

## A Combined Mechanistic and Computational Study of the Gold(I)-Catalyzed Formation of Substituted Indenes

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## Supporting Information

### Table of contents

Computational datas	S2
NMR spectra :	S8

**Table S1.** coordinate data sets and absolute energies for DFT optimized complexes.

<b>Ia</b>			<b>-732.293632a.u.</b>			<b>a</b>			<b>-2027.241044 a.u.</b>			<b>ab</b>			<b>-2027.234055 a.u.</b>		
C	1.709048	-1.690802	-0.812208	C	1.408418	-1.194733	0.161850	C	1.912288	-0.130541	0.131229						
C	1.780997	-0.703763	0.192074	N	1.187045	-2.538256	0.290704	N	2.667294	-1.269004	0.215928						
C	2.847798	-0.734813	1.115549	N	2.745482	-1.020481	0.388493	N	2.777623	0.897998	0.395443						
C	3.825248	-1.741344	1.036273	C	2.373287	-3.199955	0.597256	C	3.988362	-0.957442	0.528245						
C	3.748086	-2.722618	0.032175	C	3.355861	-2.243506	0.656826	C	4.058101	0.408343	0.642207						
C	2.688448	-2.693992	-0.892745	C	-0.107471	-3.181256	0.149370	C	2.171421	-2.618815	0.012928						
H	0.870312	-1.672306	-1.526243	C	3.442175	0.251199	0.600091	C	2.423268	2.305828	0.404143						
H	2.911416	0.044797	1.891368	H	2.408643	-4.283820	0.745000	H	4.753663	-1.731786	0.639263						
H	4.651454	-1.759740	1.764925	H	4.427320	-2.319237	0.866452	H	4.896990	1.071992	0.873793						
H	4.513257	-3.513115	-0.027019	C	-0.500279	-3.639366	-1.136697	C	2.155819	-3.143191	-1.307186						
H	2.622613	-3.462243	-1.679851	C	-1.765738	-4.254478	-1.238898	C	1.680395	-4.461329	-1.468524						
C	0.756050	0.424386	0.268679	C	-2.591216	-4.409663	-0.115911	C	1.254083	-5.220586	-0.369772						
H	0.754687	0.833562	1.302484	C	-2.168714	-3.953553	1.141069	C	1.292492	-4.676588	0.921681						
O	1.192089	1.530558	-0.609558	C	-0.914544	-3.329648	1.308986	C	1.752426	-3.362547	1.148441						
C	1.854710	2.555735	-0.004880	C	0.375020	-3.478019	-2.380719	C	2.636144	-2.353379	-2.525767						
O	2.025262	2.610170	1.189531	H	-2.108230	-4.624307	-2.218016	H	1.652118	-4.904601	-2.476409						
C	2.260268	3.595885	-1.028309	H	-3.571880	-4.900116	-0.220422	H	0.894725	-6.250664	-0.521030						
H	3.031860	3.169347	-1.702125	H	-2.823911	-4.090668	2.015557	H	0.961009	-5.286602	1.776416						
H	1.395255	3.878307	-1.660527	C	-0.476532	-2.852706	2.694429	C	1.799190	-2.805787	2.572393						
H	2.669871	4.482483	-0.512420	C	3.555671	0.986882	1.570887	C	1.986666	2.888795	1.623378						
C	-0.600829	0.044928	-0.124630	C	4.257264	2.209572	1.515590	C	1.665060	4.262264	1.600067						
C	-1.742734	-0.286613	-0.422788	C	4.818557	2.672432	0.316921	C	1.777011	5.015887	0.442925						
C	-3.114622	-0.668656	-0.759603	C	4.691449	1.926061	-0.860026	C	2.216567	4.410760	-0.763416						
H	-3.347457	-0.310124	-1.789083	C	4.002297	0.689930	-0.870351	C	2.554155	3.041679	-0.803942						
H	-3.180196	-1.780205	-0.812227	C	2.966416	0.503510	2.897015	C	1.860632	2.097701	2.926012						
C	-4.181998	-0.135400	0.224411	H	4.372414	2.806673	2.433813	H	1.327164	4.751959	2.526879						
C	-5.609484	-0.551205	-0.160629	H	5.368583	3.626449	0.301471	H	1.528105	6.088795	0.432347						
H	-4.109305	0.973852	0.269999	H	5.145812	2.292269	-1.791667	H	2.308567	5.015710	-1.679227						
H	-3.944217	-0.499492	1.248419	C	3.917074	-0.132058	-2.157059	C	3.038335	2.414450	-2.112046						
C	-6.678224	-0.024973	0.805096	H	1.349158	-3.032534	-2.059292	H	2.975575	-1.356580	-2.174274						
H	-5.828875	-0.193517	-1.192666	C	-0.251797	-2.476443	-3.375479	C	1.489976	-2.111581	-3.531290						
H	-5.665978	-1.662733	-0.211338	C	0.672319	-4.834289	-3.055120	C	3.845244	3.036251	-3.201452						
H	-7.696308	-0.345193	0.501311	H	0.537601	-2.410436	2.596648	H	2.138785	-1.750079	2.514486						
H	-6.506607	-0.393714	1.838956	C	-1.406921	-1.743231	3.229486	C	0.402830	-2.797427	3.229364						
H	-6.675558	1.085284	0.846354	C	-0.368027	-4.028296	3.690009	C	2.824826	-3.570281	3.438620						
				H	2.483669	-0.480374	2.716656	H	2.177270	1.053294	2.721914						
				C	4.065585	0.285865	3.959741	C	2.796123	2.654292	4.021226						
				C	1.869380	1.461484	3.409032	C	0.395429	2.041652	3.409128						
				H	3.237745	-0.988999	-1.968895	H	3.263818	1.345493	-1.914077						
				C	3.309682	0.674985	-3.324701	C	1.938541	2.452310	-3.194913						
				C	5.298884	-0.710460	-2.536302	C	4.344064	3.072023	-2.609727						
				H	0.413353	-2.328883	-4.251461	H	1.846778	-1.503407	-4.388302						
				H	-1.230043	-2.838669	-3.755437	H	1.097034	-3.065408	-3.941796						
				H	-0.418682	-1.486246	-2.900137	H	0.644630	-1.570928	-3.055640						
				H	1.361440	-4.695395	-3.913617	H	4.218447	-2.418106	-4.044140						
				H	1.144329	-5.548685	-2.349891	H	4.682857	-3.185358	-2.489573						
				H	-0.250555	-5.309878	-3.447484	H	3.575965	-4.031076	-3.613788						
				H	-1.047970	-1.375595	4.213032	H	0.452592	-2.335357	4.237182						
				H	-1.450660	-0.877514	2.535906	H	-0.329033	-2.224756	2.623625						
				H	-2.444140	-2.111746	3.371743	H	0.003727	-3.825135	3.357507						
				H	0.013637	-3.672998	4.669506	H	2.889408	-3.121934	4.451772						
				H	-1.355025	-4.502589	3.871630	H	2.537830	-4.635449	3.563362						
				H	0.319063	-4.817299	3.321183	H	3.839549	-3.549579	2.990485						
