Supporting Information for Nickel(II), copper(II) and zinc(II) metallo-intercalators: structural details of the DNA-binding by a combined experimental and computational investigation

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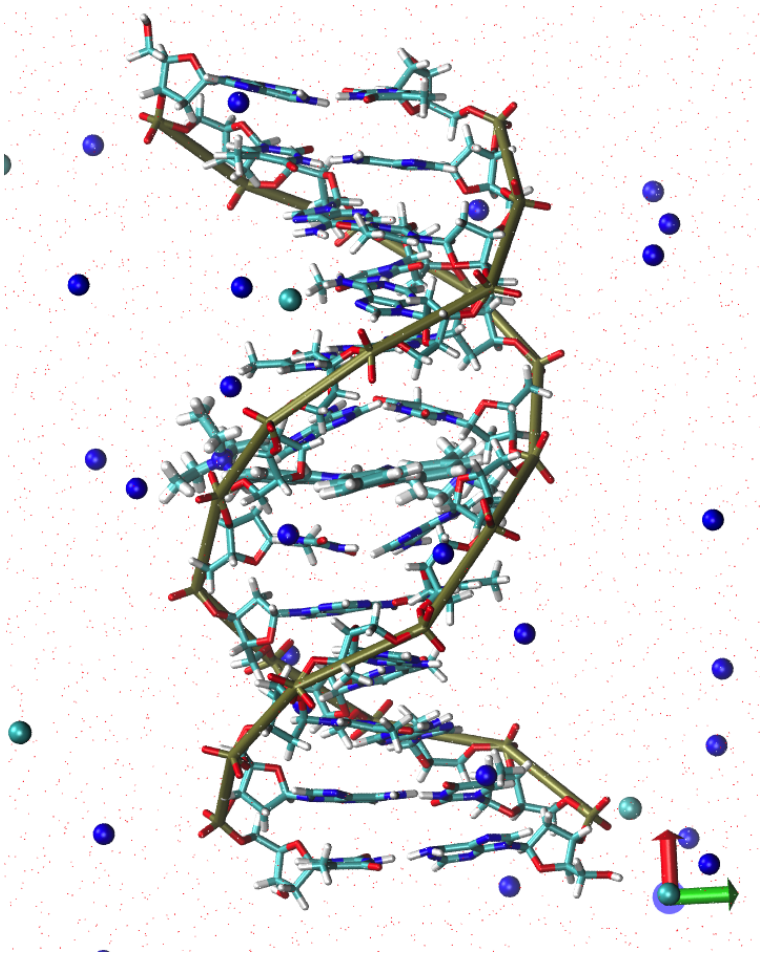
Content



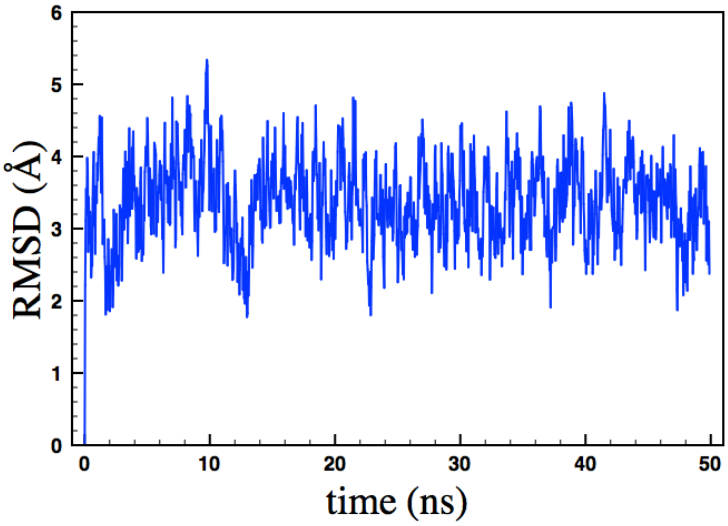


Figure S1. Top panel: Example of a MD simulation box, showing the **3**/[dodeca(dA-dT)]$_2$ intercalation complex, the solution counterions, Na^+ (in blue) and Cl^- (in cyan), and the explicit water molecules (in red). Bottom panel: Plot of the RMSD obtained for **3**/[dodeca(dA-dT)]$_2$ up to 50 ns of MD simulations.

