

Supporting Information for:

**N-Heterocyclic Carbene Derivatives to Modify Gold Superatoms Characteristics. Tailorable Electronic and Optical Properties for  $[\text{Au}_{11}(\text{PPh}_3)_7\text{LCl}_2]^+$  as Cluster from Relativistic DFT**

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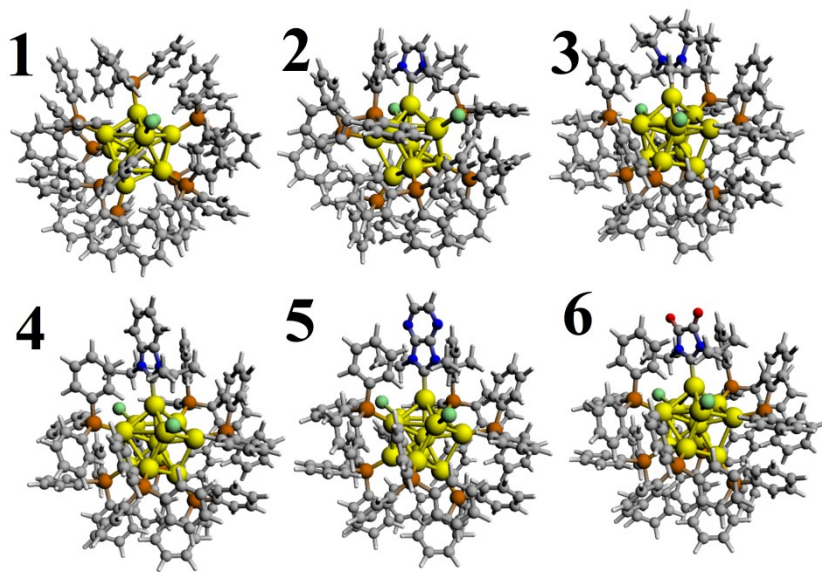


Figure S1. Representation of optimized structures for 1-6.

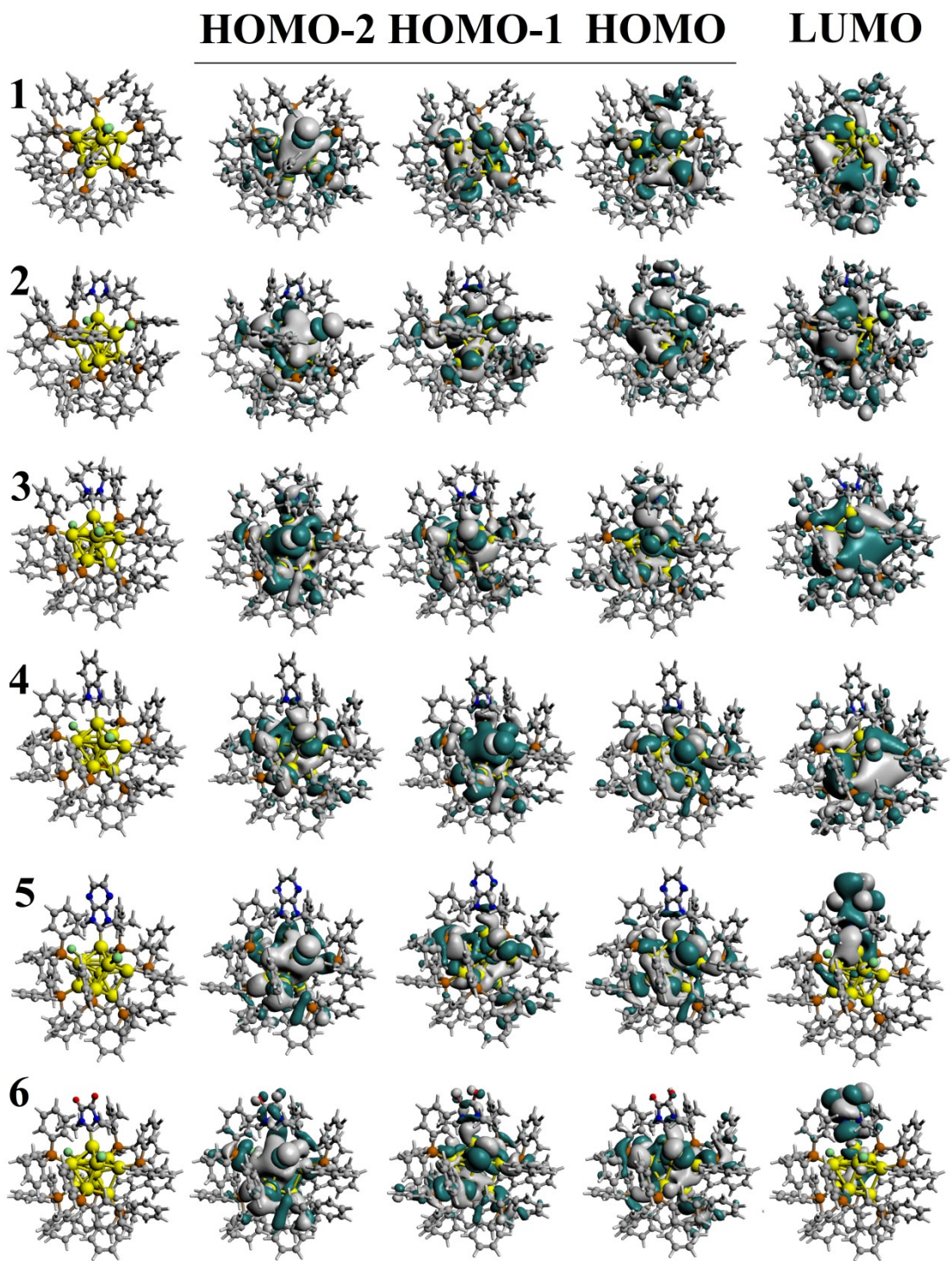


Figure S2. Isosurface representation of HOMO and LUMO for **1-6**.



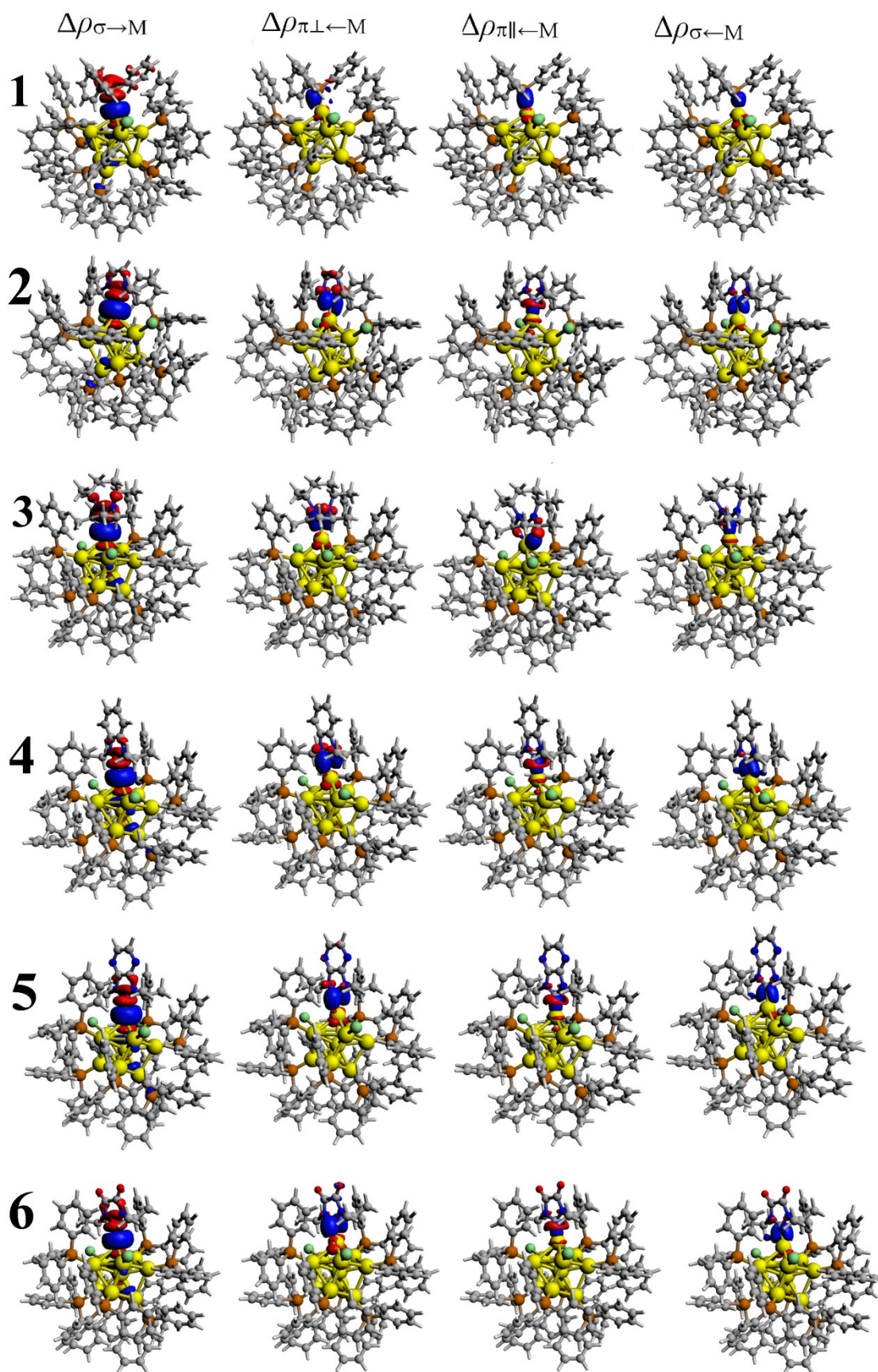


Figure S3. Isosurface representation of main deformation densities from NOCV-EDA analysis for 1-6.

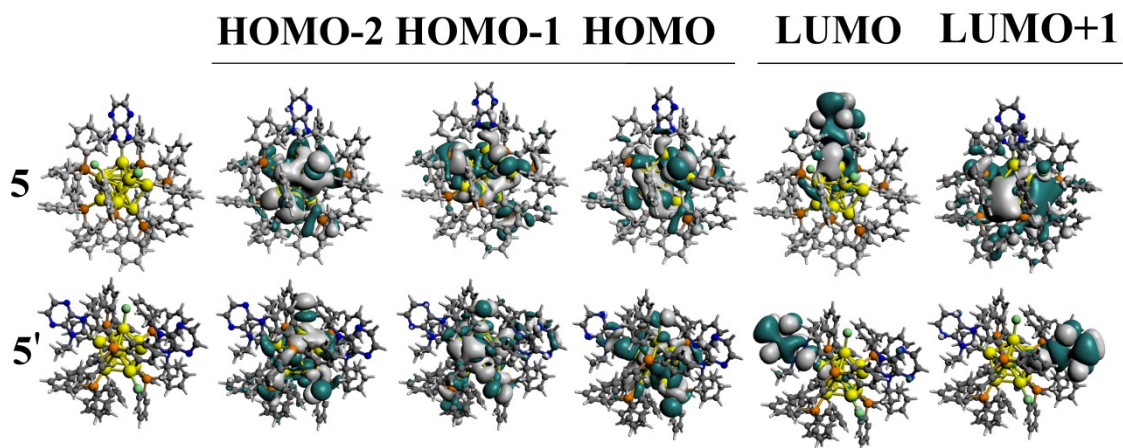


Figure S4. Isosurface representation of HOMO and LUMO for **5** and **5'**.

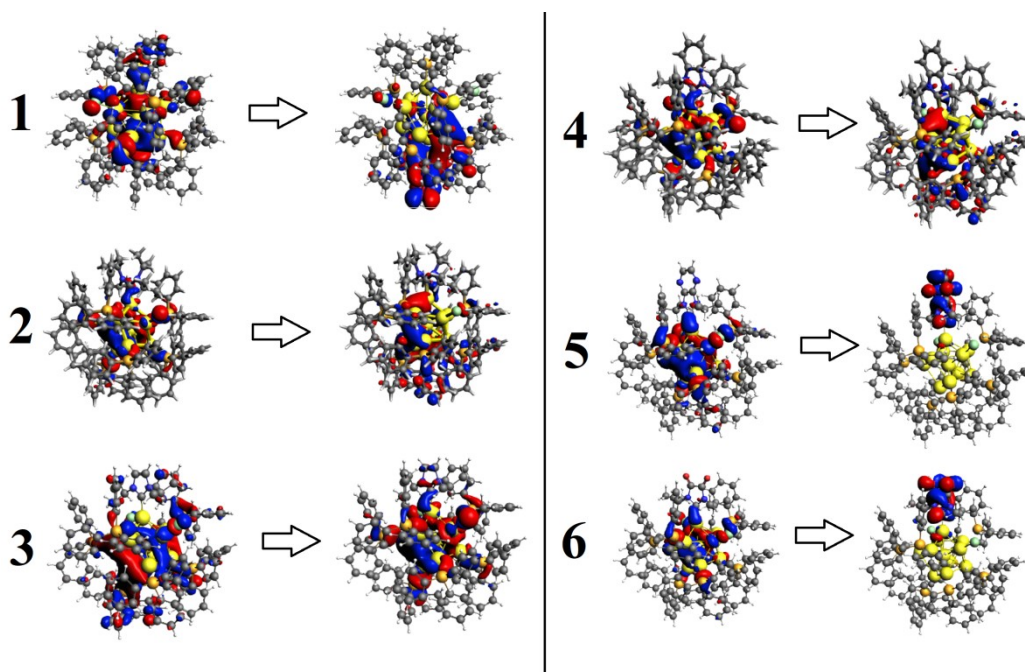


Figure S5. Isosurface representation of Natural Transition Orbitals (NTO) related to Further analysis of the optical HOMO-LUMO transition ( $S_0 \rightarrow S_1$ ) transition for **1-6**, which contribute above of 96% to the transition in all cases.

Table S1. Distances Au<sup>P/C</sup>-P/C and Au<sup>Cent</sup>-Au<sup>P/C</sup> (Å) for clusters **1** to **6** at ground state (S<sub>0</sub>), first triplet excited state (T<sub>1</sub>) and first singlet excited state (S<sub>1</sub>).