				H	3.627295	-0.127499	4.891606	H	2.734663	2.031180	4.937401						
				H	4.845278	-0.419724	3.606402	H	3.854256	2.669348	3.688400						
				H	4.570984	1.237784	4.225742	H	2.520489	3.691083	4.306387						
				H	1.414836	1.068928	4.342175	H	0.310291	1.417606	4.322811						
				H	2.279706	2.467405	3.637341	H	0.009991	3.052294	3.659604						
				H	1.059677	1.587837	2.660570	H	-0.268033	1.605722	2.632999						
				H	3.201402	0.032146	-4.222554	H	2.288383	1.953622	-4.122522						
				H	2.305615	1.070479	-3.066239	H	1.018593	1.932868	-2.853373						
				H	3.949502	1.534901	-3.613430	H	1.663656	3.494379	-3.461819						
				H	5.219747	-1.349096	-3.440442	H	4.709691	2.562936	-3.525444						
				H	6.028381	0.096438	-2.758461	H	4.193670	4.142274	-2.863193						
				H	5.724413	-1.327875	-1.718676	H	5.146974	3.019264	-1.846082						
Au	0.018477	0.208955	-0.303592	Au	-0.061232	0.008616	-0.317252	Au	-0.061232	0.008616	-0.317252						
C	-3.999925	2.193035	1.166524	C	-3.948663	-0.938414	1.365389	C	-3.948663	-0.938414	1.365389						
C	-4.033377	0.911626	0.578671	C	-3.542002	-1.799895	0.325743	C	-3.542002	-1.799895	0.325743						
C	-4.905936	-0.067966	1.102190	C	-3.773168	-3.188198	0.448532	C	-3.773168	-3.188198	0.448532						
C	-5.736288	0.230283	2.194376	C	-4.404833	-3.705744	1.590243	C	-4.404833	-3.705744	1.590243						
C	-5.695890	1.508763	2.778721	C	-4.809679	-2.840814	2.622845	C	-4.809679	-2.840814	2.622845						
C	-4.826332	2.486456	2.263881	C	-4.579651	-1.458647	2.508212	C	-4.579651	-1.458647	2.508212						
H	-3.338913	2.966487	0.749943	H	-3.770672	1.043731	1.280715	H	-3.770672	1.043731	1.280715						
H	-4.938018	-1.071060	0.645940	H	-3.458040	-3.868382	-0.359657	H	-3.458040	-3.868382	-0.359657						
H	-6.415778	-0.539313	2.592923	H	-4.580072	-4.789610	1.675464	H	-4.580072	-4.789610	1.675464						
H	-6.344471	1.743577	3.637240	H	-5.303896	-3.245766	3.519846	H	-5.303896	-3.245766	3.519846						
H	-4.795991	3.490216	2.715830	H	-4.894369	-0.778316	3.314999	H	-4.894369	-0.778316	3.314999						
C	-3.197289	0.537640	-0.643754	C	-2.911885	-1.292272	-0.967891	C	-2.911885	-1.292272	-0.967891						
H	-3.001961	-0.551821	-0.599728	H	-2.259726	-2.086245	-1.376306	H	-2.259726	-2.086245	-1.376306						
O	-3.952364	0.656250	-1.889424	O	-3.938285	-1.183788	-2.015280	O	-3.938285	-1.183788	-2.015280						
C	-4.239002	1.913420	-2.366780	C	-4.751184	-0.109188	-2.116289	C	-4.751184	-0.109188	-2.116289						
O	-3.796122	2.932843	-1.873662	O	-4.622489	0.922337	-1.458706	O	-4.622489	0.922337	-1.458706						
H	-5.169764	1.826925	-3.552121	C	-5.844475	-0.336433	-3.127941	C	-5.844475	-0.336433	-3.127941						
H	-4.864475	1.017198	-4.242856	H	-6.272216	0.632424	-3.442155	H	-6.272216	0.632424	-3.442155						
H	-6.192087	1.585459	-3.192685	H	-5.467554	-0.906255	-3.998818	H	-5.467554	-0.906255	-3.998818						
H	-5.192613	2.800003	-4.074117	H	-6.645214	-0.943545	-2.654763	H	-6.645214	-0.943545	-2.654763						
C	-1.888786	1.245069	-0.737972	C	-2.109904	-0.024248	-0.812675	C	-2.109904	-0.024248	-0.812675						
C	-1.002575	2.104872	-0.969554	C	-2.390471	1.216797	-0.895202	C	-2.390471	1.216797	-0.895202						
C	-0.289433	3.348098	-1.295259	C	-2.448018	2.669659	-0.926333	C	-2.448018	2.669659	-0.926333						
H	-1.067247	4.000146	-1.756160	H	-2.880969	2.973820	-1.906127	H	-2.880969	2.973820	-1.906127						
H	0.471710	3.153962	-2.081674	H	-1.392655	3.030281	-0.941454	H	-1.392655	3.030281	-0.941454						
C	0.360370	4.062018	-0.087483	C	-3.228905	3.323422	0.238012	C	-3.228905	3.323422	0.238012						
C	0.962218	5.422539	-0.471728	C	-3.259291	4.855663	0.129577	C	-3.259291	4.855663	0.129577						
H	1.148835	3.404813	0.342028	H	-2.765834	3.017367	1.201684	H	-2.765834	3.017367	1.201684						
H	-0.404828	4.197553	0.707902														

<b>b</b>			<b>-2027.261175 a.u.</b>	<b>bc</b>			<b>-2027.246064 a.u.</b>	<b>c</b>			<b>-2027.25651 a.u.</b>
C	-1.783472	0.561519	0.226024	C	-1.872445	0.216921	0.070361	C	-1.848760	-0.119307	-0.003047
N	-2.192178	1.813137	0.610643	N	-2.625478	1.354125	0.217833	N	-2.673975	-1.215204	0.060330
N	-2.939245	-0.165118	0.101034	N	-2.783052	-0.809288	0.087290	N	-2.694853	0.957227	0.084476
C	-3.578568	1.867518	0.726121	C	-3.978192	1.045709	0.327539	C	-4.005151	-0.830391	0.188533
C	-4.050031	0.620375	0.404275	C	-4.078361	-0.320177	0.244371	C	-4.019046	0.541284	0.201513
C	-1.308523	2.938519	0.854798	C	-2.092659	2.704547	0.239175	C	-2.240203	-2.598267	-0.025858
C	-3.035085	-1.554409	-0.306077	C	-2.473488	-2.219273	-0.053929	C	-2.307135	2.354035	0.024413
H	-4.099913	2.782500	1.023920	H	-4.741055	1.820504	0.451862	H	-4.816529	-1.562008	0.252161
H	-5.068010	0.220771	0.365466	H	-4.947252	-0.984397	0.282615	H	-4.845311	1.254947	0.276412
C	-0.992847	3.797962	-0.231145	C	-1.963576	3.999080	-0.992540	C	-1.948203	-3.296556	1.175539
C	-0.143838	4.891222	0.040577	C	-1.446910	4.711337	-0.939365	C	-1.551815	-4.644744	1.056873
C	0.361970	5.117250	1.328429	C	-1.084315	5.301153	0.279882	C	-1.451000	-5.264949	-0.196163
C	0.028435	4.251339	2.379578	C	-1.232991	4.590476	1.479361	C	-1.753084	-4.549815	-1.363240
C	-0.817135	3.141430	2.171827	C	-1.742822	3.275567	1.491344	C	-2.161306	-3.200840	-1.309352
