

Supplementary Information

Selective G-Quadruplex Stabilizers: Schiff-base Metal Complexes with Anticancer Activity

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- **Table S2.** Cartesian coordinates of the geometries of the intercalation complexes of **1**, **2** and **3** with *h-Telo*, fully optimized by DFT/MM calculations. Amber99 atom types, high and low layer labels are also shown.

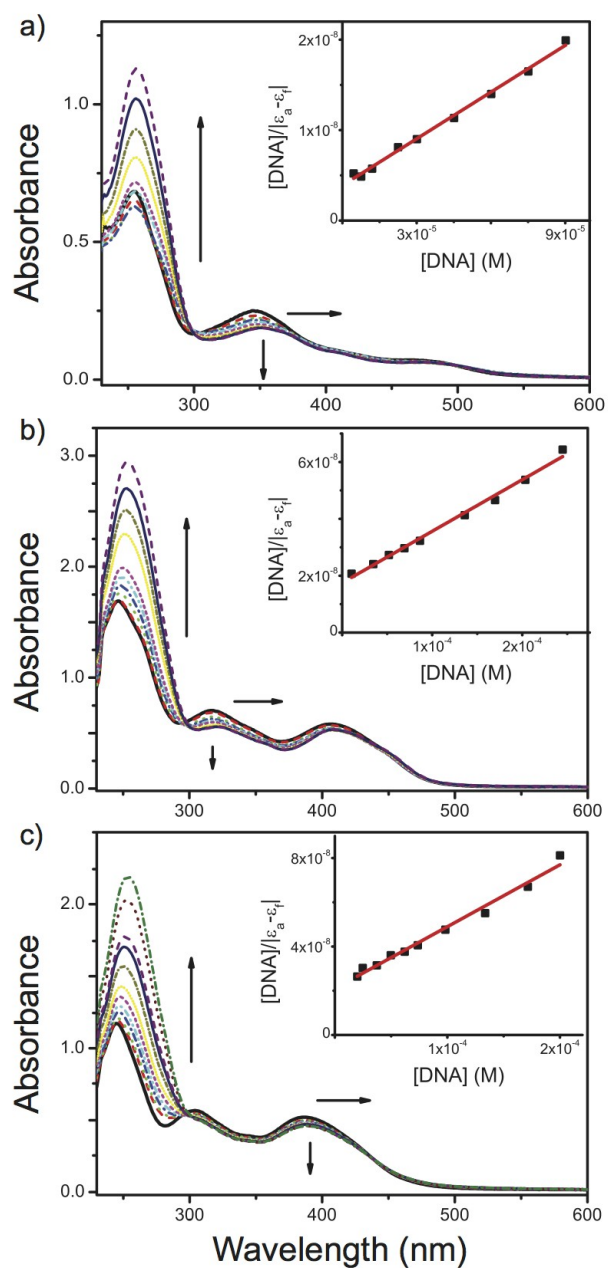


Fig S1. Absorption spectra of **1** (a), **2** (b) and **3** (c) in presence of increasing amounts of ct-DNA in Tris-HCl buffer 50 mM and KCl 100 mM. (a) $[1] = 13.1 \mu\text{M}$, (b) $[2] = 30.9 \mu\text{M}$, (c) $[3] = 23.6 \mu\text{M}$. Ratios $R = [DNA]/[ML^{2+}]$ are in the range 0.00-6.8 for **1**, 0.00-8.5 for **2** and **3**. The arrows indicate the change upon ct-DNA addition.

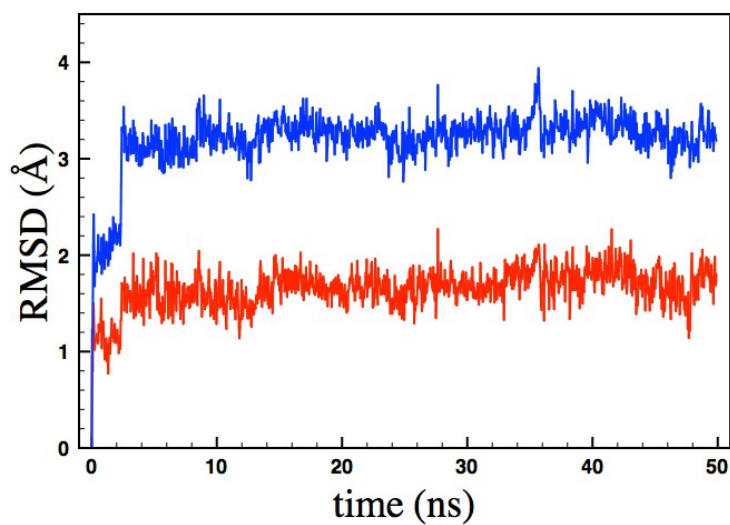
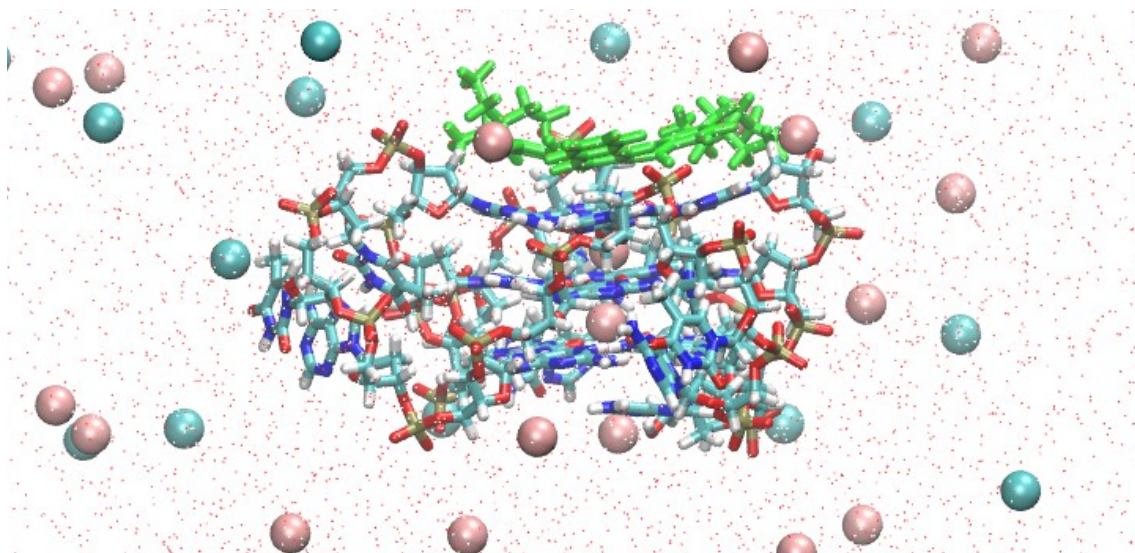


Fig S2. Top panel: Example of a MD simulation box, showing the **3/h-Telo** binding complex, the solution counterions, K^+ (in pink) and Cl^- (in cyan), and the explicit water molecules (in red). Bottom panel: Plot of the RMSD obtained for **3/h-Telo** up to 50 ns of MD simulations.

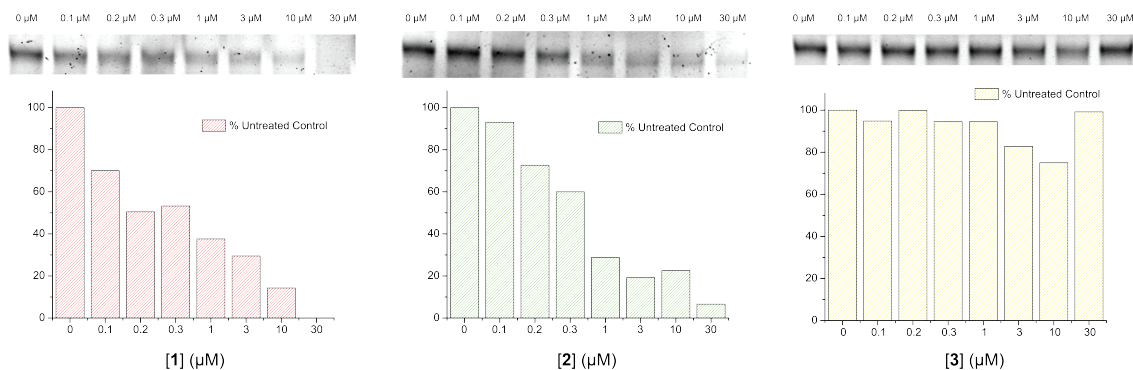


Fig S3. PCR inhibition of Pu22mu with compounds **1**, **2** and **3**.

Table S1. DFT energies (in Hartree), in vacuo and in water solution, of **1**, **2** and **3**, of the high layers of their intercalation complexes with *h-Telo*, and thermal corrections of the enthalpy and of the Gibbs free energy obtained by DFT/MM calculations of the harmonic vibration frequencies.

Model system	DFT Energy (vacuo)	DFT Energy (solution)	Thermal correction to Gibbs Free Energy (vacuo)	Thermal correction to Enthalpy (vacuo)
1	-3353.338136	-3353.521098	0.735400	0.855478
2	-3485.471036	-3485.652604	0.731248	0.854389
3	-3624.393980	-3624.586509	0.730531	0.853819
<i>h-Telo</i>	-2169.692612	-2169.767409	4.818576	5.703625
1/h-Telo	-5523.128550	-5523.352802	5.605088	6.567825
2/h-Telo	-5655.263605	-5655.484441	5.608785	6.565613
3/h-Telo	-5794.205408	-5794.421682	5.608912	6.565472

Table S2. Cartesian coordinates of the geometries of the intercalation complexes of **1**, **2** and **3** with *h-Telo*, fully optimized by DFT/MM calculations. Amber99 atom types, high and low layer labels are also indicated.

1/h-Telo

O-OH	-3.745822	-6.618299	8.997848	1
H-HO	-3.019305	-6.074136	8.655863	1
C-CT	-4.208914	-7.402979	7.905509	1
H-H1	-4.761907	-6.793471	7.185745	1
H-H1	-4.876524	-8.205118	8.235909	1
C-CT	-2.992509	-8.003332	7.202389	1
H-H1	-3.322951	-8.540410	6.310270	1
O-OS	-2.088010	-6.963812	6.846181	1
C-CT	-0.806470	-7.541236	6.781797	1
H-H2	-0.728539	-8.174796	5.890498	1
N-N*	0.297931	-6.551472	6.807638	1
C-CK	1.633996	-6.811259	6.607935	1
H-H5	2.025172	-7.800926	6.405776	1
N-NB	2.404612	-5.762766	6.669283	1
C-CB	1.521105	-4.716467	6.925123	1
C-CA	1.695895	-3.316662	7.084406	1
N-N2	2.875037	-2.688882	7.005580	1
H-H	3.718671	-3.216788	6.832971	1
H-H	2.905953	-1.688483	7.133957	1
N-NC	0.616342	-2.549929	7.327418	1
C-CQ	-0.576595	-3.134436	7.423800	1
H-H5	-1.410473	-2.474089	7.621996	1
N-NC	-0.873249	-4.427480	7.303440	1
C-CB	0.230899	-5.185568	7.033391	1
C-CT	-2.203036	-8.983638	8.075408	1
H-H1	-2.582923	-9.003106	9.103740	1
C-CT	-0.793295	-8.399710	8.036823	1
H-HC	-0.646337	-7.758299	8.905696	1
H-HC	-0.032756	-9.178181	7.993295	1
O-OS	-2.195033	-10.270280	7.479669	1
P-P	-3.338207	-11.357889	7.829972	1
O-O2	-3.533024	-11.363560	9.293860	1
O-O2	-3.019954	-12.608658	7.110464	1
O-OS	-4.643017	-10.697554	7.149597	1
C-CT	-4.962000	-10.929734	5.786480	1
H-H1	-5.309748	-11.957381	5.667982	1
H-H1	-4.068384	-10.786346	5.178224	1
C-CT	-6.051982	-9.950387	5.326124	1
H-H1	-6.915929	-10.027988	5.991587	1
O-OS	-5.482110	-8.644534	5.364483	1
C-CT	-5.348023	-8.152264	4.048410	1
H-H2	-6.183383	-7.468596	3.832946	1
N-N*	-4.052317	-7.451026	3.970702	1
C-CK	-2.852403	-7.854231	3.433001	1
H-H5	-2.670697	-8.833357	3.011089	1
N-NB	-1.921784	-6.946393	3.474947	1
C-CB	-2.547694	-5.847694	4.059145	1
C-C	-2.078075	-4.516789	4.295943	1
O-O	-0.980761	-4.031572	4.015725	1

N-NA	-3.032978	-3.698051	4.885868	1
H-H	-2.741877	-2.751339	5.080679	1
C-CA	-4.298168	-4.122739	5.216825	1
N-N2	-5.105852	-3.235871	5.771646	1
H-H	-4.816671	-2.276999	5.900278	1
H-H	-6.048204	-3.518172	5.994134	1
N-NC	-4.763191	-5.352923	4.982420	1
C-CB	-3.840514	-6.163093	4.398132	1
C-CT	-6.490388	-10.181569	3.870132	1
H-H1	-6.456547	-11.237425	3.590906	1
C-CT	-5.437680	-9.363307	3.132576	1
H-HC	-4.507683	-9.926030	3.103790	1
H-HC	-5.735833	-9.073215	2.127033	1
O-OS	-7.801930	-9.667554	3.693743	1
P-P	-8.531294	-9.589396	2.254582	1
O-O2	-9.962208	-9.904714	2.442741	1
O-O2	-7.728308	-10.326240	1.255762	1
O-OS	-8.382572	-8.006119	1.975972	1
C-CT	-9.340897	-7.112965	2.528063	1
H-H1	-9.354378	-7.217184	3.614607	1
H-H1	-10.326667	-7.387737	2.146488	1
C-CT	-9.107462	-5.638619	2.186183	1
H-H1	-10.027290	-5.090956	2.408668	1
O-OS	-8.026810	-5.065074	2.907463	1
C-CT	-7.682669	-3.844830	2.261509	1
H-H2	-7.993173	-2.972720	2.857428	1
N-N*	-6.232326	-3.799201	2.009732	1
C-CK	-5.334692	-4.825281	1.860534	1
H-H5	-5.625804	-5.865757	1.931376	1
N-NB	-4.106683	-4.429253	1.652488	1
C-CB	-4.203636	-3.035842	1.656301	1
C-C	-3.206725	-2.018801	1.495616	1
O-O	-1.992203	-2.151420	1.350116	1
N-NA	-3.730875	-0.732016	1.492967	1
H-H	-3.090447	0.043293	1.415453	1
C-CA	-5.070696	-0.458818	1.612037	1
N-N2	-5.416148	0.807108	1.464456	1
H-H	-4.700299	1.501274	1.302415	1
H-H	-6.389620	1.076977	1.460168	1
N-NC	-6.013741	-1.385470	1.797340	1
C-CB	-5.511010	-2.649799	1.825487	1
C-CT	-8.703068	-5.353660	0.750635	1
H-H1	-7.804053	-5.936520	0.532498	1
C-CT	-8.385090	-3.873695	0.906443	1
H-HC	-7.761760	-3.506607	0.093239	1
H-HC	-9.306777	-3.297328	0.955234	1
O-OS	-9.700210	-5.569046	-0.221409	1
P-P	-9.306350	-5.566168	-1.774421	1
O-O2	-10.361185	-6.236391	-2.555139	1
O-O2	-7.896860	-5.990191	-1.899936	1
O-OS	-9.327517	-4.018552	-2.149378	1
C-CT	-10.486151	-3.229706	-1.919464	1
H-H1	-10.769468	-3.277889	-0.867927	1
H-H1	-11.321038	-3.644279	-2.476671	1
C-CT	-10.286892	-1.750559	-2.293444	1
H-H1	-11.235297	-1.227967	-2.150952	1
O-OS	-9.289326	-1.178426	-1.446558	1
C-CT	-8.530036	-0.209488	-2.146309	1

H-H

H-H2	-8.577599	0.777606	-1.662893	l
N-N*	-7.149808	-0.727366	-2.164876	h
C-CK	-6.782087	-2.042720	-2.305413	h
H-H5	-7.511376	-2.830535	-2.402745	h
N-NB	-5.486568	-2.213906	-2.267309	h
C-CB	-4.981467	-0.953561	-2.091612	h
C-C	-3.607286	-0.581134	-1.903090	h
O-O	-2.656346	-1.337588	-1.835292	h
N-NA	-3.498813	0.817290	-1.739822	h
H-H	-2.536174	1.182172	-1.664409	h
C-CA	-4.567066	1.675615	-1.702940	h
N-N2	-4.282388	3.002530	-1.571117	h
H-H	-3.322599	3.296856	-1.359792	h
H-H	-5.045471	3.567281	-1.209354	h
N-NC	-5.835488	1.325414	-1.838323	h
C-CB	-5.982613	-0.008046	-2.017482	h
C-CT	-9.838136	-1.484668	-3.732613	l
H-H1	-9.164816	-2.275965	-4.044279	l
C-CT	-9.099241	-0.163502	-3.561697	l
H-HC	-8.330579	-0.027739	-4.322008	l
H-HC	-9.826534	0.648132	-3.619368	l
O-OS	-10.853147	-1.255972	-4.695402	l
P-P	-12.006184	-2.326600	-5.007232	l
O-O2	-11.408082	-3.677839	-4.968940	l
O-O2	-12.790379	-1.874886	-6.172127	l
O-OS	-12.868327	-2.086636	-3.677407	l
C-CT	-13.821792	-3.014184	-3.185426	l
H-H1	-13.406178	-4.022799	-3.158871	l
H-H1	-14.698063	-3.020298	-3.836526	l
C-CT	-14.226523	-2.601440	-1.759392	l
H-H1	-15.065791	-3.222300	-1.433786	l
O-OS	-13.147656	-2.727961	-0.833659	l
C-CT	-13.531285	-2.000630	0.316608	l
H-H2	-14.336496	-2.544169	0.833459	l
N-N*	-12.386920	-1.769064	1.246645	l
C-CM	-11.305860	-0.973409	0.913406	l
H-H4	-11.248146	-0.513773	-0.060194	l
C-CM	-10.298966	-0.727919	1.791562	l
C-CT	-9.148166	0.174794	1.376423	l
H-HC	-8.437159	-0.395301	0.779080	l
H-HC	-9.514711	1.019437	0.790637	l
H-HC	-8.630625	0.547812	2.257525	l
C-C	-10.317128	-1.334965	3.115691	l
O-O	-9.443549	-1.234060	3.971026	l
N-NA	-11.437636	-2.087898	3.386897	l
H-H	-11.511219	-2.487733	4.304764	l
C-C	-12.496546	-2.296633	2.533029	l
O-O	-13.493233	-2.880469	2.937439	l
C-CT	-14.638779	-1.132806	-1.640621	l
H-H1	-14.141731	-0.542425	-2.408571	l
C-CT	-14.100001	-0.718781	-0.278118	l
H-HC	-13.331596	0.033744	-0.403996	l
H-HC	-14.891276	-0.316178	0.337479	l
O-OS	-16.040042	-0.946461	-1.641241	l
P-P	-16.818018	-0.437969	-2.954274	l
O-O2	-18.253274	-0.305359	-2.635245	l
O-O2	-16.372121	-1.233506	-4.115412	l
O-OS	-16.196552	1.039555	-3.061063	l