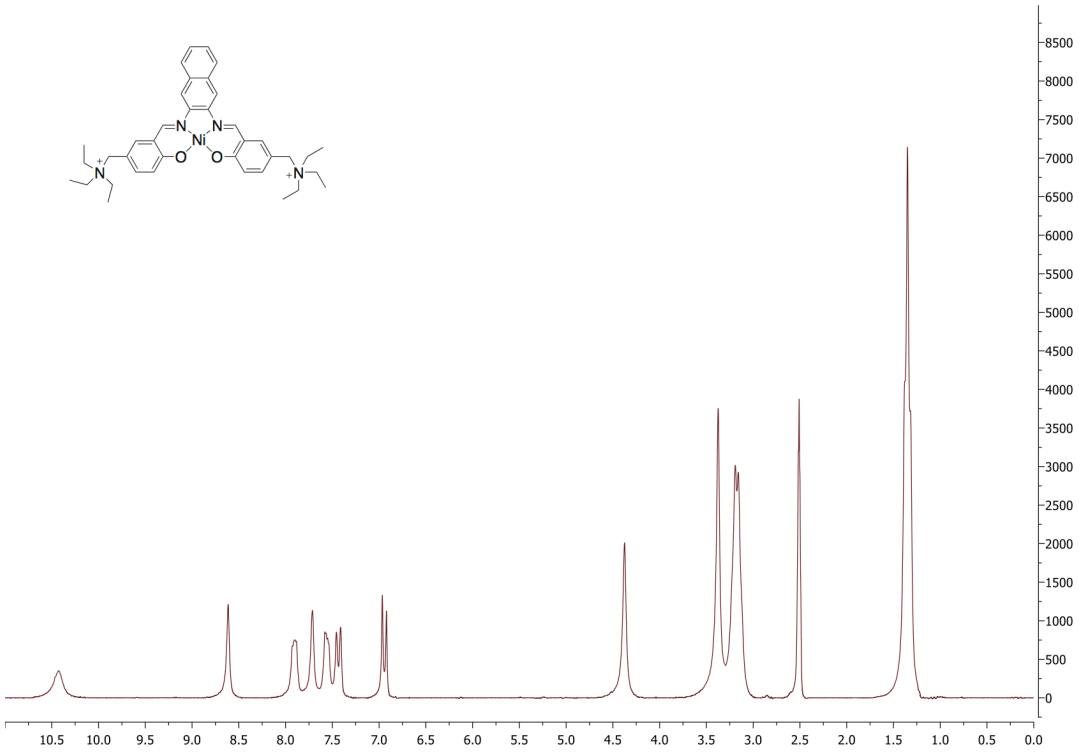


Figure S2. ^{1}H-NMR spectrum of compound **1** in DMSO, 200 MHz

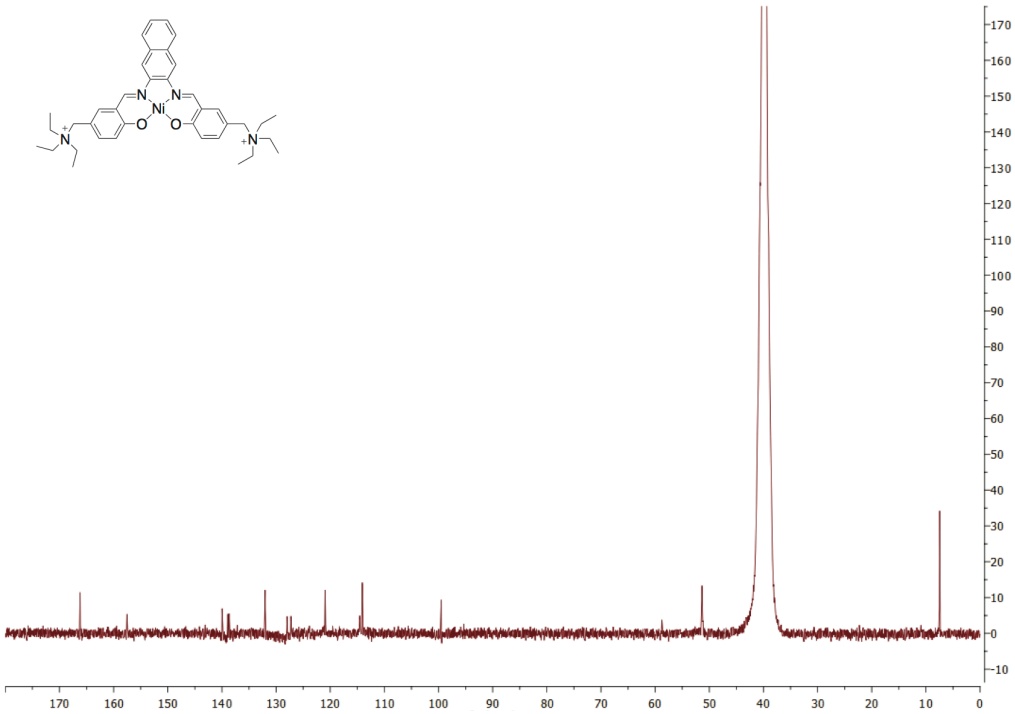


Figure S3. ^{13}C-NMR spectrum of compound **1** in DMSO, 50 MHz

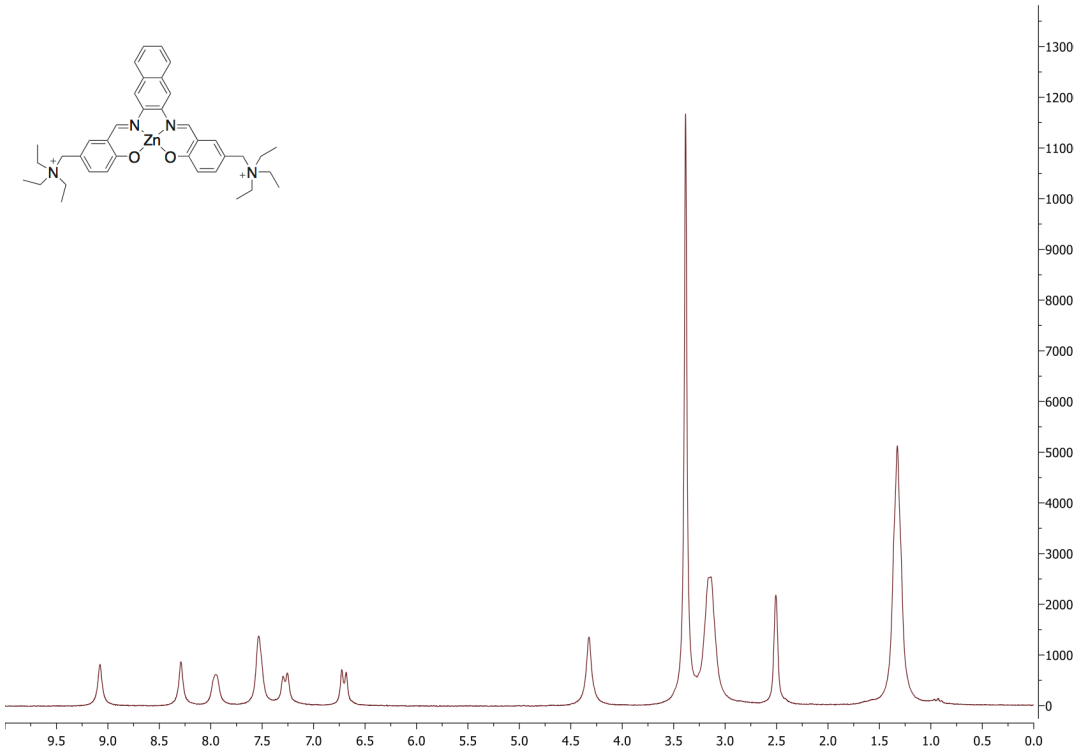


Figure S4. ^{1}H-NMR spectrum of compound **3** in DMSO, 200 MHz

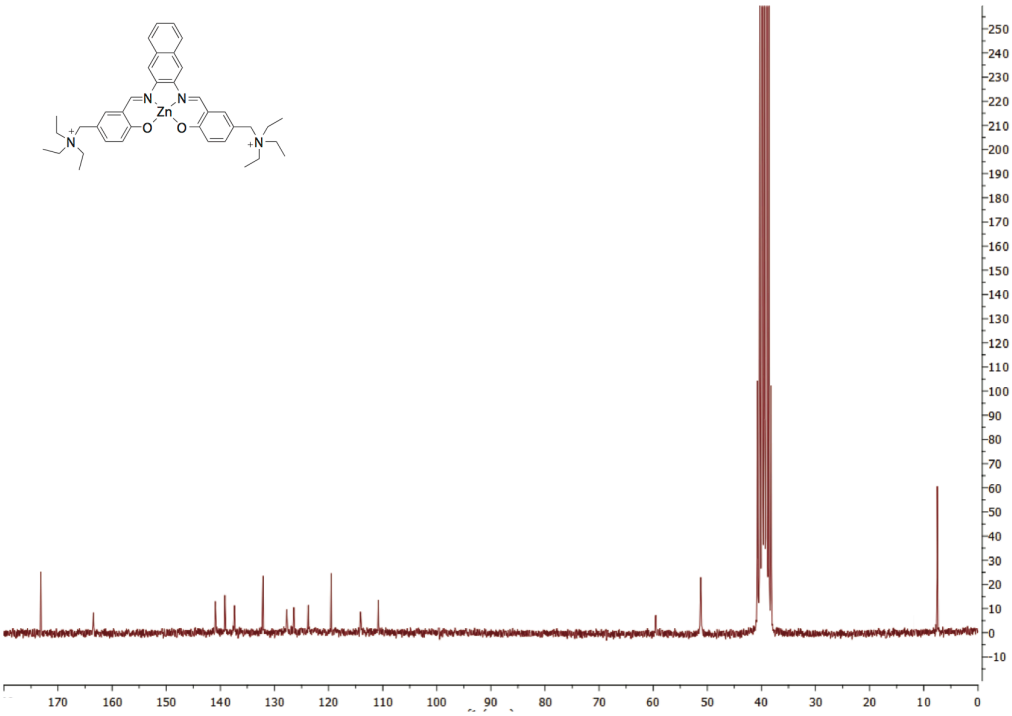


Figure S5. ^{13}C-NMR spectrum of compound **3** in DMSO, 50 MHz

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 [dodeca(dA-dT)]$_2$, 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	-3353.521875	0.735400	0.855478
2	-3485.471036	-3485.652690	0.731248	0.854389
3	-3624.393980	-3624.757209	0.730531	0.853819
[dodeca(dA-dT)]$_2$	-1842.443547	-1842.490250	5.229505	6.169698