C	-1.526409	3.582019	-1.648076	C	-2.356567	2.788445	-2.338431	C	-2.080065	-2.655318	2.557143
H	0.121492	5.582764	-0.774550	H	-1.334532	5.284227	-1.873307	H	-1.318267	-5.220733	1.965803
H	1.017692	5.982107	1.516337	H	-0.689132	6.329139	0.296358	H	-1.139127	-6.319095	-0.263146
H	0.427516	4.443906	3.387843	H	-0.951051	5.068348	2.430756	H	-1.676512	-5.051704	-2.340491
C	-1.170129	2.223084	3.342656	C	-1.888862	2.524843	2.815588	C	-2.488260	-2.451944	-2.602710
C	-2.960942	-2.561533	0.692310	C	-2.216924	-2.977266	1.119205	C	-2.229077	2.979724	-1.248216
C	-3.109723	-3.899828	0.269777	C	-1.965315	-4.355851	0.954055	C	-1.907468	4.352944	-1.271513
C	-3.336535	-4.215220	-1.077803	C	-1.980519	-4.950007	-0.316153	C	-1.680788	5.067360	-0.086846
C	-3.406973	-3.196102	-2.039308	C	-2.241957	-4.174022	-1.455161	C	-1.766563	4.420520	1.153808
C	-3.255436	-1.840055	-1.680871	C	-2.494696	-2.789484	-1.355461	C	-2.082839	3.049034	1.242213
C	-2.733820	-2.251522	2.172283	C	-2.227804	-2.367918	2.521841	C	-2.486545	2.237082	-2.560246
H	-3.061835	-4.708818	1.015614	H	-1.768128	-4.978478	1.840973	H	-1.841321	4.746657	-2.239122
H	-3.467511	-5.266127	-1.380953	H	-1.796269	-6.031203	-0.418743	H	-1.440105	6.141082	-0.130626
H	-3.590273	-3.457399	-3.093113	H	-2.260322	-4.654925	-2.445759	H	-1.591258	4.995015	2.076937
C	-3.364164	-0.749176	-2.747544	C	-2.811032	-1.978590	-2.613120	C	-2.189833	2.376142	2.611225
H	-2.189961	2.691953	-1.631399	H	-2.770765	1.776702	-2.144452	H	-2.251580	-1.567776	2.410734
C	-0.380750	3.274697	-2.637050	C	-1.126355	2.604801	-3.252969	C	-0.789997	-2.802211	3.390065
C	-2.378562	4.778314	-2.123993	C	-3.463766	3.608776	-3.035042	C	-3.303450	-3.218783	3.314750
H	-1.830722	1.418637	2.956774	H	-2.348272	1.537699	2.598226	H	-2.878379	-1.449315	-2.327508
C	0.085475	1.538558	3.923156	C	-0.510473	2.251145	3.455135	C	-1.216846	-2.262316	-3.449273
C	-1.956359	2.979242	4.436538	C	-2.830639	3.261970	3.791690	C	-3.591602	-3.161140	-3.416441
H	-2.713592	-1.147975	2.289533	H	-2.428207	-1.281133	2.418513	H	-2.733717	1.183549	-2.312565
C	-3.885676	-2.784153	3.051474	C	-3.360733	-2.964901	3.385339	C	-3.696728	2.825363	-3.317790
C	-1.363812	-2.780104	2.649071	C	-0.855963	-2.510903	3.213541	C	-1.223806	2.208866	-3.447856
H	-3.063000	2.021601	-2.279091	H	-2.857800	-0.907830	-2.323346	H	-2.388833	1.296552	2.444852
C	-2.404756	-0.993763	-3.930742	C	-1.706776	-2.111003	-3.682524	C	-0.865518	2.476047	3.397411
C	-4.823733	-0.592707	-3.231320	C	-4.194151	-2.363937	-3.184852	C	-3.371506	2.942766	3.428728
H	-0.785684	3.070342	-3.649923	H	-1.419913	2.122267	-4.208370	H	-0.887995	-2.252521	3.439686
H	0.321005	4.130623	-2.725850	H	-0.655526	3.578778	-3.503141	H	-0.580726	-3.862383	3.643917
H	0.203026	2.386661	-2.316498	H	-0.357455	1.966437	-2.769217	H	0.093534	-2.409096	2.846534
H	-2.807881	4.573635	-3.126624	H	-3.777890	3.113871	-3.977328	H	-3.418062	-2.720723	4.300138
H	-3.217559	4.987451	-1.428975	H	-4.360261	3.717868	-2.390683	H	-4.244545	-3.069859	2.746386
H	-1.773224	5.705150	-2.206674	H	-3.114798	4.629313	-3.297871	H	-3.195336	-4.308279	3.499280
H	-0.195757	0.834319	4.733570	H	-0.624521	1.659325	4.387237	H	-1.454552	-1.653196	-4.369623
H	0.627950	0.965408	3.142491	H	0.145153	1.683520	2.761679	H	-0.455197	-1.656685	-2.875494
H	0.791104	2.277802	4.357060	H	0.010125	3.195287	3.720688	H	-0.762539	-3.190270	-3.761343
H	-2.253040	2.287043	5.251684	H	-2.965631	2.671319	4.721505	H	-3.865108	-2.557592	-4.306778
H	-1.346035	3.787221	4.891634	H	-2.424400	4.252471	4.085137	H	-3.259928	-4.155259	-3.782547
H	-2.878328	3.445210	4.032111	H	-3.832373	3.430712	3.345840	H	-4.509929	-3.315669	-2.813614
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H	-4.868467	-2.386676	2.724802	H	-4.354168	-2.829394	2.910548	H	-4.613988	2.819146	-2.693795
H	-3.946461	-3.892163	3.023360	H	-3.216257	-4.052834	3.552976	H	-3.513034	3.874241	-3.631824
H	-1.190919	-2.510096	3.711620	H	-0.871497	-2.020599	4.208983	H	-1.413339	1.627811	-4.374302
H	-1.302493	-3.886157	2.571751	H	-0.586472	-3.576069	3.373882	H	-0.916525	3.230968	-3.753886
H	-0.537864	-2.347595	2.045979	H	-0.051041	-2.040158	2.612204	H	-0.369315	1.740248	-2.916487
H	-2.449644	-0.142623	-4.641388	H	-1.931467	-1.455989	-4.549626	H	-0.943647	1.925815	4.358681
H	-1.354041	-1.102157	-3.592692	H	-0.712221	-1.821560	-3.285955	H	-0.020563	2.051284	2.816778
H	-2.679230	-1.905818	-4.501887	H	-1.632030	-3.144812	-4.070379	H	-0.610869	3.528611	3.642004
H	-4.903107	0.232755	-3.968790	H	-4.438898	-1.738582	-4.068463	H	-3.465302	2.412155	4.399067
H	-5.186054	-1.519163	-3.724721	H	-4.215324	-3.425473	-3.509723	H	-3.232009	4.021754	3.649813
H	-5.516414	-0.368849	-2.393942	H	-5.002707	-2.228809	-2.437327	H	-4.334073	2.835630	2.887891
Au	0.154284	-0.004810	-0.043925	Au	0.162686	0.175722	-0.156282	Au	0.196312	-0.177980	-0.210145
C	4.610400	0.193435	-2.003267	C	4.520381	-0.081961	-1.507751	C	4.538381	-0.787878	0.073553
C	4.147530	1.033271	-0.950816	C	4.159810	1.310690	-1.309463	C	4.166631	-1.416220	-1.215890
C	4.907038	2.191072	-0.614384	C	5.167478	2.308635	-1.321281	C	5.165716	-1.978573	-2.049165
C	6.118414	2.459066	-1.260483	C	6.507672	1.917224	-1.343023	C	6.503457	-1.753130	-1.730847