C-CT	-15.207444	1.405362	-4.020142	1
H-H1	-15.673249	1.551015	-4.996655	1
H-H1	-14.452430	0.624177	-4.121826	1
C-CT	-14.524250	2.711024	-3.584955	1
H-H1	-13.652722	2.893784	-4.217847	1
O-OS	-15.464480	3.768562	-3.727109	1
C-CT	-15.665314	4.405063	-2.474939	1
H-H2	-15.077212	5.331683	-2.428115	1
N-N*	-17.110372	4.668580	-2.281162	1
C-CM	-18.063192	3.792736	-2.758500	1
H-H4	-17.748935	2.931799	-3.335159	1
C-CM	-19.383372	3.977238	-2.505248	1
C-CT	-20.382587	2.950654	-3.022740	1
H-HC	-20.393294	2.958605	-4.112767	1
H-HC	-20.112521	1.954353	-2.665875	1
H-HC	-21.385078	3.189815	-2.660811	1
C-C	-19.821023	5.131920	-1.724173	1
O-O	-20.975644	5.399390	-1.414090	1
N-NA	-18.806445	5.959662	-1.290008	1
H-H	-19.068452	6.767769	-0.754971	1
C-C	-17.463332	5.777815	-1.522292	1
O-O	-16.639176	6.550198	-1.049336	1
C-CT	-14.078599	2.674833	-2.117540	1
H-H1	-14.036439	1.651908	-1.749756	1
C-CT	-15.187460	3.427797	-1.410483	1
H-HC	-15.979882	2.726663	-1.159780	1
H-HC	-14.845706	3.934420	-0.511218	1
O-OS	-12.837802	3.331021	-1.939272	1
P-P	-11.591071	2.545028	-1.295851	1
O-O2	-10.382409	3.384978	-1.389454	1
O-O2	-11.589092	1.177817	-1.849321	1
O-OS	-12.054953	2.459106	0.239917	1
C-CT	-12.245592	3.647848	0.999480	1
H-H1	-12.739006	4.399223	0.382170	1
H-H1	-11.277229	4.056183	1.301030	1
C-CT	-13.125610	3.403680	2.235875	1
H-H1	-13.322474	4.365871	2.705557	1
O-OS	-14.373374	2.819297	1.865315	1
C-CT	-14.709485	1.891386	2.878214	1
H-H2	-15.022036	2.416138	3.791201	1
N-N*	-15.765633	0.951841	2.437210	1
C-CK	-15.910344	-0.387474	2.733814	1
H-H5	-15.214014	-0.955720	3.342170	1
N-NB	-16.937917	-0.949054	2.159309	1
C-CB	-17.572846	0.103509	1.499749	1
C-CA	-18.754800	0.200335	0.719946	1
N-N2	-19.538274	-0.837403	0.409626	1
H-H	-19.290049	-1.766809	0.714279	1
H-H	-20.346430	-0.682667	-0.173030	1
N-NC	-19.141681	1.410771	0.269581	1
C-CQ	-18.396410	2.474254	0.567506	1
H-H5	-18.759302	3.426504	0.205500	1
N-NC	-17.261239	2.516242	1.262257	1
C-CB	-16.890238	1.279303	1.705081	1
C-CT	-12.481792	2.449309	3.258366	1
H-H1	-11.435106	2.237026	3.024775	1
C-CT	-13.361733	1.220252	3.092482	1
H-HC	-13.080913	0.683232	2.191589	1

H-HC	-13.345234	0.580817	3.974351	1
O-OS	-12.651233	2.827588	4.618236	1
P-P	-11.979303	4.135504	5.282844	1
O-O2	-12.039086	3.983103	6.750740	1
O-O2	-12.533211	5.344934	4.642881	1
O-OS	-10.451210	3.988028	4.819974	1
C-CT	-9.560550	3.082804	5.445738	1
H-H1	-9.703044	2.065793	5.078872	1
H-H1	-9.703441	3.086208	6.528659	1
C-CT	-8.142134	3.565802	5.167505	1
H-H1	-8.079740	4.625443	5.428620	1
O-OS	-7.217707	2.807546	5.926170	1
C-CT	-5.931533	3.067569	5.402499	1
H-H2	-5.416439	3.849879	5.973860	1
N-N*	-5.145669	1.828264	5.397204	1
C-CK	-5.596625	0.533321	5.399864	1
H-H5	-6.648893	0.279888	5.477403	1
N-NB	-4.643072	-0.350006	5.294564	1
C-CB	-3.479320	0.413554	5.215842	1
C-C	-2.108818	0.022193	5.087406	1
O-O	-1.642947	-1.111188	5.008959	1
N-NA	-1.229995	1.094920	5.041626	1
H-H	-0.244417	0.868812	5.044928	1
C-CA	-1.630256	2.407244	5.091893	1
N-N2	-0.671363	3.317690	5.020490	1
H-H	0.302854	3.057985	4.930507	1
H-H	-0.931246	4.289911	5.066821	1
N-NC	-2.906982	2.797164	5.208044	1
C-CB	-3.779633	1.751839	5.273474	1
C-CT	-7.654855	3.383322	3.734576	1
H-H1	-7.904109	2.376365	3.398675	1
C-CT	-6.156362	3.503764	3.961569	1
H-HC	-5.636316	2.855603	3.264527	1
H-HC	-5.828003	4.535208	3.850333	1
O-OS	-8.128931	4.366795	2.833241	1
P-P	-7.735071	4.359522	1.269049	1
O-O2	-8.690477	5.222523	0.547404	1
O-O2	-7.513938	2.960974	0.843852	1
O-OS	-6.306520	5.101608	1.304979	1
C-CT	-6.203464	6.451922	1.742574	1
H-H1	-6.710487	6.566427	2.701809	1
H-H1	-6.694277	7.105358	1.016934	1
C-CT	-4.744592	6.900650	1.912028	1
H-H1	-4.739426	7.937435	2.258209	1
O-OS	-4.008026	6.103753	2.838475	1
C-CT	-2.659316	5.983436	2.391049	1
H-H2	-1.948442	6.266604	3.177042	1
N-N*	-2.442906	4.576684	1.974147	1
C-CK	-3.384955	3.596446	1.811424	1
H-H5	-4.439857	3.816274	1.868216	1
N-NB	-2.900592	2.402772	1.612069	1
C-CB	-1.524277	2.609352	1.593325	1
C-C	-0.449443	1.681139	1.403461	1
O-O	-0.502063	0.454009	1.313314	1
N-NA	0.786500	2.300308	1.285400	1
H-H	1.583326	1.711589	1.097966	1
C-CA	0.966615	3.655469	1.417375	1
N-N2	2.188997	4.099139	1.195250	1

H-H	2.934811	3.480070	0.915818	l
H-H	2.351886	5.091766	1.348182	l
N-NC	-0.010102	4.529279	1.697339	l
C-CB	-1.237671	3.946371	1.756024	l
C-CT	-3.953702	6.846312	0.617027	l
H-H1	-4.140856	5.887637	0.127298	l
C-CT	-2.550930	6.919402	1.196735	l
H-HC	-1.773308	6.616221	0.503415	l
H-HC	-2.359006	7.931521	1.544171	l
O-OS	-4.247423	7.955831	-0.204453	l
P-P	-4.163605	7.842931	-1.797682	l
O-O2	-4.805455	9.023097	-2.404710	l
O-O2	-4.598712	6.483882	-2.167907	l
O-OS	-2.595091	7.927952	-2.085748	l
C-CT	-1.827484	9.008062	-1.574346	l
H-H1	-2.056220	9.161507	-0.518662	l
H-H1	-2.090782	9.929354	-2.093307	l
C-CT	-0.318003	8.758314	-1.680948	l
H-H1	0.168597	9.553490	-1.126891	l
O-OS	0.025920	7.492359	-1.113108	l
C-CT	0.688226	6.694072	-2.080293	l
H-H2	1.770827	6.686570	-1.902986	l
N-N*	0.106971	5.339302	-1.995075	h
C-CK	-1.200225	5.045245	-1.674801	h
H-H5	-1.934260	5.823550	-1.525142	h
N-NB	-1.424892	3.761036	-1.582905	h
C-CB	-0.211256	3.186776	-1.874402	h
C-C	0.103984	1.795946	-1.998202	h
O-O	-0.654463	0.848860	-1.831639	h
N-NA	1.439216	1.606007	-2.381330	h
H-H	1.725327	0.629908	-2.545168	h
C-CA	2.300140	2.631272	-2.712523	h
N-N2	3.472639	2.247556	-3.279241	h
H-H	3.812058	1.285096	-3.167906	h
H-H	4.172850	2.973723	-3.392673	h
N-NC	2.021040	3.915294	-2.583424	h
C-CB	0.755407	4.135637	-2.153375	h
C-CT	0.226451	8.802256	-3.107043	l
H-H1	-0.465543	9.289955	-3.797214	l
C-CT	0.365588	7.326312	-3.430720	l
H-HC	-0.595684	6.970242	-3.793270	l
H-HC	1.157260	7.149796	-4.158656	l
O-OS	1.502364	9.417148	-3.140161	l
P-P	1.668862	11.013503	-3.299891	l
O-O2	0.692432	11.479375	-4.306639	l
O-O2	3.100019	11.327912	-3.463441	l
O-OS	1.209985	11.577806	-1.858965	l
C-CT	0.024919	12.357359	-1.719688	l
H-H1	-0.798010	11.874540	-2.245932	l
H-H1	0.173157	13.325783	-2.192839	l
C-CT	-0.409223	12.541146	-0.257754	l
H-H1	-1.210796	13.283470	-0.219533	l
O-OS	-0.907500	11.285822	0.208492	l
C-CT	-0.639730	11.129457	1.592225	l
H-H2	-1.576288	10.999396	2.152075	l
N-N*	0.239029	9.943804	1.796278	l
C-CM	1.376365	9.738517	1.043547	l
H-H4	1.639431	10.428921	0.260371	l

H-H

C-CM	2.167897	8.653442	1.220268	1
C-CT	3.382800	8.485561	0.321824	1
H-HC	3.068520	8.181062	-0.677312	1
H-HC	3.931610	9.420737	0.236402	1
H-HC	4.044173	7.719561	0.721278	1
C-C	1.842391	7.674135	2.250273	1
O-O	2.490288	6.671022	2.533807	1
N-NA	0.698175	7.941854	2.964434	1
H-H	0.457093	7.295654	3.691025	1
C-C	-0.130438	9.023876	2.777359	1
O-O	-1.151802	9.125882	3.446461	1
C-CT	0.668264	12.974380	0.744575	1
H-H1	1.611569	12.475230	0.522139	1
C-CT	0.039917	12.424781	2.020968	1
H-HC	0.769082	12.256766	2.809397	1
H-HC	-0.719433	13.122667	2.372958	1
O-OS	0.867474	14.366048	0.929550	1
P-P	1.563198	15.287738	-0.192557	1
O-O2	2.136357	16.475668	0.469828	1
O-O2	0.622339	15.447601	-1.318049	1
O-OS	2.788854	14.363651	-0.671476	1
C-CT	3.256181	14.381816	-2.017194	1
H-H1	3.200723	15.399586	-2.409970	1
H-H1	2.620948	13.747339	-2.634409	1
C-CT	4.721049	13.924921	-2.133304	1
H-H1	4.968505	13.779550	-3.188722	1
O-OS	5.512346	14.971864	-1.576976	1
C-CT	6.352953	14.412700	-0.586506	1
H-H2	7.290718	14.065934	-1.043773	1
N-N*	6.612381	15.370256	0.504290	1
C-CM	5.687718	16.333372	0.845227	1
H-H4	4.771048	16.412628	0.271225	1
C-CM	5.905884	17.174956	1.887400	1
C-CT	4.850598	18.216696	2.234697	1
H-HC	4.932696	19.064644	1.554730	1
H-HC	3.852402	17.783078	2.160714	1
H-HC	5.002689	18.567907	3.257284	1
C-C	7.132486	17.057737	2.674122	1
O-O	7.419073	17.714240	3.669314	1
N-NA	8.011042	16.083128	2.250445	1
H-H	8.868628	15.976254	2.759812	1
C-C	7.809115	15.225993	1.196391	1
O-O	8.652052	14.385136	0.901774	1
C-CT	5.077044	12.638581	-1.368652	1
H-H1	4.210087	11.978613	-1.260779	1
C-CT	5.562474	13.231486	-0.056961	1
H-HC	4.730560	13.578199	0.547532	1
H-HC	6.185935	12.557710	0.514884	1
O-OS	6.178214	12.001119	-2.007998	1
P-P	6.509298	10.431000	-1.823454	1
O-O2	7.680523	10.101325	-2.661361	1
O-O2	5.250146	9.674386	-1.967956	1
O-OS	6.961585	10.352984	-0.277036	1
C-CT	8.262099	10.740721	0.166322	1
H-H1	8.469636	11.776058	-0.114672	1
H-H1	9.012755	10.099142	-0.300036	1
C-CT	8.376752	10.622665	1.697167	1
H-H1	9.416274	10.779675	1.997615	1

O-OS	7.542861	11.611392	2.290400	1
C-CT	6.647384	10.997541	3.194201	1
H-H2	7.090926	10.982402	4.197563	1
N-N*	5.398675	11.789998	3.172444	1
C-CK	4.168870	11.467337	2.651466	1
H-H5	3.930096	10.505199	2.226551	1
N-NB	3.313742	12.446552	2.657180	1
C-CB	3.989775	13.474750	3.309841	1
C-CA	3.630927	14.793849	3.684581	1
N-N2	2.468573	15.374915	3.372317	1
H-H	1.826649	14.918368	2.731054	1
H-H	2.281442	16.314214	3.685006	1
N-NC	4.514646	15.529734	4.385515	1
C-CQ	5.705793	15.003525	4.679274	1
H-H5	6.383108	15.647245	5.229760	1
N-NC	6.176758	13.797445	4.357149	1
C-CB	5.253924	13.068053	3.666113	1
C-CT	7.893756	9.262189	2.218460	1
H-H1	7.908427	8.508971	1.424207	1
C-CT	6.479155	9.573353	2.674037	1
H-HC	5.826429	9.550393	1.806320	1
H-HC	6.132619	8.894260	3.451978	1
O-OS	8.613646	8.833408	3.358907	1
P-P	9.937993	7.936587	3.207478	1
O-O2	10.545419	7.745416	4.539709	1
O-O2	10.728629	8.457983	2.073300	1
O-OS	9.223901	6.569103	2.758506	1
C-CT	8.472364	5.790932	3.678901	1
H-H1	7.860210	6.429630	4.318029	1
H-H1	9.134055	5.200058	4.314734	1
C-CT	7.557095	4.864699	2.883735	1
H-H1	8.169078	4.213077	2.249126	1
O-OS	6.735114	4.098149	3.762285	1
C-CT	5.531623	3.925066	3.053345	1
H-H2	5.737264	3.301594	2.176020	1
N-N*	4.441770	3.289905	3.813170	1
C-CK	3.229979	3.806041	4.214532	1
H-H5	2.998929	4.866232	4.212677	1
N-NB	2.355407	2.899810	4.559529	1
C-CB	3.028637	1.693474	4.362323	1
C-C	2.579105	0.336422	4.468982	1
O-O	1.459410	-0.077020	4.760936	1
N-NA	3.556038	-0.597446	4.147068	1
H-H	3.299121	-1.571317	4.244407	1
C-CA	4.820330	-0.256974	3.729133	1
N-N2	5.643764	-1.249453	3.436881	1
H-H	5.360549	-2.216121	3.523775	1
H-H	6.575555	-1.030461	3.113241	1
N-NC	5.244412	1.001500	3.578790	1
C-CB	4.309716	1.928321	3.926318	1
C-CT	6.587799	5.646458	1.978944	1
H-H1	6.813968	6.711373	1.940967	1
C-CT	5.245525	5.343336	2.611216	1
H-HC	5.057658	5.985079	3.470809	1
H-HC	4.440980	5.382184	1.887313	1
O-OS	6.599678	5.051052	0.701953	1
P-P	6.044060	5.766981	-0.616921	1
O-O2	6.662917	7.102979	-0.715449	1

O-O2	4.577907	5.591255	-0.660640	l
O-OS	6.711593	4.770628	-1.682273	l
C-CT	8.116770	4.550237	-1.678602	l
H-H1	8.603330	5.188008	-0.937271	l
H-H1	8.514598	4.801772	-2.662761	l
C-CT	8.467051	3.088669	-1.362251	l
H-H1	9.554350	2.980742	-1.424084	l
O-OS	8.031775	2.648731	-0.070319	l
C-CT	7.688895	1.269969	-0.128494	l
H-H2	8.193948	0.683568	0.652113	l
N-N*	6.218846	1.109770	-0.005006	l
C-CK	5.246871	2.079213	-0.001222	l
H-H5	5.484545	3.126596	-0.139377	l
N-NB	4.037137	1.628225	0.198723	l
C-CB	4.212808	0.244552	0.291660	l
C-C	3.259724	-0.815139	0.461164	l
O-O	2.040306	-0.740028	0.596286	l
N-NA	3.829107	-2.080452	0.434286	l
H-H	3.214303	-2.867014	0.572878	l
C-CA	5.172290	-2.303492	0.268891	l
N-N2	5.538096	-3.574243	0.206826	l
H-H	4.847480	-4.306888	0.296855	l
H-H	6.513020	-3.788790	0.071653	l
N-NC	6.084949	-1.332424	0.129912	l
C-CB	5.542986	-0.080847	0.150941	l
C-CT	7.842612	2.103133	-2.339601	l
H-H1	6.773214	2.315559	-2.417474	l
C-CT	8.120869	0.846697	-1.523648	l
H-HC	7.580005	-0.025891	-1.846673	l
H-HC	9.181989	0.623390	-1.541366	l
O-OS	8.482413	2.114173	-3.602352	l
P-P	7.747473	1.582979	-4.938173	l
O-O2	8.481819	2.067884	-6.121336	l
O-O2	6.295873	1.830591	-4.798657	l
O-OS	7.950518	-0.001662	-4.848611	l
C-CT	9.220241	-0.559171	-4.551048	l
H-H1	9.720203	0.036840	-3.785973	l
H-H1	9.859000	-0.535355	-5.432800	l
C-CT	9.108121	-1.988586	-4.002257	l
H-H1	10.070363	-2.227347	-3.563088	l
O-OS	8.089032	-2.069366	-3.001739	l
C-CT	7.062448	-2.953862	-3.418336	l H-H
H-H2	7.113466	-3.886882	-2.844020	l
N-N*	5.747829	-2.287475	-3.263469	h
C-CK	5.497589	-0.933605	-3.215666	h
H-H5	6.270254	-0.201923	-3.364280	h
N-NB	4.234390	-0.651036	-3.036726	h
C-CB	3.618123	-1.879336	-3.001255	h
C-C	2.228915	-2.179090	-2.899960	h
O-O	1.298180	-1.383469	-2.770192	h
N-NA	1.999791	-3.558464	-2.998776	h
H-H	1.012597	-3.848007	-2.944975	h
C-CA	2.977979	-4.487894	-3.270073	h
N-N2	2.552533	-5.735670	-3.585136	h
H-H	1.596008	-6.036312	-3.376507	h
H-H	3.281698	-6.436445	-3.613484	h
N-NC	4.269300	-4.227506	-3.303132	h
C-CB	4.528669	-2.909033	-3.167022	h