	<b>1</b>			<b>2</b>			<b>3</b>		
	S <sub>0</sub>	T <sub>1</sub>	S <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>	S <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>	S <sub>1</sub>
Au <sup>Cent</sup> -Au <sup>C</sup>	2.807	2.718	2.887	2.787	2.750	2.742	2.786	2.721	2.730
Au <sup>Cent</sup> -Au <sup>P</sup>	2.684	2.679	2.687	2.697	2.675	2.657	2.683	2.660	2.670
	2.693	2.679	2.709	2.701	2.688	2.714	2.688	2.675	2.698
	2.709	2.692	2.714	2.701	2.694	2.716	2.696	2.676	2.698
	2.723	2.692	2.725	2.703	2.718	2.750	2.697	2.681	2.700
	2.743	2.725	2.734	2.724	2.720	2.764	2.704	2.691	2.710
	2.751	2.725	2.737	2.764	2.720	2.865	2.741	2.758	2.806
	2.753	2.763	2.749	2.769	2.765	2.865	2.760	2.759	2.821
Average Au <sup>Cent</sup> -Au <sup>P</sup>	2.722	2.708	2.722	2.723	2.711	2.762	2.710	2.700	2.729
Au <sup>Cent</sup> -Au <sup>Cl</sup>	2.803	2.818	2.798	2.795	2.797	2.788	2.807	2.844	2.878
Au <sup>Cent</sup> -Au <sup>Cl</sup>	2.815	2.837	2.830	2.806	2.869	2.836	2.836	2.954	2.892
Average Au <sup>Cent</sup> -Au <sup>Cl</sup>	2.809	2.827	2.814	2.800	2.833	2.812	2.821	2.899	2.885
	<b>4</b>			<b>5</b>			<b>6</b>		
	S <sub>0</sub>	T <sub>1</sub>	S <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>	S <sub>1</sub>	S <sub>0</sub>	T <sub>1</sub>	S <sub>1</sub>
Au <sup>Cent</sup> -Au <sup>C</sup>	2.733	2.726	2.754	2.733	2.752	2.732	2.703	2.760	2.723
Au <sup>Cent</sup> -Au <sup>P</sup>	2.673	2.663	2.669	2.676	2.677	2.674	2.676	2.671	2.672
	2.690	2.665	2.680	2.692	2.680	2.691	2.682	2.674	2.672
	2.695	2.691	2.667	2.701	2.681	2.700	2.711	2.679	2.684
	2.722	2.691	2.740	2.703	2.687	2.702	2.712	2.686	2.730
	2.739	2.714	2.753	2.710	2.702	2.708	2.717	2.698	2.731
	2.748	2.718	2.746	2.742	2.750	2.741	2.739	2.734	2.737
	2.798	2.789	2.782	2.769	2.750	2.765	2.773	2.742	2.758
Average Au <sup>Cent</sup> -Au <sup>P</sup>	2.724	2.704	2.720	2.713	2.704	2.712	2.716	2.698	2.712
Au <sup>Cent</sup> -Au <sup>Cl</sup>	2.792	2.834	2.825	2.809	2.804	2.808	2.815	2.817	2.848
Au <sup>Cent</sup> -Au <sup>Cl</sup>	2.819	2.904	2.837	2.847	2.833	2.846	2.827	2.817	2.846
Average Au <sup>Cent</sup> -Au <sup>Cl</sup>	2.805	2.869	2.831	2.828	2.819	2.827	2.821	2.817	2.847

Table S2. Energy (eV) and wavelength (nm) for the relevant transitions calculated for the studied species. 1P and 1D, stands from orbitals compromising the superatomic shell manifold; PPh<sub>3</sub> and NHC, accounts for orbitals involving mainly the PPh<sub>3</sub> and NHC ligands, respectively, whereas 5d, accountos for orbitals located at the 5d-Au block.

	E (eV)	$\lambda$ (nm)	Composition	Character
<b>1</b>	1.963	631	479a -> 480a	1P $\rightarrow$ 1D
	2.756	450	474a -> 481a	1P $\rightarrow$ 1D
	2.871	432	476a -> 489a	1P $\rightarrow$ PPh <sub>3</sub>
	3.012	412	474a -> 489a	5d $\rightarrow$ PPh <sub>3</sub>
<b>2</b>	2.140	579	464a -> 465a	1P $\rightarrow$ 1D
	2.702	459	464a -> 504a	1P $\rightarrow$ PPh <sub>3</sub>
	2.747	451	464a -> 505a	1P $\rightarrow$ PPh <sub>3</sub>
	3.032	408	464a -> 510a	5d $\rightarrow$ PPh <sub>3</sub>
<b>3</b>	2.121	585	478a -> 479a	1P $\rightarrow$ 1D
	2.777	446	477a -> 519a	1P $\rightarrow$ PPh <sub>3</sub>
	2.877	431	478a -> 522a	1P $\rightarrow$ PPh <sub>3</sub>
	2.992	414	476a -> 524a	5d $\rightarrow$ PPh <sub>3</sub>
<b>4</b>	2.127	583	473a -> 474a	1P $\rightarrow$ 1D/NHC
	2.693	460	473a -> 511a	1P $\rightarrow$ PPh <sub>3</sub>
	2.806	442	468a -> 477a	1P $\rightarrow$ PPh <sub>3</sub>
	3.082	402	466a -> 483a	5d $\rightarrow$ PPh <sub>3</sub>
<b>5</b>	1.523	814	473a -> 474a	1P $\rightarrow$ NHC
	2.632	471	473a -> 511a	1P $\rightarrow$ PPh <sub>3</sub>
	2.684	462	471a -> 511a	1P $\rightarrow$ PPh <sub>3</sub>
	3.023	410	467a -> 482a	5d $\rightarrow$ NHC
<b>6</b>	1.292	960	469a -> 470a	1P $\rightarrow$ NHC
	2.586	479	467a -> 494a	1P $\rightarrow$ PPh <sub>3</sub>
	2.622	473	467a -> 496a	1P $\rightarrow$ PPh <sub>3</sub>
	2.989	415	444a -> 470a	5d $\rightarrow$ NHC
<b>5'</b>	1.308	948	467a -> 468a	1P $\rightarrow$ NHC
	2.614	474	465a -> 500a	1P $\rightarrow$ PPh <sub>3</sub>
	2.785	445	467a -> 508a	1P $\rightarrow$ PPh <sub>3</sub>
	3.077	403	463a -> 485a	5d $\rightarrow$ NHC

Table S3. Optimized coordinates for the studied species (Å), in a multiXYZ format.

285

1 S0

Au	2.640000000	5.462400000	21.710700000
Au	1.268200000	3.497900000	20.248000000
Au	1.777600000	3.214300000	23.169600000
Au	-0.058100000	5.216700000	22.196800000
Au	0.999200000	6.641700000	19.768300000
Au	3.550600000	5.142100000	19.143000000
Au	4.159700000	3.247300000	21.362500000
Au	3.076700000	5.593400000	24.355600000
Au	1.445300000	7.627800000	22.849800000
Au	3.591700000	7.890600000	20.834700000
Au	5.264500000	5.889200000	22.136000000
Cl	1.016400000	1.281300000	24.322900000
Cl	-0.374800000	7.687200000	18.117200000
P	-0.117400000	2.088500000	19.069100000
P	-2.232600000	5.297800000	22.901400000
P	4.103600000	4.906600000	16.922300000
P	5.213200000	1.226500000	21.597200000
P	3.460800000	5.638600000	26.628600000
P	0.580000000	9.669500000	23.493500000
P	4.406500000	9.922700000	20.101200000
P	7.511800000	6.347700000	22.320000000
C	0.682800000	1.501200000	17.535900000
C	-0.002800000	1.357800000	16.321200000
H	-1.063200000	1.606900000	16.258100000
C	0.685700000	0.922600000	15.184500000
H	0.155800000	0.824900000	14.236700000
C	2.051000000	0.628300000	15.259400000
H	2.587800000	0.301400000	14.366500000
C	2.732300000	0.765000000	16.473000000
H	3.798000000	0.543600000	16.536800000
C	2.055400000	1.209200000	17.607800000
H	2.594500000	1.334900000	18.550200000
C	-0.633500000	0.574600000	19.961200000
C	-0.964900000	-0.604600000	19.272900000
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C	-1.383000000	-1.730200000	19.986000000
H	-1.640700000	-2.644600000	19.450700000
C	-1.454000000	-1.690200000	21.384200000
H	-1.764800000	-2.577200000	21.938800000
C	-1.098000000	-0.524400000	22.068000000
H	-1.100900000	-0.486900000	23.156400000
C	-0.694100000	0.608200000	21.359600000
H	-0.398900000	1.505500000	21.903400000
C	-1.671000000	2.928400000	18.572700000
C	-1.684500000	4.331200000	18.514100000
H	-0.792900000	4.902800000	18.773100000
C	-2.835100000	5.013500000	18.122200000
H	-2.809500000	6.102600000	18.084100000
C	-3.986700000	4.296400000	17.785500000
H	-4.891300000	4.827600000	17.485300000
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H	-4.884900000	2.336600000	17.599400000



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C	-2.572800000	7.305700000	21.030800000
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C	-3.564800000	5.094100000	25.385200000
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H	-0.181600000	5.403600000	24.987500000
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C	2.637400000	4.938900000	15.828500000
C	2.760200000	5.271200000	14.466400000
H	3.737100000	5.525200000	14.050500000
C	1.624000000	5.315800000	13.657400000
H	1.722600000	5.575400000	12.602500000
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C	2.479100000	-1.922700000	19.630000000
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C	2.180700000	-1.398800000	20.891800000
H	1.263700000	-1.690600000	21.403500000
C	3.039100000	-0.481900000	21.496800000
H	2.779200000	-0.055500000	22.469300000
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C	5.240800000	1.775600000	24.345200000
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C	5.530500000	1.488700000	25.680700000
H	5.407000000	2.261400000	26.438900000
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C	6.094200000	-0.791900000	25.077400000
H	6.410100000	-1.796000000	25.364100000
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H	5.926100000	-1.286300000	22.982100000
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C	7.527000000	-0.125300000	20.626200000
H	6.980100000	-1.058800000	20.756400000
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H	9.309500000	-1.101700000	19.908800000
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H	10.573800000	1.026800000	19.612800000
C	8.942500000	2.271300000	20.290200000
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H	-0.359500000	8.650300000	29.630200000
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H	6.197200000	4.748000000	26.226300000
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C	4.390100000	3.680600000	28.476400000
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H	3.386700000	9.236800000	24.066700000
C	0.360200000	10.805800000	22.078800000
C	0.066200000	10.238400000	20.828600000
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H	-0.405400000	13.092700000	19.029000000
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H	0.119900000	14.102500000	21.246100000
C	0.382400000	12.200900000	22.227200000
H	0.641400000	12.644700000	23.189200000
C	-1.045500000	9.681900000	24.339100000
C	-1.966900000	10.733100000	24.213400000
H	-1.769200000	11.558100000	23.529800000
C	-3.146900000	10.714600000	24.961800000
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C	-3.417100000	9.651800000	25.830300000
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H	-2.717300000	7.748400000	26.594000000
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C	3.469800000	12.351900000	21.225100000
H	2.764100000	12.404500000	20.395400000
C	3.494300000	13.365200000	22.189200000
H	2.803200000	14.204000000	22.100500000
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C	5.260700000	12.209400000	23.372200000
H	5.955200000	12.144300000	24.209400000
C	5.234900000	11.189400000	22.424400000
H	5.912600000	10.338600000	22.517500000
C	3.531500000	10.551600000	18.613100000
C	3.952900000	11.726500000	17.965700000
H	4.786900000	12.303400000	18.365300000
C	3.307900000	12.150400000	16.803300000
H	3.638000000	13.062600000	16.305100000
C	2.251100000	11.399300000	16.269700000
H	1.761600000	11.725800000	15.350400000
C	1.829400000	10.233800000	16.912200000
H	1.007300000	9.633900000	16.521800000
C	2.462100000	9.818500000	18.086100000
H	2.112600000	8.914700000	18.586300000
C	6.171500000	9.918900000	19.587400000
C	6.948500000	11.089800000	19.644100000
H	6.539700000	11.995000000	20.093900000
C	8.251600000	11.090300000	19.144800000
H	8.848200000	12.002400000	19.196400000
C	8.786900000	9.925000000	18.582800000
H	9.803900000	9.926300000	18.186800000
C	8.021100000	8.757600000	18.535900000
H	8.431800000	7.847000000	18.101400000
C	6.719600000	8.748500000	19.045400000
H	6.122800000	7.834900000	19.007000000
C	8.382700000	6.028100000	20.726900000
C	9.773700000	6.180500000	20.596800000
H	10.366800000	6.531800000	21.440600000
C	10.403500000	5.871400000	19.388800000
H	11.482400000	5.998100000	19.294400000
C	9.655700000	5.381700000	18.311400000
H	10.151100000	5.126500000	17.373800000
C	8.275200000	5.210900000	18.441600000
H	7.686800000	4.819900000	17.613700000
C	7.639200000	5.542500000	19.638600000
H	6.557400000	5.414700000	19.731700000
C	8.416800000	5.307900000	23.530700000
C	7.873200000	4.059000000	23.869000000
H	6.916800000	3.747900000	23.445400000
C	8.545400000	3.217900000	24.755500000
H	8.107300000	2.253500000	25.014100000
C	9.765300000	3.621400000	25.308500000
H	10.291500000	2.966800000	26.003500000
C	10.308000000	4.869400000	24.980400000
H	11.250800000	5.191800000	25.423900000
C	9.634600000	5.716300000	24.098700000
H	10.038000000	6.704400000	23.872600000
C	7.881700000	8.059500000	22.853200000
C	7.355200000	8.447300000	24.100900000

H	6.745100000	7.750300000	24.680000000
C	7.626500000	9.719700000	24.603100000
H	7.236900000	10.002200000	25.581100000
C	8.388800000	10.625300000	23.856500000
H	8.590100000	11.624300000	24.245500000
C	8.872100000	10.256200000	22.599400000
H	9.440600000	10.965000000	21.997500000
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H	8.997800000	8.700100000	21.109500000
285			
1 T1			
Au	-0.282600000	-0.403100000	0.284800000
Au	-2.228600000	-1.285600000	-1.395300000
Au	0.260400000	-2.988500000	-0.695000000
Au	-1.679100000	-2.509600000	1.400300000
Au	-2.897300000	0.352100000	1.086100000
Au	-1.393900000	1.465000000	-1.469700000
Au	0.604500000	-0.610700000	-2.247900000
Au	1.739000000	-1.611300000	1.588300000
Au	-0.581700000	-0.195400000	2.985100000
Au	-0.204200000	2.112100000	1.204600000
Au	2.032600000	0.854700000	-0.201200000
Cl	0.939700000	-5.117600000	-1.497900000
Cl	-5.097100000	0.951800000	1.830800000
P	-3.919000000	-1.904600000	-2.774000000
P	-2.366200000	3.232400000	-2.571700000
P	1.404400000	-1.091400000	-4.324500000
P	3.562600000	-2.686900000	2.462200000
P	-0.754600000	0.037200000	5.271700000
P	-0.276900000	4.297900000	1.883200000
P	4.047100000	1.842000000	-0.632400000
C	-3.421400000	-2.157400000	-4.507600000
C	-2.464200000	-1.292700000	-5.046200000
H	-2.018400000	-0.531100000	-4.405000000
C	-2.051600000	-1.440400000	-6.366500000
H	-1.309600000	-0.758600000	-6.778200000
C	-2.553000000	-2.483800000	-7.141500000
H	-2.194900000	-2.623300000	-8.162000000
C	-3.493200000	-3.361700000	-6.601800000
H	-3.878500000	-4.187100000	-7.201700000
C	-3.943600000	-3.192400000	-5.293200000
H	-4.681300000	-3.879500000	-4.877900000
C	-5.206800000	-0.616900000	-2.807200000
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H	-6.759300000	1.434800000	-0.584200000
C	-7.041900000	1.479500000	-2.741500000
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H	-7.107500000	1.277800000	-4.893200000
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C	-4.720100000	-3.468200000	-2.331800000
C	-6.105400000	-3.607100000	-2.238700000
H	-6.754700000	-2.742400000	-2.386500000