C	6.580197	1.596582	-2.275012	C	6.879537	0.540958	-1.403226	C	6.903853	-0.987027	-0.581242
C	5.820952	0.469253	-2.648504	C	5.906845	0.446590	-1.508410	C	5.962265	-0.484623	0.288541
H	3.981175	-0.646011	-2.337366	H	3.855379	-0.665685	-2.179373	H	4.244669	-1.554971	0.865923
H	4.542581	2.861954	0.180341	H	4.894739	3.370195	-1.213458	H	4.889465	-2.508786	-2.973645
H	6.707508	3.346068	-0.980673	H	7.297408	2.683042	-1.282687	H	7.287894	-2.144568	-2.398981
H	7.526097	1.817413	-2.794165	H	7.947149	0.272175	-1.423982	H	7.976760	0.825479	-0.395564
H	6.167765	-0.179847	-3.467419	H	6.196631	-1.497642	-1.667813	H	6.269059	-0.050593	1.199610
C	2.940368	0.745107	-0.194371	C	2.793812	1.488315	-0.898644	C	2.766307	-1.264678	-1.420962
H	2.541197	1.592776	0.393344	C	2.286863	2.464551	-0.949233	H	2.211295	-1.771874	-2.223866
O	1.100368	-1.646315	-2.533222	O	2.154259	-1.763968	-2.463312	O	2.874776	-1.746021	2.129654
C	1.166087	-2.672514	-1.897578	C	2.209999	-2.467803	-1.476159	C	2.778449	-0.583235	2.507901
O	2.017274	-2.806269	-0.780261	O	2.836377	-2.045166	-0.300914	O	3.043020	0.477959	1.700125
C	0.419458	-3.951485	-2.132436	C	1.679508	-3.861484	-1.323557	C	2.371201	-0.153024	3.891252
H	-0.516994	-3.927539	-1.532662	H	0.682240	-3.808180	-0.834270	H	1.286087	0.080915	3.882546
H	0.141041	-4.025127	-3.199210	H	1.556353	-4.323217	-2.319450	H	2.549030	-0.976680	4.605593
H	1.009617	-4.830503	-1.813457	H	2.338768	-4.473034	-0.679025	H	2.908299	0.763940	4.199037
C	2.208856	-0.435225	-0.221329	C	2.188499	0.333598	-0.420368	C	2.194865	-0.409171	-0.473014
C	2.694885	-1.739229	-0.263652	C	3.176602	-0.715267	-0.113564	C	3.335705	0.239774	0.303620
C	3.907143	-2.199651	0.499035	C	4.009855	-0.607623	1.164242	C	3.756125	1.618710	-0.274830
H	4.460272	-2.923879	-0.138802	H	4.855743						

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N	-1.861582	-0.281429	0.053296	C	1.779877	0.498686	-0.007633
N	-2.577682	-1.452744	0.111388	N	2.307431	1.763803	-0.106458
N	-2.808310	0.705702	0.167725	N	2.870789	-0.332905	0.007888
C	-3.938486	-1.201573	0.261318	C	3.697598	1.722174	-0.147390
C	-4.084695	0.161603	0.296305	C	4.053400	0.399986	-0.073938
C	-2.013368	-2.786346	0.007945	C	1.533057	2.990460	-0.159492
C	-2.562874	2.134942	0.141290	C	2.852975	-1.782315	0.068770
H	-4.673352	-2.009813	0.327761	H	4.303212	2.630421	-0.224539
H	-4.973943	0.791296	0.398650	H	5.033867	-0.086042	-0.072645
C	-1.596879	-3.443464	1.195684	C	1.263555	3.674647	1.055955
C	-1.071431	-4.745501	1.063022	C	0.531871	4.877511	0.969279
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C	-1.398328	-4.691849	-1.344272	C	0.381427	4.678015	-1.448648
C	-1.932616	-3.388240	-1.275730	C	1.110356	3.470402	-1.427875
C	-1.698189	-2.798970	2.578184	C	1.747981	3.173092	2.417282
H	-0.737173	-5.286630	1.962163	H	0.305298	5.382533	1.896263
H	-0.561935	-6.383911	-0.268992	H	-0.470040	6.319750	-0.309397
H	-1.320804	-5.191025	-2.322872	H	0.037984	5.083651	-2.413242
H	-2.391119	-2.685058	-2.554079	C	1.426127	2.748926	-2.738841
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C	-2.428911	4.204775	-1.096720	C	3.019700	-3.912557	-1.058666
C	-2.223345	4.901037	0.102806	C	2.945655	-4.565317	0.180168
C	-2.186254	4.209630	1.321519	C	2.828222	-3.821842	1.362582
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H	-2.460572	4.760355	-2.047038	H	3.123183	-4.507974	-1.979320
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C	-2.323403	2.085496	2.718758	C	2.696480	-1.630834	2.650910
H	-2.141483	-1.789091	2.450122	H	2.215145	2.177333	2.266020
C	-0.301473	-2.604130	3.206312	C	0.581161	2.980188	3.408677
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C	-1.202185	-2.414618	-3.501460	C	0.139933	2.348092	-3.492130
C	-3.514909	-3.468101	-3.266907	C	2.363571	3.591363	-3.631780
H	-3.068314	1.017043	-2.204927	H	3.040012	-0.727211	-2.354007
C	-3.994143	2.655504	-3.244762	C	4.393950	-2.151922	-3.229654
C	-1.512431	2.056086	-3.264117	C	1.849160	-2.177809	-3.400238
H	-2.519043	1.009275	2.529505	H	2.683063	-0.549176	2.402103
C	-0.924593	2.184262	3.364195	C	1.382312	-1.937709	3.398770
C	-3.424832	2.590811	3.674954	C	3.929853	-1.882363	3.545393
H	-0.384031	-2.078064	4.180841	H	0.951426	2.551361	4.362936
H	0.201540	-3.575741	3.395659	H	0.084709	3.942813	3.652157
H	0.355045	-2.009580	2.536505	H	-0.188903	2.293547	3.000268
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H	-3.645825	-3.712938	3.076897	H	3.693896	4.218051	2.311955
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H	-1.541517	-1.868410	-4.406154	H	0.389402	1.768883	-4.405361
H	-0.423790	-1.801078	-3.001453	H	-0.520520	1.722081	-2.856880
H	-0.728436	-3.359755	-3.841060	H	-0.440845	3.237850	-3.814422
H	-3.876956	-2.905813	-4.152531	H	2.631334	3.031689	-4.552064
H	-3.162548	-4.458000	-3.625272	H	1.881173	4.540175	-3.947502
H	-4.381176	-3.644382	-2.596634	H	3.304716	3.854164	-3.106449
H	-4.164009	2.057003	-4.163627	H	4.464171	-1.599965	-4.189774
H	-4.935569	2.654574	-2.657811	H	5.272105	-1.873851	-2.611281
H	-3.799653	3.700109	-3.566203	H	4.479070	-3.233931	-3.462731
H	-1.656359	1.488747	-4.207250	H	1.904498	-1.639454	-4.369289
H	-1.192223	3.084095	-3.535914	H	1.809651	-3.264048	-3.652972
H	-0.685628	1.578255	-2.697169	H	0.895908	-1.898144	-2.906035