C-CT	8.812444	-3.057958	-5.051715	1
H-H1	9.064955	-2.731022	-6.062267	1
C-CT	7.316148	-3.232309	-4.889678	1
H-HC	6.819736	-2.468035	-5.472635	1
H-HC	6.988604	-4.230131	-5.179302	1
O-OS	9.470470	-4.267275	-4.721786	1
P-P	10.953199	-4.598122	-5.264700	1
O-O2	10.950358	-4.396014	-6.729422	1
O-O2	11.393224	-5.885406	-4.692520	1
O-OS	11.845495	-3.432091	-4.595104	1
C-CT	12.397035	-2.388157	-5.391965	1
H-H1	11.609804	-1.911171	-5.973626	1
H-H1	13.104272	-2.812510	-6.103473	1
C-CT	13.088959	-1.307712	-4.550125	1
H-H1	13.643265	-0.635218	-5.209423	1
O-OS	12.099955	-0.573047	-3.832956	1
C-CT	12.669205	-0.024509	-2.652572	1
H-H2	12.716507	1.071661	-2.720681	1
N-N*	11.853731	-0.425516	-1.476992	1
C-CM	11.324391	-1.693512	-1.355360	1
H-H4	11.534480	-2.431510	-2.114889	1
C-CM	10.513845	-2.026850	-0.318997	1
C-CT	9.901594	-3.417548	-0.277398	1
H-HC	8.994389	-3.396671	0.326111	1
H-HC	9.637216	-3.750105	-1.283566	1
H-HC	10.607469	-4.120916	0.159831	1
C-C	10.229662	-1.053831	0.731654	1
O-O	9.497659	-1.221202	1.701760	1
N-NA	10.851085	0.166259	0.574854	1
H-H	10.717089	0.855493	1.291957	1
C-C	11.628679	0.540604	-0.496595	1
O-O	12.049741	1.688245	-0.574049	1
C-CT	14.042363	-1.815463	-3.471384	1
H-H1	13.580992	-2.656503	-2.956345	1
C-CT	14.077816	-0.600194	-2.560845	1
H-HC	14.349874	-0.870531	-1.543616	1
H-HC	14.787039	0.127864	-2.954161	1
O-OS	15.378458	-2.085878	-3.855327	1
P-P	15.812656	-3.475570	-4.541237	1
O-O2	17.242969	-3.694707	-4.250915	1
O-O2	15.311361	-3.528029	-5.926959	1
O-OS	14.965412	-4.496441	-3.639266	1
C-CT	15.101168	-5.903525	-3.760529	1
H-H1	16.138707	-6.159433	-3.990380	1
H-H1	14.457757	-6.266909	-4.564282	1
C-CT	14.736102	-6.586202	-2.432234	1
H-H1	14.738942	-7.670267	-2.572114	1
O-OS	15.739074	-6.211757	-1.490720	1
C-CT	15.117877	-5.661059	-0.345777	1
H-H2	14.921855	-6.453862	0.385577	1
N-N*	15.967062	-4.593569	0.228035	1
C-CM	16.442426	-3.570003	-0.562858	1
H-H4	16.321305	-3.642413	-1.636340	1
C-CM	17.041277	-2.480810	-0.017651	1
C-CT	17.521432	-1.352561	-0.920540	1
H-HC	17.549586	-1.665055	-1.966742	1
H-HC	16.857834	-0.495336	-0.811073	1
H-HC	18.525461	-1.053293	-0.613771	1

C-C	17.202934	-2.388572	1.431287	1
O-O	17.658597	-1.431424	2.046891	1
N-NA	16.794620	-3.500232	2.137067	1
H-H	16.945401	-3.500376	3.128459	1
C-C	16.211464	-4.623287	1.598394	1
O-O	15.941194	-5.582399	2.313487	1
C-CT	13.376546	-6.167499	-1.849346	1
H-H1	12.706879	-5.785956	-2.626464	1
C-CT	13.801566	-5.091372	-0.862889	1
H-HC	13.960550	-4.151824	-1.379998	1
H-HC	13.084634	-4.952860	-0.066028	1
O-OS	12.805581	-7.267728	-1.153866	1
P-P	11.275501	-7.273355	-0.629480	1
O-O2	10.898276	-8.662019	-0.300887	1
O-O2	10.452931	-6.460453	-1.547336	1
O-OS	11.395831	-6.463826	0.753021	1
C-CT	12.191886	-6.949468	1.825364	1
H-H1	13.162496	-7.282003	1.457040	1
H-H1	11.700944	-7.803707	2.295073	1
C-CT	12.426648	-5.848041	2.866774	1
H-H1	13.001562	-6.268015	3.697740	1
O-OS	13.152277	-4.756823	2.330024	1
C-CT	12.974584	-3.705002	3.243816	1
H-H2	13.495577	-3.913667	4.187745	1
N-N*	13.469935	-2.455331	2.644112	1
C-CK	13.520922	-2.098654	1.321716	1
H-H5	13.141343	-2.732958	0.535766	1
N-NB	14.068687	-0.937128	1.097352	1
C-CB	14.407182	-0.483393	2.371899	1
C-CA	15.016457	0.699291	2.865073	1
N-N2	15.391115	1.729962	2.098785	1
H-H	15.226179	1.706050	1.103608	1
H-H	15.823818	2.530854	2.533298	1
N-NC	15.222042	0.818153	4.192270	1
C-CQ	14.843660	-0.176469	4.996383	1
H-H5	15.037971	-0.027010	6.050911	1
N-NC	14.252205	-1.326387	4.667321	1
C-CB	14.058995	-1.415773	3.320430	1
C-CT	11.137009	-5.222041	3.415791	1
H-H1	10.299913	-5.413886	2.740843	1
C-CT	11.466052	-3.725716	3.441649	1
H-HC	10.979952	-3.226449	2.606306	1
H-HC	11.181166	-3.256066	4.382655	1
O-OS	10.829072	-5.640699	4.731662	1
P-P	10.514578	-7.180313	5.095729	1
O-O2	9.807597	-7.219507	6.391056	1
O-O2	11.740310	-7.979828	4.895704	1
O-OS	9.477428	-7.610921	3.945888	1
C-CT	8.912964	-8.914339	3.962561	1
H-H1	8.541574	-9.133013	4.967381	1
H-H1	9.681620	-9.646095	3.709495	1
C-CT	7.729456	-9.059485	3.000420	1
H-H1	7.432064	-10.110219	2.976459	1
O-OS	6.657609	-8.278936	3.515493	1
C-CT	6.137455	-7.518187	2.451898	1
H-H2	5.425665	-8.129511	1.879221	1
N-N*	5.477973	-6.310236	2.977116	1
C-CK	6.011870	-5.087624	3.304617	1

H-H5	7.073707	-4.877309	3.307000	1
N-NB	5.119290	-4.185637	3.600774	1
C-CB	3.907493	-4.867123	3.500045	1
C-C	2.560504	-4.414206	3.668799	1
O-O	2.164328	-3.273372	3.900022	1
N-NA	1.620149	-5.427282	3.526932	1
H-H	0.656019	-5.165949	3.682817	1
C-CA	1.946269	-6.725473	3.214045	1
N-N2	0.946138	-7.577188	3.073054	1
H-H	-0.015241	-7.276670	3.167726	1
H-H	1.158034	-8.517419	2.774997	1
N-NC	3.193091	-7.157102	3.001714	1
C-CB	4.126085	-6.181906	3.169744	1
C-CT	7.984345	-8.593803	1.556580	1
H-H1	9.048883	-8.571924	1.309271	1
C-CT	7.349828	-7.209906	1.588696	1
H-HC	8.021437	-6.518185	2.091154	1
H-HC	7.063887	-6.840791	0.607937	1
O-OS	7.251451	-9.464143	0.708538	1
P-P	7.352644	-9.453641	-0.904012	1
O-O2	8.086353	-10.657790	-1.341632	1
O-O2	7.739874	-8.109865	-1.377453	1
O-OS	5.791232	-9.651368	-1.222067	1
C-CT	5.101023	-10.804806	-0.762811	1
H-H1	5.248490	-10.912477	0.313466	1
H-H1	5.498357	-11.690826	-1.260370	1
C-CT	3.595375	-10.695251	-1.023152	1
H-H1	3.116049	-11.630986	-0.727653	1
O-OS	3.081288	-9.622169	-0.239713	1
C-CT	2.269119	-8.830678	-1.077099	1
H-H2	1.254623	-9.247923	-1.122623	1
N-N*	2.256622	-7.446358	-0.573124	1
C-CK	3.309479	-6.581117	-0.402498	1
H-H5	4.333471	-6.868991	-0.617205	1
N-NB	2.959191	-5.396563	0.025685	1
C-CB	1.572732	-5.502660	0.185377	1
C-C	0.600186	-4.555087	0.647721	1
O-O	0.767583	-3.385667	0.986311	1
N-NA	-0.691429	-5.061345	0.695100	1
H-H	-1.414331	-4.470812	1.076751	1
C-CA	-1.016111	-6.340092	0.321300	1
N-N2	-2.300283	-6.651103	0.370269	1
H-H	-2.982508	-5.986047	0.711122	1
H-H	-2.586651	-7.573024	0.077854	1
N-NC	-0.133537	-7.237880	-0.130119	1
C-CB	1.142228	-6.760894	-0.163326	1
C-CT	3.252522	-10.412612	-2.493118	1
H-H1	4.095220	-10.633953	-3.155351	1
C-CT	2.931169	-8.926165	-2.443353	1
H-HC	3.859449	-8.357471	-2.462319	1
H-HC	2.261089	-8.616573	-3.239983	1
O-OS	2.097426	-11.155027	-2.846966	1
P-P	1.658441	-11.389393	-4.380759	1
O-O2	1.910224	-12.801313	-4.729773	1
O-O2	2.206715	-10.296400	-5.211249	1
O-OS	0.076533	-11.159796	-4.262977	1
C-CT	-0.735667	-12.016534	-3.469835	1
H-H1	-0.308656	-12.085020	-2.467769	1

H-H1	-0.755524	-13.014335	-3.909533	l	
C-CT	-2.169083	-11.477861	-3.332068	l	
H-H1	-2.755298	-12.171888	-2.727769	l	
O-OS	-2.076528	-10.223706	-2.669368	l	
C-CT	-2.694195	-9.253141	-3.483124	l	H-H
H-H2	-3.744281	-9.154603	-3.188876	l	
N-N*	-1.958201	-7.990092	-3.335512	h	
C-CK	-0.621219	-7.778371	-3.573758	h	
H-H5	0.021212	-8.583992	-3.905836	h	
N-NB	-0.262697	-6.543273	-3.326836	h	
C-CB	-1.417773	-5.926083	-2.896191	h	
C-C	-1.634058	-4.562253	-2.500856	h	
O-O	-0.807813	-3.657761	-2.457380	h	
N-NA	-2.976986	-4.350452	-2.134381	h	
H-H	-3.234778	-3.376021	-1.927138	h	
C-CA	-3.946841	-5.326412	-2.122363	h	
N-N2	-5.148653	-4.983103	-1.586008	h	
H-H	-5.402918	-3.997357	-1.619245	h	
H-H	-5.918860	-5.636667	-1.743596	h	
N-NC	-3.763742	-6.566180	-2.533421	h	
C-CB	-2.481352	-6.803943	-2.897135	h	
C-CT	-2.887586	-11.242504	-4.675245	l	
H-H1	-2.471476	-11.864567	-5.474585	l	
C-CT	-2.612990	-9.773031	-4.914244	l	
H-HC	-1.612790	-9.648763	-5.324652	l	
H-HC	-3.357840	-9.318018	-5.561756	l	
O-OH	-4.301562	-11.368916	-4.576116	l	
H-HO	-4.538819	-12.288539	-4.412458	l	
K-K	-0.277696	-1.507240	-0.600276	l	
K-K	0.140059	-1.749098	3.135991	l	
Ni-Ni	-0.871200	-1.232997	-5.001315	h	
N-NC	0.679883	-0.151336	-5.303977	h	
N-NC	0.259196	-2.698524	-5.567604	h	
C-CA	-0.123123	-3.932758	-5.687603	h	
H-HA	0.619351	-4.705097	-5.903397	h	
C-CA	-1.492810	-4.375573	-5.660725	h	
C-CA	-2.567717	-3.478893	-5.362107	h	
O-OS	-2.418834	-2.289543	-4.906996	h	
C-CA	1.588614	-2.290572	-5.880200	h	
C-CA	1.826020	-0.893558	-5.695538	h	
C-CA	3.064893	-0.361978	-5.959185	h	
H-HA	3.299981	0.680882	-5.760814	h	
C-CA	2.580087	-3.089459	-6.407748	h	
H-HA	2.420128	-4.147545	-6.592350	h	
C-CA	3.824880	-2.531890	-6.800564	h	
C-CA	4.076951	-1.154818	-6.547269	h	
C-CA	5.304173	-0.579859	-6.974143	h	
C-CA	6.207847	-1.321428	-7.692566	h	
C-CA	5.949100	-2.691993	-7.967776	h	
C-CA	4.801315	-3.289429	-7.505314	h	
H-HA	5.504962	0.465973	-6.747112	h	
H-HA	7.128034	-0.856308	-8.031816	h	
H-HA	6.672172	-3.267590	-8.536086	h	
H-HA	4.610476	-4.340198	-7.704677	h	
C-CA	-1.777596	-5.691799	-6.077520	h	
C-CA	-3.073335	-6.127793	-6.282715	h	
C-CA	-4.142961	-5.219981	-6.100933	h	
C-CA	-3.890133	-3.943164	-5.632184	h	

H-HA	-0.949144	-6.368199	-6.276069	h
H-HA	-3.260315	-7.128488	-6.660900	h
C-CT	-5.507329	-5.603606	-6.632664	h
H-HA	-4.667087	-3.194159	-5.509911	h
C-CA	0.698716	1.141488	-5.319682	h
C-CA	-0.427443	1.991365	-5.072490	h
H-HA	1.628639	1.658001	-5.565817	h
C-CA	-1.711366	1.470017	-4.705812	h
C-CA	-2.752210	2.428180	-4.511401	h
C-CA	-2.534960	3.780186	-4.691618	h
C-CA	-1.260815	4.271777	-5.045456	h
C-CA	-0.228222	3.377453	-5.223822	h
O-OS	-1.970543	0.224182	-4.541106	h
H-HA	-3.722936	2.047824	-4.199969	h
C-CT	-3.641011	4.767471	-4.454002	h
H-HA	-1.103144	5.337181	-5.175652	h
H-HA	0.764417	3.741582	-5.481968	h
N-N3	-6.632574	-5.784399	-5.623807	h
H-HC	-5.863991	-4.850711	-7.336555	h
H-HC	-5.450973	-6.547622	-7.175217	h
H-HC	-3.223772	5.755495	-4.242039	h
H-HC	-4.248053	4.480683	-3.592785	h
N-N3	-4.608955	4.965819	-5.625523	h
C-CT	-6.836044	-4.533639	-4.791766	h
C-CT	-7.900477	-6.083900	-6.400495	h
C-CT	-6.305749	-6.910684	-4.660039	h
C-CT	-9.138326	-6.261530	-5.534969	h
H-HC	-8.044055	-5.252875	-7.091058	h
H-HC	-7.703762	-6.979122	-6.988403	h
H-HC	-7.105776	-6.897045	-3.917626	h
C-CT	-6.224040	-8.300210	-5.270674	h
H-HC	-5.381251	-6.629145	-4.152192	h
H-HC	-7.615798	-4.782972	-4.064993	h
H-HC	-5.919898	-4.376036	-4.222564	h
C-CT	-7.254006	-3.306551	-5.592958	h
H-HC	-6.671799	-3.154968	-6.500583	h
H-HC	-8.315427	-3.351561	-5.856869	h
H-HC	-7.095363	-2.431608	-4.958920	h
H-HC	-9.048430	-7.070842	-4.807194	h
H-HC	-9.402540	-5.356249	-4.978533	h
H-HC	-9.988740	-6.488354	-6.177016	h
H-HC	-7.191099	-8.644240	-5.643033	h
H-HC	-5.482024	-8.390004	-6.062580	h
H-HC	-5.938535	-8.988594	-4.470935	h
C-CT	-3.807756	5.271006	-6.873998	h
C-CT	-5.446438	3.720437	-5.849198	h
C-CT	-5.526865	6.119871	-5.261817	h
H-HC	-6.408724	6.048696	-5.898370	h
H-HC	-5.842879	5.930444	-4.233082	h
C-CT	-4.902528	7.505774	-5.342690	h
H-HC	-3.991017	7.576772	-4.743909	h
H-HC	-4.696279	7.840076	-6.357059	h
H-HC	-5.609322	8.200334	-4.883764	h
C-CT	-4.638732	5.566470	-8.114807	h
H-HC	-3.171997	6.118492	-6.609626	h
H-HC	-3.156442	4.410652	-7.030597	h
H-HC	-3.958311	5.930121	-8.886255	h
H-HC	-5.131018	4.676117	-8.505819	h

H-HC	-5.388688	6.342095	-7.946377	h
C-CT	-6.322373	3.319020	-4.670093	h
H-HC	-6.069832	3.935557	-6.716928	h
H-HC	-4.742486	2.928827	-6.108299	h
H-HC	-7.096193	4.059872	-4.454946	h
H-HC	-6.825453	2.386186	-4.930429	h
H-HC	-5.761656	3.132514	-3.751269	h