1/[dodeca(dA-dT)]$_2$	-5195.837598	-5196.053453	5.984049	7.027348

2/[dodeca(dA-dT)]$_2$	-5327.974750	-5328.187681	5.986835	7.02588
3/[dodeca(dA-dT)]$_2$	-5466.912406	-5467.269570	5.969707	7.024956

Table S2. Cartesian coordinates of the nickel(II) and copper(II) complexes **1** and **2**, fully optimized by DFT calculations.

1

Atom	X	Y	Z
C	-1.110153	5.955478	0.137006
C	0.286743	6.075124	-0.108742
C	0.861501	7.369937	-0.225909
C	0.078437	8.489693	-0.103730
C	-1.315437	8.370114	0.139257
C	-1.896993	7.133232	0.255760
H	1.927567	7.461702	-0.414320
H	0.521874	9.475688	-0.195087
H	-1.919922	9.266514	0.230545
H	-2.963478	7.041516	0.441731
C	-1.680465	4.666045	0.257516
H	-2.749568	4.608308	0.434141
C	-0.902808	3.536727	0.143342
C	0.492922	3.655824	-0.127915
C	1.066566	4.901525	-0.240541
H	2.126564	5.028253	-0.434620
N	1.169530	2.407487	-0.264467
N	-1.362876	2.192839	0.262301
C	-2.583194	1.926214	0.612315
C	2.432551	2.351748	-0.553102
Ni	0.013239	0.889772	-0.042282
C	-3.154448	0.617609	0.727894
H	-3.255589	2.753328	0.840249
C	-4.506800	0.515246	1.124500
C	-5.136481	-0.702663	1.237463
C	-4.414142	-1.881942	0.933683
C	-3.084461	-1.811356	0.573205
C	-2.395941	-0.563412	0.463019
H	-5.055182	1.425381	1.355068
H	-6.167267	-0.752122	1.577072
C	-5.091103	-3.222707	1.090158
H	-2.488335	-2.700507	0.388630
O	-1.151326	-0.572632	0.140685
H	2.979144	3.283766	-0.696427
C	3.206032	1.154914	-0.706076
C	2.628449	-0.143355	-0.556217
C	3.502427	-1.260461	-0.720839
C	4.843074	-1.102341	-1.016005
C	5.389298	0.190766	-1.191553
C	4.573291	1.288289	-1.032495
O	1.388848	-0.363064	-0.290521