H	-0.894060	1.609617	4.313972	H	1.307308	-1.324996	4.321118
H	-0.144234	1.784353	2.683446	H	0.500995	-1.711204	2.763464
H	-0.660012	3.235958	3.602894	H	1.324433	-3.004777	3.700689
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Au	0.178511	-0.167162	-0.187305	Au	-0.221121	0.134878	0.135187
C	4.602772	-0.240206	-0.129198	C	-4.655411	-0.224837	-0.410094
C	4.237231	-1.219512	-1.140413	C	-4.361817	1.162387	-0.399864
C	5.246487	-1.921590	-1.837201	C	-3.537824	2.108277	-0.706405
C	6.583624	-1.570261	-1.619695	C	-6.652653	1.642609	-1.003696
C	6.954640	-0.521630	-0.728015	C	-6.942719	0.263926	-0.996844
C	5.981492	0.174973	-0.021974	C	-5.940602	-0.687499	-0.700842
H	4.408742	-0.881179	0.951463	H	-2.052987	-0.197245	1.589120
H	4.982870	-2.692915	-2.577135	H	-5.132178	3.186127	-0.712256
H	3.736021	-2.100927	-2.171937	H	-7.449489	2.363099	-1.244133
H	8.018227	-0.269016	-0.601352	H	-7.963390	-0.077603	-1.229295
H	6.268388	0.973350	0.682352	H	-6.180150	-1.762638	-0.699896
C	2.799294	-1.259266	-1.255409	C	-2.960477	1.320521	-0.019683
H	2.265949	-2.009485	-1.857074	H	-2.471889	2.302060	0.085162
O	3.809428	-1.074286	2.183806	O	-2.360419	-0.741452	2.606840
C	3.253780	0.019002	2.428705	C	-3.229634	-1.624939	2.336554
O	3.036819	0.938491	1.496023	O	-3.710895	-1.842975	1.144505
C	2.782110	0.395822	3.799310	C	-3.784198	-2.489062	3.426311
H	1.699977	0.156896	3.872380	H	-2.970698	-2.796429	4.110716
H	3.327129	-0.190043	4.560900	H	-4.504008	-1.883098	4.017263
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C	2.188549	-0.273248	-0.497217	C	-2.323334	0.109133	0.202950
C	3.297661	0.616595	0.074739	C	-3.581002	-0.998130	-0.087901
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H	4.393232	2.443501	-0.246345	H	-3.955052	-2.587349	-1.415132
H	3.660029	1.744420	-1.708770	H	-2.793627	-1.425891	-2.089273
C	2.304250	2.975692	-0.515401	C	-1.895802	-3.013220	-0.879773
C	2.616944	4.291941	-1.249307	C	-1.726740	-4.043997	-2.009618
H	2.108599	3.184882	0.558247	H	-2.117378	-3.524349	0.068131
H	1.369532	2.525784	-0.915054	H	-0.938556	-2.466756	-0.713300
C	1.526118	5.356409	-1.089830	C	-0.698016	-5.135132	-1.695300
H	3.586465	4.696059	-0.877701	H	-2.714067	-4.514545	-2.220204
H	2.778091	4.078429	-2.330386	H	-1.443167	-3.515423	-2.947737
H	1.783552	6.284337	-1.640279	H	-0.598749	-5.808877	-2.536835
H	0.548762	4.995183	-1.472788	H	0.304905	-4.702267	-1.498152
H	1.380722	5.628979	-0.022987	H	-0.989225	-5.718509	-0.795719

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C	3.044512	2.529178	0.477558	C	2.320872	-3.036669	0.617835
C	3.511736	-0.983618	-0.272409	C	-1.248214	-2.580935	1.019755
C	0.571556	2.927107	0.511037	C	3.222153	-0.881856	-0.289548
H	4.956861	1.363806	0.247964	H	0.773282	-4.471585	1.399090
H	3.271769	3.574829	0.707343	H	3.308268	-3.508496	0.633528
C	3.678650	-1.373893	-1.627926	C	-2.083635	-3.120383	0.003637
C	4.133438	-2.687806	-1.865122	C	-3.457755	-3.232855	0.300067
C	4.416385	-3.561982	-0.806253	C	-3.969147	-2.833349	1.543592
C	4.256449	-3.138536	0.520697	C	-3.115499	-2.310796	2.525004
C	3.802384	-1.838141	0.824403	C	-1.730937	-2.174478	2.291654
C	3.398519	-0.439842	-2.806232	C	-1.539222	-3.609969	-1.339186
H	4.275037	-3.030129	-2.902153	H	-4.139588	-3.644747	-0.459262
H	4.773505	-4.582100	-1.017440	H	-5.045795	-2.936871	1.751626
H	4.494306	-3.831890	1.342376	H	-3.529588	-2.007298	3.499331
C	3.665203	-1.398733	2.283362	C	-0.822785	-1.618834	3.389562
C	-0.019255	3.051084	1.796291	C	3.993058	-0.195481	0.686675
C	-1.115080	3.931601	1.914542	C	5.061604	0.597083	0.218059
C	-1.588392	4.656016	0.811592	C	5.344020	0.700347	-1.151655
C	-0.978701	4.512369	-0.443148	C	4.567201	0.003139	-2.087560
C	0.116960	3.644172	-0.628281	C	3.492446	-0.815842	-1.682364
C	0.491568	2.299602	3.026306	C	3.721112	-0.299537	2.188927
H	-1.599799	4.059558	2.895104	H	5.689542	1.137672	0.943583
H	-2.437938	5.346170	0.932712	H	6.185767	1.323065	-1.492962
H	-1.358010	5.092256	-1.298843	H	4.809721	0.082968	-3.158657
C	0.778154	3.528784	-2.002984	C	2.688831	-1.592876	-2.726360
C	3.081654	0.542573	-2.396248	H	-0.525237	-3.173722	-1.469063
C	2.236855	-0.963143	-3.678146	C	-2.391511	-3.144046	-2.536597
C	4.669033	-0.192796	-3.648772	C	-1.386669	-5.149253	-1.336743
H	3.249388	-0.369118	2.293365	H	0.217628	-1.615237	3.001530
C	2.675606	-2.290741	3.062139	C	-1.183964	-0.158449	3.734618
C	5.042720	-1.345141	2.980982	C	-0.838003	-2.516438	4.646182
H	1.344624	1.663504	2.708733	H	2.851183	-0.974253	2.333468
C	1.021637	3.273897	4.101563	C	4.917037	-0.928461	2.936871
C	-0.585063	1.355960	3.603514	C	3.335394	1.066685	2.794989
H	1.559851	2.742255	-1.940612	H	1.959133	-2.233462	-2.187673
C	-0.223176	3.081063	-3.088358	C	1.877434	-0.641851	-3.632240
C	1.481870	4.846459	-2.397141	C	3.588540	-2.532250	-3.558234
H	2.015647	-0.251644	-4.500443	H	-1.882577	-3.404984	-3.487491
H	2.480022	-1.942662	-4.140433	H	-3.381007	-3.646927	-2.557140
H	1.311763	-1.092720	-3.077059	H	-2.572288	-2.050613	-2.572769
H	4.460601	0.535372	-4.459878	H	-0.954501	-5.499259	-2.297197
H	5.498284	0.210414	-3.032111	H	-0.727982	-5.505525	-0.518163
H	5.031289	-1.126341	-4.127533	H	-2.372172	-5.644704	-1.210002