C	-6.652400000	-4.860000000	-1.961600000
H	-7.732100000	-4.970200000	-1.867100000
C	-5.821400000	-5.966100000	-1.812800000
H	-6.243400000	-6.948600000	-1.593100000
C	-4.438700000	-5.823800000	-1.923400000
H	-3.788200000	-6.686300000	-1.811500000
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C	-1.101800000	4.389200000	-3.226100000
C	0.194100000	4.349900000	-2.689200000
H	0.417800000	3.672000000	-1.861400000
C	1.193500000	5.159200000	-3.225000000
H	2.202200000	5.111900000	-2.815200000
C	0.906700000	6.025600000	-4.278900000
H	1.695100000	6.656400000	-4.696500000
C	-0.387200000	6.087800000	-4.798000000
H	-0.615000000	6.765600000	-5.621700000
C	-1.389300000	5.264100000	-4.282400000
H	-2.386500000	5.278400000	-4.726600000
C	-3.395000000	2.889500000	-4.042900000
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H	-5.015700000	4.231900000	-3.530600000
C	-5.282000000	3.341300000	-5.477400000
H	-6.219300000	3.867700000	-5.658800000
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H	-5.315400000	2.283500000	-7.357000000
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H	-3.199800000	1.055600000	-6.906000000
C	-2.899500000	1.987300000	-4.992500000
H	-1.960600000	1.471000000	-4.808100000
C	-3.468300000	4.213000000	-1.505500000
C	-4.303600000	3.500000000	-0.641600000
H	-4.229200000	2.415000000	-0.570700000
C	-5.222000000	4.180200000	0.149100000
H	-5.849500000	3.605400000	0.826500000
C	-5.291000000	5.571700000	0.104000000
H	-5.985300000	6.104800000	0.753700000
C	-4.456400000	6.284400000	-0.754100000
H	-4.507300000	7.373500000	-0.786900000
C	-3.552200000	5.607500000	-1.570900000
H	-2.902000000	6.165000000	-2.242900000
C	3.222100000	-1.246000000	-4.310300000
C	3.767300000	-2.293100000	-3.545700000
H	3.105900000	-3.008600000	-3.054300000
C	5.149200000	-2.405400000	-3.419900000
H	5.578700000	-3.216600000	-2.833200000
C	5.988500000	-1.476100000	-4.028000000
H	7.069300000	-1.559600000	-3.903600000
C	5.444400000	-0.442000000	-4.785700000
H	6.094900000	0.282000000	-5.269300000
C	4.060300000	-0.324500000	-4.933300000
H	3.636900000	0.488800000	-5.523600000
C	0.821200000	-2.687700000	-4.987200000
C	-0.263200000	-3.326400000	-4.371800000
H	-0.717700000	-2.892200000	-3.483500000
C	-0.757000000	-4.520700000	-4.887800000

H	-1.599500000	-5.012400000	-4.400000000
C	-0.172200000	-5.083300000	-6.020100000
H	-0.562500000	-6.015400000	-6.431100000
C	0.933300000	-4.471600000	-6.616800000
H	1.414900000	-4.930800000	-7.480700000
C	1.442600000	-3.285000000	-6.092800000
H	2.339800000	-2.836800000	-6.523800000
C	1.012600000	0.214000000	-5.551300000
C	1.059200000	0.002800000	-6.937200000
H	1.311500000	-0.978500000	-7.337800000
C	0.736100000	1.036100000	-7.814300000
H	0.754800000	0.858900000	-8.891900000
C	0.386300000	2.291500000	-7.317400000
H	0.131200000	3.099300000	-8.004700000
C	0.348700000	2.511100000	-5.940000000
H	0.068200000	3.486700000	-5.545100000
C	0.649300000	1.475600000	-5.059500000
H	0.576600000	1.635500000	-3.979800000
C	4.552400000	-3.562700000	1.194600000
C	5.861000000	-3.987200000	1.448800000
H	6.364400000	-3.704300000	2.372600000
C	6.528600000	-4.763100000	0.506500000
H	7.550300000	-5.088500000	0.703700000
C	5.889800000	-5.134100000	-0.680800000
H	6.412900000	-5.757600000	-1.406800000
C	4.583500000	-4.719900000	-0.928600000
H	4.055400000	-5.028900000	-1.831800000
C	3.920700000	-3.922600000	0.000800000
H	2.896300000	-3.615200000	-0.201300000
C	4.721800000	-1.548000000	3.320300000
C	4.660300000	-0.184500000	3.000700000
H	3.927300000	0.160400000	2.266800000
C	5.519600000	0.719600000	3.620200000
H	5.466700000	1.780100000	3.367400000
C	6.450500000	0.267800000	4.558200000
H	7.120000000	0.977200000	5.047700000
C	6.515600000	-1.091000000	4.881500000
H	7.233900000	-1.445600000	5.624200000
C	5.651000000	-1.998000000	4.271300000
H	5.677000000	-3.050600000	4.559900000
C	3.285900000	-4.024900000	3.688000000
C	3.355500000	-5.374200000	3.316400000
H	3.582900000	-5.656800000	2.286200000
C	3.156200000	-6.368100000	4.276200000
H	3.195400000	-7.415300000	3.979900000
C	2.918900000	-6.027200000	5.606600000
H	2.777200000	-6.809100000	6.355800000
C	2.848000000	-4.683800000	5.974000000
H	2.656700000	-4.403200000	7.011700000
C	2.993100000	-3.687400000	5.015500000
H	2.909300000	-2.642000000	5.300900000
C	0.756700000	-0.609800000	6.071200000
C	1.976900000	-0.118400000	5.579900000
H	1.996600000	0.476500000	4.664700000
C	3.159700000	-0.390800000	6.257400000
H	4.102300000	0.006000000	5.882600000

C	3.141500000	-1.198100000	7.397200000
H	4.073900000	-1.425500000	7.915800000
C	1.937300000	-1.731900000	7.853600000
H	1.919800000	-2.366200000	8.740700000
C	0.740600000	-1.429900000	7.201300000
H	-0.209000000	-1.810400000	7.583000000
C	-2.183600000	-0.840000000	6.012700000
C	-2.430800000	-2.159100000	5.713100000
H	-0.807900000	-3.178400000	4.414500000
C	-3.461800000	-2.922700000	6.190100000
H	-3.554400000	-3.983400000	5.959000000
C	-4.404600000	-2.264300000	6.992900000
H	-5.268900000	-2.813800000	7.370300000
C	-4.223200000	-0.918200000	7.320400000
H	-4.949400000	-0.410800000	7.955200000
C	-3.119900000	-0.203300000	6.855400000
H	-2.979800000	0.843700000	7.130400000
C	-0.849200000	1.714400000	5.973400000
C	-0.158400000	2.088100000	7.131300000
H	0.453800000	1.361600000	7.668600000
C	-0.232000000	3.406200000	7.580700000
H	0.321700000	3.703600000	8.469600000
C	-0.998200000	4.346500000	6.889900000
H	-1.042700000	5.381800000	7.236100000
C	-1.709000000	3.966900000	5.753700000
H	-2.319000000	4.697300000	5.223100000
C	-1.631700000	2.654600000	5.292600000
H	-2.168400000	2.352100000	4.394300000
C	0.200500000	5.583700000	0.677200000
C	1.557600000	5.810300000	0.411500000
H	2.317900000	5.240900000	0.944400000
C	1.930200000	6.780200000	-0.513000000
H	2.988700000	6.961900000	-0.697000000
C	0.956700000	7.509000000	-1.201900000
H	1.252800000	8.267500000	-1.928900000
C	-0.393200000	7.255700000	-0.969800000
H	-1.155900000	7.811500000	-1.517800000
C	-0.774800000	6.300400000	-0.028900000
H	-1.830800000	6.115500000	0.160100000
C	0.827600000	4.583900000	3.328000000
C	1.245200000	3.469700000	4.071800000
H	0.954500000	2.467500000	3.747100000
C	2.016900000	3.640800000	5.216200000
H	2.328300000	2.768800000	5.793200000
C	2.380500000	4.925400000	5.625000000
H	2.984500000	5.062700000	6.522200000
C	1.987500000	6.035400000	4.875400000
H	2.286400000	7.038900000	5.182200000
C	1.214700000	5.868800000	3.729100000
H	0.935100000	6.738800000	3.134700000
C	-1.941000000	4.817500000	2.463900000
C	-2.196800000	6.129900000	2.891500000
H	-1.425300000	6.894500000	2.814300000
C	-3.441900000	6.462100000	3.415500000
H	-3.633900000	7.486000000	3.742700000
C	-4.428100000	5.482900000	3.548200000

H	-5.390300000	5.740500000	3.992500000
C	-4.182400000	4.182600000	3.113200000
H	-4.937100000	3.400600000	3.196500000
C	-2.952600000	3.858200000	2.548200000
H	-2.785600000	2.843100000	2.185500000
C	4.304600000	3.363400000	0.349200000
C	3.910400000	3.329000000	1.696500000
H	3.380000000	2.459200000	2.087900000
C	4.169300000	4.414300000	2.526500000
H	3.871400000	4.379300000	3.573300000
C	4.780000000	5.558100000	2.011600000
H	4.963400000	6.414700000	2.662200000
C	5.137300000	5.610400000	0.665500000
H	5.603100000	6.507700000	0.257500000
C	4.910000000	4.512300000	-0.166600000
H	5.202500000	4.553700000	-1.217100000
C	5.453000000	0.784200000	-0.157000000
C	6.530600000	1.233900000	0.613900000
H	6.563400000	2.265900000	0.968200000
C	7.556600000	0.347600000	0.946400000
H	8.381800000	0.687300000	1.574400000
C	7.524100000	-0.968600000	0.483000000
H	8.323900000	-1.664600000	0.745700000
C	6.463900000	-1.403000000	-0.315100000
H	6.441900000	-2.424500000	-0.691600000
C	5.415800000	-0.540800000	-0.616000000
H	4.568200000	-0.890700000	-1.210700000
C	4.420500000	2.307600000	-2.357700000
C	5.734200000	2.379800000	-2.822100000
H	6.558300000	2.082500000	-2.170400000
C	5.977800000	2.816900000	-4.124800000
H	6.999700000	2.876100000	-4.486700000
C	4.917600000	3.172600000	-4.966400000
H	5.105200000	3.516300000	-5.988400000
C	3.613700000	3.075500000	-4.511300000
H	2.785500000	3.328600000	-5.175200000
C	3.363400000	2.638000000	-3.209400000
H	2.346100000	2.536600000	-2.850000000
P	-2.772600000	-4.297000000	2.367500000
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C	-1.480000000	-6.871700000	5.313300000
H	-1.702900000	-7.897900000	5.607600000
C	-0.601800000	-6.097100000	6.061800000
H	-0.149600000	-6.502900000	6.969400000
C	-0.322700000	-4.796800000	5.661600000
H	0.337400000	-4.166300000	6.252500000
C	-0.893900000	-4.259800000	4.500600000
H	-0.640200000	-1.998500000	2.769600000
C	-4.418300000	-3.854800000	3.036200000
C	-5.101700000	-4.663600000	3.959500000
H	-4.672300000	-5.612900000	4.294100000
C	-6.315200000	-4.235400000	4.489100000
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C	-6.854400000	-3.001900000	4.105800000

H	-7.802500000	-2.669300000	4.530300000
C	-6.180500000	-2.193800000	3.187600000
H	-6.574900000	-1.220900000	2.883700000
C	-4.969800000	-2.620300000	2.651000000
H	-4.447400000	-1.970300000	1.943700000
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C	-4.119800000	-6.590100000	1.340800000
H	-5.026000000	-6.249600000	1.845700000
C	-4.097600000	-7.831700000	0.704200000
H	-4.985800000	-8.463000000	0.725500000
C	-2.952300000	-8.258100000	0.031700000
H	-2.939000000	-9.232300000	-0.456900000
C	-1.832600000	-7.426600000	-0.038900000
H	-0.941900000	-7.722000000	-0.596800000
C	-1.838000000	-6.197400000	0.612600000
H	-0.949600000	-5.565000000	0.560400000

285

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Au	2.630158000	5.392622000	21.668118000
Au	1.896268000	3.040191000	20.164261000
Au	2.045424000	3.130845000	23.207314000
Au	0.034644000	4.528533000	21.743776000
Au	1.292207000	6.722074000	19.558634000
Au	3.588164000	5.082864000	19.147257000
Au	4.464497000	3.387559000	21.255178000
Au	2.889954000	5.682139000	24.326481000
Au	1.145012000	7.350043000	22.809949000
Au	3.398490000	7.898608000	20.889117000
Au	5.097164000	5.950344000	22.682984000
Cl	1.345473000	1.161331000	24.359748000
Cl	-0.066449000	7.593556000	17.788513000
P	0.167134000	1.926663000	19.106578000
P	-2.038893000	5.037676000	22.543388000
P	4.212625000	5.049987000	16.934265000
P	5.521958000	1.420547000	21.755470000
P	3.259985000	5.733182000	26.603452000
P	0.323998000	9.454484000	23.320877000
P	4.387107000	9.879491000	20.270208000
P	7.317169000	6.441849000	22.504265000
C	0.643880000	1.496930000	17.394436000
C	-0.301420000	1.424519000	16.363681000
H	-1.360331000	1.566341000	16.579547000
C	0.118100000	1.221894000	15.050800000
H	-0.617791000	1.183007000	14.247700000
C	1.474693000	1.092309000	14.761278000
H	1.799973000	0.952693000	13.730435000
C	2.418377000	1.160312000	15.785413000
H	3.481719000	1.074844000	15.561691000
C	2.006285000	1.367281000	17.096726000
H	2.745181000	1.484790000	17.889372000
C	-0.410344000	0.425362000	19.959007000
C	-0.897475000	-0.692251000	19.273777000
H	-0.871221000	-0.723891000	18.183084000
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294

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H	-3.612200000	8.591000000	-1.282200000
C	-1.657700000	8.077800000	-0.498400000
H	-1.455400000	9.084600000	-0.126800000
C	-0.713400000	7.057600000	-0.311500000
H	0.226100000	7.254700000	0.207800000
C	-0.986900000	5.761900000	-0.759600000
H	-0.270400000	4.953100000	-0.570300000
C	-1.199100000	-2.429200000	-5.250500000
C	-1.053800000	-2.765400000	-6.606600000
H	-0.177900000	-3.320800000	-6.944900000
C	-2.022800000	-2.362800000	-7.531300000
H	-1.903200000	-2.622200000	-8.584200000
C	-3.132200000	-1.616300000	-7.112100000
H	-3.880100000	-1.295000000	-7.840500000
C	-3.273200000	-1.275400000	-5.762300000
H	-4.124800000	-0.693300000	-5.408100000
C	-2.309100000	-1.679900000	-4.836200000
H	-2.431300000	-1.398200000	-3.789900000
C	1.603400000	-3.085600000	-4.846300000
C	2.495700000	-2.005300000	-4.752800000
H	2.229900000	-1.147300000	-4.131800000
C	3.708600000	-2.033300000	-5.444800000
H	4.394000000	-1.188600000	-5.365300000
C	4.038400000	-3.145300000	-6.228400000
H	4.988900000	-3.171400000	-6.765200000
C	3.156800000	-4.230700000	-6.312900000
H	3.420400000	-5.106400000	-6.907400000
C	1.941600000	-4.205400000	-5.622000000
H	1.266300000	-5.062100000	-5.666800000
C	-0.466800000	-4.681100000	-3.565800000
C	-1.276500000	-5.465800000	-4.406800000

