

Supplementary Information

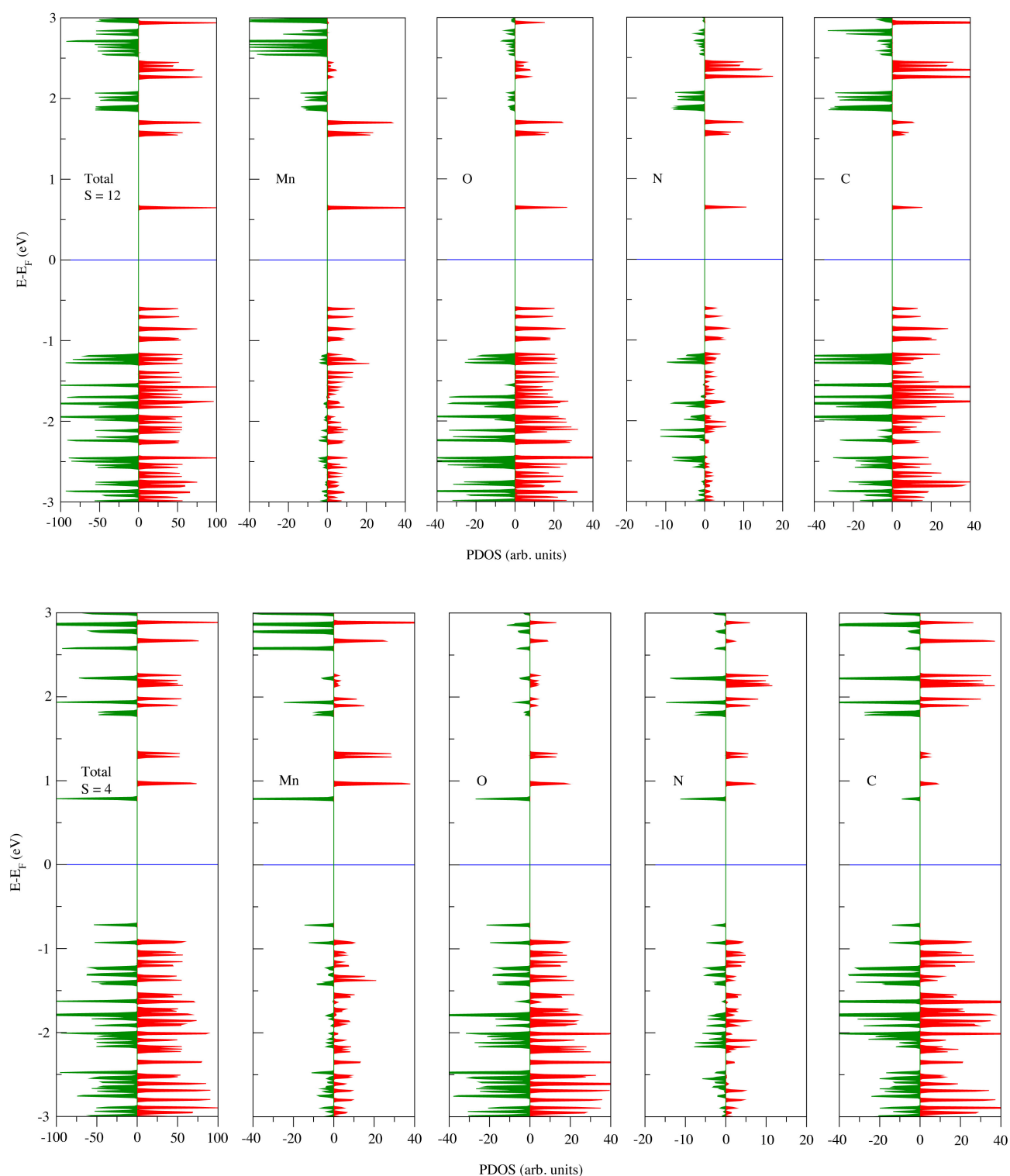


Figure S1. Total and projected density of states (red and green curves indicate alpha and beta spin states, respectively) for the $S = 12$ (above) and $S = 4$ (below) of the $[Mn_6O_2(Et-sao)_6\{O_2CPh(Me)_2\}_2(EtOH)_6]$ original SMM complex.

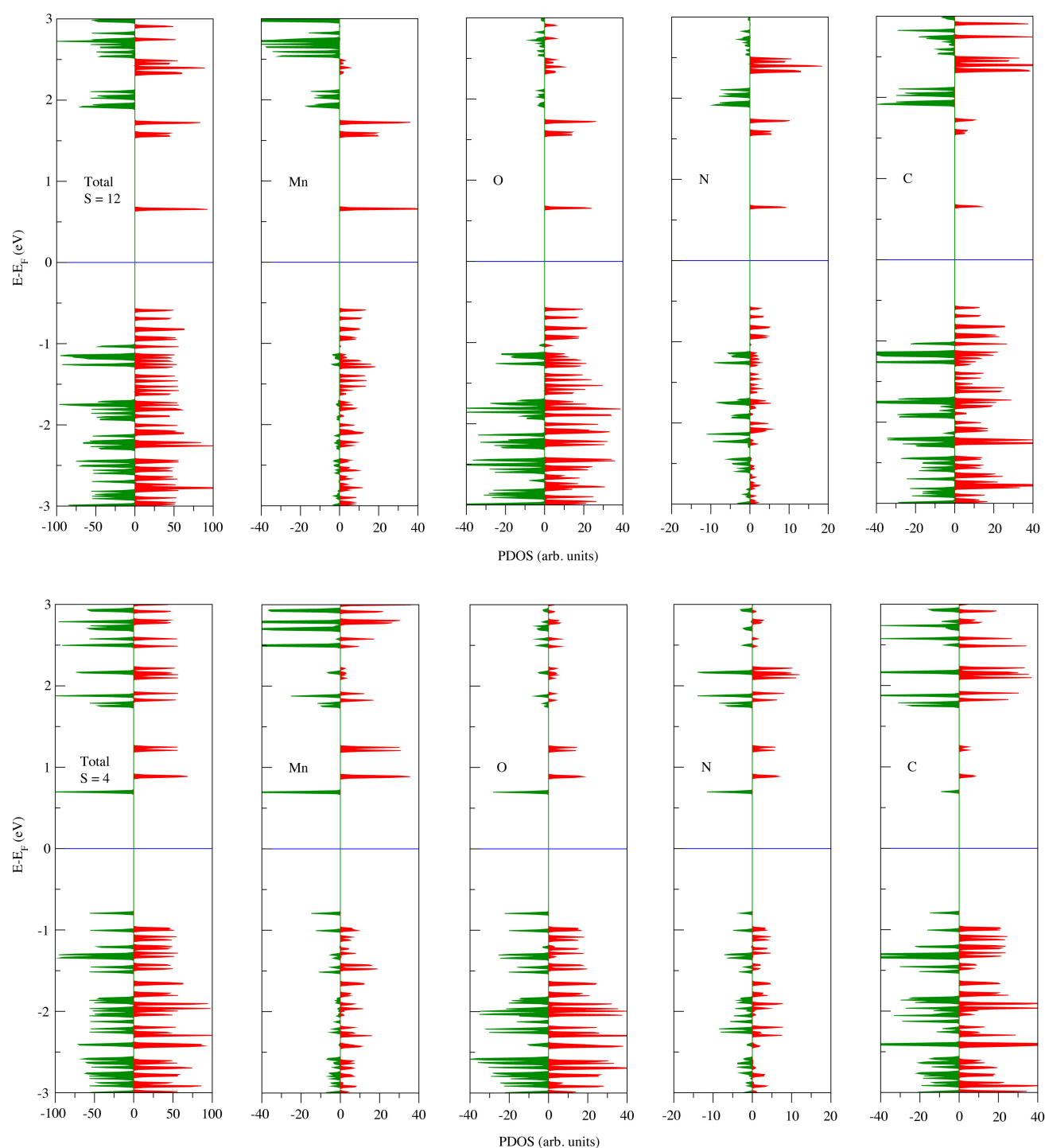


Figure S2. Total and projected density of states (red and green curves indicate alpha and beta spin states, respectively) for the $S = 12$ (above) and $S = 4$ (below) of the $[\text{Mn}_6\text{O}_2(\text{Me-sao})_6\{\text{O}_2\text{CPh}(\text{SH})\}_2(\text{MeOH})_6]$ model complex.

