-2.28719997
Ag	2.57680011	1.26400006	-0.48740000
Ag	-1.40320003	-0.80870003	-2.28719997
Ag	-2.38299990	1.59959996	-0.48740000
Ag	1.40199995	-0.81080002	-2.28719997
Ag	-0.19380000	-2.86360002	-0.48740000
P	0.80199999	-3.66810012	3.35220003
P	3.41980004	-3.18470001	1.80460000
C	4.63350010	-4.14150000	0.83279997
C	5.38789988	-3.41939998	-0.10900000
H	5.28329992	-2.33529997	-0.17240000
C	6.23689985	-4.07609987	-0.99199998
H	6.79050016	-3.50359988	-1.73759997
C	6.35620022	-5.46610022	-0.93190002
H	7.02010012	-5.98689985	-1.62300003
C	5.63259983	-6.18629980	0.01640000
H	5.73670006	-7.26989985	0.07170000
C	4.76870012	-5.53200006	0.89469999
H	4.18989992	-6.11929989	1.60619998
C	4.31599998	-2.49790001	3.24580002
C	3.72199988	-1.43340003	3.94300008
H	2.75629997	-1.03680003	3.61859989
C	4.34770012	-0.88230002	5.05429983
H	3.87490010	-0.06040000	5.59380007
C	5.59100008	-1.36479998	5.45930004
H	6.09380007	-0.91880000	6.31829977
C	6.19810009	-2.40700006	4.75860023
H	7.17500019	-2.77870011	5.06969976
C	5.56419992	-2.98110008	3.65580010
H	6.04759979	-3.79320002	3.10899997
C	2.51180005	-3.93670011	5.62470007
H	2.98320007	-4.78989983	5.13929987
C	3.03839993	-3.48070002	6.83069992
H	3.89969993	-3.98490000	7.26949978
C	2.48110008	-2.37059999	7.46099997
H	2.90639997	-2.00149989	8.39439964
C	1.38440001	-1.72619998	6.89039993
H	0.96190000	-0.85420001	7.38460016
C	0.85939997	-2.16910005	5.68079996
H	0.03120000	-1.62829995	5.21549988
C	1.42799997	-3.27789998	5.03060007
C	-0.42370000	-5.01109982	3.54150009
C	-0.35010001	-5.95459986	4.57219982
H	0.47479999	-5.92990017	5.28569984
C	-1.35650003	-6.90939999	4.70949984

H	-1.30149996	-7.64099979	5.51660013
C	-2.43759990	-6.92220020	3.82750010
H	-3.22930002	-7.66260004	3.94950008
C	-2.51760006	-5.97809982	2.80390000
H	-3.37899995	-5.96640015	2.13560009
C	-1.51839995	-5.02169991	2.66490006
H	-1.60010004	-4.25409985	1.89150000
C	2.24869990	-4.45669985	2.48810005
H	2.75729990	-5.18750000	3.13509989
H	1.82500005	-4.99879980	1.62339997
P	-3.57769990	1.13950002	3.35220003
P	-4.46789980	-1.36930001	1.80460000
C	-5.90339994	-1.94190001	0.83279997
C	-5.65520000	-2.95630002	-0.10900000
H	-4.66410017	-3.40779996	-0.17240000
C	-6.64839983	-3.36330009	-0.99199998
H	-6.42950010	-4.12900019	-1.73759997
C	-7.91190004	-2.77160001	-0.93190002
H	-8.69489956	-3.08620000	-1.62300003
C	-8.17380047	-1.78480005	0.01640000
H	-9.16429996	-1.33319998	0.07170000
C	-7.17519999	-1.36380005	0.89469999
H	-7.39440012	-0.56889999	1.60619998
C	-4.32119989	-2.48880005	3.24580002
C	-3.10229993	-2.50659990	3.94300008
H	-2.27609992	-1.86860001	3.61859989
C	-2.93790007	-3.32410002	5.05429983
H	-1.98969996	-3.32559991	5.59380007
C	-3.97749996	-4.15950012	5.45930004
H	-3.84260011	-4.81799984	6.31829977
C	-5.18359995	-4.16419983	4.75860023