2/h-Telo

O-OH	-3.838968	-6.544454	8.936434	1
H-HO	-3.096848	-6.027865	8.584722	1
C-CT	-4.309094	-7.350844	7.863090	1
H-H1	-4.850004	-6.752828	7.124902	1
H-H1	-4.989522	-8.134472	8.211116	1
C-CT	-3.097496	-7.985820	7.182536	1
H-H1	-3.429206	-8.533779	6.297336	1
O-OS	-2.172239	-6.969399	6.814471	1
C-CT	-0.899805	-7.568806	6.779581	1
H-H2	-0.821991	-8.225720	5.905366	1
N-N*	0.216675	-6.593203	6.791122	1
C-CK	1.545432	-6.866209	6.562672	1
H-H5	1.922622	-7.859370	6.351003	1
N-NB	2.326382	-5.824234	6.603052	1
C-CB	1.458627	-4.770041	6.878520	1
C-CA	1.648466	-3.371423	7.028506	1
N-N2	2.828816	-2.752602	6.909918	1
H-H	3.662434	-3.287648	6.712985	1
H-H	2.868315	-1.750176	7.020967	1
N-NC	0.582924	-2.596186	7.304106	1
C-CQ	-0.610893	-3.171148	7.439478	1
H-H5	-1.433102	-2.503468	7.661453	1
N-NC	-0.921207	-4.461867	7.329147	1
C-CB	0.168438	-5.228333	7.025013	1
C-CT	-2.332090	-8.960405	8.083673	1
H-H1	-2.726102	-8.957275	9.106789	1
C-CT	-0.914220	-8.395819	8.054861	1
H-HC	-0.772086	-7.735205	8.909989	1
H-HC	-0.162975	-9.184342	8.040827	1
O-OS	-2.332794	-10.257222	7.510758	1
P-P	-3.501243	-11.318964	7.855579	1
O-O2	-3.724799	-11.297509	9.315207	1
O-O2	-3.191969	-12.586507	7.162034	1
O-OS	-4.779820	-10.645607	7.139129	1
C-CT	-5.070640	-10.885990	5.771291	1
H-H1	-5.420064	-11.913184	5.653405	1
H-H1	-4.164252	-10.750646	5.180168	1
C-CT	-6.147278	-9.906558	5.281169	1
H-H1	-7.021441	-9.970279	5.934719	1
O-OS	-5.572683	-8.602047	5.307512	1
C-CT	-5.418659	-8.127252	3.986308	1
H-H2	-6.245163	-7.438505	3.749648	1
N-N*	-4.113979	-7.439635	3.918255	1
C-CK	-2.914015	-7.857009	3.391533	1
H-H5	-2.740963	-8.835028	2.963629	1
N-NB	-1.969981	-6.964543	3.452590	1
C-CB	-2.583558	-5.860547	4.038167	1

C-C	-2.090290	-4.542182	4.298355	1
O-O	-0.976031	-4.078596	4.047759	1
N-NA	-3.041144	-3.708680	4.875518	1
H-H	-2.734731	-2.770243	5.087758	1
C-CA	-4.321878	-4.111791	5.175146	1
N-N2	-5.125455	-3.214598	5.718492	1
H-H	-4.819753	-2.262984	5.863857	1
H-H	-6.077934	-3.480002	5.917227	1
N-NC	-4.805576	-5.331379	4.923312	1
C-CB	-3.887903	-6.155382	4.351452	1
C-CT	-6.564800	-10.161175	3.823472	1
H-H1	-6.523019	-11.221199	3.561461	1
C-CT	-5.504251	-9.351885	3.087331	1
H-HC	-4.575662	-9.917502	3.076041	1
H-HC	-5.790965	-9.075718	2.074521	1
O-OS	-7.875861	-9.657011	3.621074	1
P-P	-8.581702	-9.600342	2.169496	1
O-O2	-10.020298	-9.890065	2.339733	1
O-O2	-7.772454	-10.367831	1.199161	1
O-OS	-8.402667	-8.025275	1.867525	1
C-CT	-9.340738	-7.106035	2.410635	1
H-H1	-9.362557	-7.204671	3.497611	1
H-H1	-10.331622	-7.355974	2.024995	1
C-CT	-9.063953	-5.640751	2.065242	1
H-H1	-9.965897	-5.064779	2.290234	1
O-OS	-7.961580	-5.099714	2.778808	1
C-CT	-7.617812	-3.871169	2.149712	1
H-H2	-7.952778	-3.009242	2.747313	1
N-N*	-6.163755	-3.800140	1.925761	1
C-CK	-5.249508	-4.810348	1.768178	1
H-H5	-5.528765	-5.855709	1.805598	1
N-NB	-4.022231	-4.394110	1.595801	1
C-CB	-4.138887	-3.001992	1.634674	1
C-C	-3.153104	-1.967756	1.525110	1
O-O	-1.934617	-2.079958	1.409158	1
N-NA	-3.694389	-0.688736	1.539691	1
H-H	-3.064314	0.097257	1.482725	1
C-CA	-5.038805	-0.435121	1.632652	1
N-N2	-5.389087	0.830412	1.495736	1
H-H	-4.671844	1.527470	1.356143	1
H-H	-6.362715	1.100634	1.459999	1
N-NC	-5.973649	-1.377765	1.775479	1
C-CB	-5.454916	-2.636699	1.784083	1
C-CT	-8.652081	-5.370264	0.629114	1
H-H1	-7.765944	-5.974385	0.415768	1
C-CT	-8.299115	-3.897730	0.783697	1
H-HC	-7.652640	-3.555046	-0.020024	1
H-HC	-9.205748	-3.296165	0.811291	1
O-OS	-9.650161	-5.566533	-0.347424	1
P-P	-9.253311	-5.555290	-1.901031	1
O-O2	-10.306692	-6.217743	-2.690734	1
O-O2	-7.844067	-5.980019	-2.024715	1
O-OS	-9.272258	-4.004153	-2.261104	1
C-CT	-10.430175	-3.216431	-2.021267	1
H-H1	-10.724635	-3.289273	-0.973936	1
H-H1	-11.262134	-3.609670	-2.598130	1
C-CT	-10.216827	-1.730169	-2.352876	1
H-H1	-11.163872	-1.206177	-2.210222	1

O-OS	-9.233363	-1.184600	-1.473459	l	
C-CT	-8.460889	-0.199217	-2.134348	l	H-H
H-H2	-8.525513	0.778038	-1.633600	l	
N-N*	-7.078485	-0.711027	-2.122354	h	
C-CK	-6.703725	-2.028250	-2.218956	h	
H-H5	-7.431345	-2.818825	-2.313151	h	
N-NB	-5.408248	-2.193750	-2.154827	h	
C-CB	-4.911483	-0.925982	-2.008622	h	
C-C	-3.538788	-0.543085	-1.828912	h	
O-O	-2.586227	-1.295317	-1.755224	h	
N-NA	-3.438535	0.859744	-1.692130	h	
H-H	-2.482723	1.236111	-1.607079	h	
C-CA	-4.512222	1.713576	-1.686867	h	
N-N2	-4.231748	3.044796	-1.586580	h	
H-H	-3.281117	3.345364	-1.347084	h	
H-H	-5.004982	3.619669	-1.263247	h	
N-NC	-5.776602	1.355428	-1.829394	h	
C-CB	-5.916703	0.017139	-1.975722	h	
C-CT	-9.743951	-1.433011	-3.778650	l	
H-H1	-9.073420	-2.222466	-4.105224	l	
C-CT	-8.994613	-0.124156	-3.562027	l	
H-HC	-8.206568	0.018743	-4.300515	l	
H-HC	-9.711126	0.697206	-3.620350	l	
O-OS	-10.745193	-1.162140	-4.746312	l	
P-P	-11.926797	-2.193456	-5.089030	l	
O-O2	-11.368410	-3.561994	-5.080155	l	
O-O2	-12.689351	-1.692495	-6.248344	l	
O-OS	-12.797247	-1.965640	-3.761290	l	
C-CT	-13.760883	-2.894161	-3.290753	l	
H-H1	-13.356738	-3.907660	-3.290155	l	
H-H1	-14.637431	-2.874591	-3.941212	l	
C-CT	-14.162407	-2.516929	-1.854157	l	
H-H1	-15.008021	-3.138696	-1.547344	l	
O-OS	-13.086656	-2.680293	-0.930744	l	
C-CT	-13.474533	-1.995471	0.244216	l	
H-H2	-14.277212	-2.560654	0.741168	l	
N-N*	-12.334658	-1.788693	1.184123	l	
C-CM	-11.247868	-0.995895	0.866965	l	
H-H4	-11.186100	-0.526373	-0.101426	l	
C-CM	-10.247236	-0.763009	1.755475	l	
C-CT	-9.092975	0.144618	1.362480	l	
H-HC	-8.374662	-0.418628	0.768178	l	
H-HC	-9.453080	0.994240	0.779926	l	
H-HC	-8.587637	0.513100	2.253085	l	
C-C	-10.277229	-1.384466	3.072128	l	
O-O	-9.409481	-1.294690	3.934268	l	
N-NA	-11.403300	-2.134800	3.327474	l	
H-H	-11.485539	-2.543264	4.240846	l	
C-C	-12.458086	-2.327300	2.464435	l	
O-O	-13.462845	-2.906066	2.855997	l	
C-CT	-14.560172	-1.048905	-1.691371	l	
H-H1	-14.037692	-0.437706	-2.425623	l	
C-CT	-14.047480	-0.693873	-0.302459	l	
H-HC	-13.288174	0.075453	-0.378169	l	
H-HC	-14.855224	-0.334064	0.317745	l	
O-OS	-15.959013	-0.843408	-1.709640	l	
P-P	-16.710631	-0.276259	-3.013438	l	
O-O2	-18.145124	-0.117679	-2.702303	l	

O-O2	-16.274070	-1.048275	-4.193899	1
O-OS	-16.053381	1.188495	-3.072267	1
C-CT	-15.049348	1.556071	-4.015063	1
H-H1	-15.502877	1.729066	-4.992911	1
H-H1	-14.306624	0.764101	-4.124826	1
C-CT	-14.348398	2.840377	-3.547855	1
H-H1	-13.464170	3.017252	-4.164693	1
O-OS	-15.265683	3.918572	-3.684455	1
C-CT	-15.461684	4.546449	-2.427209	1
H-H2	-14.854297	5.459692	-2.365476	1
N-N*	-16.902881	4.837367	-2.243157	1
C-CM	-17.868464	3.981614	-2.731363	1
H-H4	-17.566184	3.118666	-3.311519	1
C-CM	-19.186555	4.187971	-2.484298	1
C-CT	-20.200841	3.182683	-3.014166	1
H-HC	-20.208050	3.200965	-4.104099	1
H-HC	-19.948225	2.178762	-2.666032	1
H-HC	-21.200336	3.434916	-2.652868	1
C-C	-19.608119	5.345563	-1.698751	1
O-O	-20.759624	5.631757	-1.393754	1
N-NA	-18.581543	6.153100	-1.254815	1
H-H	-18.832139	6.962910	-0.716920	1
C-C	-17.240574	5.949152	-1.481096	1
O-O	-16.405873	6.704951	-1.000113	1
C-CT	-13.924574	2.768907	-2.075727	1
H-H1	-13.923037	1.740324	-1.720340	1
C-CT	-15.015072	3.547292	-1.369532	1
H-HC	-15.826647	2.864218	-1.131391	1
H-HC	-14.663286	4.034973	-0.463100	1
O-OS	-12.664188	3.377812	-1.874910	1
P-P	-11.446583	2.524677	-1.265102	1
O-O2	-10.202100	3.309844	-1.358469	1
O-O2	-11.514249	1.171899	-1.848466	1
O-OS	-11.896354	2.427222	0.275106	1
C-CT	-12.040012	3.609424	1.055832	1
H-H1	-12.505083	4.388829	0.451241	1
H-H1	-11.056312	3.976200	1.359836	1
C-CT	-12.927029	3.385545	2.291861	1
H-H1	-13.083173	4.350904	2.769602	1
O-OS	-14.196342	2.854693	1.911645	1
C-CT	-14.559309	1.907658	2.897469	1
H-H2	-14.856945	2.416117	3.824621	1
N-N*	-15.642431	1.009635	2.435452	1
C-CK	-15.833619	-0.327528	2.715291	1
H-H5	-15.157718	-0.927289	3.316640	1
N-NB	-16.879170	-0.846093	2.132609	1
C-CB	-17.475963	0.235696	1.484829	1
C-CA	-18.650553	0.381906	0.701559	1
N-N2	-19.465124	-0.625691	0.372661	1
H-H	-19.247947	-1.566645	0.665550	1
H-H	-20.266077	-0.437362	-0.209996	1
N-NC	-18.995775	1.610389	0.266509	1
C-CQ	-18.217737	2.644732	0.582703	1
H-H5	-18.547640	3.613419	0.232629	1
N-NC	-17.084217	2.639539	1.281484	1
C-CB	-16.754848	1.385045	1.707562	1
C-CT	-12.323161	2.394975	3.305485	1
H-H1	-11.277037	2.165209	3.086605	1

C-CT	-13.230811	1.193147	3.093567	1
H-HC	-12.960836	0.679197	2.176068	1
H-HC	-13.234864	0.524469	3.953637	1
O-OS	-12.512152	2.733362	4.674682	1
P-P	-11.870064	4.028818	5.391177	1
O-O2	-11.932754	3.817977	6.851754	1
O-O2	-12.450059	5.249277	4.797191	1
O-OS	-10.336567	3.935076	4.932420	1
C-CT	-9.419385	3.053969	5.554598	1
H-H1	-9.549405	2.030398	5.201689	1
H-H1	-9.546846	3.068016	6.639388	1
C-CT	-8.013946	3.559187	5.249687	1
H-H1	-7.971146	4.625817	5.485423	1
O-OS	-7.063537	2.839344	6.014249	1
C-CT	-5.788365	3.089527	5.456901	1
H-H2	-5.255833	3.876912	6.005033	1
N-N*	-5.012330	1.843017	5.455349	1
C-CK	-5.478545	0.554529	5.497115	1
H-H5	-6.532083	0.317217	5.600410	1
N-NB	-4.539056	-0.343606	5.396686	1
C-CB	-3.367091	0.402185	5.281409	1
C-C	-2.004686	-0.013125	5.141241	1
O-O	-1.559205	-1.155587	5.075994	1
N-NA	-1.108937	1.043895	5.064591	1
H-H	-0.126674	0.804224	5.067959	1
C-CA	-1.490571	2.363102	5.091380	1
N-N2	-0.518537	3.256756	4.991603	1
H-H	0.450404	2.978653	4.902576	1
H-H	-0.761849	4.234126	5.017142	1
N-NC	-2.760482	2.775475	5.212375	1
C-CB	-3.648351	1.745710	5.312783	1
C-CT	-7.545811	3.356354	3.813697	1
H-H1	-7.785024	2.340290	3.496692	1
C-CT	-6.046163	3.505386	4.015442	1
H-HC	-5.523608	2.860955	3.317597	1
H-HC	-5.740920	4.541586	3.886523	1
O-OS	-8.054221	4.320862	2.910811	1
P-P	-7.694800	4.302225	1.339888	1
O-O2	-8.675027	5.149184	0.632809	1
O-O2	-7.473117	2.900321	0.927283	1
O-OS	-6.273772	5.057345	1.337098	1
C-CT	-6.177469	6.415148	1.751174	1
H-H1	-6.687718	6.542700	2.706909	1
H-H1	-6.669447	7.053981	1.013545	1
C-CT	-4.721862	6.873884	1.919754	1
H-H1	-4.725219	7.911989	2.261702	1
O-OS	-3.982301	6.085465	2.851438	1
C-CT	-2.631863	5.973407	2.409231	1
H-H2	-1.925868	6.258444	3.199072	1
N-N*	-2.402108	4.570700	1.985533	1
C-CK	-3.332816	3.582246	1.807297	1
H-H5	-4.390593	3.790820	1.850793	1
N-NB	-2.834555	2.393520	1.611396	1
C-CB	-1.459890	2.614066	1.607104	1
C-C	-0.372241	1.698377	1.428939	1
O-O	-0.408942	0.470368	1.349500	1
N-NA	0.855737	2.334787	1.312799	1
H-H	1.664456	1.763194	1.122161	1

C-CA	1.017683	3.690964	1.447244	l
N-N2	2.236605	4.145140	1.235038	l
H-H	2.983646	3.529703	0.952557	l
H-H	2.396265	5.137026	1.395638	l
N-NC	0.030704	4.552785	1.724557	l
C-CB	-1.189533	3.954232	1.773137	l
C-CT	-3.924354	6.819579	0.628734	l
H-H1	-4.100226	5.854828	0.146906	l
C-CT	-2.526715	6.914130	1.219043	l
H-HC	-1.737042	6.625808	0.533104	l
H-HC	-2.353750	7.927688	1.573194	l
O-OS	-4.222453	7.918676	-0.205025	l
P-P	-4.123951	7.796713	-1.797390	l
O-O2	-4.798099	8.952085	-2.416913	l
O-O2	-4.508610	6.421275	-2.164083	l
O-OS	-2.558970	7.926478	-2.081460	l
C-CT	-1.813007	9.011221	-1.548739	l
H-H1	-2.038676	9.138138	-0.488837	l
H-H1	-2.093414	9.938697	-2.047568	l
C-CT	-0.301505	8.782609	-1.670199	l
H-H1	0.181827	9.573238	-1.106648	l
O-OS	0.059119	7.511032	-1.126255	l
C-CT	0.701415	6.726949	-2.118333	l H-H
H-H2	1.787380	6.714640	-1.960200	l
N-N*	0.121350	5.371519	-2.040329	h
C-CK	-1.166579	5.066049	-1.659431	h
H-H5	-1.900792	5.838250	-1.480648	h
N-NB	-1.375599	3.779141	-1.561501	h
C-CB	-0.175600	3.214576	-1.919881	h
C-C	0.169402	1.824973	-1.994154	h
O-O	-0.540815	0.867922	-1.718609	h
N-NA	1.485284	1.657076	-2.457522	h
H-H	1.790355	0.693834	-2.636328	h
C-CA	2.306041	2.690980	-2.850186	h
N-N2	3.449104	2.318080	-3.484912	h
H-H	3.800692	1.363803	-3.366337	h
H-H	4.140296	3.048850	-3.621104	h
N-NC	2.019770	3.970727	-2.713939	h
C-CB	0.768882	4.174160	-2.236186	h
C-CT	0.225767	8.849867	-3.102386	l
H-H1	-0.474038	9.350503	-3.775146	l
C-CT	0.358829	7.378740	-3.454272	l
H-HC	-0.606226	7.024110	-3.810659	l
H-HC	1.141817	7.214390	-4.194410	l
O-OS	1.501492	9.465200	-3.140635	l
P-P	1.665697	11.065120	-3.263682	l
O-O2	0.674804	11.552970	-4.245551	l
O-O2	3.094252	11.384866	-3.439878	l
O-OS	1.225693	11.594597	-1.803319	l
C-CT	0.050008	12.382519	-1.632235	l
H-H1	-0.783038	11.922691	-2.163390	l
H-H1	0.204522	13.361838	-2.080337	l
C-CT	-0.369951	12.531645	-0.162353	l
H-H1	-1.167321	13.276832	-0.098202	l
O-OS	-0.869440	11.266993	0.277076	l
C-CT	-0.604192	11.085823	1.658570	l
H-H2	-1.541469	10.957104	2.217896	l
N-N*	0.264064	9.890897	1.845222	l