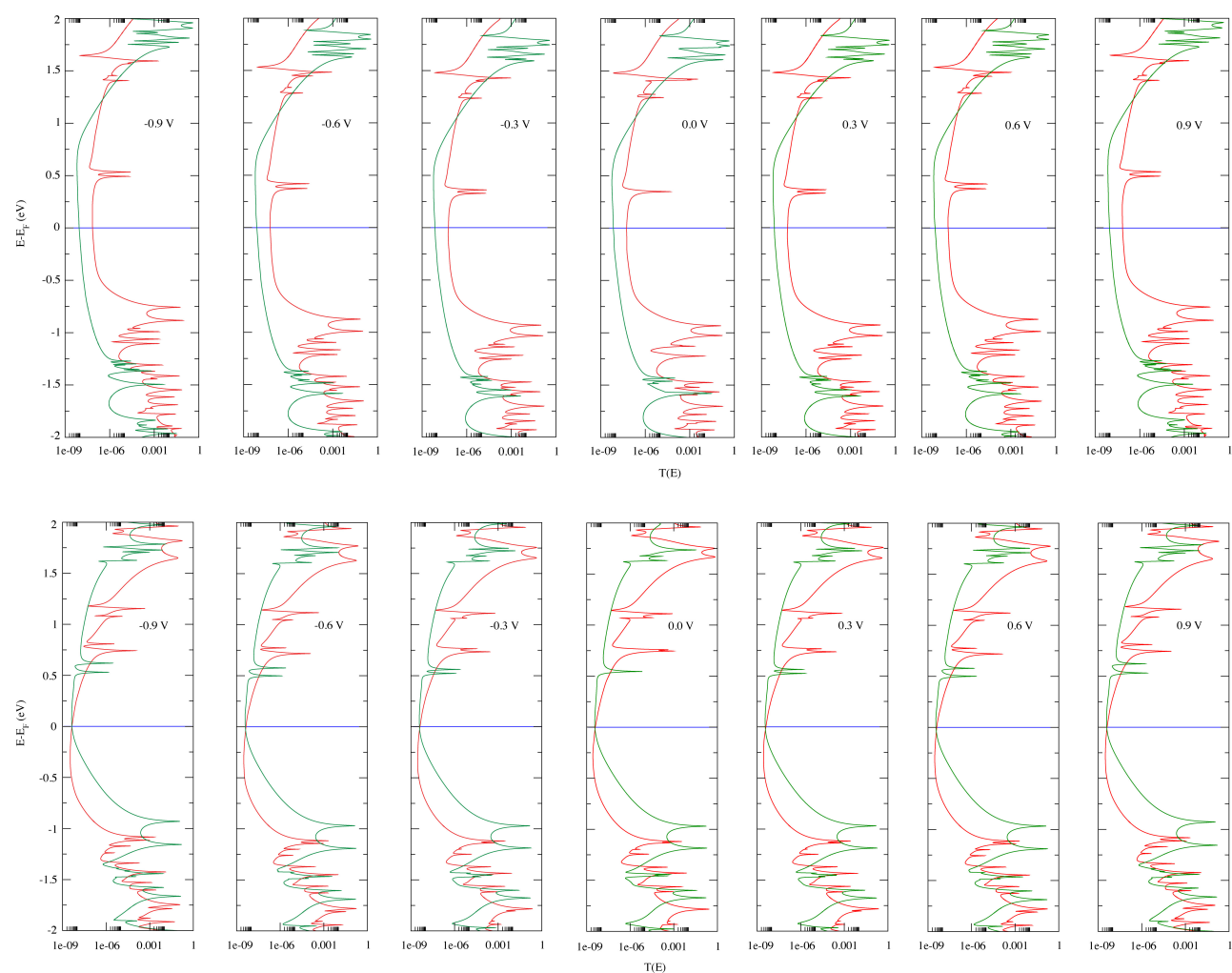


Figure S3. Transmission spectra calculated (red and green correspond to the alpha and beta contributions, respectively) at different voltages corresponding to the $S = 12$ (above) and $S = 4$ (below) ground states for the $\text{Mn}_6\text{-Au(111)}$ layers system. The total number of atoms is 880 and the supercell vectors:

12.802249	-22.174137	0.000000
17.923149	10.347931	0.000000
0.000000	0.000000	44.52210

Cartesian Coordinates of the Mn₆-Au(111) system

Au	12.802200	-19.217600	0.000000	Au	18.776600	-14.782800	2.414000	Au	11.948800	-11.826200	4.828000
Au	10.241800	-17.739300	0.000000	Au	23.897500	-14.782800	2.414000	Au	17.069700	-11.826200	4.828000
Au	15.362700	-17.739300	0.000000	Au	11.095300	-13.304500	2.414000	Au	22.190600	-11.826200	4.828000
Au	12.802200	-16.261000	0.000000	Au	16.216200	-13.304500	2.414000	Au	27.311500	-11.826200	4.828000
Au	17.923100	-16.261000	0.000000	Au	21.337100	-13.304500	2.414000	Au	14.509200	-10.347900	4.828000
Au	10.241800	-14.782800	0.000000	Au	26.458000	-13.304500	2.414000	Au	19.630100	-10.347900	4.828000
Au	15.362700	-14.782800	0.000000	Au	13.655700	-11.826200	2.414000	Au	24.751000	-10.347900	4.828000
Au	20.483600	-14.782800	0.000000	Au	18.776600	-11.826200	2.414000	Au	29.871900	-10.347900	4.828000
Au	12.802200	-13.304500	0.000000	Au	23.897500	-11.826200	2.414000	Au	9.388300	-10.347900	4.828000
Au	17.923100	-13.304500	0.000000	Au	29.018400	-11.826200	2.414000	Au	11.948800	-8.869700	4.828000
Au	23.044000	-13.304500	0.000000	Au	11.095300	-10.347900	2.414000	Au	17.069700	-8.869700	4.828000
Au	7.681300	-13.304500	0.000000	Au	16.216200	-10.347900	2.414000	Au	22.190600	-8.869700	4.828000
Au	10.241800	-11.826200	0.000000	Au	21.337100	-10.347900	2.414000	Au	27.311500	-8.869700	4.828000
Au	15.362700	-11.826200	0.000000	Au	26.458000	-10.347900	2.414000	Au	6.827900	-8.869700	4.828000
Au	20.483600	-11.826200	0.000000	Au	31.578900	-10.347900	2.414000	Au	14.509200	-7.391400	4.828000
Au	25.604500	-11.826200	0.000000	Au	13.655700	-8.869700	2.414000	Au	19.630100	-7.391400	4.828000
Au	12.802200	-10.347900	0.000000	Au	18.776600	-8.869700	2.414000	Au	24.751000	-7.391400	4.828000
Au	17.923100	-10.347900	0.000000	Au	23.897500	-8.869700	2.414000	Au	9.388300	-7.391400	4.828000
Au	23.044000	-10.347900	0.000000	Au	29.018400	-8.869700	2.414000	Au	11.948800	-5.913100	4.828000
Au	28.164900	-10.347900	0.000000	Au	8.534800	-8.869700	2.414000	Au	17.069700	-5.913100	4.828000
Au	7.681300	-10.347900	0.000000	Au	11.095300	-7.391400	2.414000	Au	22.190600	-5.913100	4.828000
Au	10.241800	-8.869700	0.000000	Au	16.216200	-7.391400	2.414000	Au	27.311500	-5.913100	4.828000
Au	15.362700	-8.869700	0.000000	Au	21.337100	-7.391400	2.414000	Au	6.827900	-5.913100	4.828000
Au	20.483600	-8.869700	0.000000	Au	26.458000	-7.391400	2.414000	Au	14.509200	-4.434800	4.828000
Au	25.604500	-8.869700	0.000000	Au	13.655700	-5.913100	2.414000	Au	19.630100	-4.434800	4.828000
Au	5.120900	-8.869700	0.000000	Au	18.776600	-5.913100	2.414000	Au	24.751000	-4.434800	4.828000
Au	12.802200	-7.391400	0.000000	Au	23.897500	-5.913100	2.414000	Au	4.267400	-4.434800	4.828000
Au	17.923100	-7.391400	0.000000	Au	29.018400	-5.913100	2.414000	Au	9.388300	-4.434800	4.828000
Au	23.044000	-7.391400	0.000000	Au	8.534800	-5.913100	2.414000	Au	11.948800	-2.956600	4.828000
Au	7.681300	-7.391400	0.000000	Au	11.095300	-4.434800	2.414000	Au	17.069700	-2.956600	4.828000
Au	10.241800	-5.913100	0.000000	Au	16.216200	-4.434800	2.414000	Au	22.190600	-2.956600	4.828000
Au	15.362700	-5.913100	0.000000	Au	21.337100	-4.434800	2.414000	Au	6.827900	-2.956600	4.828000
Au	20.483600	-5.913100	0.000000	Au	26.458000	-4.434800	2.414000	Au	14.509200	-1.478300	4.828000
Au	25.604500	-5.913100	0.000000	Au	5.974400	-4.434800	2.414000	Au	19.630100	-1.478300	4.828000
Au	5.120900	-5.913100	0.000000	Au	13.655700	-2.956600	2.414000	Au	24.751000	-1.478300	4.828000
Au	12.802200	-4.434800	0.000000	Au	18.776600	-2.956600	2.414000	Au	4.267400	-1.478300	4.828000
Au	17.923100	-4.434800	0.000000	Au	23.897500	-2.956600	2.414000	Au	9.388300	-1.478300	4.828000