H	3.041626	-2.240001	-0.625572
C	5.737529	-2.303393	-1.206836
H	6.430865	0.320065	-1.470399
H	4.985208	2.285206	-1.168608
N	-6.009061	-3.694618	-0.070800
H	-4.351274	-4.011768	1.226184
H	-5.720109	-3.202427	1.979906
H	6.600481	-2.036097	-1.821993
H	5.210904	-3.120844	-1.700460
N	6.332745	-2.890132	0.080921
C	-7.320229	-4.189032	0.529489
C	-6.257303	-2.587883	-1.077179
C	-5.378712	-4.900928	-0.750496
C	-7.128056	-2.996967	-2.255329
H	-6.710595	-1.762943	-0.530016
H	-5.277330	-2.244560	-1.409105
H	-6.137603	-5.320196	-1.411743
C	-4.104927	-4.612714	-1.524122
H	-5.200554	-5.627342	0.045794
H	-7.838278	-4.743941	-0.253299
H	-7.033786	-4.902942	1.305745
C	-8.223671	-3.104499	1.090739
H	-9.070241	-3.597340	1.573503
H	-7.733860	-2.491765	1.850323
H	-8.626162	-2.453088	0.313485
H	-7.260159	-2.113935	-2.884069
H	-6.669569	-3.768564	-2.876468
H	-8.123932	-3.328658	-1.953719
H	-3.721243	-5.566177	-1.893431
H	-4.278168	-3.972542	-2.390760
H	-3.328626	-4.161026	-0.906222
C	7.391929	-3.895219	-0.364338
C	6.958246	-1.741505	0.858422
C	5.257717	-3.542515	0.922835
H	5.758002	-3.924989	1.812622
H	4.585506	-2.739789	1.233164
C	4.485581	-4.654338	0.224962
H	3.886046	-5.165912	0.980891
H	3.798139	-4.280215	-0.533824
H	5.134027	-5.401379	-0.236060
C	7.788183	-4.981055	0.629586
H	7.004420	-4.361048	-1.272468
H	8.258414	-3.293860	-0.651283
H	8.595951	-5.550802	0.163968
H	8.164237	-4.598864	1.576146
H	6.978274	-5.682158	0.832598
C	7.820508	-2.102833	2.057612
H	7.552398	-1.184099	0.130359
H	6.125249	-1.105824	1.161484
H	8.071986	-1.163420	2.555289
H	7.305726	-2.725222	2.791623
H	8.761039	-2.574631	1.772282

2

Atom	X	Y	Z

C	-1.225169	5.888477	0.112089
C	0.164279	6.051896	-0.149815
C	0.689644	7.361860	-0.314075
C	-0.132221	8.456203	-0.214719
C	-1.518141	8.293363	0.045217
C	-2.053646	7.039512	0.201264
H	1.749684	7.486463	-0.516983
H	0.274837	9.454306	-0.338029
H	-2.154562	9.169252	0.116079
H	-3.114969	6.914419	0.397110
C	-1.748990	4.580447	0.252878
H	-2.820338	4.478047	0.397380
C	-0.933009	3.475402	0.172369
C	0.465585	3.639966	-0.092838
C	0.983902	4.903017	-0.262771
H	2.029085	5.054678	-0.514438
N	1.204641	2.431001	-0.210921
N	-1.373968	2.128371	0.274547
C	-2.543738	1.820053	0.738238
C	2.499400	2.417810	-0.240457
Cu	0.049032	0.792449	-0.187025
C	-3.102714	0.496445	0.795622
H	-3.186991	2.616689	1.119862
C	-4.406368	0.369809	1.327672
C	-5.054074	-0.842662	1.391790
C	-4.403617	-1.994537	0.890257
C	-3.117587	-1.906522	0.397933
C	-2.404444	-0.668711	0.341210
H	-4.903506	1.260824	1.703786
H	-6.041325	-0.909345	1.840988
C	-5.087492	-3.337280	0.990460
H	-2.567914	-2.782775	0.065548
O	-1.194753	-0.680534	-0.101571
H	3.039060	3.360138	-0.122203
C	3.327142	1.255527	-0.422063
C	2.798569	-0.067306	-0.574236
C	3.744606	-1.111717	-0.806679
C	5.105201	-0.875536	-0.865117
C	5.607070	0.436682	-0.713497
C	4.721291	1.468402	-0.495068
O	1.548033	-0.375300	-0.516135
H	3.322002	-2.100739	-0.960885
C	6.072516	-1.998799	-1.150566
H	6.670982	0.637814	-0.797050
H	5.100365	2.482297	-0.392452
N	-6.162972	-3.674298	-0.077226
H	-4.356421	-4.145081	0.939244
H	-5.591335	-3.407526	1.954395
H	6.999281	-1.599899	-1.570677
H	5.657482	-2.711090	-1.864423
N	6.509403	-2.818971	0.070593
C	-7.361422	-4.285098	0.639102
C	-6.575129	-2.449445	-0.870775
C	-5.631558	-4.755758	-1.006393
C	-7.605793	-2.725188	-1.955136
H	-6.955101	-1.725481	-0.152192
H	-5.661483	-2.027375	-1.289439