C-CM	1.399017	9.688957	1.088935	1
H-H4	1.651213	10.376614	0.299071	1
C-CM	2.206221	8.618186	1.280924	1
C-CT	3.424764	8.455413	0.388239	1
H-HC	3.127516	8.032485	-0.571748	1
H-HC	3.904114	9.415203	0.206862	1
H-HC	4.140208	7.779903	0.852964	1
C-C	1.899537	7.651376	2.328256	1
O-O	2.568009	6.667802	2.631995	1
N-NA	0.747695	7.907572	3.033805	1
H-H	0.515750	7.267182	3.768399	1
C-C	-0.096266	8.974728	2.832897	1
O-O	-1.120897	9.069873	3.497683	1
C-CT	0.718644	12.934732	0.840633	1
H-H1	1.656309	12.432497	0.600833	1
C-CT	0.095029	12.363689	2.109573	1
H-HC	0.831513	12.170822	2.885995	1
H-HC	-0.652504	13.062170	2.485003	1
O-OS	0.929478	14.320152	1.057283	1
P-P	1.614120	15.266853	-0.050333	1
O-O2	2.206734	16.432697	0.634010	1
O-O2	0.657029	15.462964	-1.156293	1
O-OS	2.824706	14.347382	-0.572886	1
C-CT	3.279299	14.407962	-1.921366	1
H-H1	3.224647	15.438049	-2.280861	1
H-H1	2.636242	13.795292	-2.552462	1
C-CT	4.740793	13.949014	-2.063668	1
H-H1	4.976977	13.827283	-3.124620	1
O-OS	5.543218	14.978461	-1.491148	1
C-CT	6.396039	14.390473	-0.528265	1
H-H2	7.323602	14.047859	-1.008902	1
N-N*	6.680690	15.321000	0.579387	1
C-CM	5.768605	16.281904	0.958227	1
H-H4	4.841823	16.378801	0.403558	1
C-CM	6.011486	17.099776	2.013724	1
C-CT	4.969309	18.139615	2.403652	1
H-HC	5.052007	19.006954	1.748645	1
H-HC	3.966338	17.717304	2.328094	1
H-HC	5.136113	18.458709	3.434475	1
C-C	7.252023	16.958884	2.774179	1
O-O	7.561232	17.592402	3.777402	1
N-NA	8.116317	15.988200	2.313513	1
H-H	8.982932	15.865924	2.803922	1
C-C	7.889094	15.154642	1.245717	1
O-O	8.720691	14.314867	0.917657	1
C-CT	5.096732	12.643853	-1.332025	1
H-H1	4.225280	11.989597	-1.225909	1
C-CT	5.605145	13.202905	-0.013776	1
H-HC	4.784067	13.541199	0.610413	1
H-HC	6.232094	12.512290	0.534064	1
O-OS	6.181851	12.011762	-2.003051	1
P-P	6.501427	10.435345	-1.857702	1
O-O2	7.653494	10.112499	-2.724415	1
O-O2	5.232475	9.692845	-1.993173	1
O-OS	6.983339	10.324872	-0.322591	1
C-CT	8.294698	10.693923	0.103866	1
H-H1	8.502461	11.735342	-0.153366	1
H-H1	9.032513	10.060859	-0.393546	1

C-CT	8.436657	10.533818	1.628501	1
H-H1	9.482211	10.678025	1.914260	1
O-OS	7.618529	11.510700	2.262434	1
C-CT	6.736565	10.878883	3.166931	1
H-H2	7.197739	10.837186	4.161538	1
N-N*	5.490376	11.676427	3.186463	1
C-CK	4.247709	11.367665	2.687748	1
H-H5	3.996577	10.413509	2.252979	1
N-NB	3.395979	12.349336	2.728512	1
C-CB	4.090967	13.363589	3.383459	1
C-CA	3.746327	14.677736	3.787680	1
N-N2	2.580792	15.269274	3.508828	1
H-H	1.923201	14.826015	2.874634	1
H-H	2.405059	16.204257	3.840600	1
N-NC	4.647584	15.397589	4.482934	1
C-CQ	5.842013	14.861336	4.743206	1
H-H5	6.533274	15.492124	5.291365	1
N-NC	6.300961	13.659399	4.390111	1
C-CB	5.360837	12.945913	3.705826	1
C-CT	7.956283	9.161073	2.120374	1
H-H1	7.947523	8.431751	1.303648	1
C-CT	6.553494	9.469179	2.613973	1
H-HC	5.884160	9.472878	1.758696	1
H-HC	6.217876	8.771912	3.380446	1
O-OS	8.699670	8.692122	3.230077	1
P-P	10.025154	7.807368	3.019979	1
O-O2	10.677062	7.596823	4.327963	1
O-O2	10.775365	8.353650	1.870256	1
O-OS	9.309831	6.441200	2.569841	1
C-CT	8.607207	5.633172	3.503017	1
H-H1	8.040146	6.250220	4.202537	1
H-H1	9.300220	5.012766	4.073707	1
C-CT	7.637314	4.748069	2.726530	1
H-H1	8.202564	4.126929	2.021739	1
O-OS	6.865790	3.942977	3.617293	1
C-CT	5.618591	3.812403	2.976029	1
H-H2	5.762351	3.229657	2.058498	1
N-N*	4.565330	3.157749	3.769585	1
C-CK	3.365806	3.667297	4.214620	1
H-H5	3.130157	4.726742	4.228647	1
N-NB	2.505461	2.757297	4.579961	1
C-CB	3.173738	1.554891	4.349727	1
C-C	2.725017	0.199196	4.461857	1
O-O	1.615612	-0.210906	4.796630	1
N-NA	3.685522	-0.734238	4.091163	1
H-H	3.424936	-1.707937	4.172122	1
C-CA	4.937858	-0.394853	3.635265	1
N-N2	5.743978	-1.391727	3.303035	1
H-H	5.451210	-2.357257	3.372022	1
H-H	6.664573	-1.176340	2.941581	1
N-NC	5.360651	0.866047	3.485287	1
C-CB	4.439476	1.792995	3.871813	1
C-CT	6.619961	5.579179	1.924945	1
H-H1	6.854298	6.642778	1.917503	1
C-CT	5.319852	5.255562	2.626044	1
H-HC	5.193685	5.854844	3.526658	1
H-HC	4.474821	5.341600	1.954459	1
O-OS	6.532858	5.036596	0.629217	1

P-P	5.944047	5.820443	-0.630971	l
O-O2	6.545848	7.167336	-0.657072	l
O-O2	4.479331	5.630986	-0.651884	l
O-OS	6.599237	4.906766	-1.775343	l
C-CT	8.001776	4.671607	-1.791298	l
H-H1	8.505751	5.315650	-1.067705	l
H-H1	8.385207	4.907440	-2.784871	l
C-CT	8.347109	3.209437	-1.468392	l
H-H1	9.434685	3.100707	-1.520017	l
O-OS	7.900170	2.760096	-0.183380	l
C-CT	7.569717	1.381170	-0.249743	l
H-H2	8.078908	0.798339	0.527540	l
N-N*	6.108440	1.173754	-0.122311	l
C-CK	5.096497	2.101200	-0.096550	l
H-H5	5.283403	3.159121	-0.246763	l
N-NB	3.917197	1.595054	0.153477	l
C-CB	4.156554	0.219337	0.243186	l
C-C	3.264183	-0.884900	0.457298	l
O-O	2.054037	-0.867533	0.666554	l
N-NA	3.886101	-2.123764	0.381402	l
H-H	3.321236	-2.944654	0.532862	l
C-CA	5.228256	-2.284043	0.154365	l
N-N2	5.643922	-3.536995	0.053822	l
H-H	4.990869	-4.297362	0.178949	l
H-H	6.619695	-3.707111	-0.129162	l
N-NC	6.089210	-1.270957	-0.005992	l
C-CB	5.491559	-0.046018	0.046087	l
C-CT	7.732299	2.228233	-2.455032	l
H-H1	6.662384	2.436060	-2.540019	l
C-CT	8.009247	0.971256	-1.643248	l
H-HC	7.469364	0.104096	-1.975592	l
H-HC	9.070046	0.747884	-1.655083	l
O-OS	8.383429	2.236866	-3.712235	l
P-P	7.688701	1.636415	-5.039044	l
O-O2	8.451816	2.065949	-6.225535	l
O-O2	6.231859	1.877635	-4.954696	l
O-OS	7.898693	0.060753	-4.866166	l
C-CT	9.170259	-0.479590	-4.541196	l
H-H1	9.660288	0.141098	-3.789659	l
H-H1	9.816720	-0.477404	-5.417640	l
C-CT	9.055888	-1.896059	-3.957492	l
H-H1	10.006838	-2.119157	-3.482158	l
O-OS	8.003986	-1.961594	-2.990308	l
C-CT	6.989516	-2.847707	-3.428428	l
H-H2	7.032308	-3.776186	-2.847333	l
N-N*	5.660638	-2.200909	-3.311725	h
C-CK	5.372417	-0.854028	-3.291836	h
H-H5	6.126865	-0.104594	-3.454250	h
N-NB	4.098511	-0.604367	-3.133138	h
C-CB	3.513377	-1.848674	-3.081450	h
C-C	2.134092	-2.199548	-3.023760	h
O-O	1.160891	-1.434135	-2.950304	h
N-NA	1.959287	-3.581945	-3.090240	h
H-H	0.985591	-3.911023	-3.023769	h
C-CA	2.970010	-4.484645	-3.330945	h
N-N2	2.588249	-5.746159	-3.629126	h
H-H	1.628711	-6.061246	-3.453690	h
H-H	3.332377	-6.430961	-3.646676	h

H-H

N-NC	4.251443	-4.179260	-3.345604	h
C-CB	4.459999	-2.853827	-3.219344	h
C-CT	8.788561	-2.983289	-4.997254	l
H-H1	9.079959	-2.676966	-6.003703	l
C-CT	7.285340	-3.138391	-4.888443	l
H-HC	6.817084	-2.371628	-5.492523	l
H-HC	6.955608	-4.134272	-5.181677	l
O-OS	9.420302	-4.194349	-4.625178	l
P-P	10.916376	-4.548721	-5.111794	l
O-O2	10.972492	-4.350023	-6.575911	l
O-O2	11.314495	-5.841290	-4.521235	l
O-OS	11.797774	-3.394060	-4.410023	l
C-CT	12.376753	-2.347037	-5.183343	l
H-H1	11.609702	-1.865045	-5.787163	l
H-H1	13.103919	-2.769590	-5.874997	l
C-CT	13.043827	-1.271423	-4.315178	l
H-H1	13.627767	-0.602577	-4.952223	l
O-OS	12.030008	-0.530315	-3.642053	l
C-CT	12.551248	0.007644	-2.435672	l
H-H2	12.614679	1.102973	-2.499848	l
N-N*	11.670645	-0.388713	-1.307548	l
C-CM	11.171945	-1.669288	-1.188453	l
H-H4	11.437069	-2.414380	-1.923469	l
C-CM	10.314990	-2.007926	-0.192476	l
C-CT	9.744633	-3.416691	-0.165882	l
H-HC	8.853857	-3.438146	0.461003	l
H-HC	9.468537	-3.731495	-1.174314	l
H-HC	10.487089	-4.104578	0.235855	l
C-C	9.937440	-1.021539	0.816196	l
O-O	9.155694	-1.186459	1.748156	l
N-NA	10.521253	0.217778	0.659545	l
H-H	10.313116	0.923070	1.343017	l
C-C	11.347380	0.593424	-0.374048	l
O-O	11.722664	1.755974	-0.463184	l
C-CT	13.953602	-1.784906	-3.200757	l
H-H1	13.476841	-2.633817	-2.712698	l
C-CT	13.948123	-0.582408	-2.271370	l
H-HC	14.159484	-0.867531	-1.241755	l
H-HC	14.684707	0.144154	-2.613916	l
O-OS	15.303209	-2.049444	-3.542105	l
P-P	15.757872	-3.423623	-4.246460	l
O-O2	17.172780	-3.666616	-3.903151	l
O-O2	15.314778	-3.436229	-5.652884	l
O-OS	14.861399	-4.453996	-3.405081	l
C-CT	14.932815	-5.856751	-3.597517	l
H-H1	15.954094	-6.145985	-3.858076	l
H-H1	14.260718	-6.152535	-4.405473	l
C-CT	14.558680	-6.584169	-2.295796	l
H-H1	14.524163	-7.660258	-2.485168	l
O-OS	15.583901	-6.287376	-1.351253	l
C-CT	14.989421	-5.769710	-0.176585	l
H-H2	14.773517	-6.592858	0.514523	l
N-N*	15.869629	-4.756034	0.440939	l
C-CM	16.490098	-3.800797	-0.334035	l
H-H4	16.427749	-3.878633	-1.412381	l
C-CM	17.168248	-2.769687	0.228207	l
C-CT	17.820798	-1.736553	-0.680732	l
H-HC	18.721585	-2.160088	-1.127110	l

H-HC	17.134494	-1.440148	-1.475248	1
H-HC	18.099361	-0.853543	-0.101804	1
C-C	17.263554	-2.668722	1.683554	1
O-O	17.815578	-1.772829	2.311599	1
N-NA	16.666867	-3.699051	2.381297	1
H-H	16.751671	-3.684736	3.380893	1
C-C	15.991878	-4.761456	1.826731	1
O-O	15.527484	-5.645093	2.538662	1
C-CT	13.223270	-6.152833	-1.665899	1
H-H1	12.539365	-5.735095	-2.410835	1
C-CT	13.694078	-5.122500	-0.650047	1
H-HC	13.891818	-4.172544	-1.136259	1
H-HC	12.994108	-4.976457	0.163006	1
O-OS	12.664835	-7.273060	-0.993768	1
P-P	11.138184	-7.317214	-0.469430	1
O-O2	10.821881	-8.708362	-0.091428	1
O-O2	10.281748	-6.574853	-1.416370	1
O-OS	11.218684	-6.456061	0.881729	1
C-CT	11.998312	-6.884759	1.990369	1
H-H1	13.012015	-7.129374	1.675591	1
H-H1	11.555888	-7.780960	2.429852	1
C-CT	12.074652	-5.777823	3.047973	1
H-H1	12.635476	-6.153103	3.909377	1
O-OS	12.721893	-4.611109	2.563904	1
C-CT	12.343251	-3.577874	3.441380	1
H-H2	12.804841	-3.711311	4.427953	1
N-N*	12.728044	-2.276844	2.863390	1
C-CK	13.525231	-2.029510	1.773544	1
H-H5	13.939144	-2.821583	1.166265	1
N-NB	13.745628	-0.764947	1.541410	1
C-CB	13.040837	-0.118701	2.559472	1
C-CA	12.830176	1.243795	2.902591	1
N-N2	13.323359	2.281338	2.218978	1
H-H	13.841561	2.121585	1.367153	1
H-H	13.113161	3.220228	2.521322	1
N-NC	12.062617	1.535761	3.971815	1
C-CQ	11.532617	0.536686	4.677874	1
H-H5	10.927618	0.827178	5.527553	1
N-NC	11.652258	-0.774297	4.468669	1
C-CB	12.422537	-1.038172	3.374127	1
C-CT	10.691991	-5.304686	3.516821	1
H-H1	9.917797	-5.605662	2.808047	1
C-CT	10.837446	-3.782566	3.525470	1
H-HC	10.367053	-3.357883	2.642769	1
H-HC	10.421738	-3.334690	4.427574	1
O-OS	10.369629	-5.739120	4.823301	1
P-P	10.178172	-7.298904	5.188120	1
O-O2	9.459204	-7.388935	6.474593	1
O-O2	11.468192	-7.995671	5.010520	1
O-OS	9.195183	-7.817993	4.025946	1
C-CT	8.636117	-9.121443	4.110288	1
H-H1	8.191726	-9.256688	5.099864	1
H-H1	9.425621	-9.863219	3.980480	1
C-CT	7.527824	-9.366927	3.080208	1
H-H1	7.223789	-10.413809	3.148911	1
O-OS	6.426826	-8.537395	3.424739	1
C-CT	6.023902	-7.833300	2.272527	1
H-H2	5.294873	-8.435959	1.711791	1