Au	23.044000	-4.434800	0.000000	Au	8.534800	-2.956600	2.414000	Au	11.948800	0.000000	4.828000
Au	2.560400	-4.434800	0.000000	Au	11.095300	-1.478300	2.414000	Au	17.069700	0.000000	4.828000
Au	7.681300	-4.434800	0.000000	Au	16.216200	-1.478300	2.414000	Au	1.707000	0.000000	4.828000
Au	10.241800	-2.956600	0.000000	Au	21.337100	-1.478300	2.414000	Au	22.190600	0.000000	4.828000
Au	15.362700	-2.956600	0.000000	Au	26.458000	-1.478300	2.414000	Au	6.827900	0.000000	4.828000
Au	20.483600	-2.956600	0.000000	Au	5.974400	-1.478300	2.414000	Au	14.509200	1.478300	4.828000
Au	5.120900	-2.956600	0.000000	Au	13.655700	0.000000	2.414000	Au	19.630100	1.478300	4.828000
Au	12.802200	-1.478300	0.000000	Au	18.776600	0.000000	2.414000	Au	4.267400	1.478300	4.828000
Au	17.923100	-1.478300	0.000000	Au	23.897500	0.000000	2.414000	Au	9.388300	1.478300	4.828000
Au	23.044000	-1.478300	0.000000	Au	3.413900	0.000000	2.414000	Au	11.948800	2.956600	4.828000
Au	2.560400	-1.478300	0.000000	Au	8.534800	0.000000	2.414000	Au	17.069700	2.956600	4.828000
Au	7.681300	-1.478300	0.000000	Au	11.095300	1.478300	2.414000	Au	22.190600	2.956600	4.828000
Au	0.000000	0.000000	0.000000	Au	16.216200	1.478300	2.414000	Au	6.827900	2.956600	4.828000
Au	10.241800	0.000000	0.000000	Au	21.337100	1.478300	2.414000	Au	14.509200	4.434800	4.828000
Au	15.362700	0.000000	0.000000	Au	5.974400	1.478300	2.414000	Au	19.630100	4.434800	4.828000
Au	20.483600	0.000000	0.000000	Au	13.655700	2.956600	2.414000	Au	9.388300	4.434800	4.828000
Au	5.120900	0.000000	0.000000	Au	18.776600	2.956600	2.414000	Au	11.948800	5.913100	4.828000
Au	12.802200	1.478300	0.000000	Au	23.897500	2.956600	2.414000	Au	17.069700	5.913100	4.828000
Au	17.923100	1.478300	0.000000	Au	8.534800	2.956600	2.414000	Au	14.509200	7.391400	4.828000
Au	2.560400	1.478300	0.000000	Au	11.095300	4.434800	2.414000	Au	19.630100	7.391400	4.828000
Au	7.681300	1.478300	0.000000	Au	16.216200	4.434800	2.414000	Au	17.069700	8.869700	4.828000
Au	10.241800	2.956600	0.000000	Au	21.337100	4.434800	2.414000	Au	12.802200	-19.217600	7.242100
Au	15.362700	2.956600	0.000000	Au	13.655700	5.913100	2.414000	Au	10.241800	-17.739300	7.242100
Au	20.483600	2.956600	0.000000	Au	18.776600	5.913100	2.414000	Au	15.362700	-17.739300	7.242100
Au	5.120900	2.956600	0.000000	Au	16.216200	7.391400	2.414000	Au	12.802200	-16.261000	7.242100
Au	12.802200	4.434800	0.000000	Au	21.337100	7.391400	2.414000	Au	17.923100	-16.261000	7.242100
Au	17.923100	4.434800	0.000000	Au	18.776600	8.869700	2.414000	Au	10.241800	-14.782800	7.242100
Au	7.681300	4.434800	0.000000	Au	14.509200	-19.217600	4.828000	Au	15.362700	-14.782800	7.242100
Au	10.241800	5.913100	0.000000	Au	11.948800	-17.739300	4.828000	Au	20.483600	-14.782800	7.242100
Au	15.362700	5.913100	0.000000	Au	17.069700	-17.739300	4.828000	Au	12.802200	-13.304500	7.242100
Au	12.802200	7.391400	0.000000	Au	14.509200	-16.261000	4.828000	Au	17.923100	-13.304500	7.242100
Au	17.923100	7.391400	0.000000	Au	19.630100	-16.261000	4.828000	Au	23.044000	-13.304500	7.242100
Au	15.362700	8.869700	0.000000	Au	11.948800	-14.782800	4.828000	Au	7.681300	-13.304500	7.242100
Au	16.216200	-19.217600	2.414000	Au	17.069700	-14.782800	4.828000	Au	10.241800	-11.826200	7.242100
Au	13.655700	-17.739300	2.414000	Au	22.190600	-14.782800	4.828000	Au	15.362700	-11.826200	7.242100
Au	18.776600	-17.739300	2.414000	Au	14.509200	-13.304500	4.828000	Au	20.483600	-11.826200	7.242100
Au	16.216200	-16.261000	2.414000	Au	19.630100	-13.304500	4.828000	Au	25.604500	-11.826200	7.242100
Au	21.337100	-16.261000	2.414000	Au	24.751000	-13.304500	4.828000	Au	12.802200	-10.347900	7.242100
Au	13.655700	-14.782800	2.414000	Au	9.388300	-13.304500	4.828000	Au	17.923100	-10.347900	7.242100

Au	23.044000	-10.347900	7.242100	Au	16.216200	-7.391400	9.656100	H	19.529700	-3.199600	18.290500
Au	28.164900	-10.347900	7.242100	Au	21.337100	-7.391400	9.656100	H	22.602000	-6.967100	18.320700
Au	7.681300	-10.347900	7.242100	Au	26.458000	-7.391400	9.656100	H	16.221700	-10.473900	18.339800
Au	10.241800	-8.869700	7.242100	Au	13.655700	-5.913100	9.656100	O	16.993500	-1.533400	18.353100
Au	15.362700	-8.869700	7.242100	Au	18.776600	-5.913100	9.656100	H	20.322700	-1.172000	18.356800