H	-5.99389982	-4.82429981	5.06969976
C	-5.36390018	-3.32820010	3.65580010
H	-6.30880022	-3.34080005	3.10899997
C	-4.66510010	-0.20690000	5.62470007
H	-5.63980007	-0.18860000	5.13929987
C	-4.53359985	-0.89099997	6.83069992
H	-5.40089989	-1.38469994	7.26949978
C	-3.29349995	-0.96340001	7.46099997
H	-3.18659997	-1.51629996	8.39439964
C	-2.18709993	-0.33579999	6.89039993
H	-1.22070003	-0.40590000	7.38460016
C	-2.30819988	0.34020001	5.68079996
H	-1.42579997	0.78710002	5.21549988
C	-3.55270004	0.40220001	5.03060007
C	-4.12790012	2.87249994	3.54150009
C	-4.98180008	3.28049994	4.57219982
H	-5.37279987	2.55380011	5.28569984
C	-5.30550003	4.62949991	4.70949984
H	-5.96649981	4.94759989	5.51660013
C	-4.77600002	5.57219982	3.82750010
H	-5.02129984	6.62790012	3.94950008
C	-3.91840005	5.16940022	2.80390000
H	-3.47760010	5.90959978	2.13560009
C	-3.58969998	3.82579994	2.66490006
H	-2.88420010	3.51279998	1.89150000
C	-4.98400021	0.28090000	2.48810005
H	-5.87120008	0.20580000	3.13509989
H	-5.24160004	0.91890001	1.62339997
P	2.77570009	2.52859998	3.35220003
P	1.04809999	4.55389977	1.80460000
C	1.26989996	6.08349991	0.83279997
C	0.26730001	6.37570000	-0.10900000
H	-0.61919999	5.74319983	-0.17240000
C	0.41159999	7.43930006	-0.99199998
H	-0.36109999	7.63259983	-1.73759997
C	1.55569994	8.23770046	-0.93190002
H	1.67470002	9.07310009	-1.62300003

C	2.54119992	7.97109985	0.01640000
H	3.42759991	8.60309982	0.07170000
C	2.40650010	6.89580011	0.89469999
H	3.20449996	6.68820000	1.60619998
C	0.00520000	4.98670006	3.24580002
C	-0.61970001	3.94000006	3.94300008
H	-0.48019999	2.90549994	3.61859989
C	-1.40980005	4.20639992	5.05429983
H	-1.88520002	3.38599992	5.59380007
C	-1.61350000	5.52440023	5.45930004
H	-2.25119996	5.73680019	6.31829977
C	-1.01460004	6.57119989	4.75860023
H	-1.18099999	7.60309982	5.06969976
C	-0.20039999	6.30929995	3.65580010
H	0.26120001	7.13399982	3.10899997
C	2.15339994	4.14359999	5.62470007
H	2.65660000	4.97849989	5.13929987
C	1.49520004	4.37169981	6.83069992
H	1.50119996	5.36969995	7.26949978
C	0.81239998	3.33400011	7.46099997
H	0.28020000	3.51780009	8.39439964
C	0.80269998	2.06200004	6.89039993
H	0.25880000	1.26010001	7.38460016
C	1.44879997	1.82879996	5.68079996
H	1.39450002	0.84119999	5.21549988
C	2.12470007	2.87570000	5.03060007
C	4.55159998	2.13870001	3.54150009
C	5.33190012	2.67409992	4.57219982
H	4.89799976	3.37610006	5.28569984
C	6.66200018	2.27999997	4.70949984
H	7.26800013	2.69339991	5.51660013
C	7.21360016	1.35000002	3.82750010
H	8.25059986	1.03460002	3.94950008
C	6.43599987	0.80879998	2.80390000
H	6.85659981	0.05690000	2.13560009
C	5.10809994	1.19589996	2.66490006
H	4.48420000	0.74140000	1.89150000
C	2.73519993	4.17579985	2.48810005
H	3.11389995	4.98169994	3.13509989
H	3.41659999	4.07980013	1.62339997
P	0.80199999	3.66810012	-3.35220003