H	-6.478274	-5.100347	-1.600531
C	-4.490791	-4.325928	-1.910539
H	-5.331241	-5.580704	-0.356259
H	-7.978359	-4.760248	-0.124239
H	-6.950910	-5.075955	1.271851
C	-8.193438	-3.307925	1.452410
H	-8.935313	-3.886037	2.007402
H	-7.606155	-2.750352	2.185525
H	-8.736201	-2.601460	0.822602
H	-7.852521	-1.768700	-2.420642
H	-7.229381	-3.378983	-2.743830
H	-8.536143	-3.141586	-1.562798
H	-4.167566	-5.204923	-2.472473
H	-4.795215	-3.568865	-2.635144
H	-3.630148	-3.952519	-1.355761
C	7.657320	-3.706155	-0.406073
C	6.979297	-1.837035	1.134318
C	5.355854	-3.636371	0.610790
H	5.744546	-4.179608	1.472163
H	4.616201	-2.918891	0.972449
C	4.730374	-4.598580	-0.390718
H	4.056187	-5.258066	0.159796
H	4.136680	-4.091493	-1.151312
H	5.464679	-5.229964	-0.893869
C	7.954579	-4.962032	0.405022
H	7.415934	-3.989030	-1.432500
H	8.531582	-3.051262	-0.445238
H	8.837164	-5.423274	-0.044633
H	8.185930	-4.769192	1.450172
H	7.149869	-5.695730	0.355151
C	7.691334	-2.416094	2.346138
H	7.641833	-1.139231	0.616571
H	6.088478	-1.284901	1.437060
H	7.841157	-1.590093	3.045265
H	7.110793	-3.176848	2.870833
H	8.677945	-2.811564	2.103737

Table S3. Amber atom types and Cartesian coordinates of the zinc(II) complex **3**, fully optimized by DFT calculations, and Mulliken charges used as atomic partial charges in the Amber99 force field for the MD simulations.

type	X	Y	Z	charge
CA	17.391775	-5.658697	-13.110883	0.242326
CA	17.286945	-4.281122	-12.941348	0.263069
CA	16.301417	-3.590418	-13.705707	-0.314848
CA	15.504556	-4.222150	-14.570664	-0.270629
CA	15.621626	-5.656235	-14.750102	-0.266011
CA	16.526271	-6.344849	-14.050350	-0.324820
HA	16.213493	-2.513372	-13.570944	0.251561
HA	14.766609	-3.660427	-15.141473	0.273890
HA	14.971603	-6.171559	-15.455674	0.272927