Au	20.483600	-8.869700	7.242100	Au	23.897500	-5.913100	9.656100	C	12.941300	-3.325300	18.487700
Au	25.604500	-8.869700	7.242100	Au	29.018400	-5.913100	9.656100	C	20.901600	-1.950700	18.565800
Au	5.120900	-8.869700	7.242100	Au	8.534800	-5.913100	9.656100	C	14.104000	-4.287300	18.578000
Au	12.802200	-7.391400	7.242100	Au	11.095300	-4.434800	9.656100	C	24.053400	-5.657000	18.815800
Au	17.923100	-7.391400	7.242100	Au	16.216200	-4.434800	9.656100	C	22.790500	-6.211200	18.864500
Au	23.044000	-7.391400	7.242100	Au	21.337100	-4.434800	9.656100	O	20.077300	-3.070300	18.890500
Au	7.681300	-7.391400	7.242100	Au	26.458000	-4.434800	9.656100	H	12.171200	-3.697200	18.901200
Au	10.241800	-5.913100	7.242100	Au	5.974400	-4.434800	9.656100	H	13.187700	-2.474000	18.922100
Au	15.362700	-5.913100	7.242100	Au	13.655700	-2.956600	9.656100	C	20.268000	-7.714000	19.095500
Au	20.483600	-5.913100	7.242100	Au	18.776600	-2.956600	9.656100	H	17.666700	4.010000	19.114000
Au	25.604500	-5.913100	7.242100	Au	23.897500	-2.956600	9.656100	H	21.127000	-8.198200	19.129700
Au	5.120900	-5.913100	7.242100	Au	8.534800	-2.956600	9.656100	H	17.120100	-8.580300	19.222100
Au	12.802200	-4.434800	7.242100	Au	11.095300	-1.478300	9.656100	H	15.363800	3.643600	19.244800
Au	17.923100	-4.434800	7.242100	Au	16.216200	-1.478300	9.656100	O	15.578100	-6.725300	19.298600
Au	23.044000	-4.434800	7.242100	Au	21.337100	-1.478300	9.656100	O	17.514000	-9.280400	19.308000
Au	2.560400	-4.434800	7.242100	Au	26.458000	-1.478300	9.656100	H	21.477400	-1.733000	19.338500
Au	7.681300	-4.434800	7.242100	Au	5.974400	-1.478300	9.656100	N	15.101300	-4.025100	19.354800
Au	10.241800	-2.956600	7.242100	Au	13.655700	0.000000	9.656100	C	17.334600	3.194200	19.468100
Au	15.362700	-2.956600	7.242100	Au	18.776600	0.000000	9.656100	C	15.970100	2.965400	19.513800
Au	20.483600	-2.956600	7.242100	Au	23.897500	0.000000	9.656100	H	25.190000	-4.147400	19.578800
Au	5.120900	-2.956600	7.242100	Au	3.413900	0.000000	9.656100	C	24.327300	-4.544700	19.603200
Au	12.802200	-1.478300	7.242100	Au	8.534800	0.000000	9.656100	Mn	16.700700	-5.197800	19.631900
Au	17.923100	-1.478300	7.242100	Au	11.095300	1.478300	9.656100	H	19.594500	-8.196700	19.635200
Au	23.044000	-1.478300	7.242100	Au	16.216200	1.478300	9.656100	C	20.448100	-6.338200	19.672100
Au	2.560400	-1.478300	7.242100	Au	21.337100	1.478300	9.656100	C	21.769800	-5.692800	19.683900
Au	7.681300	-1.478300	7.242100	Au	5.974400	1.478300	9.656100	H	19.140300	2.441100	19.931300
Au	0.000000	0.000000	7.242100	Au	13.655700	2.956600	9.656100	H	14.197400	-12.945300	19.932800
Au	10.241800	0.000000	7.242100	Au	18.776600	2.956600	9.656100	C	18.208800	2.247900	19.934300
Au	15.362700	0.000000	7.242100	Au	23.897500	2.956600	9.656100	C	15.501200	1.745700	19.945700
Au	20.483600	0.000000	7.242100	Au	8.534800	2.956600	9.656100	H	14.564600	1.583700	19.962100
Au	5.120900	0.000000	7.242100	Au	11.095300	4.434800	9.656100	O	15.025300	-2.897000	20.121800
Au	12.802200	1.478300	7.242100	Au	16.216200	4.434800	9.656100	N	19.427000	-5.672600	20.125600
Au	17.923100	1.478300	7.242100	Au	21.337100	4.434800	9.656100	O	18.198400	-6.324000	20.174700
Au	2.560400	1.478300	7.242100	Au	13.655700	5.913100	9.656100	O	17.611300	-3.695800	20.293000
Au	7.681300	1.478300	7.242100	Au	18.776600	5.913100	9.656100	C	16.379800	0.740200	20.370800
Au	10.241800	2.956600	7.242100	Au	16.216200	7.391400	9.656100	H	13.512600	-11.589800	20.400300
Au	15.362700	2.956600	7.242100	Au	21.337100	7.391400	9.656100	C	17.767100	0.999200	20.410600
Au	20.483600	2.956600	7.242100	Au	18.776600	8.869700	9.656100	C	23.355900	-4.015700	20.421200
Au	5.120900	2.956600	7.242100	S	17.069800	-5.913300	10.963100	C	22.070700	-4.572100	20.493700
Au	12.802200	4.434800	7.242100	H	18.730300	-4.078200	12.280900	O	14.779200	-9.758300	20.509900
Au	17.923100	4.434800	7.242100	C	17.270500	-5.490400	12.598200	Mn	16.700700	-2.053900	20.510200
Au	7.681300	4.434800	7.242100	C	18.195600	-4.510700	12.936200	C	14.068900	-12.362100	20.671700
Au	10.241800	5.913100	7.242100	H	15.883900	-6.814200	13.290400	H	20.520300	1.046800	20.694000
Au	15.362700	5.913100	7.242100	C	16.507400	-6.148300	13.555500	O	12.950300	-7.763200	20.757200