P	3.41980004	3.18470001	-1.80460000
C	4.63350010	4.14150000	-0.83279997
C	5.38789988	3.41939998	0.10900000
H	5.28329992	2.33529997	0.17240000
C	6.23689985	4.07609987	0.99199998
H	6.79050016	3.50359988	1.73759997
C	6.35620022	5.46610022	0.93190002
H	7.02010012	5.98689985	1.62300003
C	5.63259983	6.18629980	-0.01640000
H	5.73670006	7.26989985	-0.07170000
C	4.76870012	5.53200006	-0.89469999
H	4.18989992	6.11929989	-1.60619998
C	4.31599998	2.49790001	-3.24580002
C	3.72199988	1.43340003	-3.94300008
H	2.75629997	1.03680003	-3.61859989
C	4.34770012	0.88230002	-5.05429983
H	3.87490010	0.06040000	-5.59380007
C	5.59100008	1.36479998	-5.45930004
H	6.09380007	0.91880000	-6.31829977
C	6.19810009	2.40700006	-4.75860023
H	7.17500019	2.77870011	-5.06969976
C	5.56419992	2.98110008	-3.65580010
H	6.04759979	3.79320002	-3.10899997
C	2.51180005	3.93670011	-5.62470007
H	2.98320007	4.78989983	-5.13929987
C	3.03839993	3.48070002	-6.83069992
H	3.89969993	3.98490000	-7.26949978

C	2.48110008	2.37059999	-7.46099997
H	2.90639997	2.00149989	-8.39439964
C	1.38440001	1.72619998	-6.89039993
H	0.96190000	0.85420001	-7.38460016
C	0.85939997	2.16910005	-5.68079996
H	0.03120000	1.62829995	-5.21549988
C	1.42799997	3.27789998	-5.03060007
C	-0.42370000	5.01109982	-3.54150009
C	-0.35010001	5.95459986	-4.57219982
H	0.47479999	5.92990017	-5.28569984
C	-1.35650003	6.90939999	-4.70949984
H	-1.30149996	7.64099979	-5.51660013
C	-2.43759990	6.92220020	-3.82750010
H	-3.22930002	7.66260004	-3.94950008
C	-2.51760006	5.97809982	-2.80390000
H	-3.37899995	5.96640015	-2.13560009
C	-1.51839995	5.02169991	-2.66490006
H	-1.60010004	4.25409985	-1.89150000
C	2.24869990	4.45669985	-2.48810005
H	2.75729990	5.18750000	-3.13509989
H	1.82500005	4.99879980	-1.62339997
P	-3.57769990	-1.13950002	-3.35220003
P	-4.46789980	1.36930001	-1.80460000
C	-5.90339994	1.94190001	-0.83279997
C	-5.65520000	2.95630002	0.10900000
H	-4.66410017	3.40779996	0.17240000
C	-6.64839983	3.36330009	0.99199998
H	-6.42950010	4.12900019	1.73759997
C	-7.91190004	2.77160001	0.93190002
H	-8.69489956	3.08620000	1.62300003
C	-8.17380047	1.78480005	-0.01640000
H	-9.16429996	1.33319998	-0.07170000
C	-7.17519999	1.36380005	-0.89469999
H	-7.39440012	0.56889999	-1.60619998
C	-4.32119989	2.48880005	-3.24580002
C	-3.10229993	2.50659990	-3.94300008
H	-2.27609992	1.86860001	-3.61859989
C	-2.93790007	3.32410002	-5.05429983
H	-1.98969996	3.32559991	-5.59380007
C	-3.97749996	4.15950012	-5.45930004
H	-3.84260011	4.81799984	-6.31829977
C	-5.18359995	4.16419983	-4.75860023
H	-5.99389982	4.82429981	-5.06969976
C	-5.36390018	3.32820010	-3.65580010
H	-6.30880022	3.34080005	-3.10899997
C	-4.66510010	0.20690000	-5.62470007
H	-5.63980007	0.18860000	-5.13929987
C	-4.53359985	0.89099997	-6.83069992
H	-5.40089989	1.38469994	-7.26949978