H	-1.686800000	-5.043700000	-5.327900000
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H	-2.214900000	-7.390400000	-4.710500000
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C	0.023600000	-5.221000000	-2.365800000
H	0.616200000	-4.594300000	-1.692200000
C	3.039800000	-5.092100000	-0.663800000
C	3.414900000	-4.221300000	-1.702300000
H	3.298200000	-3.141000000	-1.578800000
C	3.911400000	-4.739500000	-2.895800000
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C	3.599900000	-6.996800000	-2.059500000
H	3.651700000	-8.078500000	-2.203900000
C	3.133600000	-6.482000000	-0.847000000
H	2.835300000	-7.160100000	-0.044900000
C	1.624400000	-5.711400000	1.778700000
C	0.264900000	-5.945000000	1.499700000
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C	-0.391600000	-7.019100000	2.101800000
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C	1.636400000	-7.604400000	3.298000000
H	2.169200000	-8.241800000	4.005100000
C	2.305700000	-6.542400000	2.684900000
H	3.358500000	-6.352200000	2.908900000
C	4.026600000	-4.111700000	1.866100000
C	5.211700000	-4.779600000	1.521300000
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C	6.348800000	-4.640600000	2.319000000
H	7.272800000	-5.147000000	2.041600000
C	6.297200000	-3.852800000	3.469200000
H	7.183600000	-3.741500000	4.095600000
C	5.114200000	-3.192600000	3.814600000
H	5.076900000	-2.572000000	4.706300000
C	3.979900000	-3.300400000	3.010600000
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C	5.536300000	2.907400000	-0.443400000
H	5.341200000	2.244000000	-1.287200000
C	5.946500000	4.221500000	-0.669300000
H	6.063700000	4.574700000	-1.695000000
C	6.196800000	5.075800000	0.411500000
H	6.512900000	6.105100000	0.233400000
C	6.025500000	4.612500000	1.720200000
H	6.206600000	5.278200000	2.565500000
C	5.629300000	3.291700000	1.956500000
H	5.504800000	2.934300000	2.980400000
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C	5.536400000	-1.606400000	-0.261700000
H	4.514000000	-1.905400000	-0.020700000

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H	6.014400000	-3.466100000	-1.235000000
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H	8.101300000	-0.109800000	4.829900000
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H	6.329100000	-0.398400000	6.562500000
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C	4.347600000	0.187800000	3.845400000
H	3.291100000	0.254400000	3.579700000
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C	6.875200000	1.400900000	-3.659200000
H	7.949600000	1.213000000	-3.628400000
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H	3.011200000	0.519200000	-8.419100000
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H	0.630000000	-0.177200000	-8.702400000
C	0.061800000	0.393700000	-6.697600000
H	-0.978700000	0.092400000	-6.817000000
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H	2.322400000	3.832200000	-6.154300000
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H	1.567200000	4.233700000	-1.924700000
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H	0.166300000	-3.784700000	5.078900000
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H	-5.079800000	-2.385200000	0.780400000

294

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Au	-2.068800000	0.724400000	1.780400000
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Au	-1.709800000	-2.069200000	1.121600000
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Au	0.390800000	2.146700000	1.692900000
Au	-1.185200000	2.147900000	-0.890000000
Au	0.017600000	-1.488100000	-2.155400000
Au	1.284900000	-2.392800000	0.591500000
Au	2.566500000	0.252400000	0.532100000
Au	1.238600000	1.056200000	-1.945400000
Cl	-4.478100000	-0.311900000	-2.522400000
Cl	1.159000000	-0.983100000	5.232800000
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P	1.114500000	3.930100000	2.895300000



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H	-7.100200000	-1.775700000	2.012100000
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H	2.336300000	3.883200000	0.248100000
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H	3.372100000	5.656700000	-1.150000000
C	3.119600000	7.200600000	0.329600000
H	3.577800000	7.975000000	-0.287400000
C	2.655400000	7.513000000	1.604400000
H	2.747800000	8.529500000	1.987300000
C	2.049700000	6.531300000	2.385800000
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H	0.665900000	-4.669400000	-1.930900000
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C	3.299600000	-4.272200000	-1.710900000
H	3.326000000	-3.190200000	-1.567700000
C	3.672000000	-4.822200000	-2.929800000
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H	2.261800000	-7.933100000	4.330900000
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C	6.642500000	-3.578000000	2.713200000
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C	4.271300000	-3.112900000	2.669700000
H	3.410200000	-2.548600000	3.036600000
C	5.240200000	2.464600000	0.848800000
C	5.427100000	2.934700000	-0.456900000
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C	5.813100000	4.253300000	-0.670800000
H	5.974900000	4.603100000	-1.689500000
C	5.982000000	5.119300000	0.410700000
H	6.272700000	6.156100000	0.241100000
C	5.757300000	4.662300000	1.707100000
H	5.876100000	5.341000000	2.552000000
C	5.395500000	3.335500000	1.933200000
H	5.239000000	2.978300000	2.951000000
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C	5.519200000	-1.550000000	-0.268000000
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C	6.408200000	-2.399900000	-0.917100000
H	6.070300000	-3.384500000	-1.243600000
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H	9.155900000	-0.385300000	-0.942900000
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H	7.563200000	1.149500000	0.173300000
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C	6.540900000	0.440700000	3.245000000
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H	7.923000000	0.233800000	4.879000000
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H	6.147700000	-0.306000000	6.541200000
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2 S1

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C	0.832339000	0.007570000	-7.425944000
H	0.487440000	-0.514626000	-8.319462000
C	-0.058573000	0.253489000	-6.382898000
H	-1.100553000	-0.047790000	-6.466100000
C	0.373456000	0.884802000	-5.223034000
H	-0.327004000	1.054605000	-4.400796000
C	1.899934000	3.882186000	-3.815121000
C	2.024767000	4.478314000	-5.076745000
H	2.289416000	3.871578000	-5.943903000
C	1.776622000	5.839673000	-5.223400000
H	1.864203000	6.303513000	-6.206424000
C	1.407956000	6.607328000	-4.116210000
H	1.204471000	7.672670000	-4.233379000
C	1.271611000	6.011641000	-2.865180000
H	0.965721000	6.603950000	-2.003088000
C	1.503383000	4.646519000	-2.713844000
H	1.343483000	4.166748000	-1.746421000
N	-2.582651000	-4.214325000	2.816221000
N	-3.646646000	-4.355849000	0.693963000
C	-2.775982000	-3.765295000	1.554020000
C	-1.459565000	-3.582378000	3.594019000
H	-0.729343000	-3.266135000	2.835901000
C	-1.952191000	-2.342867000	4.334612000
H	-1.081011000	-1.832045000	4.764460000
H	-2.635883000	-2.583886000	5.164117000
H	-2.465624000	-1.659869000	3.642094000
C	-4.211679000	-3.503986000	-0.402330000
H	-3.659003000	-2.559203000	-0.297377000
C	-3.671937000	-4.721690000	3.722522000
H	-3.357386000	-4.329753000	4.696538000
C	-3.728578000	-6.242911000	3.906139000
C	-5.017922000	-4.073747000	3.433459000
H	-4.915188000	-2.978017000	3.413597000
H	-5.443922000	-4.394893000	2.477936000
H	-5.725760000	-4.345303000	4.231489000
H	-4.351158000	-6.747394000	3.155097000
H	-4.175659000	-6.459790000	4.888879000
H	-2.717969000	-6.675040000	3.892708000
C	-3.774778000	-5.839316000	0.655325000
H	-3.380201000	-6.166285000	1.618140000
C	-2.867002000	-6.462144000	-0.414855000
C	-5.207519000	-6.344238000	0.523767000
H	-5.872533000	-5.930266000	1.293934000
H	-5.626556000	-6.104488000	-0.463662000
H	-5.205261000	-7.441435000	0.625991000

H	-3.305413000	-6.432566000	-1.418704000
H	-2.683908000	-7.520670000	-0.167148000
H	-1.901682000	-5.943509000	-0.456733000
C	-3.946191000	-3.972316000	-1.824831000
H	-2.877797000	-4.166331000	-1.986932000
H	-4.525372000	-4.862100000	-2.104959000
H	-4.246588000	-3.150900000	-2.491740000
C	-0.753758000	-4.557603000	4.525455000
H	-1.400770000	-4.897394000	5.349979000
H	-0.372613000	-5.433262000	3.985581000
H	0.099353000	-4.023917000	4.973058000
C	-5.673685000	-3.153687000	-0.138626000
H	-5.955073000	-2.342589000	-0.828229000
H	-6.355052000	-4.003243000	-0.297661000
H	-5.788945000	-2.789502000	0.891524000

278

3 S0

Au	0.054300000	0.064600000	0.001100000
Au	-2.046000000	0.871000000	1.599400000
Au	-2.475000000	-0.347600000	-1.144500000
Au	-1.508200000	-1.984800000	1.060800000
Au	0.560700000	-0.520500000	2.729400000
Au	0.423400000	2.359800000	1.453300000
Au	-1.177900000	2.233200000	-1.042000000
Au	0.035000000	-1.513500000	-2.186200000
Au	1.339000000	-2.284600000	0.316900000
Au	2.641100000	0.414700000	0.642900000
Au	1.449700000	1.240500000	-1.966200000
Cl	-4.650000000	-0.684500000	-2.070300000
Cl	1.009600000	-1.118300000	5.001200000
P	-3.729000000	1.369600000	3.050800000
P	0.952000000	4.133100000	2.812000000
P	-2.499800000	3.830800000	-2.018300000
P	-0.132500000	-2.824200000	-4.078800000
P	2.341600000	-4.317700000	0.670800000
P	4.838700000	0.730400000	1.217300000
P	2.488400000	2.136900000	-3.814400000
C	-4.711200000	2.853500000	2.644500000
C	-4.093700000	3.891400000	1.931800000
H	-3.045100000	3.799900000	1.638500000
C	-4.832200000	5.019500000	1.570400000
H	-4.350000000	5.809400000	0.996400000
C	-6.183400000	5.116200000	1.912300000
H	-6.762800000	5.991200000	1.611200000
C	-6.802800000	4.081200000	2.624500000
H	-7.860700000	4.149000000	2.884500000
C	-6.071100000	2.948900000	2.989500000
H	-6.556000000	2.131300000	3.525800000
C	-3.139500000	1.558700000	4.771700000
C	-2.101800000	0.713300000	5.201000000
H	-1.682700000	-0.037200000	4.527000000
C	-1.566600000	0.858200000	6.480600000
H	-0.746600000	0.205100000	6.778700000
C	-2.059400000	1.850400000	7.339100000
H	-1.630300000	1.975200000	8.336000000
C	-3.090000000	2.694100000	6.913900000

H	-3.466700000	3.476500000	7.575200000
C	-3.631300000	2.554700000	5.630300000
H	-4.415500000	3.230800000	5.288700000
C	-4.926400000	-0.018300000	3.035500000
C	-5.462900000	-0.560500000	4.212000000
H	-5.175000000	-0.147800000	5.181100000
C	-6.354900000	-1.636400000	4.138900000
H	-6.764400000	-2.060000000	5.058000000
C	-6.722300000	-2.161000000	2.895000000
H	-7.419400000	-2.999800000	2.843100000
C	-6.192900000	-1.612300000	1.718400000
H	-6.472600000	-2.008900000	0.741400000
C	-5.286800000	-0.555500000	1.784100000
H	-4.849900000	-0.169300000	0.859500000
C	1.924100000	5.427900000	1.950400000
C	2.603300000	5.090700000	0.768600000
H	2.575800000	4.060300000	0.402800000
C	3.302500000	6.071700000	0.063100000
H	3.824700000	5.802800000	-0.852700000
C	3.331000000	7.389400000	0.529400000
H	3.870300000	8.153400000	-0.033000000
C	2.665300000	7.727000000	1.714000000
H	2.683600000	8.753800000	2.081200000
C	1.961000000	6.750600000	2.422700000
H	1.420300000	7.015700000	3.332300000
C	-0.451200000	5.057100000	3.549900000
C	-0.675700000	5.118000000	4.934400000
H	-0.020600000	4.586900000	5.623800000
C	-1.747600000	5.865400000	5.434300000
H	-1.921700000	5.900600000	6.510800000
C	-2.580700000	6.572300000	4.565000000
H	-3.408200000	7.165000000	4.958700000
C	-2.355300000	6.511600000	3.183900000
H	-3.000300000	7.055100000	2.495400000
C	-1.311900000	5.740500000	2.674900000
H	-1.157700000	5.676000000	1.596400000
C	1.931400000	3.571000000	4.244800000
C	1.413600000	2.491000000	4.981300000
H	0.511700000	1.974700000	4.647300000
C	2.057300000	2.076000000	6.144800000
H	1.649700000	1.230900000	6.697000000
C	3.235800000	2.706400000	6.558500000
H	3.747100000	2.367100000	7.460300000
C	3.777700000	3.750100000	5.801100000
H	4.709500000	4.225900000	6.111600000
C	3.123700000	4.191600000	4.647500000
H	3.537600000	5.014200000	4.062400000
C	-2.275000000	3.793800000	-3.831900000
C	-2.823900000	2.683700000	-4.505000000
H	-3.404100000	1.939800000	-3.950800000
C	-2.618700000	2.542600000	-5.875900000
H	-3.043700000	1.683900000	-6.395100000
C	-1.848700000	3.482900000	-6.577500000
H	-1.678000000	3.356300000	-7.648000000
C	-1.285800000	4.568400000	-5.902900000
H	-0.673500000	5.293200000	-6.442200000