Au	12.802200	7.391400	7.242100	C	18.327500	-4.167400	14.280400	O	15.846800	-0.417000	20.776100
Au	17.923100	7.391400	7.242100	H	18.947500	-3.489800	14.536300	Mn	19.413500	-3.806800	20.848100
Au	15.362700	8.869700	7.242100	C	16.682500	-5.806900	14.891600	C	18.755500	0.059700	20.942400
Au	16.216200	-19.217600	9.656100	H	12.535200	-6.818200	15.202900	H	23.560400	-3.253800	20.949200
Au	13.655700	-17.739300	9.656100	C	17.581800	-4.811900	15.253400	N	18.449100	-1.205500	21.000900
Au	18.776600	-17.739300	9.656100	H	16.185600	-6.257000	15.564100	N	15.697600	-10.593500	21.103400
Au	16.216200	-16.261000	9.656100	C	13.067300	-6.796900	15.987700	H	10.586400	-8.545100	21.155200
Au	21.337100	-16.261000	9.656100	H	13.531600	-8.778300	16.003100	C	15.391300	-11.858600	21.161900
Au	13.655700	-14.782800	9.656100	H	12.804700	-4.839900	16.367900	Mn	14.733300	-7.992100	21.256200
Au	18.776600	-14.782800	9.656100	C	13.675900	-7.955400	16.453300	O	18.299800	-11.381900	21.328200
Au	23.897500	-14.782800	9.656100	C	13.246500	-5.623900	16.675600	O	21.196500	-4.035700	21.347200
Au	11.095300	-13.304500	9.656100	C	17.740800	-4.417000	16.702800	H	13.626500	-12.845700	21.410400
Au	16.216200	-13.304500	9.656100	H	16.335000	-0.421000	16.868200	C	20.077800	0.563200	21.432700
Au	21.337100	-13.304500	9.656100	O	18.368700	-3.342700	16.931000	Mn	17.446000	-9.744900	21.594100
Au	26.458000	-13.304500	9.656100	H	15.498200	-1.770300	17.072100	O	19.367500	-2.040500	21.594400
Au	13.655700	-11.826200	9.656100	H	17.245700	-9.669200	17.360400	C	12.076100	-7.226800	21.610600
Au	18.776600	-11.826200	9.656100	C	15.968600	-1.011400	17.516000	C	10.790900	-7.783200	21.683100
Au	23.897500	-11.826200	9.656100	H	12.746000	-3.084700	17.548700	C	16.379700	-12.798100	21.693800
Au	29.018400	-11.826200	9.656100	C	14.490100	-7.911400	17.565700	H	20.634100	-0.209000	21.704000
Au	11.095300	-10.347900	9.656100	O	17.239900	-5.168000	17.570100	C	17.766900	-12.539000	21.733600
Au	16.216200	-10.347900	9.656100	H	21.441900	-2.158900	17.812700	O	16.535400	-8.103000	21.811400
Au	21.337100	-10.347900	9.656100	C	14.060600	-5.539600	17.820500	O	15.948300	-5.474900	21.929700
Au	26.458000	-10.347900	9.656100	H	14.896900	-8.713600	17.875400	N	14.719800	-6.126300	21.978800
Au	31.578900	-10.347900	9.656100	H	17.463300	-2.061000	17.929700	O	19.121400	-8.901900	21.982600
Au	13.655700	-8.869700	9.656100	H	15.301000	-0.532400	18.092200	H	19.582000	-13.382700	22.142200
Au	18.776600	-8.869700	9.656100	H	19.971600	-7.648800	18.195300	C	18.645500	-13.544500	22.158600
Au	23.897500	-8.869700	9.656100	H	17.745000	-10.910400	18.213500	C	15.938000	-14.046800	22.170000
Au	29.018400	-8.869700	9.656100	C	17.160200	-10.161800	18.218300	H	19.949300	1.146400	22.171500
Au	8.534800	-8.869700	9.656100	C	14.733500	-6.708000	18.242100	H	15.006400	-14.240000	22.173000
Au	11.095300	-7.391400	9.656100	H	24.723900	-6.030800	18.254000	C	12.376800	-6.106200	22.420400

C	13.698700	-5.460700	22.432200	Au	23.897900	-11.825900	32.452000	Au	22.191000	-8.869400	34.866000
H	14.552200	-3.602300	22.469100	Au	29.018800	-11.825900	32.452000	Au	27.311900	-8.869400	34.866000
Mn	17.446000	-6.601100	22.472400	Au	11.095700	-10.347600	32.452000	Au	6.828300	-8.869400	34.866000
C	9.819400	-7.254100	22.501200	Au	16.216600	-10.347600	32.452000	Au	14.509600	-7.391100	34.866000
H	8.956800	-7.651400	22.525600	Au	21.337500	-10.347600	32.452000	Au	19.630500	-7.391100	34.866000
C	18.176600	-14.764200	22.590600	Au	26.458400	-10.347600	32.452000	Au	24.751400	-7.391100	34.866000
C	16.812100	-14.993000	22.636200	Au	31.579300	-10.347600	32.452000	Au	9.388700	-7.391100	34.866000
N	19.045500	-7.773800	22.749600	Au	13.656100	-8.869400	32.452000	Au	11.949200	-5.912800	34.866000
H	12.669300	-10.065800	22.765900	Au	18.777000	-8.869400	32.452000	Au	17.070100	-5.912800	34.866000
O	16.632700	-2.518400	22.796400	Au	23.897900	-8.869400	32.452000	Au	22.191000	-5.912800	34.866000
O	18.568600	-5.073600	22.805700	Au	29.018800	-8.869400	32.452000	Au	27.311900	-5.912800	34.866000
H	18.782900	-15.442500	22.859500	Au	8.535200	-8.869400	32.452000	Au	6.828300	-5.912800	34.866000