C	-3.29349995	0.96340001	-7.46099997
H	-3.18659997	1.51629996	-8.39439964
C	-2.18709993	0.33579999	-6.89039993
H	-1.22070003	0.40590000	-7.38460016
C	-2.30819988	-0.34020001	-5.68079996
H	-1.42579997	-0.78710002	-5.21549988
C	-3.55270004	-0.40220001	-5.03060007
C	-4.12790012	-2.87249994	-3.54150009
C	-4.98180008	-3.28049994	-4.57219982
H	-5.37279987	-2.55380011	-5.28569984
C	-5.30550003	-4.62949991	-4.70949984
H	-5.96649981	-4.94759989	-5.51660013
C	-4.77600002	-5.57219982	-3.82750010
H	-5.02129984	-6.62790012	-3.94950008
C	-3.91840005	-5.16940022	-2.80390000
H	-3.47760010	-5.90959978	-2.13560009
C	-3.58969998	-3.82579994	-2.66490006
H	-2.88420010	-3.51279998	-1.89150000
C	-4.98400021	-0.28090000	-2.48810005

H	-5.87120008	-0.20580000	-3.13509989
H	-5.24160004	-0.91890001	-1.62339997
P	2.77570009	-2.52859998	-3.35220003
P	1.04809999	-4.55389977	-1.80460000
C	1.26989996	-6.08349991	-0.83279997
C	0.26730001	-6.37570000	0.10900000
H	-0.61919999	-5.74319983	0.17240000
C	0.41159999	-7.43930006	0.99199998
H	-0.36109999	-7.63259983	1.73759997
C	1.55569994	-8.23770046	0.93190002
H	1.67470002	-9.07310009	1.62300003
C	2.54119992	-7.97109985	-0.01640000
H	3.42759991	-8.60309982	-0.07170000
C	2.40650010	-6.89580011	-0.89469999
H	3.20449996	-6.68820000	-1.60619998
C	0.00520000	-4.98670006	-3.24580002
C	-0.61970001	-3.94000006	-3.94300008
H	-0.48019999	-2.90549994	-3.61859989
C	-1.40980005	-4.20639992	-5.05429983
H	-1.88520002	-3.38599992	-5.59380007
C	-1.61350000	-5.52440023	-5.45930004
H	-2.25119996	-5.73680019	-6.31829977
C	-1.01460004	-6.57119989	-4.75860023
H	-1.18099999	-7.60309982	-5.06969976
C	-0.20039999	-6.30929995	-3.65580010
H	0.26120001	-7.13399982	-3.10899997
C	2.15339994	-4.14359999	-5.62470007
H	2.65660000	-4.97849989	-5.13929987
C	1.49520004	-4.37169981	-6.83069992
H	1.50119996	-5.36969995	-7.26949978
C	0.81239998	-3.33400011	-7.46099997
H	0.28020000	-3.51780009	-8.39439964
C	0.80269998	-2.06200004	-6.89039993
H	0.25880000	-1.26010001	-7.38460016
C	1.44879997	-1.82879996	-5.68079996
H	1.39450002	-0.84119999	-5.21549988
C	2.12470007	-2.87570000	-5.03060007
C	4.55159998	-2.13870001	-3.54150009
C	5.33190012	-2.67409992	-4.57219982
H	4.89799976	-3.37610006	-5.28569984
C	6.66200018	-2.27999997	-4.70949984
H	7.26800013	-2.69339991	-5.51660013
C	7.21360016	-1.35000002	-3.82750010
H	8.25059986	-1.03460002	-3.94950008
C	6.43599987	-0.80879998	-2.80390000
H	6.85659981	-0.05690000	-2.13560009
C	5.10809994	-1.19589996	-2.66490006
H	4.48420000	-0.74140000	-1.89150000
C	2.73519993	-4.17579985	-2.48810005
H	3.11389995	-4.98169994	-3.13509989
H	3.41659999	-4.07980013	-1.62339997

307

Cu13 (dppm) 6 q= +3

Cu	0.00000000	0.00000000	0.00000000
Cu	-0.02320000	-1.44809997	2.00040007
Cu	2.17400002	-1.16410005	0.49520001
Cu	-1.24249995	0.74419999	2.00040007