C	-1.494700000	4.728900000	-4.527700000
H	-1.046800000	5.575100000	-4.002900000
C	-4.295800000	3.585200000	-1.795700000
C	-4.755200000	2.634600000	-0.873200000
H	-4.040300000	2.034200000	-0.310100000
C	-6.125400000	2.438200000	-0.689000000
H	-6.469100000	1.684300000	0.020900000
C	-7.041000000	3.201500000	-1.415200000
H	-8.112100000	3.054700000	-1.266300000
C	-6.588900000	4.142300000	-2.354600000
H	-7.304100000	4.722300000	-2.940400000
C	-5.220800000	4.325200000	-2.558200000
H	-4.867700000	5.024000000	-3.320400000
C	-2.094900000	5.516000000	-1.408500000
C	-3.057000000	6.518900000	-1.207900000
H	-4.099900000	6.336600000	-1.466000000
C	-2.686100000	7.743200000	-0.644400000
H	-3.442900000	8.510800000	-0.475600000
C	-1.354300000	7.983400000	-0.291400000
H	-1.071200000	8.933000000	0.164500000
C	-0.390400000	6.991600000	-0.496600000
H	0.642100000	7.155600000	-0.187600000
C	-0.760400000	5.760200000	-1.037600000
H	-0.022700000	4.962800000	-1.138500000
C	-1.360900000	-2.223300000	-5.303600000
C	-1.262600000	-2.499400000	-6.676700000
H	-0.412000000	-3.059500000	-7.064200000
C	-2.244200000	-2.030100000	-7.552400000
H	-2.159700000	-2.240900000	-8.619300000
C	-3.324700000	-1.284300000	-7.065600000
H	-4.086600000	-0.916200000	-7.754700000
C	-3.426800000	-1.014500000	-5.696000000
H	-4.265100000	-0.446400000	-5.292000000
C	-2.446400000	-1.479600000	-4.819300000
H	-2.538300000	-1.258800000	-3.754900000
C	1.445600000	-3.008400000	-4.993400000
C	2.410800000	-2.001100000	-4.850500000
H	2.205500000	-1.154700000	-4.192200000
C	3.617400000	-2.081000000	-5.546200000
H	4.357600000	-1.290100000	-5.427400000
C	3.869200000	-3.172000000	-6.384800000
H	4.813200000	-3.235900000	-6.928100000
C	2.916400000	-4.187900000	-6.517100000
H	3.118900000	-5.048100000	-7.156300000
C	1.708200000	-4.111900000	-5.820500000
H	0.976000000	-4.915600000	-5.904500000
C	-0.652200000	-4.545800000	-3.713600000
C	-1.606400000	-5.237000000	-4.476300000
H	-2.089700000	-4.750300000	-5.325800000
C	-1.948600000	-6.550700000	-4.135000000
H	-2.695400000	-7.082000000	-4.726900000
C	-1.338900000	-7.178300000	-3.041400000
H	-1.609200000	-8.202900000	-2.777300000
C	-0.390300000	-6.487500000	-2.278500000
H	0.076800000	-6.960100000	-1.413000000
C	-0.056500000	-5.173900000	-2.606500000

H	0.660900000	-4.621900000	-1.997900000
C	2.951400000	-5.095200000	-0.869900000
C	3.407800000	-4.256500000	-1.900500000
H	3.354900000	-3.172400000	-1.780600000
C	3.894000000	-4.808100000	-3.084800000
H	4.236200000	-4.151700000	-3.884500000
C	3.906800000	-6.196100000	-3.256800000
H	4.265500000	-6.622700000	-4.194800000
C	3.442100000	-7.034400000	-2.238800000
H	3.441200000	-8.116400000	-2.376000000
C	2.967800000	-6.487200000	-1.044100000
H	2.598500000	-7.138700000	-0.250800000
C	1.182700000	-5.542400000	1.385000000
C	-0.152200000	-5.516800000	0.945400000
H	-0.472800000	-4.774500000	0.214700000
C	-1.076700000	-6.423200000	1.464600000
H	-2.111800000	-6.381900000	1.127400000
C	-0.678100000	-7.352500000	2.433100000
H	-1.403500000	-8.052900000	2.851800000
C	0.647600000	-7.375400000	2.879200000
H	0.956500000	-8.090900000	3.642200000
C	1.580300000	-6.472400000	2.358200000
H	2.610600000	-6.480100000	2.715500000
C	3.792400000	-4.268700000	1.777800000
C	4.899100000	-5.107100000	1.569900000
H	4.905100000	-5.808400000	0.733200000
C	5.999200000	-5.031500000	2.428200000
H	6.862000000	-5.676900000	2.259200000
C	5.993000000	-4.124300000	3.493900000
H	6.855800000	-4.057500000	4.159200000
C	4.889300000	-3.290900000	3.702200000
H	4.890800000	-2.574700000	4.523500000
C	3.788400000	-3.351600000	2.845300000
H	2.937000000	-2.683600000	3.002800000
C	5.462600000	2.418500000	0.887400000
C	5.577700000	2.839300000	-0.451300000
H	5.310500000	2.160500000	-1.262700000
C	6.055700000	4.116700000	-0.741400000
H	6.158700000	4.422900000	-1.784100000
C	6.397800000	4.991800000	0.297700000
H	6.770800000	5.991000000	0.067900000
C	6.242300000	4.590200000	1.628600000
H	6.488300000	5.274900000	2.441200000
C	5.776000000	3.306200000	1.928300000
H	5.658200000	2.994600000	2.968200000
C	5.959500000	-0.385600000	0.280200000
C	5.468600000	-1.650800000	-0.082500000
H	4.431800000	-1.911900000	0.142900000
C	6.301100000	-2.572300000	-0.720000000
H	5.908400000	-3.553400000	-0.989300000
C	7.627300000	-2.232800000	-1.009000000
H	8.277600000	-2.952500000	-1.509700000
C	8.116700000	-0.967900000	-0.662200000
H	9.147300000	-0.696900000	-0.894900000
C	7.287600000	-0.044500000	-0.019900000
H	7.668200000	0.945800000	0.233500000

C	5.228900000	0.396700000	2.978400000
C	6.562000000	0.303700000	3.419200000
H	7.383800000	0.447700000	2.717100000
C	6.834100000	0.014800000	4.757000000
H	7.869700000	-0.057300000	5.094400000
C	5.781300000	-0.196400000	5.658300000
H	5.998500000	-0.440500000	6.700500000
C	4.457700000	-0.109000000	5.219300000
H	3.623600000	-0.301000000	5.892900000
C	4.179700000	0.196700000	3.883900000
H	3.141300000	0.251200000	3.552700000
C	4.289500000	1.813000000	-3.766600000
C	4.698600000	0.546100000	-3.309700000
H	3.952600000	-0.175900000	-2.971900000
C	6.053200000	0.226800000	-3.249200000
H	6.359800000	-0.752300000	-2.881400000
C	7.012500000	1.179100000	-3.613400000
H	8.072800000	0.936800000	-3.534200000
C	6.612000000	2.443800000	-4.054200000
H	7.359300000	3.189400000	-4.328500000
C	5.252300000	2.761700000	-4.138400000
H	4.939100000	3.748700000	-4.482200000
C	1.934300000	1.390300000	-5.384100000
C	2.817800000	1.140300000	-6.444900000
H	3.878500000	1.370700000	-6.337700000
C	2.337500000	0.579500000	-7.630600000
H	3.026700000	0.371600000	-8.449200000
C	0.977800000	0.279400000	-7.761400000
H	0.603400000	-0.167300000	-8.684200000
C	0.097600000	0.541800000	-6.708500000
H	-0.961700000	0.312700000	-6.807100000
C	0.570800000	1.084800000	-5.514800000
H	-0.117000000	1.269800000	-4.686700000
C	2.306800000	3.941000000	-4.071900000
C	2.272600000	4.503700000	-5.356600000
H	2.360000000	3.862200000	-6.233700000
C	2.100200000	5.881600000	-5.510300000
H	2.066700000	6.312900000	-6.511100000
C	1.958000000	6.702600000	-4.387100000
H	1.807900000	7.776800000	-4.508200000
C	1.994800000	6.143900000	-3.106700000
H	1.872900000	6.777400000	-2.230500000
C	2.163000000	4.767000000	-2.947500000
H	2.159500000	4.319300000	-1.953100000
C	-1.905900000	-3.252400000	4.196100000
N	-2.818400000	-3.773400000	3.146500000
N	-3.758200000	-4.059700000	1.209800000
C	-2.786000000	-3.351900000	1.855600000
C	-3.781200000	-4.754900000	3.310000000
H	-3.974100000	-5.232100000	4.260600000
C	-4.377500000	-4.931300000	2.094500000
H	-5.189600000	-5.583300000	1.807300000
C	-4.149300000	-3.790500000	-0.205400000
H	-4.303300000	-2.707400000	-0.261900000
C	-3.034900000	-4.161700000	-1.175800000
H	-2.802800000	-5.230900000	-1.137300000

H	-2.124900000	-3.591200000	-0.959000000
H	-3.341500000	-3.899900000	-2.198000000
C	-2.655300000	-3.027700000	5.508400000
H	-2.942700000	-3.979800000	5.983900000
H	-1.988700000	-2.493600000	6.199700000
H	-3.555000000	-2.416000000	5.349300000
H	-1.578200000	-2.277800000	3.809900000
C	-5.456900000	-4.485800000	-0.558400000
H	-5.758500000	-4.154900000	-1.564600000
H	-5.337700000	-5.577500000	-0.582700000
H	-6.266100000	-4.229600000	0.139600000
C	-0.682000000	-4.147600000	4.327800000
H	-0.020400000	-3.723100000	5.091600000
H	-0.964200000	-5.180700000	4.598600000
H	-0.126200000	-4.174100000	3.381300000

278

3 T1

Au	-0.060900000	-0.014300000	0.002900000
Au	-2.211300000	1.026500000	1.380500000
Au	-2.458200000	-0.572700000	-1.420800000
Au	-1.507800000	-2.017500000	1.141700000
Au	0.528800000	-0.579800000	2.841900000
Au	0.234900000	2.366500000	1.366300000
Au	-1.187900000	2.081300000	-1.186600000
Au	-0.030000000	-1.614200000	-2.160700000
Au	1.181000000	-2.352100000	0.388300000
Au	2.404600000	0.538700000	0.899600000
Au	1.341600000	1.174900000	-1.941300000
Cl	-4.798600000	-0.870600000	-1.563900000
Cl	0.752900000	-0.920200000	5.216200000
P	-3.871000000	1.401000000	2.893100000
P	0.973100000	4.047800000	2.737600000
P	-2.506600000	3.758100000	-1.987400000
P	-0.158800000	-2.783400000	-4.150900000
P	2.300100000	-4.328900000	0.654600000
P	4.631900000	0.776900000	1.347800000
P	2.523200000	2.082600000	-3.671500000
C	-5.078100000	2.653500000	2.369100000
C	-4.604600000	3.791000000	1.697300000
H	-3.538400000	3.877900000	1.483200000
C	-5.498000000	4.764500000	1.265700000
H	-5.122000000	5.641000000	0.738900000
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278			
3 S1			
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284

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H	5.641400000	-4.168200000	5.211800000
C	3.702500000	-3.704200000	4.384200000
H	3.305400000	-3.265700000	5.296700000
C	2.897300000	-3.734400000	3.253500000
H	1.893700000	-3.310300000	3.294300000
C	5.359700000	2.483500000	0.999500000
C	5.500200000	2.949700000	-0.320200000
H	5.294700000	2.282800000	-1.158100000
C	5.920800000	4.257600000	-0.557900000
H	6.038300000	4.601500000	-1.586100000
C	6.179900000	5.120300000	0.513900000
H	6.501100000	6.146100000	0.326300000
C	6.010800000	4.668000000	1.825400000
H	6.199200000	5.338300000	2.665200000
C	5.601900000	3.353600000	2.072500000
H	5.468400000	3.005800000	3.096700000
C	5.934200000	-0.281200000	0.295800000
C	5.499100000	-1.558100000	-0.097100000
H	4.472900000	-1.869300000	0.115400000
C	6.377200000	-2.427300000	-0.747800000
H	6.031900000	-3.417700000	-1.045100000
C	7.691000000	-2.026300000	-1.018300000
H	8.373900000	-2.707300000	-1.529200000
C	8.124600000	-0.751600000	-0.637300000
H	9.145300000	-0.432400000	-0.851800000
C	7.250800000	0.119600000	0.018500000
H	7.587600000	1.117500000	0.302200000

C	5.173900000	0.356400000	3.001900000
C	6.483000000	0.498100000	3.490300000
H	7.265700000	0.883700000	2.842300000
C	6.780600000	0.143500000	4.805300000
H	7.795700000	0.255700000	5.180500000
C	5.779500000	-0.363200000	5.638200000
H	6.016700000	-0.643400000	6.666700000
C	4.484600000	-0.509400000	5.151700000
H	3.687700000	-0.896600000	5.781000000
C	4.178600000	-0.149600000	3.836500000
H	3.160200000	-0.269300000	3.471000000
C	4.181700000	2.006500000	-3.657600000
C	4.639900000	0.745200000	-3.233200000
H	3.922600000	-0.019700000	-2.931100000
C	6.005300000	0.480600000	-3.164400000
H	6.348600000	-0.497600000	-2.826700000
C	6.927500000	1.484200000	-3.483200000
H	7.996300000	1.284000000	-3.401600000
C	6.477600000	2.746700000	-3.879900000
H	7.195200000	3.533300000	-4.115500000
C	5.106900000	3.009500000	-3.975000000
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C	1.945800000	1.450000000	-5.377800000
C	2.902300000	1.237800000	-6.383600000
H	3.949100000	1.487800000	-6.205200000
C	2.511900000	0.691500000	-7.608400000
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H	0.864000000	-0.063400000	-8.787700000
C	0.218700000	0.586300000	-6.831900000
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C	0.601100000	1.112900000	-5.599000000
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C	2.026800000	3.997200000	-4.028600000
C	2.273900000	4.614800000	-5.266600000
H	2.678200000	4.029900000	-6.095600000
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H	1.192500000	7.766800000	-4.525900000
C	1.178200000	6.095700000	-3.160600000
H	0.745700000	6.663600000	-2.342300000
C	1.466400000	4.739800000	-2.981700000
H	1.240000000	4.250800000	-2.034500000
N	-2.809200000	-3.960600000	2.853100000
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C	-2.818200000	-3.461800000	1.587200000
C	-3.786300000	-4.946700000	2.982400000
C	-4.423500000	-5.045700000	1.722800000
C	-1.877000000	-3.456500000	3.896500000
H	-1.292600000	-2.692200000	3.364700000
C	-0.907300000	-4.536200000	4.363300000
H	-0.405600000	-5.005100000	3.505900000
H	-1.405600000	-5.321400000	4.950300000
H	-0.144500000	-4.055700000	4.993000000
C	-4.115900000	-3.798000000	-0.523600000

C	-5.534800000	-3.255400000	-0.668400000
H	-3.423000000	-2.980600000	-0.771600000
H	-6.297900000	-4.000300000	-0.405600000
H	-5.670800000	-2.367300000	-0.040000000
C	-4.173200000	-5.760000000	4.052600000
C	-5.455900000	-5.964200000	1.503900000
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C	-5.835300000	-6.773600000	2.575400000
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H	-6.635700000	-7.499400000	2.436000000
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H	-5.686500000	-2.936300000	-1.706500000
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H	-3.292300000	-1.983700000	4.631600000
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H	-3.965300000	-4.675300000	-2.480700000