H	17.026700	-3.218600	22.882200	Au	11.095700	-7.391100	32.452000	Au	14.509600	-4.434500	34.866000
H	13.019800	-3.600700	22.974600	Au	16.216600	-7.391100	32.452000	Au	19.630500	-4.434500	34.866000
H	16.480000	-15.808800	22.990400	Au	21.337500	-7.391100	32.452000	Au	24.751400	-4.434500	34.866000
C	13.878600	-4.084900	23.008800	Au	26.458400	-7.391100	32.452000	Au	4.267800	-4.434500	34.866000
H	20.959100	-9.324900	23.182200	Au	13.656100	-5.912800	32.452000	Au	9.388700	-4.434500	34.866000
H	21.975600	-8.101600	23.203200	Au	18.777000	-5.912800	32.452000	Au	11.949200	-2.956300	34.866000
O	14.069400	-8.728500	23.213800	Au	23.897900	-5.912800	32.452000	Au	17.070100	-2.956300	34.866000
C	11.356300	-5.587700	23.239800	Au	29.018800	-5.912800	32.452000	Au	22.191000	-2.956300	34.866000
C	10.093300	-6.141800	23.288500	Au	8.535200	-5.912800	32.452000	Au	6.828300	-2.956300	34.866000
C	20.042700	-7.511600	23.526300	Au	11.095700	-4.434500	32.452000	Au	14.509600	-1.478000	34.866000
C	13.245100	-9.848100	23.538500	Au	16.216600	-4.434500	32.452000	Au	19.630500	-1.478000	34.866000
C	21.205400	-8.473600	23.616700	Au	21.337500	-4.434500	32.452000	Au	24.751400	-1.478000	34.866000
H	13.824000	-10.626900	23.747500	Au	26.458400	-4.434500	32.452000	Au	4.267800	-1.478000	34.866000
O	17.153300	-10.265600	23.751200	Au	5.974800	-4.434500	32.452000	Au	9.388700	-1.478000	34.866000
H	17.925000	-1.325000	23.764600	Au	13.656100	-2.956300	32.452000	Au	11.949200	0.000300	34.866000
H	11.544700	-4.831700	23.783600	Au	18.777000	-2.956300	32.452000	Au	17.070100	0.000300	34.866000
H	14.617100	-8.599300	23.813800	Au	23.897900	-2.956300	32.452000	Au	1.707400	0.000300	34.866000
H	9.422800	-5.768100	23.850300	Au	8.535200	-2.956300	32.452000	Au	22.191000	0.000300	34.866000
C	19.413300	-5.090900	23.862300	Au	11.095700	-1.478000	32.452000	Au	6.828300	0.000300	34.866000
C	16.986500	-1.637100	23.886000	Au	16.216600	-1.478000	32.452000	Au	14.509600	1.478600	34.866000
H	16.401700	-0.888500	23.890800	Au	21.337500	-1.478000	32.452000	Au	19.630500	1.478600	34.866000
H	14.175100	-4.150100	23.909000	Au	26.458400	-1.478000	32.452000	Au	4.267800	1.478600	34.866000
H	18.845800	-11.266500	24.012100	Au	5.974800	-1.478000	32.452000	Au	9.388700	1.478600	34.866000
H	16.683400	-9.737800	24.174600	Au	13.656100	0.000300	32.452000	Au	11.949200	2.956900	34.866000
H	19.249800	-3.085200	24.229000	Au	18.777000	0.000300	32.452000	Au	17.070100	2.956900	34.866000
C	20.086200	-6.259300	24.283800	Au	23.897900	0.000300	32.452000	Au	22.191000	2.956900	34.866000
H	12.704800	-9.639900	24.291600	Au	3.414300	0.000300	32.452000	Au	6.828300	2.956900	34.866000
O	16.906800	-6.630800	24.534300	Au	8.535200	0.000300	32.452000	Au	14.509600	4.435100	34.866000
C	19.656600	-3.887500	24.538700	Au	11.095700	1.478600	32.452000	Au	19.630500	4.435100	34.866000
H	21.400800	-8.714200	24.555600	Au	16.216600	1.478600	32.452000	Au	9.388700	4.435100	34.866000
C	18.178100	-10.787400	24.588300	Au	21.337500	1.478600	32.452000	Au	11.949200	5.913400	34.866000
H	16.901000	-2.129700	24.743900	Au	5.974800	1.478600	32.452000	Au	17.070100	5.913400	34.866000
H	18.648500	-10.028700	25.032200	Au	13.656100	2.956900	32.452000	Au	14.509600	7.391700	34.866000
O	15.777900	-8.456300	25.173400	Au	18.777000	2.956900	32.452000	Au	19.630500	7.391700	34.866000
H	17.811700	-11.377900	25.236100	Au	23.897900	2.956900	32.452000	Au	17.070100	8.870000	34.866000
C	16.406000	-7.381900	25.401600	Au	8.535200	2.956900	32.452000	Au	12.802600	-19.217300	37.280100
C	20.900300	-6.175000	25.428800	Au	11.095700	4.435100	32.452000	Au	10.242200	-17.739000	37.280100
C	20.470800	-3.843400	25.651000	Au	16.216600	4.435100	32.452000	Au	15.363100	-17.739000	37.280100
H	21.342000	-6.958900	25.736400	Au	21.337500	4.435100	32.452000	Au	12.802600	-16.260700	37.280100
H	20.615100	-3.020500	26.101200	Au	13.656100	5.913400	32.452000	Au	17.923500	-16.260700	37.280100
C	21.079400	-5.001900	26.116600	Au	18.777000	5.913400	32.452000	Au	10.242200	-14.782500	37.280100
H	17.961200	-5.541900	26.540200	Au	16.216600	7.391700	32.452000	Au	15.363100	-14.782500	37.280100
C	16.565000	-6.987000	26.851000	Au	21.337500	7.391700	32.452000	Au	20.484000	-14.782500	37.280100