Cu	-2.09509993	-1.30069995	0.49520001
Cu	1.26569998	0.70400000	2.00040007
Cu	-0.07890000	2.46479988	0.49520001
Cu	-0.02320000	1.44809997	-2.00040007
Cu	2.17400002	1.16410005	-0.49520001
Cu	-1.24249995	-0.74419999	-2.00040007
Cu	-2.09509993	1.30069995	-0.49520001
Cu	1.26569998	-0.70400000	-2.00040007
Cu	-0.07890000	-2.46479988	-0.49520001
P	0.51010001	-3.38330007	3.02620006
P	3.17580009	-2.85240006	1.69620001

C	4.46649981	-3.74029994	0.76639998
C	5.32889986	-2.94129992	0.00190000
H	5.21040010	-1.85790002	0.02070000
C	6.28669977	-3.52099991	-0.82040000
H	6.92600012	-2.88930011	-1.43830001
C	6.40380001	-4.91190004	-0.86820000
H	7.15040016	-5.37319994	-1.51559997
C	5.57410002	-5.71120024	-0.08160000
H	5.68300009	-6.79610014	-0.10380000
C	4.60470009	-5.13129997	0.73640001
H	3.95370007	-5.77010012	1.33150005
C	4.01859999	-2.37910008	3.24580002
C	3.46770000	-1.35490000	4.02510023
H	2.54940009	-0.86470002	3.68429995
C	4.08309984	-0.96539998	5.20819998
H	3.65849996	-0.15920000	5.80740023
C	5.26140022	-1.59189999	5.61380005
H	5.75610018	-1.27559996	6.53299999
C	5.81470013	-2.61400008	4.84289980
H	6.73890018	-3.10010004	5.15880013
C	5.19820023	-3.01099992	3.65750003
H	5.65040016	-3.79489994	3.04819989
C	2.06850004	-3.97410011	5.34049988
H	2.53439999	-4.78779984	4.78660011
C	2.51349998	-3.71190000	6.63269997
H	3.30900002	-4.31930017	7.06409979
C	1.94780004	-2.67030001	7.36639977
H	2.29450011	-2.46269989	8.37969971
C	0.93900001	-1.89400005	6.80009985
H	0.48510000	-1.09720004	7.38360023
C	0.51239997	-2.12809992	5.49660015
H	-0.23670000	-1.47829998	5.03770018
C	1.07379997	-3.17849994	4.75719976
C	-0.78600001	-4.67159986	3.10590005
C	-0.79619998	-5.66660023	4.08890009
H	0.01950000	-5.74259996	4.80900002
C	-1.88059998	-6.53730011	4.18050003
H	-1.89380002	-7.30569983	4.95419979
C	-2.95860004	-6.41260004	3.30299997
H	-3.81620002	-7.07999992	3.39630008
C	-2.94950008	-5.42490005	2.31780005
H	-3.80500007	-5.31400013	1.64970005
C	-1.86749995	-4.55709982	2.22289991
H	-1.85880005	-3.75180006	1.47839999
C	1.96669996	-4.16720009	2.19269991
H	2.42790008	-4.95590019	2.80399990
H	1.57679999	-4.62500000	1.26979995
P	-3.18499994	1.24989998	3.02620006
P	-4.05810022	-1.32410002	1.69620001
C	-5.47249985	-1.99790001	0.76639998
C	-5.21169996	-3.14429998	0.00190000
H	-4.21420002	-3.58340001	0.02070000
C	-6.19259977	-3.68400002	-0.82040000
H	-5.96519995	-4.55340004	-1.43830001
C	-7.45569992	-3.08990002	-0.86820000
H	-8.22850037	-3.50580001	-1.51559997
C	-7.73309994	-1.97169995	-0.08160000
H	-8.72710037	-1.52359998	-0.10380000
C	-6.74620008	-1.42209995	0.73640001
H	-6.97389984	-0.53890002	1.33150005
C	-4.06969976	-2.29069996	3.24580002
C	-2.90720010	-2.32570004	4.02510023
H	-2.02349997	-1.77550006	3.68429995
C	-2.87759995	-3.05329990	5.20819998