N-N*	5.424416	-6.554895	2.702410	1
C-CK	6.008177	-5.332044	2.934903	1
H-H5	7.071829	-5.149966	2.859375	1
N-NB	5.163096	-4.393603	3.260611	1
C-CB	3.930193	-5.046437	3.276048	1
C-C	2.610394	-4.556482	3.540577	1
O-O	2.260160	-3.404348	3.791464	1
N-NA	1.634471	-5.544596	3.475886	1
H-H	0.688618	-5.258559	3.686781	1
C-CA	1.905502	-6.856997	3.170061	1
N-N2	0.875786	-7.681364	3.100770	1
H-H	-0.069977	-7.348024	3.231261	1
H-H	1.045544	-8.631387	2.807779	1
N-NC	3.124240	-7.329108	2.894919	1
C-CB	4.091150	-6.375932	2.969609	1
C-CT	7.895643	-9.065284	1.619250	1
H-H1	8.976441	-9.078654	1.459732	1
C-CT	7.292177	-7.676204	1.447316	1
H-HC	7.961528	-6.944472	1.892076	1
H-HC	7.071640	-7.427223	0.412407	1
O-OS	7.232329	-10.038555	0.826193	1
P-P	7.367753	-10.148399	-0.780999	1
O-O2	7.857660	-11.499470	-1.120955	1
O-O2	8.026701	-8.943531	-1.322533	1
O-OS	5.804722	-10.063700	-1.141439	1
C-CT	4.911714	-11.073907	-0.695073	1
H-H1	4.985894	-11.173324	0.389711	1
H-H1	5.182916	-12.026963	-1.152211	1
C-CT	3.460228	-10.735439	-1.043939	1
H-H1	2.828393	-11.590788	-0.795116	1
O-OS	3.057174	-9.604000	-0.277712	1
C-CT	2.319468	-8.774559	-1.143871	1
H-H2	1.305050	-9.175455	-1.271326	1
N-N*	2.269839	-7.398395	-0.622545	1
C-CK	3.284240	-6.487255	-0.455919	1
H-H5	4.317125	-6.714051	-0.688682	1
N-NB	2.889201	-5.328279	-0.000250	1
C-CB	1.511493	-5.500351	0.174393	1
C-C	0.506949	-4.607995	0.670536	1
O-O	0.640412	-3.447202	1.046916	1
N-NA	-0.765527	-5.162967	0.705205	1
H-H	-1.514680	-4.607965	1.088898	1
C-CA	-1.044080	-6.439239	0.290124	1
N-N2	-2.319011	-6.789889	0.313053	1
H-H	-3.021001	-6.148515	0.657265	1
H-H	-2.576045	-7.708653	-0.014438	1
N-NC	-0.127451	-7.292147	-0.179306	1
C-CB	1.129749	-6.765786	-0.199920	1
C-CT	3.251994	-10.390425	-2.528098	1
H-H1	4.108969	-10.686243	-3.141631	1
C-CT	3.079466	-8.879857	-2.454863	1
H-HC	4.056477	-8.406055	-2.370585	1
H-HC	2.505764	-8.483855	-3.287751	1
O-OS	2.045534	-10.985765	-2.978147	1
P-P	1.711629	-11.175694	-4.543330	1
O-O2	2.048565	-12.559455	-4.930058	1
O-O2	2.256505	-10.025421	-5.294019	1
O-OS	0.118063	-11.015419	-4.511666	1

C-CT	-0.701028	-11.926134	-3.790272	l	
H-H1	-0.299974	-12.044293	-2.782064	l	
H-H1	-0.695032	-12.897550	-4.285636	l	
C-CT	-2.143598	-11.410592	-3.659792	l	
H-H1	-2.734843	-12.141978	-3.106817	l	
O-OS	-2.080513	-10.192583	-2.929448	l	
C-CT	-2.671874	-9.178983	-3.710244	l	H-H
H-H2	-3.726944	-9.083842	-3.433444	l	
N-N*	-1.928241	-7.931359	-3.484522	h	
C-CK	-0.584841	-7.719781	-3.685460	h	
H-H5	0.062211	-8.516040	-4.034232	h	
N-NB	-0.224013	-6.499436	-3.375529	h	
C-CB	-1.384011	-5.890256	-2.947846	h	
C-C	-1.590160	-4.556010	-2.454662	h	
O-O	-0.751456	-3.673528	-2.317298	h	
N-NA	-2.938706	-4.351275	-2.102932	h	
H-H	-3.200028	-3.386543	-1.862480	h	
C-CA	-3.912594	-5.320712	-2.151818	h	
N-N2	-5.115374	-5.005729	-1.598784	h	
H-H	-5.363930	-4.019277	-1.567290	h	
H-H	-5.887256	-5.643462	-1.805851	h	
N-NC	-3.733806	-6.535859	-2.631697	h	
C-CB	-2.452033	-6.760917	-3.005647	h	
C-CT	-2.834754	-11.110582	-5.004106	l	
H-H1	-2.398814	-11.689421	-5.824612	l	
C-CT	-2.565609	-9.628924	-5.163681	l	
H-HC	-1.560749	-9.479552	-5.553529	l	
H-HC	-3.302608	-9.145195	-5.799398	l	
O-OH	-4.248587	-11.253902	-4.941282	l	
H-HO	-4.479582	-12.183285	-4.834793	l	
K-K	-0.216976	-1.528448	-0.623147	l	
K-K	0.212662	-1.812375	3.221199	l	
Cu-Cu	-0.510405	-1.238805	-4.739176	h	
N-NC	1.001513	-0.100829	-5.432387	h	
N-NC	0.561544	-2.705838	-5.665600	h	
C-CA	0.124087	-3.898182	-5.921075	h	
H-HA	0.792499	-4.632587	-6.379374	h	
C-CA	-1.241264	-4.336686	-5.762805	h	
C-CA	-2.279416	-3.485362	-5.251447	h	
O-OS	-2.088150	-2.373164	-4.646932	h	
C-CA	1.864416	-2.275167	-6.039506	h	
C-CA	2.102046	-0.864708	-5.891644	h	
C-CA	3.335516	-0.341101	-6.197386	h	
H-HA	3.568938	0.705459	-6.010529	h	
C-CA	2.864222	-3.082230	-6.539047	h	
H-HA	2.721809	-4.153985	-6.646442	h	
C-CA	4.101370	-2.533551	-6.966868	h	
C-CA	4.344863	-1.145347	-6.773709	h	
C-CA	5.571912	-0.582746	-7.216798	h	
C-CA	6.491874	-1.353980	-7.881884	h	
C-CA	6.243028	-2.736950	-8.095589	h	
C-CA	5.088870	-3.317139	-7.625999	h	
H-HA	5.762255	0.473874	-7.035961	h	
H-HA	7.414671	-0.902012	-8.230864	h	
H-HA	6.977853	-3.335410	-8.623759	h	
H-HA	4.905233	-4.376825	-7.780145	h	
C-CA	-1.581831	-5.597521	-6.294308	h	
C-CA	-2.895126	-6.001955	-6.448094	h	

C-CA	-3.935871	-5.106296	-6.105239	h
C-CA	-3.627185	-3.904979	-5.491538	h
H-HA	-0.782763	-6.251537	-6.637706	h
H-HA	-3.121392	-6.950726	-6.925820	h
C-CT	-5.314242	-5.397091	-6.666187	h
H-HA	-4.374613	-3.163011	-5.225695	h
C-CA	0.977612	1.184854	-5.555330	h
C-CA	-0.124431	2.037543	-5.193624	h
H-HA	1.835527	1.698828	-5.997982	h
C-CA	-1.370839	1.540154	-4.672707	h
C-CA	-2.398516	2.512750	-4.471388	h
C-CA	-2.204416	3.854846	-4.731003	h
C-CA	-0.955590	4.329435	-5.183770	h
C-CA	0.053610	3.417678	-5.415457	h
O-OS	-1.617502	0.315730	-4.383519	h
H-HA	-3.347259	2.152100	-4.079777	h
C-CT	-3.326921	4.824199	-4.492797	h
H-HA	-0.797675	5.388501	-5.360957	h
H-HA	1.020490	3.768011	-5.771215	h
N-N3	-6.468079	-5.594895	-5.696202	h
H-HC	-5.625173	-4.585812	-7.326039	h
H-HC	-5.287522	-6.304466	-7.269715	h
H-HC	-2.941556	5.825620	-4.282790	h
H-HC	-3.928988	4.520945	-3.633060	h
N-N3	-4.302963	4.986074	-5.668949	h
C-CT	-6.643616	-4.390833	-4.793181	h
C-CT	-7.727798	-5.798368	-6.518317	h
C-CT	-6.209058	-6.791126	-4.799112	h
C-CT	-8.993669	-5.973141	-5.692234	h
H-HC	-7.819579	-4.927974	-7.167890	h
H-HC	-7.551572	-6.669304	-7.147904	h
H-HC	-7.027320	-6.793325	-4.076529	h
C-CT	-6.162703	-8.141150	-5.496376	h
H-HC	-5.288877	-6.576407	-4.252965	h
H-HC	-7.467560	-4.642027	-4.117538	h
H-HC	-5.747540	-4.325656	-4.177055	h
C-CT	-6.949746	-3.092488	-5.527498	h
H-HC	-6.259377	-2.880622	-6.342446	h
H-HC	-7.973992	-3.084736	-5.911585	h
H-HC	-6.852463	-2.280807	-4.803644	h
H-HC	-8.951663	-6.823606	-5.007898	h
H-HC	-9.239921	-5.090381	-5.093719	h
H-HC	-9.835104	-6.133664	-6.365724	h
H-HC	-7.134765	-8.428880	-5.902084	h
H-HC	-5.412216	-8.204960	-6.283323	h
H-HC	-5.910319	-8.888679	-4.739691	h
C-CT	-3.515420	5.334556	-6.914552	h
C-CT	-5.080360	3.703550	-5.902088	h
C-CT	-5.277022	6.092083	-5.306508	h
H-HC	-6.143705	5.988744	-5.959582	h
H-HC	-5.603965	5.875744	-4.286581	h
C-CT	-4.715873	7.505607	-5.360033	h
H-HC	-3.825353	7.612168	-4.735742	h
H-HC	-4.498957	7.859102	-6.365604	h
H-HC	-5.466575	8.161952	-4.914719	h
C-CT	-4.354810	5.616597	-8.153207	h
H-HC	-2.909727	6.200988	-6.641150	h
H-HC	-2.834608	4.499681	-7.082252	h

H-HC	-3.684175	6.007847	-8.919741	h
H-HC	-4.819400	4.716319	-8.554989	h
H-HC	-5.127739	6.367854	-7.979313	h
C-CT	-5.980543	3.285099	-4.747444	h
H-HC	-5.681478	3.879594	-6.793964	h
H-HC	-4.335496	2.938613	-6.123072	h
H-HC	-6.814482	3.975203	-4.600457	h
H-HC	-6.400267	2.306026	-4.984046	h
H-HC	-5.450912	3.185595	-3.797223	h

3/h-Telo

O-OH	-3.919176	-6.527523	8.886170	l
H-HO	-3.174879	-6.010384	8.539773	l
C-CT	-4.367820	-7.348924	7.814996	l
H-H1	-4.901211	-6.762808	7.061951	l
H-H1	-5.048440	-8.133024	8.161462	l
C-CT	-3.141836	-7.983352	7.160160	l
H-H1	-3.455543	-8.541816	6.275121	l
O-OS	-2.217463	-6.965338	6.795680	l
C-CT	-0.940848	-7.556135	6.790355	l
H-H2	-0.843107	-8.223131	5.925828	l
N-N*	0.165524	-6.569660	6.807791	l
C-CK	1.497576	-6.827730	6.581846	l
H-H5	1.886259	-7.816371	6.369699	l
N-NB	2.266341	-5.776767	6.623587	l
C-CB	1.386276	-4.732768	6.898837	l
C-CA	1.559370	-3.332092	7.049111	l
N-N2	2.731579	-2.698940	6.927494	l
H-H	3.570848	-3.223620	6.727182	l
H-H	2.757852	-1.695305	7.032039	l
N-NC	0.485215	-2.569985	7.327898	l
C-CQ	-0.701427	-3.159278	7.464769	l
H-H5	-1.531087	-2.501842	7.689507	l
N-NC	-0.996701	-4.453322	7.352507	l
C-CB	0.101748	-5.206227	7.045759	l
C-CT	-2.384795	-8.943908	8.083267	l
H-H1	-2.797363	-8.936073	9.099005	l
C-CT	-0.971380	-8.367470	8.075209	l
H-HC	-0.851283	-7.695265	8.924662	l
H-HC	-0.213240	-9.149435	8.084714	l
O-OS	-2.364797	-10.245138	7.520743	l
P-P	-3.534824	-11.311127	7.846825	l
O-O2	-3.790560	-11.281209	9.301012	l
O-O2	-3.203688	-12.581484	7.168742	l
O-OS	-4.801161	-10.649663	7.098148	l
C-CT	-5.059497	-10.897951	5.725170	l
H-H1	-5.398012	-11.928419	5.604020	l
H-H1	-4.141666	-10.757423	5.153166	l
C-CT	-6.133291	-9.929252	5.208260	l
H-H1	-7.019214	-9.995938	5.845476	l
O-OS	-5.569707	-8.619693	5.237870	l
C-CT	-5.393690	-8.149911	3.917388	l
H-H2	-6.219878	-7.467347	3.662087	l
N-N*	-4.091386	-7.455074	3.866856	l
C-CK	-2.883877	-7.864589	3.350891	l
H-H5	-2.701304	-8.839809	2.920576	l

N-NB	-1.944523	-6.968290	3.424924	1
C-CB	-2.569031	-5.869184	4.007688	1
C-C	-2.082658	-4.550454	4.279070	1
O-O	-0.965265	-4.084147	4.047729	1
N-NA	-3.044483	-3.720400	4.842829	1
H-H	-2.743460	-2.781503	5.060654	1
C-CA	-4.328304	-4.128089	5.123092	1
N-N2	-5.143803	-3.233024	5.651991	1
H-H	-4.842206	-2.281602	5.806513	1
H-H	-6.098522	-3.501579	5.835467	1
N-NC	-4.804056	-5.349475	4.864402	1
C-CB	-3.876192	-6.169832	4.303798	1
C-CT	-6.521805	-10.195840	3.744785	1
H-H1	-6.464854	-11.256665	3.489049	1
C-CT	-5.455130	-9.380393	3.024369	1
H-HC	-4.522437	-9.939266	3.033053	1
H-HC	-5.724495	-9.111512	2.004970	1
O-OS	-7.834660	-9.706956	3.519015	1
P-P	-8.513861	-9.649103	2.054905	1
O-O2	-9.952619	-9.953130	2.196252	1
O-O2	-7.679523	-10.401259	1.093865	1
O-OS	-8.343487	-8.069860	1.772144	1
C-CT	-9.289041	-7.164969	2.325707	1
H-H1	-9.316530	-7.283114	3.410638	1
H-H1	-10.276454	-7.413218	1.930196	1
C-CT	-9.018594	-5.692392	2.009239	1
H-H1	-9.924636	-5.126565	2.243500	1
O-OS	-7.920986	-5.157791	2.735091	1
C-CT	-7.585122	-3.915260	2.129088	1
H-H2	-7.919826	-3.066275	2.745105	1
N-N*	-6.133310	-3.833518	1.895740	1
C-CK	-5.214629	-4.835858	1.714989	1
H-H5	-5.487662	-5.883333	1.737144	1
N-NB	-3.990513	-4.409750	1.544180	1
C-CB	-4.115614	-3.019079	1.605744	1
C-C	-3.136926	-1.977165	1.510177	1
O-O	-1.917962	-2.081062	1.396685	1
N-NA	-3.685848	-0.701579	1.537736	1
H-H	-3.061008	0.089466	1.491552	1
C-CA	-5.031062	-0.457383	1.643560	1
N-N2	-5.390555	0.808050	1.529570	1
H-H	-4.679241	1.512009	1.393876	1
H-H	-6.366097	1.072121	1.505887	1
N-NC	-5.958539	-1.408093	1.780936	1
C-CB	-5.432608	-2.663884	1.766999	1
C-CT	-8.605161	-5.390749	0.579949	1
H-H1	-7.710904	-5.979722	0.358443	1
C-CT	-8.272564	-3.917310	0.766352	1
H-HC	-7.635884	-3.544765	-0.032006	1
H-HC	-9.187432	-3.329773	0.813511	1
O-OS	-9.596769	-5.579825	-0.403663	1
P-P	-9.191858	-5.545190	-1.954360	1
O-O2	-10.252403	-6.177102	-2.759466	1
O-O2	-7.788728	-5.988811	-2.081292	1
O-OS	-9.186605	-3.986974	-2.285203	1
C-CT	-10.339431	-3.192682	-2.043674	1
H-H1	-10.649799	-3.287017	-1.002745	1
H-H1	-11.166635	-3.564890	-2.640555	1

C-CT	-10.110187	-1.701350	-2.337160	1	
H-H1	-11.055310	-1.175538	-2.190087	1	
O-OS	-9.126801	-1.185599	-1.438414	1	
C-CT	-8.339616	-0.192790	-2.071851	1	H-H
H-H2	-8.393341	0.771557	-1.545364	1	
N-N*	-6.959641	-0.714211	-2.079410	h	
C-CK	-6.589882	-2.029918	-2.211541	h	
H-H5	-7.322111	-2.817797	-2.303055	h	
N-NB	-5.292867	-2.197741	-2.182993	h	
C-CB	-4.788916	-0.933603	-2.025389	h	
C-C	-3.411559	-0.548465	-1.894496	h	
O-O	-2.450479	-1.298868	-1.886976	h	
N-NA	-3.308972	0.846151	-1.718033	h	
H-H	-2.352981	1.225592	-1.665787	h	
C-CA	-4.382927	1.701330	-1.671310	h	
N-N2	-4.099651	3.027031	-1.556081	h	
H-H	-3.143025	3.325952	-1.341086	h	
H-H	-4.869856	3.610651	-1.242950	h	
N-NC	-5.650123	1.343753	-1.787094	h	
C-CB	-5.793427	0.009238	-1.950339	h	
C-CT	-9.627555	-1.371524	-3.751660	1	
H-H1	-8.959629	-2.156563	-4.092109	1	
C-CT	-8.873341	-0.072542	-3.496478	1	
H-HC	-8.084942	0.088900	-4.230750	1	
H-HC	-9.586686	0.753016	-3.530288	1	
O-OS	-10.620589	-1.071649	-4.719136	1	
P-P	-11.798631	-2.092156	-5.103330	1	
O-O2	-11.240630	-3.460637	-5.129093	1	
O-O2	-12.549949	-1.557512	-6.254963	1	
O-OS	-12.683564	-1.905401	-3.779256	1	
C-CT	-13.651708	-2.849072	-3.349617	1	
H-H1	-13.243824	-3.860862	-3.368279	1	
H-H1	-14.517287	-2.816181	-4.013883	1	
C-CT	-14.077858	-2.510491	-1.910924	1	
H-H1	-14.922358	-3.146400	-1.631270	1	
O-OS	-13.013149	-2.687589	-0.977565	1	
C-CT	-13.420277	-2.031629	0.206998	1	
H-H2	-14.223585	-2.613942	0.682709	1	
N-N*	-12.292040	-1.836687	1.162753	1	
C-CM	-11.207456	-1.030714	0.872818	1	
H-H4	-11.138103	-0.541013	-0.085110	1	
C-CM	-10.218551	-0.809082	1.776907	1	
C-CT	-9.068756	0.116322	1.415524	1	
H-HC	-8.335885	-0.430854	0.824380	1	
H-HC	-9.429075	0.970129	0.839193	1	
H-HC	-8.581466	0.476884	2.319381	1	
C-C	-10.256696	-1.459311	3.079366	1	
O-O	-9.397056	-1.384093	3.950909	1	
N-NA	-11.380361	-2.221742	3.307732	1	
H-H	-11.469136	-2.649679	4.211518	1	
C-C	-12.425233	-2.402390	2.430313	1	
O-O	-13.429973	-2.995800	2.799302	1	
C-CT	-14.490341	-1.050087	-1.719670	1	
H-H1	-13.964204	-0.418015	-2.433308	1	
C-CT	-13.997609	-0.722659	-0.316938	1	
H-HC	-13.244665	0.055283	-0.365536	1	
H-HC	-14.816276	-0.384964	0.301266	1	
O-OS	-15.890706	-0.855662	-1.749125	1	