284

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Au	-2.144700000	0.832600000	1.454000000
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Au	0.331200000	2.384400000	1.369200000
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Au	2.454400000	0.512300000	0.828300000
Au	1.370800000	1.257200000	-1.947100000
Cl	-4.691100000	-0.733200000	-2.199800000
Cl	0.724800000	-0.986900000	5.090800000
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P	1.027000000	4.054300000	2.776900000
P	-2.515400000	3.753900000	-2.055600000
P	-0.124900000	-2.750200000	-4.198900000
P	2.277300000	-4.343400000	0.654100000
P	4.667000000	0.735200000	1.311300000
P	2.528800000	2.226100000	-3.649000000
C	-4.897700000	2.714000000	2.301500000
C	-4.311100000	3.778400000	1.604200000
H	-3.239400000	3.757500000	1.401100000
C	-5.099700000	4.820300000	1.131700000
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C	-6.481300000	4.785000000	1.317200000
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H	-1.226300000	3.182000000	7.657300000
C	-2.720000000	3.648900000	6.172300000
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H	-5.182600000	0.759000000	5.412900000
C	-6.081200000	-1.184400000	5.127000000
H	-6.471200000	-1.233100000	6.144100000
C	-6.270800000	-2.253400000	4.250400000
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C	-5.050900000	-1.072000000	2.528100000
H	-4.620200000	-1.038400000	1.524800000
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C	2.585600000	5.001100000	0.667900000
H	2.531100000	3.972300000	0.301800000
C	3.249600000	5.977000000	-0.070700000
H	3.704300000	5.711600000	-1.022100000
C	3.324300000	7.286100000	0.400100000
H	3.838000000	8.049500000	-0.186900000
C	2.740100000	7.623200000	1.619000000
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C	2.055100000	6.656900000	2.355700000
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H	2.018200000	1.116300000	6.548000000
C	3.543300000	2.647700000	6.364500000
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H	-0.973700000	5.610000000	-3.811200000
C	-4.304500000	3.439900000	-1.961100000
C	-4.782200000	2.455600000	-1.090300000
H	-4.083000000	1.861700000	-0.505000000
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C	-7.043100000	2.974600000	-1.740200000
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H	-1.822800000	-1.991900000	-8.836400000
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H	-2.491000000	-1.105300000	-3.995400000
C	1.470500000	-2.973500000	-5.056300000
C	2.437000000	-1.972900000	-4.910700000
H	2.222700000	-1.114300000	-4.273600000
C	3.652400000	-2.078600000	-5.578800000
H	4.403700000	-1.299500000	-5.454300000
C	3.903900000	-3.177400000	-6.400900000
H	4.856700000	-3.257400000	-6.924600000
C	2.944800000	-4.180800000	-6.538900000
H	3.146800000	-5.045000000	-7.172100000
C	1.733000000	-4.088100000	-5.860000000
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C	-1.775700000	-5.025300000	-4.676000000
H	-2.239300000	-4.465300000	-5.487800000
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H	-3.010600000	-6.764200000	-4.981500000
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H	0.569400000	-4.694200000	-2.229300000
C	2.663400000	-5.122500000	-0.944200000
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H	3.216500000	-3.218000000	-1.812800000
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H	0.892800000	-7.673000000	4.109000000
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H	7.038700000	-5.580200000	1.322800000
C	6.423000000	-3.963400000	2.614600000
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H	5.532300000	-2.394100000	3.790200000
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H	6.238700000	4.562400000	-1.379300000
C	6.173700000	5.050600000	0.725800000
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C	5.881400000	4.588000000	2.006500000
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H	5.240300000	2.914000000	3.205900000
C	5.768500000	-0.353600000	0.330400000
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H	4.175900000	-1.768800000	-0.021100000
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C	-5.493800000	-3.667000000	-0.540000000
H	-3.437600000	-3.112600000	-0.630200000
H	-6.155600000	-4.486600000	-0.224900000
H	-5.777200000	-2.748000000	-0.007900000
C	-3.945800000	-5.602000000	4.364800000
C	-5.176200000	-6.094700000	1.838700000
C	-4.872500000	-6.626700000	4.198200000
C	-5.477500000	-6.870600000	2.956000000
H	-3.470600000	-5.430000000	5.326300000
H	-5.128900000	-7.255300000	5.051000000
H	-6.194600000	-7.685100000	2.860500000
H	-5.638900000	-6.298600000	0.877100000
H	-5.653200000	-3.476300000	-1.609400000
C	-2.668300000	-2.566300000	5.227100000
H	-3.441200000	-1.891200000	4.844000000
H	-3.156500000	-3.329400000	5.843500000
H	-1.982700000	-1.988300000	5.862800000
C	-3.519800000	-5.184000000	-1.117700000
H	-2.466100000	-5.381400000	-0.883200000
H	-4.100000000	-6.099000000	-0.925600000
H	-3.580500000	-4.953700000	-2.190300000

282

5 S0

Au	0.021200000	0.047100000	-0.066200000
Au	-2.071600000	0.825700000	1.571400000
Au	-2.492100000	-0.335800000	-1.260700000
Au	-1.507800000	-1.992400000	0.918400000
Au	0.545100000	-0.549400000	2.667900000
Au	0.414200000	2.335000000	1.392600000
Au	-1.228900000	2.229100000	-1.058400000
Au	0.033700000	-1.485000000	-2.301600000
Au	1.343700000	-2.291800000	0.211000000
Au	2.610100000	0.380400000	0.591000000
Au	1.381000000	1.240300000	-2.037800000
Cl	-4.513000000	-0.649800000	-2.460900000
Cl	1.005200000	-1.196700000	4.931900000
P	-3.688600000	1.344800000	3.098100000
P	1.032800000	4.095800000	2.739100000
P	-2.567600000	3.818000000	-2.023000000
P	-0.053500000	-2.799700000	-4.200900000
P	2.308600000	-4.335300000	0.596500000
P	4.805800000	0.691400000	1.191800000
P	2.432300000	2.180100000	-3.859100000
C	-4.770200000	2.741600000	2.634200000
C	-4.222400000	3.757600000	1.839100000
H	-3.190500000	3.671700000	1.494600000
C	-5.004500000	4.849300000	1.462000000
H	-4.571600000	5.624200000	0.830600000
C	-6.341300000	4.924100000	1.858300000
H	-6.958500000	5.767600000	1.543500000

C	-6.897300000	3.904500000	2.639500000
H	-7.944600000	3.952900000	2.940500000
C	-6.115300000	2.815000000	3.032300000
H	-6.550200000	2.017600000	3.635700000
C	-2.921000000	1.774800000	4.698800000
C	-1.950100000	0.887000000	5.197700000
H	-1.659700000	0.002600000	4.628600000
C	-1.332600000	1.147800000	6.418600000
H	-0.575000000	0.451600000	6.780000000
C	-1.665500000	2.301800000	7.139700000
H	-1.172900000	2.513400000	8.091000000
C	-2.616400000	3.194200000	6.634500000
H	-2.867000000	4.101800000	7.185100000
C	-3.248600000	2.935400000	5.412700000
H	-3.983800000	3.636600000	5.011900000
C	-4.782400000	-0.071100000	3.481000000
C	-5.319700000	-0.234900000	4.769100000
H	-5.082300000	0.488000000	5.551600000
C	-6.126900000	-1.338400000	5.054900000
H	-6.529300000	-1.468500000	6.060400000
C	-6.405200000	-2.277900000	4.056900000
H	-7.030400000	-3.144500000	4.280600000
C	-5.877700000	-2.113200000	2.771800000
H	-6.099200000	-2.848000000	1.998600000
C	-5.059800000	-1.018300000	2.479000000
H	-4.616700000	-0.908300000	1.485200000
C	1.979100000	5.392500000	1.848300000
C	2.571800000	5.076600000	0.615500000
H	2.519000000	4.052400000	0.234800000
C	3.219600000	6.069900000	-0.120900000
H	3.669400000	5.819200000	-1.080000000
C	3.282800000	7.378400000	0.365800000
H	3.777500000	8.154100000	-0.220300000
C	2.712000000	7.693300000	1.604600000
H	2.760500000	8.712900000	1.989300000
C	2.058300000	6.705600000	2.343700000
H	1.586000000	6.956100000	3.294600000
C	-0.316900000	5.035500000	3.548900000
C	-0.252200000	5.418100000	4.897900000
H	0.588300000	5.102500000	5.515700000
C	-1.270100000	6.200000000	5.449500000
H	-1.217600000	6.490300000	6.499100000
C	-2.348800000	6.607200000	4.660800000
H	-3.144600000	7.216400000	5.092500000
C	-2.415000000	6.223500000	3.317800000
H	-3.258300000	6.530400000	2.702900000
C	-1.409400000	5.431100000	2.763800000
H	-1.460800000	5.126200000	1.717700000
C	2.061400000	3.531800000	4.135700000
C	1.543600000	2.473300000	4.901900000
H	0.623300000	1.970600000	4.599000000
C	2.206100000	2.069800000	6.058100000
H	1.799400000	1.241100000	6.636500000
C	3.399100000	2.694500000	6.438300000
H	3.924500000	2.365200000	7.336100000
C	3.937600000	3.718500000	5.651900000

H	4.880500000	4.188200000	5.934900000
C	3.267900000	4.144700000	4.501000000
H	3.678100000	4.950000000	3.890000000
C	-2.299200000	3.811900000	-3.830600000
C	-2.756900000	2.671200000	-4.523500000
H	-3.300700000	1.886600000	-3.990800000
C	-2.507500000	2.553000000	-5.888200000
H	-2.859600000	1.671900000	-6.424400000
C	-1.785200000	3.544700000	-6.563100000
H	-1.575700000	3.432600000	-7.627500000
C	-1.319400000	4.664700000	-5.870100000
H	-0.746600000	5.432600000	-6.389300000
C	-1.573600000	4.803000000	-4.500700000
H	-1.201100000	5.674100000	-3.958200000
C	-4.361900000	3.518400000	-1.855500000
C	-4.821200000	2.533400000	-0.971900000
H	-4.109200000	1.942000000	-0.396400000
C	-6.190100000	2.293000000	-0.839100000
H	-6.533500000	1.514000000	-0.158500000
C	-7.105200000	3.043900000	-1.578100000
H	-8.175700000	2.859200000	-1.471600000
C	-6.652200000	4.017400000	-2.479300000
H	-7.365000000	4.583300000	-3.079900000
C	-5.284800000	4.244700000	-2.631800000
H	-4.929000000	4.963000000	-3.371800000
C	-2.212700000	5.492800000	-1.361800000
C	-3.182300000	6.503400000	-1.252100000
H	-4.195700000	6.329200000	-1.613700000
C	-2.860200000	7.721900000	-0.647300000
H	-3.625400000	8.493700000	-0.549500000
C	-1.567600000	7.949600000	-0.163500000
H	-1.323900000	8.897700000	0.318400000
C	-0.595600000	6.951900000	-0.277700000
H	0.407700000	7.111100000	0.117900000
C	-0.920100000	5.726400000	-0.859900000
H	-0.177900000	4.926900000	-0.893400000
C	-1.216600000	-2.225900000	-5.499000000
C	-1.059000000	-2.558400000	-6.854400000
H	-0.199000000	-3.145000000	-7.179400000
C	-1.995900000	-2.116300000	-7.791000000
H	-1.866100000	-2.370000000	-8.843900000
C	-3.092300000	-1.346000000	-7.381700000
H	-3.820500000	-1.000300000	-8.117900000
C	-3.251700000	-1.020000000	-6.030800000
H	-4.105900000	-0.434700000	-5.689000000
C	-2.312900000	-1.452000000	-5.093200000
H	-2.450300000	-1.186900000	-4.044900000
C	1.573400000	-2.981000000	-5.030600000
C	2.505500000	-1.941900000	-4.890200000
H	2.251700000	-1.079400000	-4.271500000
C	3.737500000	-2.009200000	-5.542800000
H	4.450400000	-1.192200000	-5.431200000
C	4.048900000	-3.120700000	-6.333100000
H	5.013200000	-3.174800000	-6.841700000
C	3.131500000	-4.170000000	-6.458100000
H	3.380900000	-5.046200000	-7.057100000

C	1.897300000	-4.106100000	-5.805800000
H	1.190900000	-4.933900000	-5.885600000
C	-0.564300000	-4.524700000	-3.843400000
C	-1.512900000	-5.221000000	-4.606000000
H	-2.008100000	-4.733800000	-5.446400000
C	-1.825300000	-6.546500000	-4.284500000
H	-2.568400000	-7.082600000	-4.876200000
C	-1.191400000	-7.180600000	-3.212400000
H	-1.437200000	-8.214200000	-2.965000000
C	-0.247000000	-6.485300000	-2.449100000
H	0.244400000	-6.963300000	-1.602900000
C	0.053100000	-5.159000000	-2.752800000
H	0.773000000	-4.607100000	-2.146900000
C	3.042200000	-5.089400000	-0.902600000
C	3.509200000	-4.233400000	-1.914500000
H	3.401600000	-3.152200000	-1.803100000
C	4.079200000	-4.762500000	-3.071900000
H	4.429400000	-4.090900000	-3.855400000
C	4.165200000	-6.148000000	-3.237700000
H	4.590100000	-6.560400000	-4.154600000
C	3.691500000	-7.005200000	-2.238500000
H	3.748400000	-8.086700000	-2.370000000
C	3.133300000	-6.479900000	-1.070500000
H	2.757800000	-7.148100000	-0.293800000
C	1.136900000	-5.593700000	1.232700000
C	-0.190900000	-5.572500000	0.778500000
H	-0.512700000	-4.799700000	0.079500000
C	-1.098600000	-6.530700000	1.232900000
H	-2.126300000	-6.513900000	0.871500000
C	-0.695100000	-7.498900000	2.155700000
H	-1.413000000	-8.233800000	2.522800000
C	0.624300000	-7.515500000	2.619500000
H	0.938900000	-8.260400000	3.350800000
C	1.541000000	-6.567000000	2.160000000
H	2.565700000	-6.569800000	2.533000000
C	3.653200000	-4.273600000	1.826100000
C	4.851400000	-4.987600000	1.659300000
H	5.003200000	-5.600300000	0.768000000
C	5.849500000	-4.908200000	2.636300000
H	6.783800000	-5.456300000	2.499300000
C	5.649700000	-4.127000000	3.780500000
H	6.432600000	-4.059900000	4.539000000
C	4.450500000	-3.422700000	3.949300000
H	4.292600000	-2.806000000	4.833800000
C	3.456200000	-3.478500000	2.971400000
H	2.535400000	-2.902500000	3.105000000
C	5.404000000	2.399700000	0.919200000
C	5.514600000	2.868100000	-0.404100000
H	5.265100000	2.212100000	-1.240800000
C	5.970900000	4.162400000	-0.647000000
H	6.071200000	4.507700000	-1.677500000
C	6.287500000	5.009600000	0.424500000
H	6.637800000	6.025100000	0.233700000
C	6.136500000	4.559500000	1.740300000
H	6.364800000	5.221600000	2.577500000
C	5.696700000	3.256400000	1.992700000