H	-1.96710002	-3.08870006	5.80740023
C	-4.00939989	-3.76060009	5.61380005
H	-3.98270011	-4.34709978	6.53299999
C	-5.17119980	-3.72869992	4.84289980



H	-6.05420017	-4.28599977	5.15880013
C	-5.20669985	-2.99629998	3.65750003
H	-6.11170006	-2.99589992	3.04819989
C	-4.47590017	0.19570000	5.34049988
H	-5.41349983	0.19910000	4.78660011
C	-4.47139978	-0.32080001	6.63269997
H	-5.39510012	-0.70599997	7.06409979
C	-3.28649998	-0.35170001	7.36639977
H	-3.27990007	-0.75569999	8.37969971
C	-2.10969996	0.13380000	6.80009985
H	-1.19280005	0.12850000	7.38360023
C	-2.09920001	0.62019998	5.49660015
H	-1.16190004	0.94410002	5.03770018
C	-3.28959990	0.65939999	4.75719976
C	-3.65269995	3.01650000	3.10590005
C	-4.50930023	3.52279997	4.08890009
H	-4.98299980	2.85450006	4.80900002
C	-4.72119999	4.89729977	4.18050003
H	-5.38000011	5.29290009	4.95419979
C	-4.07420015	5.76849985	3.30299997
H	-4.22340012	6.84490013	3.39630008
C	-3.22340012	5.26679993	2.31780005
H	-2.69950008	5.95219994	1.64970005
C	-3.01279998	3.89580011	2.22289991
H	-2.31979990	3.48569989	1.47839999
C	-4.59229994	0.38029999	2.19269991
H	-5.50589991	0.37529999	2.80399990
H	-4.79379988	0.94690001	1.26979995
P	2.67490005	2.13339996	3.02620006
P	0.88230002	4.17649984	1.69620001
C	1.00600004	5.73829985	0.76639998
C	-0.11720000	6.08559990	0.00190000
H	-0.99620003	5.44129992	0.02070000
C	-0.09410000	7.20499992	-0.82040000
H	-0.96079999	7.44269991	-1.43830001
C	1.05190003	8.00179958	-0.86820000
H	1.07819998	8.87899971	-1.51559997
C	2.15899992	7.68289995	-0.08160000
H	3.04410005	8.31970024	-0.10380000
C	2.14150000	6.55340004	0.73640001
H	3.02020001	6.30900002	1.33150005
C	0.05100000	4.66979980	3.24580002
C	-0.56050003	3.68050003	4.02510023
H	-0.52590001	2.64019990	3.68429995
C	-1.20550001	4.01879978	5.20819998
H	-1.69140005	3.24790001	5.80740023
C	-1.25209999	5.35249996	5.61380005
H	-1.77339995	5.62270021	6.53299999
C	-0.64349997	6.34270000	4.84289980
H	-0.68470001	7.38609982	5.15880013
C	0.00850000	6.00719976	3.65750003
H	0.46129999	6.79090023	3.04819989
C	2.40739989	3.77839994	5.34049988
H	2.87919998	4.58869982	4.78660011
C	1.95790005	4.03270006	6.63269997
H	2.08620000	5.02530003	7.06409979
C	1.33870006	3.02200007	7.36639977
H	0.98549998	3.21840000	8.37969971
C	1.17079997	1.76020002	6.80009985
H	0.70770001	0.96869999	7.38360023
C	1.58669996	1.50779998	5.49660015
H	1.39859998	0.53420001	5.03770018
C	2.21580005	2.51920009	4.75719976
C	4.43870020	1.65509999	3.10590005
C	5.30550003	2.14369988	4.08890009
H	4.96350002	2.88820004	4.80900002
C	6.60179996	1.63999999	4.18050003
H	7.27379990	2.01279998	4.95419979

C	7.03280020	0.64410001	3.30299997
H	8.03960037	0.23510000	3.39630008
C	6.17280006	0.15809999	2.31780005
H	6.50449991	-0.63830000	1.64970005
C	4.88030005	0.66130000	2.22289991