H	2.560880	-1.924272	4.103258	H	-0.482362	0.247344	4.492714
H	1.672542	-2.289981	2.587350	H	-1.137728	0.493924	2.837647
C	3.025700	-3.342576	3.118935	H	-2.208393	-0.080638	4.154875
H	4.939203	-0.971190	4.020661	H	-0.126075	-2.132496	5.406037
H	5.510508	-2.350442	3.032484	H	-1.842693	-2.543462	5.117273
H	5.748741	-0.676995	2.446260	H	-0.552576	-3.561666	4.407998
H	1.438792	2.711300	4.962362	H	4.678354	-1.056236	4.012987
H	1.821390	3.931440	3.703078	H	5.182669	-1.923920	2.525449
H	0.214486	3.928180	4.492458	H	5.821520	-0.288443	2.871024
H	-0.177022	0.782741	4.461524	H	3.105346	0.959397	3.875379
H	-1.468203	1.918516	3.971762	H	4.160894	1.803169	2.703677
H	-0.939617	0.629210	2.843268	H	2.442451	1.494808	2.294976
H	0.295479	2.945468	-4.059944	H	1.266082	-1.217798	-3.457644
H	-0.708383	2.119823	-2.820908	H	1.188832	-0.009586	-3.031580
H	-1.024685	3.832527	-3.245925	H	2.541065	0.033368	-4.211984
H	2.003217	4.733906	-3.370281	H	2.972642	-3.144122	-4.249287
H	0.755013	5.678945	-2.501717	H	4.314295	-1.965776	-4.178582
H	2.233132	5.154114	-1.641036	H	4.166886	-3.224467	-9.212660
Au	0.150395	-0.524622	-0.212081	Au	-0.095363	0.334110	-0.350738
C	-3.180460	-1.721941	0.775686	C	-1.598512	3.017293	0.611026
C	-2.002854	-2.395018	1.200912	C	-2.845008	2.339124	0.525994
C	-1.906321	-2.960107	2.483029	C	-3.831043	2.522649	1.498720
C	-3.013409	-2.856267	3.345247	C	-3.565284	3.402347	2.569237
C	-4.187640	-2.205464	2.921854	C	-2.333973	4.080713	2.656898
C	-4.281448	-1.632443	1.634102	C	-1.338065	3.894588	1.680216
H	-1.304339	-1.896958	-2.071560	H	-1.327204	1.544440	-2.419344
H	-0.994366	-3.489939	2.799426	H	-4.802481	2.010195	1.423131
H	-2.967984	-3.300867	4.351351	H	-4.333573	3.569629	3.340242
H	-5.053559	-2.153019	3.600255	H	-2.149851	4.768487	3.496625
H	-5.219063	-1.156169	1.312396	H	-0.383279	4.435311	1.756626
C	-1.059240	-2.450873	0.071315	C	-2.891508	1.500567	-0.735654
H	-0.216498	-3.159926	0.019560	H	-3.101807	0.424468	-0.546898
O	-3.423607	-3.884375	-1.251142	O	-3.927431	2.017046	-1.609549
C	-4.161632	-3.064605	-1.758944	C	-4.301195	1.188419	-2.639528
O	-4.017745	-1.708611	-1.582581	O	-3.771628	0.111360	-2.839608
C	-5.350522	-3.359429	-2.642983	C	-5.428924	1.796530	-3.346498
H	-5.379186	-2.677180	-3.514721	H	-6.340082	1.860860	-2.806682
H	-5.310875	-4.412894	-2.972209	H	-5.174555	2.830487	-3.743414
H	-6.285101	-3.196397	-2.066445	H	-5.634576	1.712420	-4.322925
C	-1.604124	-1.765440	-1.020032	H	-1.500470	1.725487	-1.346019
C	-3.002951	-1.209958	-0.660258	C	-0.789087	2.682964	-0.591731
C	-3.081449	0.329472	-0.820072	C	0.383506	3.490052	-1.089080
H	-2.996709	0.786317	-0.174970	H	0.000146	4.534030	-1.182057
H	-2.791451	0.550455	-1.871424	H	0.634669	3.161147	-2.119681
C	-4.446849	0.971429	-0.526213	C	1.668179	3.511464	-0.234715
C	-4.524984	2.436671	-0.986227	C	2.713493	4.946041	-0.785289
H	-4.659132	0.923693	0.564075	C	2.096053	2.483766	-0.200535
H	-5.242924	0.384721	-1.032900	H	1.429358	3.772265	0.817854
C	-5.873061	3.096953	-0.672374	C	3.995405	4.561285	0.052266
H	-3.701357	3.014859	-0.509783	H	2.962297	4.213938	-1.833160
H	-4.331909	2.484125	-2.082177	H	2.257309	5.100022	-0.848790
H	-5.905310	4.146883	-1.028912	H	4.721783	5.280921	-0.376960
H	-6.712272	2.555573	-1.158439	H	3.784303	4.883938	1.094011
H	-6.076119	3.109162	0.419728	H	4.493617	3.570475	0.102953
C	1.734838	0.526300	0.131429	C	1.734838	0.526300	0.131429
N	2.925564	-0.149159	0.042459	N	2.925564	-0.149159	0.042459
N	2.072056	1.773552	0.589537	N	2.072056	1.773552	0.589537
C	3.986663	0.661819	0.437574	C	3.986663	0.661819	0.437574
C	3.448443	1.875282	0.783105	C	3.448443	1.875282	0.783105
C	3.071833	-1.527326	-0.388130	C	3.071833	-1.527326	-0.388130
C	1.141051	2.856584	0.845607	C	1.141051	2.856584	0.845607
H	5.020978	0.304330	0.435215	H	5.020978	0.304330	0.435215
H	3.914816	2.796736	1.145302	H	3.914816	2.796736	1.145302
C	3.241643	-1.793202	-1.772501	C	3.241643	-1.793202	-1.772501
C	3.385977	-3.143322	-2.155498	C	3.385977	-3.143322	-2.155498
C	3.372692	-4.174339	-1.205502	C	3.372692	-4.174339	-1.205502
C	3.216464	-3.876865	0.155869	C	3.216464	-3.876865	0.155869
C	3.062581	-2.547242	0.600542	C	3.062581	-2.547242	0.600542
C	3.272889	-0.692071	-2.833685	C	3.272889	-0.692071	-2.833685
H	3.519851	-3.390176	-3.220357	H	3.519851	-3.390176	-3.220357
H	3.494679	-5.220178	-1.528815	H	3.494679	-5.220178	-1.528815
H	3.219698	-4.694818	0.893488	H	3.219698	-4.694818	0.893488
C	2.922173	-2.251117	2.094169	C	2.922173	-2.251117	2.094169
C	0.584449	2.976082	2.146711	C	0.584449	2.976082	2.146711
C	-0.296917	4.054083	2.372887	C	-0.296917	4.054083	2.372887
C	-0.600098	4.969911	1.355116	C	-0.600098	4.969911	1.355116
C	-0.028107	4.827003	0.082885	C	-0.028107	4.827003	0.082885
C	0.858721	3.768702	-0.205305	C	0.858721	3.768702	-0.205305
C	0.895782	1.991165	3.274551	C	0.895782	1.991165	3.274551
H	-0.747704	4.183582	3.369321	H	-0.747704	4.183582	3.369321
H	-1.283341	5.809571	1.558169	H	-1.283341	5.809571	1.558169
H	-0.270243	5.558127	-0.704228	H	-0.270243	5.558127	-0.704228
C	1.459071	3.632821	-1.605115	C	1.459071	3.632821	-1.605115
H	3.200937	0.285012	-2.311086	H	3.200937	0.285012	-2.311086

IVa	-732.348727 a.u.	IIIa	-732.344002 a.u.	IIIa-IVa	-732.292346 a.u.		