H	5.584900000	2.905500000	3.020400000
C	5.951000000	-0.378700000	0.230200000
C	5.498800000	-1.657500000	-0.135600000
H	4.475700000	-1.957700000	0.103700000
C	6.354800000	-2.543800000	-0.790000000
H	5.994000000	-3.535300000	-1.065600000
C	7.665700000	-2.157600000	-1.091100000
H	8.332500000	-2.850000000	-1.607200000
C	8.117400000	-0.881200000	-0.737700000
H	9.135400000	-0.572500000	-0.978500000
C	7.264300000	0.008100000	-0.079700000
H	7.614000000	1.008000000	0.180900000
C	5.207800000	0.310500000	2.939200000
C	6.545600000	0.199100000	3.359600000
H	7.359000000	0.342800000	2.647700000
C	6.832800000	-0.108000000	4.689400000
H	7.871400000	-0.197300000	5.010900000
C	5.789700000	-0.314600000	5.603300000
H	6.017600000	-0.572000000	6.639900000
C	4.462900000	-0.204300000	5.184900000
H	3.636400000	-0.388200000	5.870500000
C	4.169000000	0.112500000	3.856000000
H	3.127400000	0.184300000	3.541700000
C	4.239800000	1.910300000	-3.764800000
C	4.669400000	0.641500000	-3.333200000
H	3.935800000	-0.107300000	-3.029200000
C	6.028900000	0.348000000	-3.261000000
H	6.351000000	-0.635100000	-2.917300000
C	6.973000000	1.329000000	-3.585400000
H	8.037100000	1.106700000	-3.497500000
C	6.551400000	2.597100000	-3.996800000
H	7.285500000	3.366000000	-4.239600000
C	5.186700000	2.888900000	-4.094700000
H	4.856700000	3.876900000	-4.419700000
C	1.960200000	1.433600000	-5.455300000
C	2.888300000	1.233300000	-6.490200000
H	3.938400000	1.490800000	-6.340900000
C	2.465400000	0.690600000	-7.705800000
H	3.188600000	0.524300000	-8.505700000
C	1.118600000	0.358600000	-7.892000000
H	0.787200000	-0.070300000	-8.839600000
C	0.194900000	0.565300000	-6.862700000
H	-0.854600000	0.309200000	-7.005700000
C	0.610900000	1.090500000	-5.639700000
H	-0.110300000	1.235900000	-4.831100000
C	2.185200000	3.978100000	-4.105900000
C	2.266600000	4.566500000	-5.378200000
H	2.478800000	3.948200000	-6.251300000
C	2.044600000	5.937300000	-5.527300000
H	2.098100000	6.388200000	-6.519600000
C	1.737000000	6.725100000	-4.412600000
H	1.549300000	7.793100000	-4.532700000
C	1.653500000	6.140500000	-3.145600000
H	1.403700000	6.745800000	-2.275100000
C	1.871000000	4.770400000	-2.992400000
H	1.779000000	4.301200000	-2.011000000



N	-3.681500000	-4.130800000	0.998600000
N	-2.692200000	-3.893900000	2.969400000
C	-2.701800000	-3.451700000	1.676300000
C	-4.290700000	-5.028500000	1.862400000
C	-3.656200000	-4.874100000	3.125800000
C	-3.983800000	-3.920100000	-0.447500000
H	-3.343700000	-3.071400000	-0.728700000
C	-5.439100000	-3.513000000	-0.651600000
H	-5.657800000	-2.573900000	-0.128100000
H	-6.126200000	-4.301400000	-0.316300000
H	-5.598200000	-3.319100000	-1.719600000
C	-1.755100000	-3.372600000	4.003700000
C	-0.757700000	-4.445900000	4.422900000
H	-1.208900000	-2.578700000	3.476000000
H	-1.259100000	-5.265700000	4.955100000
H	-0.233900000	-4.850500000	3.546800000
N	-5.267100000	-5.897400000	1.630300000
N	-3.977600000	-5.583000000	4.200900000
C	-5.601800000	-6.616900000	2.724600000
C	-4.975600000	-6.463300000	3.971300000
H	-6.400600000	-7.349400000	2.599000000
H	-5.287500000	-7.076400000	4.818200000
H	-0.014800000	-3.980700000	5.083700000
C	-2.516800000	-2.751700000	5.167900000
H	-3.240700000	-2.011400000	4.811600000
H	-3.047200000	-3.517500000	5.750600000
H	-1.791100000	-2.249400000	5.817000000
C	-3.570700000	-5.142100000	-1.259900000
H	-2.503300000	-5.361500000	-1.130800000
H	-4.160500000	-6.025100000	-0.976700000
H	-3.735600000	-4.938200000	-2.326200000

282

5 T1

Au	-0.023100000	-0.005200000	-0.082800000
Au	-2.148900000	0.738900000	1.494500000
Au	-2.553300000	-0.387900000	-1.229700000
Au	-1.545800000	-2.015800000	1.017500000
Au	0.477700000	-0.552800000	2.651400000
Au	0.386600000	2.248800000	1.438400000
Au	-1.262300000	2.142000000	-1.104700000
Au	-0.018700000	-1.467800000	-2.324800000
Au	1.263300000	-2.353900000	0.280200000
Au	2.572800000	0.337400000	0.520300000
Au	1.346900000	1.165400000	-2.066300000
Cl	-4.570000000	-0.738900000	-2.410600000
Cl	0.810400000	-0.956800000	4.981800000
P	-3.811400000	1.242200000	2.963600000
P	1.079000000	3.950900000	2.770200000
P	-2.499000000	3.844200000	-1.963200000
P	-0.139900000	-2.757000000	-4.195100000
P	2.318200000	-4.341700000	0.601200000
P	4.746100000	0.703100000	1.136500000
P	2.487000000	2.161000000	-3.797700000
C	-4.998200000	2.498000000	2.386200000
C	-4.484100000	3.625200000	1.730400000
H	-3.410100000	3.696400000	1.555700000

C	-5.344200000	4.617500000	1.275000000
H	-4.938800000	5.486800000	0.758100000
C	-6.721600000	4.473200000	1.430500000
H	-7.396600000	5.236200000	1.041000000
C	-7.237400000	3.337700000	2.054600000
H	-8.315300000	3.213000000	2.160100000
C	-6.380700000	2.352100000	2.544100000
H	-6.786700000	1.465300000	3.033500000
C	-3.073800000	1.868500000	4.507500000
C	-2.113000000	1.040600000	5.111000000
H	-1.838800000	0.083400000	4.663300000
C	-1.487800000	1.450300000	6.281300000
H	-0.740600000	0.796700000	6.732400000
C	-1.800800000	2.691700000	6.844500000
H	-1.299400000	3.019300000	7.756700000
C	-2.749100000	3.515500000	6.238700000
H	-2.996000000	4.483600000	6.677400000
C	-3.390500000	3.111100000	5.067400000
H	-4.129000000	3.760600000	4.592900000
C	-4.793300000	-0.204400000	3.489300000
C	-5.296100000	-0.284000000	4.794700000
H	-5.106200000	0.523100000	5.505200000
C	-5.997300000	-1.419300000	5.199400000
H	-6.360400000	-1.493300000	6.224900000
C	-6.206500000	-2.466900000	4.302500000
H	-6.729400000	-3.369500000	4.622500000
C	-5.734400000	-2.373700000	2.993800000
H	-5.918000000	-3.190300000	2.296700000
C	-5.017300000	-1.251500000	2.583000000
H	-4.609200000	-1.194300000	1.572100000
C	2.042900000	5.218300000	1.871000000
C	2.582000000	4.905600000	0.615300000
H	2.474500000	3.894600000	0.212300000
C	3.243500000	5.887800000	-0.114900000
H	3.648900000	5.646800000	-1.096700000
C	3.388000000	7.172800000	0.406900000
H	3.899300000	7.940400000	-0.175600000
C	2.876200000	7.479700000	1.668900000
H	2.986600000	8.484800000	2.078500000
C	2.192900000	6.508500000	2.397900000
H	1.750100000	6.762500000	3.362500000
C	-0.307300000	4.886600000	3.507900000
C	-0.229100000	5.420400000	4.801800000
H	0.625500000	5.193100000	5.442100000
C	-1.251400000	6.242700000	5.269100000
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C	2.165500000	2.081800000	6.189300000

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282

5 S1

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278

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C	5.822300000	-0.207500000	5.682200000
H	6.047100000	-0.441000000	6.724700000
C	4.496200000	-0.131200000	5.250800000
H	3.666900000	-0.321800000	5.930500000
C	4.208400000	0.162800000	3.915100000
H	3.167000000	0.214100000	3.593800000
C	4.291700000	1.861800000	-3.686500000
C	4.727100000	0.597400000	-3.247700000
H	3.996900000	-0.150600000	-2.932500000
C	6.087900000	0.307200000	-3.183900000
H	6.414400000	-0.673600000	-2.836800000
C	7.028100000	1.287800000	-3.522000000
H	8.093600000	1.067400000	-3.445300000
C	6.600800000	2.553000000	-3.935700000
H	7.331700000	3.322000000	-4.189100000
C	5.234700000	2.840600000	-4.026400000
H	4.901300000	3.826300000	-4.355100000
C	2.025200000	1.354000000	-5.380500000
C	2.963400000	1.146400000	-6.406400000
H	4.012100000	1.405700000	-6.249700000
C	2.552400000	0.592400000	-7.620500000
H	3.283800000	0.420000000	-8.412000000
C	1.207100000	0.259100000	-7.816500000
H	0.885500000	-0.176600000	-8.764000000
C	0.274100000	0.472200000	-6.796100000
H	-0.773200000	0.213300000	-6.947700000
C	0.678600000	1.005400000	-5.572600000

H	-0.049100000	1.152100000	-4.769800000
C	2.225900000	3.913100000	-4.047500000
C	2.388500000	4.502000000	-5.313300000
H	2.660100000	3.883300000	-6.172100000
C	2.172600000	5.872600000	-5.474000000
H	2.291400000	6.324000000	-6.459100000
C	1.788600000	6.659300000	-4.379500000
H	1.606400000	7.728400000	-4.508300000
C	1.623000000	6.073400000	-3.122800000
H	1.314400000	6.679800000	-2.271600000
C	1.835800000	4.703200000	-2.954900000
H	1.682400000	4.234000000	-1.980700000
N	-2.610600000	-3.702600000	3.200700000
N	-3.395900000	-4.260600000	1.180400000
C	-2.540500000	-3.431800000	1.865600000
C	-3.541200000	-4.718900000	3.460700000
O	-3.814000000	-5.236000000	4.524500000
C	-4.127500000	-5.061700000	2.063800000
O	-5.016700000	-5.847200000	1.809300000
C	-1.706500000	-3.087400000	4.213400000
C	-3.562400000	-4.217700000	-0.301400000
H	-2.715700000	-3.601400000	-0.642400000
C	-4.863300000	-3.516800000	-0.673100000
H	-4.929700000	-3.426300000	-1.764400000
H	-4.881700000	-2.497100000	-0.278700000
H	-5.729400000	-4.083100000	-0.307100000
H	-1.188200000	-2.296000000	3.654600000
C	-0.673500000	-4.109700000	4.675100000
H	-0.111600000	-4.503800000	3.813800000
H	0.033800000	-3.608100000	5.348500000
H	-1.155000000	-4.942600000	5.205900000
C	-3.435600000	-5.614200000	-0.897100000
H	-2.459100000	-6.054500000	-0.670200000
H	-4.228200000	-6.277500000	-0.529600000
H	-3.511000000	-5.537800000	-1.987500000
C	-2.492300000	-2.449500000	5.349600000
H	-3.238300000	-1.747400000	4.961100000
H	-2.999500000	-3.207000000	5.961200000
H	-1.786100000	-1.893100000	5.976700000

278

6 T1

Au	-0.010300000	0.026600000	0.034800000
Au	-2.163200000	0.865400000	1.497100000
Au	-2.508300000	-0.380700000	-1.202900000
Au	-1.636500000	-1.972000000	1.023400000
Au	0.481900000	-0.327500000	2.786200000
Au	0.342300000	2.299100000	1.527900000
Au	-1.289900000	2.153400000	-1.022600000
Au	0.057000000	-1.483900000	-2.185600000
Au	1.287800000	-2.282500000	0.373400000
Au	2.568800000	0.413100000	0.647300000
Au	1.362700000	1.121600000	-1.981100000
Cl	-4.501300000	-0.688800000	-2.416500000
Cl	0.904800000	-0.841100000	5.074300000
P	-3.849500000	1.295700000	2.967100000
P	0.976900000	4.132900000	2.735500000



P	-2.514000000	3.839500000	-1.939700000
P	-0.111600000	-2.768300000	-4.086100000
P	2.282100000	-4.300300000	0.763800000
P	4.752500000	0.781600000	1.224200000
P	2.503500000	2.079400000	-3.712500000
C	-5.093000000	2.489400000	2.380600000
C	-4.639100000	3.658600000	1.755700000
H	-3.569000000	3.809300000	1.615800000
C	-5.552400000	4.598000000	1.295500000
H	-5.197800000	5.506200000	0.811800000
C	-6.921200000	4.356800000	1.409800000
H	-7.636800000	5.079300000	1.016500000
C	-7.375000000	3.179800000	2.002800000
H	-8.444200000	2.982000000	2.082500000
C	-6.465300000	2.247600000	2.500800000
H	-6.819500000	1.329700000	2.972400000
C	-3.127000000	1.974600000	4.496300000
C	-2.086100000	1.230500000	5.073200000
H	-1.747900000	0.300600000	4.618400000
C	-1.471100000	1.681100000	6.232900000
H	-0.665000000	1.087100000	6.663800000
C	-1.874100000	2.884100000	6.812700000
H	-1.379400000	3.247400000	7.713500000
C	-2.905300000	3.623800000	6.237700000
H	-3.225200000	4.560400000	6.692000000
C	-3.537200000	3.175900000	5.077700000
H	-4.342600000	3.759500000	4.629000000
C	-4.731800000	-0.204200000	3.489800000
C	-5.136000000	-0.376000000	4.819700000
H	-4.965000000	0.413300000	5.552200000
C	-5.705000000	-1.583600000	5.216000000
H	-5.982800000	-1.731100000	6.260200000
C	-5.881200000	-2.609100000	4.289900000
H	-6.282300000	-3.571300000	4.606000000
C	-5.522800000	-2.420800000	2.955000000
H	-5.688200000	-3.218700000	2.235000000
C	-4.934300000	-1.227400000	2.551700000
H	-4.610000000	-1.093000000	1.519300000
C	1.926200000	5.396100000	1.819200000
C	2.540000000	5.033400000	0.614000000
H	2.475900000	4.000200000	0.261800000
C	3.223400000	5.992300000	-0.128000000
H	3.685600000	5.712000000	-1.072800000
C	3.315100000	7.303700000	0.334600000
H	3.845900000	8.053300000	-0.255000000
C	2.727700000	7.660900000	1.548900000
H	2.800400000	8.686600000	1.912300000
C	2.024400000	6.712000000	2.288600000
H	1.528500000	7.000100000	3.216900000
C	-0.413600000	5.054500000	3.482400000
C	-0.336600000	5.592800000	4.773800000
H	0.539400000	5.404300000	5.396700000
C	-1.390600000	6.361800000	5.261900000
H	-1.332900000	6.777400000	6.269100000
C	-2.521000000	6.583700000	4.475300000
H	-3.348500000	7.177900000	4.865300000