H	4.17859983	0.26620001	1.47839999
C	2.62549996	3.78679991	2.19269991
H	3.07800007	4.58059978	2.80399990
H	3.21690011	3.67810011	1.26979995
P	0.51010001	3.38330007	-3.02620006
P	3.17580009	2.85240006	-1.69620001
C	4.46649981	3.74029994	-0.76639998
C	5.32889986	2.94129992	-0.00190000
H	5.21040010	1.85790002	-0.02070000
C	6.28669977	3.52099991	0.82040000
H	6.92600012	2.88930011	1.43830001
C	6.40380001	4.91190004	0.86820000
H	7.15040016	5.37319994	1.51559997
C	5.57410002	5.71120024	0.08160000
H	5.68300009	6.79610014	0.10380000
C	4.60470009	5.13129997	-0.73640001
H	3.95370007	5.77010012	-1.33150005
C	4.01859999	2.37910008	-3.24580002
C	3.46770000	1.35490000	-4.02510023
H	2.54940009	0.86470002	-3.68429995
C	4.08309984	0.96539998	-5.20819998
H	3.65849996	0.15920000	-5.80740023
C	5.26140022	1.59189999	-5.61380005
H	5.75610018	1.27559996	-6.53299999
C	5.81470013	2.61400008	-4.84289980
H	6.73890018	3.10010004	-5.15880013
C	5.19820023	3.01099992	-3.65750003
H	5.65040016	3.79489994	-3.04819989
C	2.06850004	3.97410011	-5.34049988
H	2.53439999	4.78779984	-4.78660011
C	2.51349998	3.71190000	-6.63269997
H	3.30900002	4.31930017	-7.06409979
C	1.94780004	2.67030001	-7.36639977
H	2.29450011	2.46269989	-8.37969971
C	0.93900001	1.89400005	-6.80009985
H	0.48510000	1.09720004	-7.38360023
C	0.51239997	2.12809992	-5.49660015
H	-0.23670000	1.47829998	-5.03770018
C	1.07379997	3.17849994	-4.75719976
C	-0.78600001	4.67159986	-3.10590005
C	-0.79619998	5.66660023	-4.08890009
H	0.01950000	5.74259996	-4.80900002
C	-1.88059998	6.53730011	-4.18050003
H	-1.89380002	7.30569983	-4.95419979
C	-2.95860004	6.41260004	-3.30299997
H	-3.81620002	7.07999992	-3.39630008
C	-2.94950008	5.42490005	-2.31780005
H	-3.80500007	5.31400013	-1.64970005
C	-1.86749995	4.55709982	-2.22289991
H	-1.85880005	3.75180006	-1.47839999
C	1.96669996	4.16720009	-2.19269991
H	2.42790008	4.95590019	-2.80399990
H	1.57679999	4.62500000	-1.26979995
P	-3.18499994	-1.24989998	-3.02620006
P	-4.05810022	1.32410002	-1.69620001
C	-5.47249985	1.99790001	-0.76639998
C	-5.21169996	3.14429998	-0.00190000
H	-4.21420002	3.58340001	-0.02070000
C	-6.19259977	3.68400002	0.82040000
H	-5.96519995	4.55340004	1.43830001
C	-7.45569992	3.08990002	0.86820000
H	-8.22850037	3.50580001	1.51559997
C	-7.73309994	1.97169995	0.08160000

H	-8.72710037	1.52359998	0.10380000
C	-6.74620008	1.42209995	-0.73640001
H	-6.97389984	0.53890002	-1.33150005
C	-4.06969976	2.29069996	-3.24580002
C	-2.90720010	2.32570004	-4.02510023
H	-2.02349997	1.77550006	-3.68429995
C	-2.87759995	3.05329990	-5.20819998
H	-1.96710002	3.08870006	-5.80740023
C	-4.00939989	3.76060009	-5.61380005
H	-3.98270011	4.34709978	-6.53299999
C	-5.17119980	3.72869992	-4.84289980
H	-6.05420017	4.28599977	-5.15880013
C	-5.20669985	2.99629998	-3.65750003
H	-6.11170006	2.99589992	-3.04819989