P-P	-16.635159	-0.274011	-3.050712	1
O-O2	-18.072805	-0.127552	-2.748195	1
O-O2	-16.185754	-1.026825	-4.238722	1
O-OS	-15.985739	1.194922	-3.084118	1
C-CT	-14.974694	1.580344	-4.012246	1
H-H1	-15.419912	1.766085	-4.991554	1
H-H1	-14.227457	0.793263	-4.126871	1
C-CT	-14.283708	2.860347	-3.519419	1
H-H1	-13.394973	3.050579	-4.125781	1
O-OS	-15.204763	3.936478	-3.647203	1
C-CT	-15.412968	4.545194	-2.382508	1
H-H2	-14.810097	5.460047	-2.302822	1
N-N*	-16.856887	4.826967	-2.205210	1
C-CM	-17.814802	3.974202	-2.713362	1
H-H4	-17.504187	3.121754	-3.304529	1
C-CM	-19.135603	4.170294	-2.472495	1
C-CT	-20.141130	3.168327	-3.024880	1
H-HC	-20.139994	3.202521	-4.114455	1
H-HC	-19.886554	2.160576	-2.689473	1
H-HC	-21.144542	3.410755	-2.667753	1
C-C	-19.568423	5.313634	-1.672340	1
O-O	-20.723461	5.589506	-1.371192	1
N-NA	-18.549010	6.119309	-1.208949	1
H-H	-18.807358	6.919600	-0.660571	1
C-C	-17.205474	5.925381	-1.428785	1
O-O	-16.377994	6.677776	-0.930358	1
C-CT	-13.872092	2.767777	-2.045034	1
H-H1	-13.870978	1.734172	-1.704708	1
C-CT	-14.970222	3.532589	-1.336039	1
H-HC	-15.780985	2.843262	-1.113749	1
H-HC	-14.626604	4.008354	-0.420146	1
O-OS	-12.614797	3.376046	-1.825241	1
P-P	-11.399776	2.516059	-1.219795	1
O-O2	-10.155323	3.302512	-1.298769	1
O-O2	-11.464023	1.170127	-1.818892	1
O-OS	-11.856907	2.399927	0.317062	1
C-CT	-12.008948	3.572787	1.110128	1
H-H1	-12.472995	4.357494	0.511645	1
H-H1	-11.028407	3.939320	1.423861	1
C-CT	-12.902057	3.332382	2.338614	1
H-H1	-13.064430	4.292212	2.825175	1
O-OS	-14.166870	2.800806	1.944731	1
C-CT	-14.531138	1.839304	2.915885	1
H-H2	-14.837513	2.334526	3.847340	1
N-N*	-15.606956	0.942143	2.435118	1
C-CK	-15.794560	-0.399022	2.697792	1
H-H5	-15.120220	-1.003340	3.296319	1
N-NB	-16.834258	-0.914765	2.102191	1
C-CB	-17.430814	0.172079	1.462712	1
C-CA	-18.599850	0.322493	0.671928	1
N-N2	-19.407251	-0.684642	0.324432	1
H-H	-19.188491	-1.628066	0.608069	1
H-H	-20.204338	-0.492776	-0.262377	1
N-NC	-18.946896	1.554477	0.248433	1
C-CQ	-18.175742	2.588284	0.582685	1
H-H5	-18.507001	3.559590	0.241239	1
N-NC	-17.047539	2.579599	1.290001	1
C-CB	-16.715990	1.321628	1.704015	1

C-CT	-12.300223	2.333236	3.345192	1
H-H1	-11.251322	2.111893	3.131116	1
C-CT	-13.200147	1.129187	3.112036	1
H-HC	-12.921649	0.627713	2.190130	1
H-HC	-13.206537	0.449906	3.963731	1
O-OS	-12.500440	2.653014	4.717500	1
P-P	-11.879191	3.947648	5.454292	1
O-O2	-11.946214	3.715957	6.911538	1
O-O2	-12.474035	5.167730	4.874439	1
O-OS	-10.341744	3.883006	5.002840	1
C-CT	-9.412524	3.015862	5.626806	1
H-H1	-9.532043	1.989515	5.278402	1
H-H1	-9.538879	3.032678	6.711684	1
C-CT	-8.012225	3.533852	5.318273	1
H-H1	-7.976639	4.600383	5.555612	1
O-OS	-7.053805	2.819073	6.077929	1
C-CT	-5.782106	3.074285	5.514429	1
H-H2	-5.249380	3.863211	6.060147	1
N-N*	-5.002516	1.829778	5.507941	1
C-CK	-5.466021	0.540424	5.551237	1
H-H5	-6.517757	0.301432	5.667502	1
N-NB	-4.527122	-0.356065	5.432738	1
C-CB	-3.357825	0.391917	5.305040	1
C-C	-1.997517	-0.021174	5.140455	1
O-O	-1.553551	-1.162726	5.054425	1
N-NA	-1.102836	1.036958	5.064683	1
H-H	-0.120467	0.798582	5.056643	1
C-CA	-1.485136	2.355598	5.107967	1
N-N2	-0.514783	3.250845	5.006106	1
H-H	0.453406	2.974397	4.904794	1
H-H	-0.758709	4.227745	5.042467	1
N-NC	-2.753976	2.766052	5.246515	1
C-CB	-3.639828	1.734911	5.350424	1
C-CT	-7.548701	3.336878	3.880102	1
H-H1	-7.786906	2.321296	3.560726	1
C-CT	-6.048365	3.489035	4.073947	1
H-HC	-5.529634	2.843974	3.373531	1
H-HC	-5.745161	4.525734	3.941467	1
O-OS	-8.063030	4.302551	2.982231	1
P-P	-7.714809	4.283777	1.409079	1
O-O2	-8.700448	5.130995	0.709888	1
O-O2	-7.496051	2.881600	0.995519	1
O-OS	-6.294383	5.038615	1.395569	1
C-CT	-6.197194	6.400749	1.793491	1
H-H1	-6.698377	6.537785	2.752708	1
H-H1	-6.696920	7.030125	1.052982	1
C-CT	-4.740621	6.862346	1.941823	1
H-H1	-4.740318	7.906201	2.265617	1
O-OS	-3.995197	6.088139	2.880745	1
C-CT	-2.647638	5.970638	2.431322	1
H-H2	-1.936248	6.267406	3.211962	1
N-N*	-2.418735	4.564046	2.022099	1
C-CK	-3.348558	3.573339	1.852933	1
H-H5	-4.406320	3.779280	1.906230	1
N-NB	-2.848905	2.386850	1.647674	1
C-CB	-1.475206	2.611588	1.628243	1
C-C	-0.387333	1.700704	1.430203	1
O-O	-0.423286	0.474156	1.334245	1

N-NA	0.839162	2.340309	1.316117	1	
H-H	1.649656	1.772452	1.121328	1	
C-CA	0.997880	3.696146	1.456779	1	
N-N2	2.213539	4.155453	1.239532	1	
H-H	2.961418	3.542927	0.953569	1	
H-H	2.368988	5.148120	1.398481	1	
N-NC	0.010630	4.554061	1.743170	1	
C-CB	-1.206839	3.951253	1.799317	1	
C-CT	-3.951836	6.782334	0.646511	1	
H-H1	-4.128951	5.806905	0.187254	1	
C-CT	-2.550763	6.891293	1.224894	1	
H-HC	-1.766219	6.592993	0.536811	1	
H-HC	-2.378654	7.911092	1.560546	1	
O-OS	-4.251360	7.859549	-0.214048	1	
P-P	-4.132069	7.699790	-1.801522	1	
O-O2	-4.803211	8.837718	-2.455744	1	
O-O2	-4.507572	6.314763	-2.139770	1	
O-OS	-2.564089	7.829984	-2.070731	1	
C-CT	-1.833638	8.936408	-1.561225	1	
H-H1	-2.055480	9.075939	-0.502236	1	
H-H1	-2.135522	9.850735	-2.071827	1	
C-CT	-0.318630	8.738194	-1.690012	1	
H-H1	0.150199	9.541550	-1.132122	1	
O-OS	0.074507	7.477352	-1.144001	1	
C-CT	0.737849	6.708711	-2.135213	1	H-H
H-H2	1.824435	6.727231	-1.981806	1	
N-N*	0.196711	5.338429	-2.049618	h	
C-CK	-1.076278	5.000484	-1.649141	h	
H-H5	-1.826043	5.755873	-1.458894	h	
N-NB	-1.251909	3.708371	-1.554444	h	
C-CB	-0.044455	3.174149	-1.933850	h	
C-C	0.331747	1.793666	-2.025283	h	
O-O	-0.354507	0.815857	-1.756696	h	
N-NA	1.648012	1.663445	-2.496229	h	
H-H	1.993491	0.715326	-2.671186	h	
C-CA	2.433518	2.718210	-2.903363	h	
N-N2	3.576939	2.370662	-3.547827	h	
H-H	3.933158	1.418507	-3.468087	h	
H-H	4.250233	3.108604	-3.723244	h	
N-NC	2.117588	3.989237	-2.762698	h	
C-CB	0.870413	4.158793	-2.262431	h	
C-CT	0.198456	8.812417	-3.125487	1	
H-H1	-0.518049	9.290819	-3.796777	1	
C-CT	0.370554	7.344185	-3.472263	1	
H-HC	-0.585643	6.960501	-3.822403	1	
H-HC	1.154642	7.198381	-4.215221	1	
O-OS	1.456299	9.462336	-3.172854	1	
P-P	1.575374	11.065799	-3.297575	1	
O-O2	0.561921	11.524875	-4.270298	1	
O-O2	2.992849	11.423917	-3.488778	1	
O-OS	1.134559	11.584616	-1.832809	1	
C-CT	-0.053185	12.353289	-1.655276	1	
H-H1	-0.880960	11.879802	-2.182756	1	
H-H1	0.082834	13.334952	-2.104242	1	
C-CT	-0.471182	12.496447	-0.184278	1	
H-H1	-1.281817	13.227121	-0.119009	1	
O-OS	-0.946299	11.223517	0.257828	1	
C-CT	-0.687150	11.056650	1.642291	1	

H-H2	-1.625510	10.920026	2.197962	1
N-N*	0.195654	9.875059	1.840975	1
C-CM	1.332160	9.680375	1.085539	1
H-H4	1.576319	10.366081	0.290962	1
C-CM	2.150664	8.619702	1.285308	1
C-CT	3.370473	8.464089	0.393714	1
H-HC	3.075380	8.043355	-0.567614	1
H-HC	3.846012	9.426265	0.215503	1
H-HC	4.087630	7.789540	0.857035	1
C-C	1.854915	7.657150	2.339759	1
O-O	2.532676	6.681530	2.648472	1
N-NA	0.702648	7.908066	3.046448	1
H-H	0.479428	7.271882	3.787437	1
C-C	-0.152295	8.964990	2.838528	1
O-O	-1.176387	9.055890	3.504618	1
C-CT	0.611361	12.919731	0.816915	1
H-H1	1.556027	12.429477	0.579477	1
C-CT	-0.005339	12.345726	2.087907	1
H-HC	0.733232	12.166488	2.865632	1
H-HC	-0.762370	13.035669	2.460152	1
O-OS	0.801800	14.308749	1.029985	1
P-P	1.469460	15.263816	-0.080540	1
O-O2	2.046996	16.439204	0.600377	1
O-O2	0.507028	15.443963	-1.184578	1
O-OS	2.691654	14.360919	-0.603886	1
C-CT	3.141310	14.424343	-1.953710	1
H-H1	3.081383	15.454425	-2.312342	1
H-H1	2.498460	13.809865	-2.583112	1
C-CT	4.603921	13.970807	-2.100810	1
H-H1	4.835857	13.845798	-3.162345	1
O-OS	5.403775	15.006083	-1.535926	1
C-CT	6.261152	14.427087	-0.571733	1
H-H2	7.190284	14.088836	-1.052386	1
N-N*	6.540700	15.366166	0.529993	1
C-CM	5.621100	16.321032	0.906172	1
H-H4	4.690094	16.403968	0.356293	1
C-CM	5.862097	17.150702	1.952837	1
C-CT	4.811840	18.183424	2.340066	1
H-HC	4.883832	19.047050	1.678903	1
H-HC	3.812475	17.751457	2.271569	1
H-HC	4.980037	18.511086	3.367981	1
C-C	7.108711	17.029193	2.706646	1
O-O	7.417785	17.674850	3.702100	1
N-NA	7.979768	16.062855	2.249527	1
H-H	8.850856	15.954156	2.735193	1
C-C	7.754374	15.217364	1.190751	1
O-O	8.592057	14.382628	0.865431	1
C-CT	4.968776	12.670356	-1.365189	1
H-H1	4.100554	12.012632	-1.253822	1
C-CT	5.479521	13.236088	-0.050567	1
H-HC	4.659045	13.570914	0.576309	1
H-HC	6.112995	12.550495	0.496291	1
O-OS	6.053948	12.040712	-2.038310	1
P-P	6.378794	10.465604	-1.891450	1
O-O2	7.525462	10.143584	-2.765575	1
O-O2	5.111046	9.718981	-2.015614	1
O-OS	6.872539	10.361737	-0.359538	1
C-CT	8.184430	10.742248	0.055438	1

H-H1	8.382076	11.784376	-0.206847	1
H-H1	8.923205	10.113398	-0.445917	1
C-CT	8.340335	10.588465	1.579237	1
H-H1	9.387118	10.741455	1.855812	1
O-OS	7.520456	11.561694	2.216481	1
C-CT	6.652574	10.927625	3.132883	1
H-H2	7.123334	10.894734	4.123316	1
N-N*	5.400088	11.715498	3.159345	1
C-CK	4.155081	11.392983	2.675443	1
H-H5	3.907001	10.432817	2.252692	1
N-NB	3.296521	12.368735	2.714035	1
C-CB	3.989539	13.393746	3.353967	1
C-CA	3.638219	14.708732	3.749414	1
N-N2	2.466143	15.289086	3.474324	1
H-H	1.806524	14.835140	2.850029	1
H-H	2.285749	16.225474	3.799606	1
N-NC	4.539367	15.441035	4.431639	1
C-CQ	5.739779	14.915883	4.687055	1
H-H5	6.430281	15.556344	5.224856	1
N-NC	6.205211	13.714607	4.340145	1
C-CB	5.265128	12.988246	3.669486	1
C-CT	7.874520	9.213494	2.078788	1
H-H1	7.860115	8.483321	1.262901	1
C-CT	6.475739	9.513936	2.587926	1
H-HC	5.797518	9.509325	1.740011	1
H-HC	6.153731	8.817014	3.360564	1
O-OS	8.634408	8.749501	3.179247	1
P-P	9.965142	7.876550	2.952350	1
O-O2	10.633466	7.668822	4.252469	1
O-O2	10.697798	8.431873	1.795661	1
O-OS	9.257626	6.504721	2.506748	1
C-CT	8.575614	5.686530	3.446298	1
H-H1	8.009102	6.295606	4.153234	1
H-H1	9.282581	5.073922	4.008282	1
C-CT	7.607694	4.790345	2.680057	1
H-H1	8.171823	4.175581	1.968933	1
O-OS	6.856340	3.976729	3.580711	1
C-CT	5.601397	3.835801	2.957152	1
H-H2	5.737733	3.254776	2.037340	1
N-N*	4.562405	3.172741	3.762678	1
C-CK	3.359848	3.671942	4.211454	1
H-H5	3.114535	4.729228	4.225178	1
N-NB	2.508089	2.754948	4.578825	1
C-CB	3.186280	1.558358	4.347940	1
C-C	2.748217	0.199397	4.461009	1
O-O	1.641643	-0.218570	4.796288	1
N-NA	3.716502	-0.726465	4.091147	1
H-H	3.461344	-1.701738	4.169085	1
C-CA	4.966313	-0.377703	3.634574	1
N-N2	5.779386	-1.368937	3.300687	1
H-H	5.493248	-2.336408	3.369951	1
H-H	6.698043	-1.147614	2.936462	1
N-NC	5.378277	0.886809	3.482512	1
C-CB	4.449625	1.806764	3.868625	1
C-CT	6.571907	5.610166	1.890071	1
H-H1	6.796898	6.675809	1.874643	1
C-CT	5.286642	5.277198	2.612743	1
H-HC	5.170587	5.875418	3.515469	1

H-HC	4.431114	5.357856	1.954522	1
O-OS	6.466154	5.061015	0.598182	1
P-P	5.856803	5.835403	-0.658192	1
O-O2	6.447237	7.187135	-0.695918	1
O-O2	4.393518	5.634688	-0.662180	1
O-OS	6.507165	4.923529	-1.807170	1
C-CT	7.910982	4.696627	-1.832762	1
H-H1	8.416534	5.349730	-1.118437	1
H-H1	8.285692	4.927030	-2.830937	1
C-CT	8.268113	3.239364	-1.500553	1
H-H1	9.356824	3.140240	-1.547544	1
O-OS	7.820665	2.791535	-0.215534	1
C-CT	7.505866	1.409245	-0.275997	1
H-H2	8.021930	0.836979	0.503941	1
N-N*	6.048127	1.184479	-0.140864	1
C-CK	5.027173	2.100932	-0.092163	1
H-H5	5.199527	3.160840	-0.249749	1
N-NB	3.861451	1.582166	0.194992	1
C-CB	4.118367	0.209197	0.283998	1
C-C	3.247912	-0.904466	0.539768	1
O-O	2.048335	-0.901412	0.805148	1
N-NA	3.879371	-2.136670	0.438996	1
H-H	3.329977	-2.963315	0.613608	1
C-CA	5.214689	-2.282613	0.166917	1
N-N2	5.640092	-3.531057	0.051391	1
H-H	4.999630	-4.299101	0.193756	1
H-H	6.610927	-3.690414	-0.164585	1
N-NC	6.058694	-1.260282	-0.022176	1
C-CB	5.449071	-0.041925	0.044033	1
C-CT	7.666553	2.248600	-2.485349	1
H-H1	6.595198	2.445908	-2.575935	1
C-CT	7.951743	0.997898	-1.666637	1
H-HC	7.419597	0.125078	-1.995399	1
H-HC	9.014548	0.782659	-1.673860	1
O-OS	8.326581	2.262361	-3.738183	1
P-P	7.656833	1.641559	-5.068349	1
O-O2	8.429708	2.070635	-6.248616	1
O-O2	6.196520	1.863207	-5.005456	1
O-OS	7.885060	0.071961	-4.876971	1
C-CT	9.163183	-0.447207	-4.543908	1
H-H1	9.640987	0.185271	-3.794336	1
H-H1	9.812880	-0.441576	-5.417994	1
C-CT	9.065467	-1.860936	-3.952048	1
H-H1	10.017002	-2.069516	-3.471586	1
O-OS	8.010552	-1.931931	-2.988952	1
C-CT	7.010065	-2.833171	-3.426141	1
H-H2	7.068409	-3.760184	-2.844006	1
N-N*	5.670162	-2.209085	-3.307790	h
C-CK	5.350777	-0.867586	-3.295052	h
H-H5	6.088459	-0.106130	-3.482711	h
N-NB	4.075472	-0.641745	-3.115580	h
C-CB	3.519171	-1.900414	-3.045160	h
C-C	2.159156	-2.291570	-2.984323	h
O-O	1.168101	-1.531166	-2.887340	h
N-NA	2.004817	-3.664940	-3.060809	h
H-H	1.034136	-4.009174	-3.015980	h
C-CA	3.033284	-4.548477	-3.307423	h
N-N2	2.677035	-5.813496	-3.597365	h