HA	16.614195	-7.421895	-14.185114	0.256000
CA	18.332329	-6.383338	-12.385102	-0.491089
HA	18.401224	-7.468535	-12.563513	0.239093
CA	19.184456	-5.751622	-11.460298	0.344126
CA	19.076145	-4.322894	-11.284985	0.344280
CA	18.122429	-3.621027	-12.045410	-0.485846
HA	18.025624	-2.527042	-11.955615	0.240277
NC	19.970653	-3.700576	-10.375089	-0.432137
NC	20.176702	-6.434983	-10.709436	-0.431751
CA	20.210079	-7.740315	-10.607356	-0.118403
CA	19.815923	-2.466855	-9.964837	-0.124214
Zn	21.403723	-5.071323	-9.702868	0.923825
CA	21.201018	-8.504343	-9.888491	0.055698
HA	19.425732	-8.363380	-11.103538	0.211974
CA	21.034661	-9.911711	-9.885858	-0.325258
CA	21.915620	-10.746564	-9.240345	-0.402788
CA	23.025183	-10.196080	-8.551683	0.388393
CA	23.218519	-8.837527	-8.523869	-0.505728
CA	22.304631	-7.933627	-9.190017	0.407703
HA	20.168394	-10.346315	-10.414182	0.249852
HA	21.748259	-11.832749	-9.234908	0.258873
CT	23.914391	-11.102938	-7.757291	-0.615562
HA	24.052472	-8.372170	-7.976373	0.267434
OS	22.590639	-6.670742	-9.093811	-0.579810
HA	18.939856	-1.864409	-10.309944	0.210080
CA	20.700837	-1.759546	-9.069626	0.052078
CA	21.895037	-2.310772	-8.519403	0.415594
CA	22.682830	-1.466806	-7.647881	-0.523082
CA	22.286817	-0.186952	-7.343623	0.355794
CA	21.092304	0.340975	-7.888453	-0.309240
CA	20.328231	-0.436563	-8.727743	-0.335670
OS	22.367597	-3.501747	-8.731358	-0.578261
HA	23.597764	-1.911117	-7.226591	0.284272
CT	23.071608	0.620711	-6.356797	-0.508183
HA	20.762018	1.353640	-7.618388	0.199194
HA	19.393969	-0.021634	-9.144242	0.244586
NA	25.001337	-11.832834	-8.526204	-0.174542
HC	24.414129	-10.503352	-6.940517	0.339276
HC	23.261832	-11.878365	-7.256623	0.332255
HC	23.762730	1.321879	-6.908196	0.347502
HC	23.676926	-0.074701	-5.703871	0.296783
NA	22.241323	1.463549	-5.403256	-0.189503
CT	24.901458	-13.317039	-8.246398	-0.434618
CT	24.886903	-11.564214	-10.000737	-0.477035
CT	26.358093	-11.395729	-8.017794	-0.431421
CT	25.923953	-12.238944	-10.873281	-0.638214
HC	23.855206	-11.896445	-10.319224	0.324482
HC	24.949178	-10.444614	-10.137215	0.335784
HC	27.127230	-12.081033	-8.479734	0.297508
CT	26.739520	-9.962438	-8.315505	-0.642248
HC	26.362034	-11.567524	-6.902417	0.310000
HC	25.823696	-13.802486	-8.680534	0.298728
HC	24.933216	-13.440549	-7.125033	0.314867
CT	23.679003	-14.015506	-8.799953	-0.655903
HC	23.705171	-15.077386	-8.441532	0.308889
HC	22.725665	-13.554853	-8.445315	0.225977
HC	23.681196	-14.027987	-9.917276	0.236102

HC	25.708035	-11.952486	-11.934972	0.293729
HC	26.960877	-11.902928	-10.630196	0.232950
HC	25.874091	-13.352322	-10.800356	0.233086
HC	27.683832	-9.737593	-7.756296	0.298735
HC	26.936461	-9.809066	-9.404891	0.237384
HC	25.956080	-9.237647	-7.986650	0.223963
CT	23.191418	2.414864	-4.715107	-0.456031
CT	21.228156	2.216260	-6.232998	-0.414076
CT	21.524833	0.583878	-4.416675	-0.422286
HC	20.914015	1.261525	-3.753003	0.289857
HC	20.817594	-0.066590	-5.011623	0.325589
CT	22.404750	-0.303337	-3.558941	-0.664601
HC	21.772557	-0.705289	-2.725775	0.294378
HC	22.804847	-1.172550	-4.136074	0.246647
HC	23.264971	0.247422	-3.107934	0.234315
CT	22.758272	2.979249	-3.378270	-0.644197
HC	24.164731	1.862334	-4.558183	0.312077
HC	23.378634	3.262853	-5.435643	0.309496
HC	23.526279	3.736696	-3.072404	0.301034
HC	21.767184	3.489894	-3.420073	0.245959
HC	22.716768	2.192332	-2.586170	0.232753
CT	20.417985	3.281940	-5.532351	-0.651916
HC	21.797204	2.689037	-7.086660	0.330908
HC	20.528343	1.443373	-6.669144	0.221766
HC	19.642257	3.643489	-6.256573	0.293746
HC	19.888730	2.893934	-4.629127	0.228350
HC	21.049654	4.156712	-5.242532	0.232138

Table S4. Cartesian coordinates of the geometries of the intercalation complexes of **1**, **2** and **3** with [dodeca(dA-dT)]$_2$, fully optimized by DFT/MM calculations. Amber99 atom types, high and low layer labels are also indicated.