C	-4.47590017	-0.19570000	-5.34049988
H	-5.41349983	-0.19910000	-4.78660011
C	-4.47139978	0.32080001	-6.63269997
H	-5.39510012	0.70599997	-7.06409979
C	-3.28649998	0.35170001	-7.36639977
H	-3.27990007	0.75569999	-8.37969971
C	-2.10969996	-0.13380000	-6.80009985
H	-1.19280005	-0.12850000	-7.38360023
C	-2.09920001	-0.62019998	-5.49660015
H	-1.16190004	-0.94410002	-5.03770018
C	-3.28959990	-0.65939999	-4.75719976
C	-3.65269995	-3.01650000	-3.10590005
C	-4.50930023	-3.52279997	-4.08890009
H	-4.98299980	-2.85450006	-4.80900002
C	-4.72119999	-4.89729977	-4.18050003
H	-5.38000011	-5.29290009	-4.95419979
C	-4.07420015	-5.76849985	-3.30299997
H	-4.22340012	-6.84490013	-3.39630008
C	-3.22340012	-5.26679993	-2.31780005
H	-2.69950008	-5.95219994	-1.64970005
C	-3.01279998	-3.89580011	-2.22289991
H	-2.31979990	-3.48569989	-1.47839999
C	-4.59229994	-0.38029999	-2.19269991
H	-5.50589991	-0.37529999	-2.80399990
H	-4.79379988	-0.94690001	-1.26979995
P	2.67490005	-2.13339996	-3.02620006
P	0.88230002	-4.17649984	-1.69620001
C	1.00600004	-5.73829985	-0.76639998
C	-0.11720000	-6.08559990	-0.00190000
H	-0.99620003	-5.44129992	-0.02070000
C	-0.09410000	-7.20499992	0.82040000
H	-0.96079999	-7.44269991	1.43830001
C	1.05190003	-8.00179958	0.86820000
H	1.07819998	-8.87899971	1.51559997
C	2.15899992	-7.68289995	0.08160000
H	3.04410005	-8.31970024	0.10380000
C	2.14150000	-6.55340004	-0.73640001
H	3.02020001	-6.30900002	-1.33150005
C	0.05100000	-4.66979980	-3.24580002
C	-0.56050003	-3.68050003	-4.02510023
H	-0.52590001	-2.64019990	-3.68429995
C	-1.20550001	-4.01879978	-5.20819998
H	-1.69140005	-3.24790001	-5.80740023
C	-1.25209999	-5.35249996	-5.61380005
H	-1.77339995	-5.62270021	-6.53299999
C	-0.64349997	-6.34270000	-4.84289980
H	-0.68470001	-7.38609982	-5.15880013
C	0.00850000	-6.00719976	-3.65750003
H	0.46129999	-6.79090023	-3.04819989
C	2.40739989	-3.77839994	-5.34049988
H	2.87919998	-4.58869982	-4.78660011
C	1.95790005	-4.03270006	-6.63269997
H	2.08620000	-5.02530003	-7.06409979
C	1.33870006	-3.02200007	-7.36639977

H	0.98549998	-3.21840000	-8.37969971
C	1.17079997	-1.76020002	-6.80009985
H	0.70770001	-0.96869999	-7.38360023
C	1.58669996	-1.50779998	-5.49660015
H	1.39859998	-0.53420001	-5.03770018
C	2.21580005	-2.51920009	-4.75719976
C	4.43870020	-1.65509999	-3.10590005
C	5.30550003	-2.14369988	-4.08890009
H	4.96350002	-2.88820004	-4.80900002
C	6.60179996	-1.63999999	-4.18050003
H	7.27379990	-2.01279998	-4.95419979
C	7.03280020	-0.64410001	-3.30299997
H	8.03960037	-0.23510000	-3.39630008
C	6.17280006	-0.15809999	-2.31780005
H	6.50449991	0.63830000	-1.64970005
C	4.88030005	-0.66130000	-2.22289991
H	4.17859983	-0.26620001	-1.47839999
C	2.62549996	-3.78679991	-2.19269991
H	3.07800007	-4.58059978	-2.80399990
H	3.21690011	-3.67810011	-1.26979995