H-H

H-H	1.710708	-6.134134	-3.477657	h
H-H	3.429705	-6.485056	-3.664249	h
N-NC	4.307864	-4.212960	-3.319913	h
C-CB	4.487684	-2.886912	-3.195332	h
C-CT	8.813937	-2.955703	-4.987937	l
H-H1	9.106680	-2.651074	-5.994531	l
C-CT	7.311730	-3.123617	-4.884604	l
H-HC	6.838730	-2.361575	-5.490612	l
H-HC	6.991650	-4.122883	-5.176948	l
O-OS	9.455418	-4.159175	-4.608035	l
P-P	10.959078	-4.498788	-5.081821	l
O-O2	11.026864	-4.297077	-6.545025	l
O-O2	11.363678	-5.788653	-4.489733	l
O-OS	11.822873	-3.337032	-4.369969	l
C-CT	12.396326	-2.281109	-5.135399	l
H-H1	11.629675	-1.808165	-5.746816	l
H-H1	13.136228	-2.692913	-5.819980	l
C-CT	13.039752	-1.198156	-4.258305	l
H-H1	13.624772	-0.522793	-4.887445	l
O-OS	12.009208	-0.468357	-3.598235	l
C-CT	12.508768	0.075639	-2.385402	l
H-H2	12.562433	1.171436	-2.450119	l
N-N*	11.617201	-0.327827	-1.268217	l
C-CM	11.131806	-1.613806	-1.151348	l
H-H4	11.413629	-2.357633	-1.881431	l
C-CM	10.267996	-1.959989	-0.163702	l
C-CT	9.714104	-3.375201	-0.139138	l
H-HC	8.814532	-3.404421	0.474786	l
H-HC	9.457047	-3.697680	-1.150131	l
H-HC	10.458844	-4.051981	0.276875	l
C-C	9.868205	-0.975998	0.838708	l
O-O	9.078504	-1.147642	1.763026	l
N-NA	10.439507	0.269520	0.684935	l
H-H	10.217012	0.973538	1.365218	l
C-C	11.270949	0.652851	-0.341493	l
O-O	11.631657	1.820037	-0.430485	l
C-CT	13.939934	-1.701868	-3.131808	l
H-H1	13.465332	-2.555569	-2.650107	l
C-CT	13.909371	-0.499944	-2.202199	l
H-HC	14.109545	-0.783409	-1.169880	l
H-HC	14.643072	0.234283	-2.534430	l
O-OS	15.296443	-1.952950	-3.455757	l
P-P	15.773175	-3.321864	-4.156022	l
O-O2	17.185012	-3.553490	-3.792792	l
O-O2	15.350484	-3.335708	-5.568698	l
O-OS	14.873064	-4.360618	-3.328907	l
C-CT	14.956258	-5.762400	-3.523105	l
H-H1	15.982131	-6.044022	-3.773722	l
H-H1	14.294435	-6.061502	-4.338288	l
C-CT	14.574005	-6.494274	-2.226181	l
H-H1	14.550291	-7.570376	-2.417133	l
O-OS	15.587026	-6.190105	-1.270785	l
C-CT	14.975975	-5.679166	-0.101745	l
H-H2	14.759353	-6.505476	0.585224	l
N-N*	15.840802	-4.659687	0.527668	l
C-CM	16.462673	-3.698361	-0.238498	l
H-H4	16.413622	-3.775153	-1.317558	l
C-CM	17.125621	-2.662576	0.333150	l

C-CT	17.780165	-1.622762	-0.566695	1
H-HC	18.687511	-2.039466	-1.006182	1
H-HC	17.099268	-1.328216	-1.366544	1
H-HC	18.048057	-0.739770	0.017276	1
C-C	17.202724	-2.562972	1.789671	1
O-O	17.739838	-1.663537	2.425508	1
N-NA	16.605899	-3.598990	2.478859	1
H-H	16.678780	-3.585438	3.479409	1
C-C	15.945975	-4.665884	1.914835	1
O-O	15.479372	-5.553835	2.619984	1
C-CT	13.228607	-6.074870	-1.609165	1
H-H1	12.548343	-5.662449	-2.360291	1
C-CT	13.680832	-5.041302	-0.588192	1
H-HC	13.876626	-4.089664	-1.071805	1
H-HC	12.971307	-4.900499	0.217380	1
O-OS	12.673528	-7.200528	-0.943052	1
P-P	11.142914	-7.258756	-0.431237	1
O-O2	10.836789	-8.652675	-0.055313	1
O-O2	10.287105	-6.525193	-1.385625	1
O-OS	11.203811	-6.396712	0.920533	1
C-CT	11.980530	-6.816463	2.034723	1
H-H1	12.998855	-7.050324	1.727147	1
H-H1	11.545104	-7.717412	2.471512	1
C-CT	12.037795	-5.708682	3.092703	1
H-H1	12.600858	-6.076439	3.955889	1
O-OS	12.669911	-4.532014	2.612754	1
C-CT	12.272595	-3.505669	3.490211	1
H-H2	12.730767	-3.634918	4.478933	1
N-N*	12.644605	-2.198963	2.916336	1
C-CK	13.458555	-1.940797	1.841426	1
H-H5	13.896048	-2.727323	1.243376	1
N-NB	13.664290	-0.673334	1.611686	1
C-CB	12.930429	-0.036593	2.615056	1
C-CA	12.692703	1.323126	2.951595	1
N-N2	13.184643	2.366870	2.276525	1
H-H	13.723623	2.213401	1.436516	1
H-H	12.955320	3.303137	2.572968	1
N-NC	11.898556	1.605199	4.003909	1
C-CQ	11.369302	0.599263	4.700784	1
H-H5	10.741981	0.881813	5.536877	1
N-NC	11.513757	-0.710102	4.497004	1
C-CB	12.309905	-0.964230	3.418754	1
C-CT	10.646699	-5.256215	3.556412	1
H-H1	9.880003	-5.568458	2.844495	1
C-CT	10.769377	-3.731977	3.566186	1
H-HC	10.297596	-3.313393	2.681174	1
H-HC	10.342515	-3.291023	4.466489	1
O-OS	10.326332	-5.697008	4.861321	1
P-P	10.160219	-7.260304	5.224795	1
O-O2	9.433975	-7.363160	6.506223	1
O-O2	11.463466	-7.934244	5.056098	1
O-OS	9.194912	-7.796072	4.055437	1
C-CT	8.648293	-9.104855	4.140056	1
H-H1	8.200112	-9.241803	5.127686	1
H-H1	9.445332	-9.839500	4.016090	1
C-CT	7.546695	-9.362742	3.105607	1
H-H1	7.245707	-10.410039	3.181033	1
O-OS	6.441961	-8.533816	3.438779	1

C-CT	6.050111	-7.829733	2.282676	1
H-H2	5.321331	-8.430658	1.719830	1
N-N*	5.453063	-6.548579	2.707642	1
C-CK	6.036565	-5.323433	2.929056	1
H-H5	7.099355	-5.140308	2.845667	1
N-NB	5.192348	-4.384109	3.254986	1
C-CB	3.960377	-5.038795	3.281064	1
C-C	2.641202	-4.549371	3.549375	1
O-O	2.291550	-3.396844	3.798573	1
N-NA	1.665300	-5.537887	3.489373	1
H-H	0.719684	-5.251804	3.700766	1
C-CA	1.936415	-6.851378	3.188441	1
N-N2	0.906937	-7.676253	3.121523	1
H-H	-0.039076	-7.343326	3.250864	1
H-H	1.077426	-8.627363	2.832310	1
N-NC	3.154912	-7.324034	2.913671	1
C-CB	4.121162	-6.369583	2.980516	1
C-CT	7.919523	-9.070999	1.643924	1
H-H1	9.000566	-9.091052	1.486947	1
C-CT	7.322687	-7.680259	1.462604	1
H-HC	7.992539	-6.948685	1.906601	1
H-HC	7.107786	-7.435382	0.425526	1
O-OS	7.252743	-10.045113	0.854647	1
P-P	7.396130	-10.168255	-0.750793	1
O-O2	7.892362	-11.520554	-1.076447	1
O-O2	8.054435	-8.966096	-1.299239	1
O-OS	5.834536	-10.091653	-1.120113	1
C-CT	4.943032	-11.104203	-0.675443	1
H-H1	5.010133	-11.198459	0.410287	1
H-H1	5.222223	-12.057840	-1.126504	1
C-CT	3.491996	-10.775313	-1.036227	1
H-H1	2.863895	-11.635726	-0.795578	1
O-OS	3.074510	-9.649037	-0.270027	1
C-CT	2.339205	-8.820280	-1.139055	1
H-H2	1.327254	-9.224454	-1.275083	1
N-N*	2.282005	-7.445350	-0.614109	1
C-CK	3.294652	-6.535573	-0.429230	1
H-H5	4.330231	-6.762317	-0.649374	1
N-NB	2.894922	-5.378405	0.027273	1
C-CB	1.514723	-5.550029	0.181647	1
C-C	0.504765	-4.659886	0.671075	1
O-O	0.635342	-3.503857	1.063170	1
N-NA	-0.769852	-5.210845	0.677568	1
H-H	-1.523804	-4.659917	1.057807	1
C-CA	-1.044267	-6.484042	0.250617	1
N-N2	-2.319931	-6.832883	0.255492	1
H-H	-3.024971	-6.190454	0.590840	1
H-H	-2.574528	-7.748535	-0.082680	1
N-NC	-0.121999	-7.336315	-0.208938	1
C-CB	1.136421	-6.812335	-0.207021	1
C-CT	3.295221	-10.427640	-2.521296	1
H-H1	4.161591	-10.712881	-3.126559	1
C-CT	3.109028	-8.919087	-2.444645	1
H-HC	4.081315	-8.437108	-2.353040	1
H-HC	2.537679	-8.526582	-3.280574	1
O-OS	2.099838	-11.032083	-2.988954	1
P-P	1.783427	-11.208876	-4.559954	1
O-O2	2.103995	-12.595848	-4.949263	1

O-O2	2.356586	-10.064088	-5.297988	l	
O-OS	0.191997	-11.024476	-4.551368	l	
C-CT	-0.650970	-11.931860	-3.853713	l	
H-H1	-0.273576	-12.057777	-2.837349	l	
H-H1	-0.641005	-12.900949	-4.353507	l	
C-CT	-2.092609	-11.407257	-3.753743	l	
H-H1	-2.700622	-12.136397	-3.216137	l	
O-OS	-2.037071	-10.192637	-3.017891	l	
C-CT	-2.603774	-9.172799	-3.808350	l	H-H
H-H2	-3.663867	-9.071663	-3.554098	l	
N-N*	-1.857808	-7.930948	-3.559893	h	
C-CK	-0.512281	-7.720143	-3.743607	h	
H-H5	0.136800	-8.514339	-4.093300	h	
N-NB	-0.151671	-6.503919	-3.417067	h	
C-CB	-1.315505	-5.896600	-2.995433	h	
C-C	-1.533454	-4.563132	-2.512970	h	
O-O	-0.695783	-3.672338	-2.379981	h	
N-NA	-2.880154	-4.358906	-2.175035	h	
H-H	-3.153040	-3.390139	-1.966407	h	
C-CA	-3.853228	-5.330626	-2.231383	h	
N-N2	-5.056316	-5.020976	-1.677863	h	
H-H	-5.300219	-4.035160	-1.624394	h	
H-H	-5.830569	-5.654658	-1.888123	h	
N-NC	-3.669333	-6.543172	-2.713545	h	
C-CB	-2.384949	-6.765429	-3.075377	h	
C-CT	-2.753031	-11.098006	-5.111534	l	
H-H1	-2.303661	-11.677188	-5.924510	l	
C-CT	-2.470706	-9.617694	-5.261010	l	
H-HC	-1.457019	-9.474194	-5.629627	l	
H-HC	-3.191865	-9.126211	-5.909447	l	
O-OH	-4.168896	-11.232614	-5.078603	l	
H-HO	-4.407497	-12.161165	-4.982431	l	
K-K	-0.172742	-1.554171	-0.579780	l	
K-K	0.236679	-1.822043	3.221907	l	
Zn-Zn	-0.440292	-1.365079	-4.258508	h	
N-NC	1.025689	-0.186710	-5.363305	h	
N-NC	0.598016	-2.802629	-5.584693	h	
C-CA	0.117864	-3.921960	-6.014872	h	
H-HA	0.727174	-4.563986	-6.660626	h	
C-CA	-1.245089	-4.374271	-5.839018	h	
C-CA	-2.272873	-3.537772	-5.280834	h	
O-OS	-2.070263	-2.462448	-4.621864	h	
C-CA	1.882507	-2.359633	-5.991705	h	
C-CA	2.110667	-0.945050	-5.857085	h	
C-CA	3.338587	-0.418640	-6.185573	h	
H-HA	3.566091	0.631084	-6.006413	h	
C-CA	2.889066	-3.165235	-6.482288	h	
H-HA	2.756651	-4.242310	-6.550521	h	
C-CA	4.115559	-2.612670	-6.937544	h	
C-CA	4.346947	-1.219083	-6.769596	h	
C-CA	5.563104	-0.651043	-7.236260	h	
C-CA	6.482654	-1.422862	-7.901900	h	
C-CA	6.245787	-2.811542	-8.089858	h	
C-CA	5.103866	-3.396117	-7.595455	h	
H-HA	5.744827	0.410352	-7.073286	h	
H-HA	7.395771	-0.967353	-8.271155	h	
H-HA	6.979532	-3.410791	-8.618741	h	
H-HA	4.929080	-4.459869	-7.731718	h	

C-CA	-1.597431	-5.603035	-6.428470	h
C-CA	-2.914512	-6.000675	-6.581694	h
C-CA	-3.944283	-5.110058	-6.202072	h
C-CA	-3.623967	-3.929345	-5.553405	h
H-HA	-0.804783	-6.240486	-6.815853	h
H-HA	-3.150412	-6.928755	-7.094381	h
C-CT	-5.328285	-5.381083	-6.752616	h
H-HA	-4.363935	-3.187116	-5.268215	h
C-CA	0.980829	1.083570	-5.580676	h
C-CA	-0.093621	1.962880	-5.188275	h
H-HA	1.786462	1.569765	-6.141964	h
C-CA	-1.331512	1.492050	-4.621377	h
C-CA	-2.350240	2.481080	-4.450123	h
C-CA	-2.140506	3.817203	-4.732474	h
C-CA	-0.891154	4.268259	-5.203869	h
C-CA	0.096897	3.333104	-5.444649	h
O-OS	-1.572778	0.283464	-4.278363	h
H-HA	-3.304173	2.142164	-4.052003	h
C-CT	-3.251677	4.800170	-4.502498	h
H-HA	-0.717935	5.322072	-5.398269	h
H-HA	1.058602	3.661016	-5.835109	h
N-N3	-6.467842	-5.585907	-5.767161	h
H-HC	-5.644450	-4.558960	-7.396268	h
H-HC	-5.316984	-6.280735	-7.368176	h
H-HC	-2.859641	5.800450	-4.301506	h
H-HC	-3.855534	4.507953	-3.640973	h
N-N3	-4.230331	4.956764	-5.677595	h
C-CT	-6.635327	-4.387518	-4.855442	h
C-CT	-7.735649	-5.788818	-6.576049	h
C-CT	-6.192431	-6.782272	-4.875312	h
C-CT	-8.992422	-5.975511	-5.740247	h
H-HC	-7.837645	-4.912465	-7.216334	h
H-HC	-7.562097	-6.653097	-7.215367	h
H-HC	-7.013972	-6.801870	-4.156218	h
C-CT	-6.113073	-8.127198	-5.578683	h
H-HC	-5.277298	-6.554451	-4.325719	h
H-HC	-7.458248	-4.639507	-4.179368	h
H-HC	-5.736979	-4.332760	-4.242268	h
C-CT	-6.934809	-3.079647	-5.574846	h
H-HC	-6.250130	-2.866680	-6.394031	h
H-HC	-7.963402	-3.056165	-5.947117	h
H-HC	-6.818327	-2.276592	-4.843878	h
H-HC	-8.943860	-6.835553	-5.068774	h
H-HC	-9.230582	-5.100205	-5.127892	h
H-HC	-9.840676	-6.124997	-6.407521	h
H-HC	-7.068807	-8.422770	-6.016218	h
H-HC	-5.335866	-8.176680	-6.340212	h
H-HC	-5.876351	-8.876149	-4.818390	h
C-CT	-3.443039	5.266423	-6.933648	h
C-CT	-5.028029	3.681341	-5.879981	h
C-CT	-5.184996	6.084208	-5.334712	h
H-HC	-6.049900	5.988258	-5.991354	h
H-HC	-5.522643	5.886646	-4.314663	h
C-CT	-4.598331	7.486645	-5.401441	h
H-HC	-3.724467	7.590815	-4.753804	h
H-HC	-4.347459	7.815087	-6.407598	h
H-HC	-5.350819	8.163759	-4.991901	h
C-CT	-4.284276	5.549724	-8.170533	h

H-HC	-2.814578	6.121729	-6.677468	h
H-HC	-2.783840	4.412668	-7.092169	h
H-HC	-3.607788	5.898259	-8.952392	h
H-HC	-4.784933	4.657672	-8.546865	h
H-HC	-5.028112	6.332055	-8.007522	h
C-CT	-5.925330	3.297385	-4.710825	h
H-HC	-5.634109	3.848163	-6.770276	h
H-HC	-4.295713	2.901603	-6.090861	h
H-HC	-6.745678	4.004148	-4.566323	h
H-HC	-6.364299	2.322447	-4.928545	h
H-HC	-5.389009	3.201848	-3.763643	h