H	21.611500	-4.980700	26.901500	Au	18.777000	8.870000	32.452000	Au	12.802600	-13.304200	37.280100
C	17.464200	-5.992000	27.212700	Au	14.509600	-19.217300	34.866000	Au	17.923500	-13.304200	37.280100
H	15.199300	-8.309100	27.568000	Au	11.949200	-17.739000	34.866000	Au	23.044400	-13.304200	37.280100
C	15.819300	-7.631500	27.824000	Au	17.070100	-17.739000	34.866000	Au	7.681700	-13.304200	37.280100
C	17.639300	-5.650700	28.548900	Au	14.509600	-16.260700	34.866000	Au	10.242200	-11.825900	37.280100
H	18.262800	-4.984800	28.813900	Au	19.630500	-16.260700	34.866000	Au	15.363100	-11.825900	37.280100
C	15.951100	-7.288100	29.168100	Au	11.949200	-14.782500	34.866000	Au	20.484000	-11.825900	37.280100
C	16.876300	-6.308500	29.506200	Au	17.070100	-14.782500	34.866000	Au	25.604900	-11.825900	37.280100
H	15.416400	-7.720700	29.823400	Au	22.191000	-14.782500	34.866000	Au	12.802600	-10.347600	37.280100
S	17.069800	-5.913300	31.144400	Au	14.509600	-13.304200	34.866000	Au	17.923500	-10.347600	37.280100
Au	16.216600	-19.217300	32.452000	Au	19.630500	-13.304200	34.866000	Au	23.044400	-10.347600	37.280100
Au	13.656100	-17.739000	32.452000	Au	24.751400	-13.304200	34.866000	Au	28.165300	-10.347600	37.280100
Au	18.777000	-17.739000	32.452000	Au	9.388700	-13.304200	34.866000	Au	7.681700	-10.347600	37.280100
Au	16.216600	-16.260700	32.452000	Au	11.949200	-11.825900	34.866000	Au	10.242200	-8.869400	37.280100
Au	21.337500	-16.260700	32.452000	Au	17.070100	-11.825900	34.866000	Au	15.363100	-8.869400	37.280100
Au	13.656100	-14.782500	32.452000	Au	22.191000	-11.825900	34.866000	Au	20.484000	-8.869400	37.280100
Au	18.777000	-14.782500	32.452000	Au	27.311900	-11.825900	34.866000	Au	25.604900	-8.869400	37.280100
Au	23.897900	-14.782500	32.452000	Au	14.509600	-10.347600	34.866000	Au	5.121300	-8.869400	37.280100
Au	11.095700	-13.304200	32.452000	Au	19.630500	-10.347600	34.866000	Au	12.802600	-7.391100	37.280100
Au	16.216600	-13.304200	32.452000	Au	24.751400	-10.347600	34.866000	Au	17.923500	-7.391100	37.280100
Au	21.337500	-13.304200	32.452000	Au	29.872300	-10.347600	34.866000	Au	23.044400	-7.391100	37.280100
Au	26.458400	-13.304200	32.452000	Au	9.388700	-10.347600	34.866000	Au	7.681700	-7.391100	37.280100
Au	13.656100	-11.825900	32.452000	Au	11.949200	-8.869400	34.866000	Au	10.242200	-5.912800	37.280100
Au	18.777000	-11.825900	32.452000	Au	17.070100	-8.869400	34.866000	Au	15.363100	-5.912800	37.280100

Au	20.484000	-5.912800	37.280100	Au	18.777000	-8.869400	39.694100	Au	11.949200	-11.825900	42.108100
Au	25.604900	-5.912800	37.280100	Au	23.897900	-8.869400	39.694100	Au	17.070100	-11.825900	42.108100
Au	5.121300	-5.912800	37.280100	Au	29.018800	-8.869400	39.694100	Au	22.191000	-11.825900	42.108100
Au	12.802600	-4.434500	37.280100	Au	8.535200	-8.869400	39.694100	Au	27.311900	-11.825900	42.108100
Au	17.923500	-4.434500	37.280100	Au	11.095700	-7.391100	39.694100	Au	14.509600	-10.347600	42.108100
Au	23.044400	-4.434500	37.280100	Au	16.216600	-7.391100	39.694100	Au	19.630500	-10.347600	42.108100
Au	2.560800	-4.434500	37.280100	Au	21.337500	-7.391100	39.694100	Au	24.751400	-10.347600	42.108100
Au	7.681700	-4.434500	37.280100	Au	26.458400	-7.391100	39.694100	Au	29.872300	-10.347600	42.108100
Au	10.242200	-2.956300	37.280100	Au	13.656100	-5.912800	39.694100	Au	9.388700	-10.347600	42.108100
Au	15.363100	-2.956300	37.280100	Au	18.777000	-5.912800	39.694100	Au	11.949200	-8.869400	42.108100
Au	20.484000	-2.956300	37.280100	Au	23.897900	-5.912800	39.694100	Au	17.070100	-8.869400	42.108100
Au	5.121300	-2.956300	37.280100	Au	29.018800	-5.912800	39.694100	Au	22.191000	-8.869400	42.108100
Au	12.802600	-1.478000	37.280100	Au	8.535200	-5.912800	39.694100	Au	27.311900	-8.869400	42.108100
Au	17.923500	-1.478000	37.280100	Au	11.095700	-4.434500	39.694100	Au	6.828300	-8.869400	42.108100
Au	23.044400	-1.478000	37.280100	Au	16.216600	-4.434500	39.694100	Au	14.509600	-7.391100	42.108100
Au	2.560800	-1.478000	37.280100	Au	21.337500	-4.434500	39.694100	Au	19.630500	-7.391100	42.108100
Au	7.681700	-1.478000	37.280100	Au	26.458400	-4.434500	39.694100	Au	24.751400	-7.391100	42.108100