C	0.017466	1.167461	0.422736	C	0.721872	-0.965810	0.285879
C	-1.386155	0.954146	0.430539	C	2.049360	-0.527003	0.553202
C	-2.263457	1.869508	-0.153494	C	3.150343	-1.162621	-0.016917
C	-1.725701	3.022400	-0.767190	C	2.920853	-2.278330	-0.862271
C	-0.337198	3.252804	-0.764170	C	1.616611	-2.721125	-1.120299
C	0.546056	2.329815	-0.164452	C	0.497664	-2.061233	-0.548435
H	-0.108344	-1.803938	2.031052	H	0.231246	1.469071	2.623853
H	-3.351982	1.697438	-0.142289	H	4.175200	-0.812378	0.183111
H	-2.398486	3.751270	-1.246389	H	3.776403	-2.801683	-1.317682
H	0.065216	4.160785	-1.237460	H	1.453876	-3.591359	-1.775478
H	1.630749	2.522886	-0.163716	H	-0.519225	-2.419589	-0.767191
C	-1.667754	-0.316107	1.217562	C	1.940742	0.621178	1.479491
H	-2.154469	-0.040501	2.181805	H	2.802655	1.161318	1.893278
O	-2.635050	-1.237432	0.649899	O	1.876210	2.038770	-0.213411
C	-2.339251	-1.801954	-0.560316	C	0.702398	2.209582	-0.676507
O	-1.318212	-1.586985	-1.180644	O	-0.266536	1.375089	-0.581560
C	-3.468605	-2.714276	-0.998397	C	0.404330	3.528795	-1.382690
H	-3.694714	-3.458561	-0.208586	H	-0.058119	4.236694	-0.661840
H	-4.392040	-2.121070	-1.159946	H	1.341667	3.979981	-1.763912
H	-3.185827	-3.224896	-1.935955	H	-0.313443	3.370507	-2.212409
C	-0.280173	-0.856243	1.499831	C	0.620338	0.717028	1.924751
C	0.679701	0.023570	1.095154	C	-0.191945	-0.064785	1.055762
C	2.169738	-0.132294	1.233913	C	-1.667526	-0.248067	1.247536
H	2.609617	0.819890	1.611076	H	-1.767652	-1.171806	1.871434
H	2.388924	-0.901789	2.005572	H	-2.039362	0.580743	1.888192
C	2.873218	-0.523531	-0.086629	C	-2.574484	-0.379654	0.008999
C	4.394312	-0.680530	0.060743	C	-4.052837	-0.557664	0.387311
H	2.650404	0.236833	-0.868133	H	-2.251827	-1.237284	-0.620188
H	2.428270	-1.471872	-0.461623	H	-2.437971	0.524066	-0.617502
C	5.097750	-1.071697	-1.244746	C	-4.980738	-0.667993	-0.828649
H	4.825646	0.271655	0.446819	H	-4.168043	-1.461969	1.028818
H	4.609178	-1.443065	0.844223	H	-4.373266	0.299838	1.022600
H	6.193414	-1.178752	-1.103534	H	-6.041447	-0.787709	-0.525073
H	4.715196	-2.038257	-1.637026	H	-4.915092	0.237059	-1.469419
H	4.935649	-0.309134	-2.036440	H	-4.714865	-1.540160	-1.463794
C	0.827279	-0.542201	-0.069372	C	1.902984	-0.936579	0.773310
C	2.824018	-1.905649	0.343756	C	2.677514	-2.457230	-0.945290
C	2.677514	-2.457230	-0.945290	C	1.629798	-2.044088	-1.787641
C	0.690559	-1.082244	-1.350454	C	0.690559	-1.082244	-1.350454
H	0.481935	1.442088	2.713750	H	0.481935	1.442088	2.713750
H	3.655633	-2.218860	0.995340	H	3.655633	-2.218860	0.995340
H	3.397669	-3.211512	-1.300748	H	1.540561	-2.471511	-2.799019
H	1.540561	-2.471511	-2.799019	H	-0.119154	-0.756671	-2.022071
H	-0.119154	-0.756671	-2.022071	C	1.838184	-0.142799	2.010145
C	1.838184	-0.142799	2.010145	C	2.555431	-0.227189	2.839857
C	2.555431	-0.227189	2.839857	O	1.782073	2.262381	-0.339833
O	1.782073	2.262381	-0.339833	C	0.599767	2.463751	-0.525051
C	0.599767	2.463751	-0.525051	O	-0.400898	1.656429	-0.059818
O	-0.400898	1.656429	-0.059818	C	0.010749	3.623711	-1.305397
C	0.010749	3.623711	-1.305397	H	-0.781847	4.129035	-0.718361
H	-0.781847	4.129035	-0.718361	H	0.813227	4.337555	-1.563155
H	0.813227	4.337555	-1.563155	H	-0.461710	3.247956	-2.236491
H	-0.461710	3.247956	-2.236491	C	0.789468	0.715816	1.947388
C	0.789468	0.715816	1.947388	C	-0.045816	0.457650	0.694540
C	-0.045816	0.457650	0.694540	C	-1.414075	-0.139619	1.130670
C	-1.414075	-0.139619	1.130670	H	-1.200331	-1.046187	1.736594
H	-1.200331	-1.046187	1.736594	H	-1.882668	0.597832	1.820476
H	-1.882668	0.597832	1.820476	C	-2.402482	-0.474226	0.004729
C	-2.402482	-0.474226	0.004729	C	-3.766633	-0.947912	0.533906
C	-3.766633	-0.947912	0.533906	H	-1.972368	1.264230	-0.649146
H	-1.972368	1.264230	-0.649146	H	-2.543583	0.423415	-0.635899
H	-2.543583	0.423415	-0.635899	C	-4.766069	-1.288404	-0.578512
C	-4.766069	-1.288404	-0.578512	H	-3.618787	-1.837747	1.187659
H	-3.618787	-1.837747	1.187659	H	-4.197651	-0.160790	1.194158
H	-4.197651	-0.160790	1.194158	H	-5.740846	-1.621549	-0.165546
H	-5.740846	-1.621549	-0.165546	H	-4.961724	-0.409244	-1.229260
H	-4.961724	-0.409244	-1.229260	H	-4.384651	-2.102734	-1.231302
H	-4.384651	-2.102734	-1.231302				

<b>ac'</b>	<b>-2027.212726 a.u.</b>			<b>b-Htransfer</b>	<b>-2027.191018 a.u.</b>		
C	1.817625	0.719780	0.101374	C	-1.837387	-0.072586	0.574935
N	3.031664	0.097804	0.239737	N	-2.337639	-1.150144	1.260503
N	2.114478	2.054774	0.004403	N	-2.762028	0.924454	0.755263
C	4.068393	1.028666	0.232409	C	-3.555250	-0.830045	1.857256
C	3.489619	2.263660	0.083993	C	-3.821521	0.477712	1.540894
C	3.227992	-1.335122	0.355408	C	-1.720320	-2.461313	1.339152
C	1.138670	3.116186	-0.160672	C	-2.674919	2.258756	0.190190
H	5.116358	0.729932	0.334070	H	-4.121623	-1.560591	2.442855
H	3.927107	3.265279	0.027679	H	-4.662896	1.127508	1.800672
C	3.471653	-2.080948	-0.828559	C	-0.930425	-2.772280	2.478522
C	3.682042	-3.468547	-0.683773	C	-0.364708	-4.062711	2.537183
C	3.649276	-4.081240	0.577225	C	-0.577116	-4.997068	1.513470
C	3.406819	-3.316192	1.726738	C	-1.369745	-4.662405	0.407437
C	3.196224	-1.923854	1.647606	C	-1.966780	-3.389312	0.292619
C	3.528046	-1.442084	-2.217259	C	-0.722725	-1.789225	3.632395
H	3.883708	-4.079648	-1.577853	H	0.251164	-4.343283	3.405489