C	-2.609300000	6.023900000	3.199900000
H	-3.501200000	6.178900000	2.593600000
C	-1.561800000	5.255700000	2.702900000
H	-1.621200000	4.816800000	1.704400000
C	2.030800000	3.659900000	4.143200000
C	1.557700000	2.626900000	4.963500000
H	0.617400000	2.128600000	4.730900000
C	2.296900000	2.229400000	6.069100000
H	1.923700000	1.415300000	6.689300000
C	3.525700000	2.829600000	6.341200000
H	4.119500000	2.493300000	7.191700000
C	4.008600000	3.841200000	5.512800000
H	4.975700000	4.299600000	5.718500000
C	3.260000000	4.267500000	4.416400000
H	3.636300000	5.060400000	3.770400000
C	-2.089800000	3.939600000	-3.709700000
C	-2.422200000	2.810600000	-4.481400000
H	-2.994500000	1.992700000	-4.037400000
C	-2.016500000	2.742800000	-5.805700000
H	-2.273300000	1.869900000	-6.405300000
C	-1.263700000	3.776900000	-6.361200000
H	-0.924500000	3.704700000	-7.393500000
C	-0.944900000	4.896800000	-5.597300000
H	-0.371400000	5.711300000	-6.033800000
C	-1.353800000	4.984300000	-4.268100000
H	-1.098800000	5.860400000	-3.669500000
C	-4.308900000	3.556700000	-1.916400000
C	-4.833800000	2.515100000	-1.145000000
H	-4.175400000	1.886100000	-0.550100000
C	-6.201400000	2.263800000	-1.153200000
H	-6.594900000	1.432600000	-0.569700000
C	-7.049400000	3.067500000	-1.908100000
H	-8.123300000	2.876100000	-1.909100000
C	-6.530200000	4.106400000	-2.685900000
H	-7.194400000	4.720500000	-3.295000000
C	-5.159400000	4.342300000	-2.709300000
H	-4.745500000	5.117600000	-3.356600000
C	-2.174700000	5.450100000	-1.152900000
C	-3.175800000	6.377500000	-0.843400000
H	-4.208300000	6.184300000	-1.133600000
C	-2.853900000	7.541600000	-0.147400000
H	-3.641000000	8.249300000	0.112700000
C	-1.533000000	7.803400000	0.211400000
H	-1.284700000	8.708900000	0.765100000
C	-0.530000000	6.892100000	-0.113900000
H	0.500000000	7.088500000	0.176600000
C	-0.850400000	5.708000000	-0.765600000
H	-0.083500000	4.953900000	-0.940600000
C	-1.202700000	-2.078500000	-5.384700000
C	-1.092300000	-2.461600000	-6.727300000
H	-0.297300000	-3.135900000	-7.046400000
C	-1.991500000	-1.959100000	-7.664600000
H	-1.905600000	-2.259600000	-8.709200000
C	-2.998000000	-1.073900000	-7.270300000
H	-3.703100000	-0.687500000	-8.008000000
C	-3.103900000	-0.689500000	-5.934300000

H	-3.898000000	-0.018900000	-5.604800000
C	-2.204600000	-1.185200000	-4.994600000
H	-2.304900000	-0.885100000	-3.953800000
C	1.481300000	-3.065300000	-4.937300000
C	2.470500000	-2.080000000	-4.834600000
H	2.283900000	-1.197800000	-4.221500000
C	3.678100000	-2.229600000	-5.509100000
H	4.447800000	-1.462000000	-5.416500000
C	3.899800000	-3.361200000	-6.295600000
H	4.845200000	-3.479700000	-6.827500000
C	2.921800000	-4.353500000	-6.385400000
H	3.102400000	-5.247500000	-6.983400000
C	1.717000000	-4.215800000	-5.698500000
H	0.968000000	-5.009800000	-5.736100000
C	-0.766100000	-4.445800000	-3.770700000
C	-1.764900000	-5.037800000	-4.556100000
H	-2.236400000	-4.482400000	-5.372500000
C	-2.165800000	-6.346700000	-4.281800000
H	-2.949200000	-6.805500000	-4.889500000
C	-1.579400000	-7.059000000	-3.229400000
H	-1.905500000	-8.077400000	-3.011100000
C	-0.599800000	-6.458500000	-2.433600000
H	-0.158600000	-7.000800000	-1.591600000
C	-0.199900000	-5.153200000	-2.694000000
H	0.559200000	-4.677800000	-2.069000000
C	2.711100000	-5.126700000	-0.804300000
C	3.234300000	-4.333000000	-1.836400000
H	3.322200000	-3.252200000	-1.703700000
C	3.603600000	-4.919900000	-3.038600000
H	4.017900000	-4.303200000	-3.834200000
C	3.417800000	-6.289000000	-3.234800000
H	3.679800000	-6.738600000	-4.193300000
C	2.887900000	-7.077000000	-2.215500000
H	2.736500000	-8.145700000	-2.371200000
C	2.547000000	-6.501900000	-0.991600000
H	2.140300000	-7.117700000	-0.187100000
C	1.275400000	-5.510800000	1.672700000
C	-0.061400000	-5.689400000	1.279600000
H	-0.481000000	-5.097100000	0.463900000
C	-0.854600000	-6.618000000	1.947900000
H	-1.895200000	-6.758100000	1.657200000
C	-0.329800000	-7.349800000	3.013700000
H	-0.967800000	-8.051500000	3.553600000
C	0.997300000	-7.172700000	3.400900000
H	1.405100000	-7.739500000	4.238300000
C	1.806400000	-6.254100000	2.731500000
H	2.841700000	-6.104000000	3.041500000
C	3.884900000	-4.144200000	1.616500000
C	4.982200000	-4.926700000	1.235300000
H	4.871300000	-5.687400000	0.460900000
C	6.225800000	-4.708800000	1.822800000
H	7.082600000	-5.305800000	1.507700000
C	6.372800000	-3.724800000	2.797600000
H	7.349300000	-3.543600000	3.247200000
C	5.274600000	-2.964800000	3.197900000
H	5.391500000	-2.211000000	3.972500000

C	4.030800000	-3.159100000	2.605300000
H	3.181400000	-2.536600000	2.900100000
C	5.353900000	2.481300000	0.955500000
C	5.602500000	2.914900000	-0.353400000
H	5.476100000	2.222100000	-1.183500000
C	6.034100000	4.216400000	-0.582600000
H	6.245000000	4.541000000	-1.601700000
C	6.186300000	5.103000000	0.484900000
H	6.511700000	6.128000000	0.303500000
C	5.902700000	4.683700000	1.783100000
H	6.007600000	5.379200000	2.615800000
C	5.493500000	3.373700000	2.025100000
H	5.285100000	3.042000000	3.042600000
C	5.907300000	-0.305600000	0.303300000
C	5.424000000	-1.552300000	-0.119800000
H	4.371200000	-1.797900000	0.024800000
C	6.283300000	-2.469500000	-0.717500000
H	5.898200000	-3.437000000	-1.041400000
C	7.629100000	-2.147300000	-0.896600000
H	8.304900000	-2.869800000	-1.356400000
C	8.106900000	-0.896600000	-0.503400000
H	9.154300000	-0.638100000	-0.661800000
C	7.249400000	0.027700000	0.091300000
H	7.622500000	1.013400000	0.373400000
C	5.129100000	0.449900000	2.985400000
C	6.455400000	0.418700000	3.438800000
H	7.279200000	0.610000000	2.752900000
C	6.725000000	0.126300000	4.771400000
H	7.757600000	0.100700000	5.120900000
C	5.678300000	-0.157800000	5.651900000
H	5.896200000	-0.418800000	6.688600000
C	4.362100000	-0.128200000	5.201400000
H	3.531100000	-0.375400000	5.860900000
C	4.083900000	0.192800000	3.874500000
H	3.047100000	0.217600000	3.540500000
C	4.302300000	1.825800000	-3.544100000
C	4.724200000	0.546900000	-3.146400000
H	3.988900000	-0.216000000	-2.882100000
C	6.080100000	0.259400000	-3.064100000
H	6.401500000	-0.734800000	-2.756600000
C	7.023400000	1.250200000	-3.340900000
H	8.086100000	1.026400000	-3.245400000
C	6.607000000	2.525700000	-3.717800000
H	7.344000000	3.302000000	-3.925100000
C	5.246900000	2.816300000	-3.828500000
H	4.923300000	3.814300000	-4.127700000
C	2.125100000	1.294600000	-5.309600000
C	3.115300000	0.997300000	-6.253100000
H	4.162300000	1.221100000	-6.042000000
C	2.760400000	0.385800000	-7.453200000
H	3.534300000	0.127300000	-8.176900000
C	1.422800000	0.100500000	-7.722500000
H	1.146800000	-0.383800000	-8.659600000
C	0.436900000	0.423800000	-6.791200000
H	-0.607700000	0.214500000	-7.008400000
C	0.783100000	0.996100000	-5.574600000

H	0.015300000	1.207200000	-4.827200000
C	2.264600000	3.864300000	-4.000700000
C	2.491500000	4.438200000	-5.256700000
H	2.764800000	3.808900000	-6.103000000
C	2.352300000	5.813400000	-5.421600000
H	2.535200000	6.261900000	-6.397100000
C	1.965900000	6.613000000	-4.348000000
H	1.844300000	7.688200000	-4.485500000
C	1.708200000	6.037600000	-3.106200000
H	1.382200000	6.659000000	-2.273400000
C	1.857600000	4.664600000	-2.930900000
H	1.651800000	4.198100000	-1.966800000
N	-2.368700000	-3.899900000	3.233700000
N	-3.305500000	-4.411400000	1.311000000
C	-2.380500000	-3.612900000	1.910300000
C	-3.333000000	-4.879000000	3.560700000
O	-3.559100000	-5.322000000	4.689200000
C	-3.988700000	-5.206300000	2.262000000
O	-4.935300000	-5.962600000	2.022400000
C	-1.490100000	-3.244600000	4.224200000
C	-3.610300000	-4.382700000	-0.135500000
H	-2.799200000	-3.778100000	-0.573100000
C	-4.934000000	-3.687300000	-0.399900000
H	-5.107300000	-3.621900000	-1.480800000
H	-4.913700000	-2.659600000	-0.024600000
H	-5.758500000	-4.244100000	0.068500000
H	-0.882000000	-2.550000000	3.628800000
C	-0.561200000	-4.251200000	4.879500000
H	0.068000000	-4.737300000	4.117900000
H	0.096300000	-3.713800000	5.585200000
H	-1.139200000	-5.017300000	5.418800000
C	-3.540600000	-5.787200000	-0.718100000
H	-2.552400000	-6.225800000	-0.548000000
H	-4.303100000	-6.437000000	-0.273900000
H	-3.702100000	-5.727800000	-1.800000000
C	-2.320000000	-2.444000000	5.215200000
H	-2.941700000	-1.723700000	4.680100000
H	-2.976600000	-3.106600000	5.797900000
H	-1.645600000	-1.902600000	5.891700000

278

6 S1

Au	-0.010609000	0.011760000	0.068554000
Au	-2.243490000	0.750994000	1.451894000
Au	-2.459709000	-0.425881000	-1.318254000
Au	-1.654911000	-2.023600000	0.822609000
Au	0.785972000	-0.229213000	2.789667000
Au	0.284823000	2.304025000	1.574033000
Au	-1.342190000	2.213759000	-0.845723000
Au	0.070249000	-1.475908000	-2.227569000
Au	1.323088000	-2.313397000	0.201659000
Au	2.634746000	0.323100000	0.667108000
Au	1.445473000	1.192535000	-1.835151000
Cl	-4.333876000	-0.299403000	-2.748701000
Cl	1.093347000	-1.005739000	5.002569000
P	-3.768767000	1.292166000	3.036606000
P	1.008070000	4.121131000	2.764758000

P	-2.600135000	3.727746000	-2.005052000
P	0.032930000	-2.774058000	-4.129099000
P	2.241430000	-4.347317000	0.654817000
P	4.832670000	0.642125000	1.263403000
P	2.470735000	2.166995000	-3.612614000
C	-4.888724000	2.626125000	2.498807000
C	-4.324313000	3.691985000	1.783787000
H	-3.257448000	3.675751000	1.559264000
C	-5.128613000	4.723179000	1.315204000
H	-4.681475000	5.536029000	0.741118000
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H	-7.143757000	5.474137000	1.136463000
C	-7.074340000	3.614647000	2.227390000
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C	-6.269788000	2.585917000	2.719301000
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C	-2.914360000	1.881495000	4.533010000
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C	-1.217123000	1.431738000	6.192581000
H	-0.435382000	0.774601000	6.572500000
C	-1.508484000	2.646931000	6.811540000
H	-0.950993000	2.952482000	7.696604000
C	-2.502142000	3.475162000	6.292822000
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H	2.476772000	3.925124000	0.270599000
C	3.161994000	5.918089000	-0.209508000
H	3.614635000	5.612586000	-1.150677000
C	3.218011000	7.250750000	0.191065000
H	3.714644000	7.988547000	-0.440924000
C	2.636461000	7.643198000	1.396694000
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C	3.614876000	2.958135000	6.370571000
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C	3.338942000	4.303812000	4.379399000
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279

2-NHC-S0

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279

2-NHC\_T1

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H	5.283708	2.883970	3.390260
C	6.275236	-0.096666	0.494156
C	6.094057	-1.433187	0.121474
H	5.133040	-1.920462	0.292864
C	7.141397	-2.139032	-0.458344
H	6.992823	-3.180204	-0.743426
C	8.371648	-1.517313	-0.668016
H	9.193698	-2.073677	-1.119748
C	8.550701	-0.185930	-0.302505
H	9.512195	0.301247	-0.466999
C	7.505382	0.529149	0.275959
H	7.643009	1.576916	0.545244
C	5.220166	0.241775	3.111920
C	6.502975	0.370799	3.657320
H	7.318685	0.775954	3.059671
C	6.740548	-0.030056	4.967854
H	7.737877	0.081726	5.392503
C	5.712151	-0.583794	5.730601
H	5.906830	-0.904342	6.755773
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H	3.621615	-1.163531	5.755686

C	4.195149	-0.311246	3.879841
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C	3.399062	1.287158	-6.218693
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C	2.348763	6.129691	-3.164379
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C	-0.828637	-4.384590	4.852979
H	-0.209690	-4.651404	3.985493
H	-1.312226	-5.290460	5.250919
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H	-3.508144	-5.164446	-1.851588
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279

2-NHC\_S1

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H	2.175577	7.323420	0.787410
H	1.338797	6.679128	-0.657408
C	2.135598	2.540598	4.900150
C	0.874164	2.757799	5.724093
H	2.000132	1.656028	4.260565
H	0.955791	3.681845	6.320171
H	-0.015186	2.817439	5.077714
N	2.772974	7.057495	3.116065
N	3.430443	5.335679	5.341750
C	3.458127	7.474957	4.208666
C	3.777150	6.644122	5.278698
H	3.753057	8.526426	4.222832
H	4.328456	7.038034	6.134911
H	0.747847	1.903266	6.400498
C	3.360117	2.349149	5.782097
H	3.488240	3.190889	6.473612
H	3.212665	1.424775	6.357563
H	4.280506	2.233862	5.192081