Au	0.000400	0.000300	37.280100	Au	5.974800	-4.434500	39.694100	Au	9.388700	-7.391100	42.108100
Au	10.242200	0.000300	37.280100	Au	13.656100	-2.956300	39.694100	Au	11.949200	-5.912800	42.108100
Au	15.363100	0.000300	37.280100	Au	18.777000	-2.956300	39.694100	Au	17.070100	-5.912800	42.108100
Au	20.484000	0.000300	37.280100	Au	23.897900	-2.956300	39.694100	Au	22.191000	-5.912800	42.108100
Au	5.121300	0.000300	37.280100	Au	8.535200	-2.956300	39.694100	Au	27.311900	-5.912800	42.108100
Au	12.802600	1.478600	37.280100	Au	11.095700	-1.478000	39.694100	Au	6.828300	-5.912800	42.108100
Au	17.923500	1.478600	37.280100	Au	16.216600	-1.478000	39.694100	Au	14.509600	-4.434500	42.108100
Au	2.560800	1.478600	37.280100	Au	21.337500	-1.478000	39.694100	Au	19.630500	-4.434500	42.108100
Au	7.681700	1.478600	37.280100	Au	26.458400	-1.478000	39.694100	Au	24.751400	-4.434500	42.108100
Au	10.242200	2.956900	37.280100	Au	5.974800	-1.478000	39.694100	Au	4.267800	-4.434500	42.108100
Au	15.363100	2.956900	37.280100	Au	13.656100	0.000300	39.694100	Au	9.388700	-4.434500	42.108100
Au	20.484000	2.956900	37.280100	Au	18.777000	0.000300	39.694100	Au	11.949200	-2.956300	42.108100
Au	5.121300	2.956900	37.280100	Au	23.897900	0.000300	39.694100	Au	17.070100	-2.956300	42.108100
Au	12.802600	4.435100	37.280100	Au	3.414300	0.000300	39.694100	Au	22.191000	-2.956300	42.108100
Au	17.923500	4.435100	37.280100	Au	8.535200	0.000300	39.694100	Au	6.828300	-2.956300	42.108100
Au	7.681700	4.435100	37.280100	Au	11.095700	1.478600	39.694100	Au	14.509600	-1.478000	42.108100
Au	10.242200	5.913400	37.280100	Au	16.216600	1.478600	39.694100	Au	19.630500	-1.478000	42.108100
Au	15.363100	5.913400	37.280100	Au	21.337500	1.478600	39.694100	Au	24.751400	-1.478000	42.108100
Au	12.802600	7.391700	37.280100	Au	5.974800	1.478600	39.694100	Au	4.267800	-1.478000	42.108100
Au	17.923500	7.391700	37.280100	Au	13.656100	2.956900	39.694100	Au	9.388700	-1.478000	42.108100
Au	15.363100	8.870000	37.280100	Au	18.777000	2.956900	39.694100	Au	11.949200	0.000300	42.108100
Au	16.216600	-19.217300	39.694100	Au	23.897900	2.956900	39.694100	Au	17.070100	0.000300	42.108100
Au	13.656100	-17.739000	39.694100	Au	8.535200	2.956900	39.694100	Au	1.707400	0.000300	42.108100
Au	18.777000	-17.739000	39.694100	Au	11.095700	4.435100	39.694100	Au	22.191000	0.000300	42.108100
Au	16.216600	-16.260700	39.694100	Au	16.216600	4.435100	39.694100	Au	6.828300	0.000300	42.108100
Au	21.337500	-16.260700	39.694100	Au	21.337500	4.435100	39.694100	Au	14.509600	1.478600	42.108100
Au	13.656100	-14.782500	39.694100	Au	13.656100	5.913400	39.694100	Au	19.630500	1.478600	42.108100
Au	18.777000	-14.782500	39.694100	Au	18.777000	5.913400	39.694100	Au	4.267800	1.478600	42.108100
Au	23.897900	-14.782500	39.694100	Au	16.216600	7.391700	39.694100	Au	9.388700	1.478600	42.108100
Au	11.095700	-13.304200	39.694100	Au	21.337500	7.391700	39.694100	Au	11.949200	2.956900	42.108100
Au	16.216600	-13.304200	39.694100	Au	18.777000	8.870000	39.694100	Au	17.070100	2.956900	42.108100
Au	21.337500	-13.304200	39.694100	Au	14.509600	-19.217300	42.108100	Au	22.191000	2.956900	42.108100
Au	26.458400	-13.304200	39.694100	Au	11.949200	-17.739000	42.108100	Au	6.828300	2.956900	42.108100
Au	13.656100	-11.825900	39.694100	Au	17.070100	-17.739000	42.108100	Au	14.509600	4.435100	42.108100
Au	18.777000	-11.825900	39.694100	Au	14.509600	-16.260700	42.108100	Au	19.630500	4.435100	42.108100
Au	23.897900	-11.825900	39.694100	Au	19.630500	-16.260700	42.108100	Au	9.388700	4.435100	42.108100
Au	29.018800	-11.825900	39.694100	Au	11.949200	-14.782500	42.108100	Au	11.949200	5.913400	42.108100
Au	11.095700	-10.347600	39.694100	Au	17.070100	-14.782500	42.108100	Au	17.070100	5.913400	42.108100
Au	16.216600	-10.347600	39.694100	Au	22.191000	-14.782500	42.108100	Au	14.509600	7.391700	42.108100
Au	21.337500	-10.347600	39.694100	Au	14.509600	-13.304200	42.108100	Au	19.630500	7.391700	42.108100
Au	26.458400	-10.347600	39.694100	Au	19.630500	-13.304200	42.108100	Au	17.070100	8.870000	42.108100
Au	31.579300	-10.347600	39.694100	Au	24.751400	-13.304200	42.108100				
Au	13.656100	-8.869400	39.694100	Au	9.388700	-13.304200	42.108100				