H	3.821612	-5.165506	0.665995	H	-0.127297	-5.999970	1.583698
H	3.387718	-3.809576	2.711111	H	-1.539121	-5.409611	-0.383676
C	2.935887	-1.116837	2.920037	C	-2.852902	-3.073402	-0.913267
C	0.606888	3.734089	1.002048	C	-3.277331	2.498439	-1.073557
C	-0.329024	4.771920	0.809745	C	-3.179314	3.805417	-1.595011
C	-0.712447	5.175161	-0.477201	C	-2.520987	4.822547	-0.889873
C	-0.165429	4.547292	-1.605622	C	-1.951149	4.556940	0.363294
C	0.777591	3.506016	-1.478109	C	-2.018364	3.270917	0.938652
C	0.997728	3.310783	2.418222	C	-4.027424	1.420147	-1.857184
H	-0.762483	5.277405	1.686991	H	-3.634320	4.031467	-2.572194
H	-1.438675	5.993785	-0.602611	H	-2.459535	5.835706	-1.317330
H	-0.470483	4.877479	-2.610818	H	-1.447294	5.368230	0.911756
C	1.344571	2.829794	-2.727284	C	-1.388955	3.011549	2.307696
H	3.282677	-0.365178	-2.105946	H	-1.044558	-0.784641	3.283692
C	2.475077	-2.047128	-3.169764	C	0.757038	-1.671831	4.049502
C	4.948210	-1.532082	-2.818053	C	-1.606183	-2.169076	4.842990
H	2.909021	-0.042454	2.641052	H	-3.214633	-2.028989	-0.807048
C	1.555741	-1.464683	3.519583	C	-2.057416	-3.145010	-2.233859
C	4.064779	-1.290121	3.957988	C	-4.097053	-3.987571	-0.952701
H	1.775103	2.522727	2.333826	H	-3.950628	0.469488	-1.288779
C	1.615807	4.477126	3.218647	C	-5.528898	1.761369	-1.981093
C	-0.202192	2.685015	3.161880	C	-3.390523	1.170941	-3.240526
H	2.171913	2.162704	-2.405777	H	-1.648861	1.975585	2.611676
C	0.277801	1.937765	-3.400142	C	0.150768	3.088484	2.228229
C	1.942511	3.845882	-3.722733	C	-1.949428	3.956697	3.391344
H	2.500303	-1.531395	-4.152137	H	0.880544	-0.874194	4.810992
H	2.666097	-3.124112	-3.360602	H	1.136950	-2.612097	4.500742
H	1.449003	-1.947879	-2.759077	H	1.405813	-1.427765	3.183698
H	4.990044	-1.014130	-3.798690	H	-1.489706	-1.429290	5.662232
H	5.705715	-1.067541	-2.153865	H	-2.681389	-2.211773	4.574005
H	5.253130	-2.586597	-2.984575	H	-1.324625	-3.165400	5.243908
H	1.352502	-0.847595	4.419565	H	-2.702182	-2.861650	-3.091543
H	0.745266	-1.278603	2.782554	H	-1.186275	-2.456899	-2.215178
H	1.503985	-2.531498	3.823418	H	-1.677867	-4.170216	-2.428107
H	3.885450	-0.636023	4.836363	H	-4.756547	-3.707991	-1.800378
H	4.125602	-2.333421	4.332349	H	-3.816775	-5.053192	-1.087666
H	5.055646	-1.027595	3.533880	H	-4.691060	-3.913728	-0.018680
H	1.952732	4.126111	4.216098	H	-6.073025	0.943572	-2.497634
H	2.491843	4.914264	2.696935	H	-6.000044	1.911033	-0.987876
H	0.884088	5.294848	3.387240	H	-5.686904	2.689976	-2.568597
H	0.105244	2.329393	4.167358	H	-3.916803	0.347769	-3.767027
H	-1.020878	3.421415	3.305201	H	-3.452006	2.069704	-3.889401
H	-0.614661	1.820415	2.600211	H	-2.321062	0.890377	-3.146992
H	0.703496	1.415260	-4.281998	H	0.605439	2.845074	3.211374
H	-0.102804	1.166796	-2.696325	H	0.545005	2.375154	1.473859
H	-0.586880	2.539598	-3.751774	H	0.491480	4.106052	1.943056
H	2.417726	3.316633	-4.574365	H	-1.535083	3.693557	4.386673
H	1.166590	4.516825	-4.147345	H	-1.682126	5.015683	3.193565
H	2.713161	4.483944	-3.243678	H	-3.055234	3.896186	3.455049
Au	-0.032821	-0.143584	0.069119	Au	-0.177185	0.019216	-0.584030
C	-4.261887	-1.929574	-0.613467	C	1.388767	0.068390	-2.043924
C	-3.673336	-2.609561	0.506407	C	2.041048	-1.162334	-2.438082
C	-4.475846	-3.125354	1.522849	C	2.034686	-1.586657	-3.786086
C	-5.874577	-2.923525	1.473094	C	1.546673	-0.713365	-4.768663
C	-6.470817	-2.208950	0.413448	C	1.084386	0.576850	-4.420918
C	-5.675190	-1.728483	-0.634425	C	1.026155	0.979221	-3.075729
H	-3.733864	-2.039347	-1.584810	H	2.225221	0.141308	-0.860967
H	-4.021593	-3.628049	2.391615	H	2.513528	-2.536683	-4.071932
H	-6.503687	-3.299653	2.295764	H	1.579417	-1.012105	-5.828214
H	-7.561132	-2.058585	0.398357	H	0.733533	1.259802	-5.210742
H	-6.144905	-1.252619	-1.510298	H	0.608157	1.967299	-2.824030
C	-2.149671	-2.464297	0.601482	C	2.911316	-1.704870	-1.410070
H	-1.839433	-2.503054	1.664748	H	3.244211	-2.756873	-1.389457
O	-1.398809	-3.570187	0.035434	O	5.639595	-0.280910	-1.972516
C	-1.367440	-3.759810	-1.319760	C	6.192753	-0.520326	-0.931266
O	-1.991029	-3.080632	-2.117216	O	5.522927	-0.492105	0.321810
C	-0.446788	-4.903161	-1.669504	C	7.643360	-0.840327	-0.698747
H	0.603503	-4.593713	-1.487402	H	8.165567	-0.904669	-1.669395
H	-0.646315	-5.779722	-1.022467	H	8.109717	-0.052381	-0.072421
H	-0.574405	-5.168486	-2.733838	H	7.741482	-1.794457	-0.142298
C	-1.874910	-1.071363	0.050068	C	3.265049	-0.765286	-0.486879
C	-2.947442	-0.453082	-0.418837	C	4.163228	-0.372309	0.462715
C	-3.509257	0.828831	-0.881914	C	3.770147	0.325222	1.735907
H	-3.949161	0.715228	-1.898316	H	2.689207	0.140278	1.898782
H	-2.612611	1.482460	-1.000760	H	4.317611	-0.164765	2.572166
C	-4.515893	1.515912	0.066741	C	4.038050	1.855099	1.770469
C	-4.980591	2.885689	-0.452904	C	5.508194	2.285255	1.893587
H	-4.049484	1.624327	1.070450	H	3.473755	2.256276	2.641359
H	-5.396777	0.849026	0.205270	H	3.577861	2.324751	0.872177
C	-6.002672	3.564319	0.466904	C	5.668655	3.804466	2.034030
H	-4.093531	3.545916	-0.581023	H	5.963163	1.775827	2.772944
H	-5.414941	2.763391	-1.471160	H	6.082266	1.931656	1.010824
H	-6.313440	4.550721	0.066758	H	6.735764	4.091291	2.128019
H	-6.919869	2.948307	0.581047	H	5.256386	4.340306	1.152624
H	-5.586972	3.732087	1.483043	H	5.140672	4.187557	2.933141



