1/[dodeca(dA-dT)]$_2$

H-HO	22.049880	-0.764563	7.250822	l
O-OH	22.302615	-0.313539	8.070048	l
C-CT	21.601154	0.922188	8.096392	l
H-H1	21.981444	1.589061	7.318279	l
H-H1	21.720455	1.413737	9.067581	l

C-CT	20.118249	0.652967	7.829547	1
H-H1	19.563455	1.595085	7.796259	1
O-OS	19.989326	-0.006846	6.580075	1
C-CT	18.765002	-0.694271	6.658149	1
H-H2	17.938331	0.028076	6.696097	1
N-N*	18.597792	-1.616819	5.514928	1
C-CK	18.103230	-2.900628	5.500840	1
H-H5	17.858142	-3.456183	6.396140	1
N-NB	17.954936	-3.407827	4.309493	1
C-CB	18.358529	-2.378776	3.459667	1
C-CA	18.412063	-2.237837	2.048272	1
N-N2	18.066927	-3.183835	1.167936	1
H-H	18.121847	-2.999953	0.167792	1
H-H	17.730688	-4.076137	1.495635	1
N-NC	18.822458	-1.065174	1.535621	1
C-CQ	19.169781	-0.072461	2.354381	1
H-H5	19.473773	0.855246	1.879263	1
N-NC	19.171625	-0.079576	3.685710	1
C-CB	18.752167	-1.278620	4.187100	1
C-CT	19.472615	-0.282585	8.870234	1
H-H1	20.220798	-0.662826	9.574476	1
C-CT	18.924301	-1.405138	7.994258	1
H-HC	19.673643	-2.190823	7.899152	1
H-HC	17.978808	-1.793465	8.370486	1
O-OS	18.373031	0.298114	9.552058	1
P-P	18.561240	1.538519	10.563888	1
O-O2	17.423413	1.559732	11.505849	1
O-O2	19.954967	1.545273	11.053618	1
O-OS	18.381932	2.738043	9.511494	1
C-CT	17.097626	3.081783	9.022172	1
H-H1	16.698056	3.897657	9.625578	1
H-H1	16.423864	2.224222	9.083030	1
C-CT	17.210734	3.499424	7.556001	1
H-H1	18.096890	4.129242	7.431976	1
O-OS	17.287533	2.314877	6.753166	1
C-CT	16.460101	2.533514	5.626955	1
H-H2	16.939443	3.243963	4.937496	1
N-N*	16.099510	1.281582	4.925165	1
C-CM	15.570050	0.199795	5.596395	1
H-H4	15.478276	0.240666	6.672682	1
C-CM	15.168729	-0.914108	4.930637	1
C-CT	14.597944	-2.087118	5.712256	1
H-HC	15.118811	-2.203273	6.662137	1
H-HC	14.720065	-3.000059	5.124098	1
H-HC	13.534628	-1.923667	5.886598	1
C-C	15.284407	-0.977619	3.476274	1
O-O	14.944350	-1.909205	2.754469	1
N-NA	15.840346	0.132618	2.889276	1
H-H	15.931793	0.137105	1.887939	1
C-C	16.243843	1.270531	3.539227	1
O-O	16.694639	2.212428	2.895664	1
C-CT	15.980017	4.277098	7.058943	1
H-H1	15.368331	4.670024	7.874991	1
C-CT	15.254107	3.192686	6.270448	1
H-HC	14.747772	2.505376	6.946458	1
H-HC	14.560551	3.585696	5.534237	1
O-OS	16.430598	5.331924	6.218515	1

P-P	15.419360	6.280492	5.396778	1
O-O2	14.083299	6.221463	6.023906	1
O-O2	16.070966	7.579254	5.135410	1
O-OS	15.343531	5.457890	4.012034	1
C-CT	16.286783	5.641029	2.957966	1
H-H1	16.686585	4.671378	2.652034	1
H-H1	17.126511	6.246975	3.303391	1
C-CT	15.669772	6.294823	1.706996	1
H-H1	16.453834	6.852256	1.189930	1
O-OS	15.188593	5.267588	0.849131	1
C-CT	13.772992	5.218061	0.885736	1
H-H2	13.363448	5.444283	-0.109288	1
N-N*	13.430171	3.835343	1.278566	1
C-CK	13.531494	3.224815	2.505428	1
H-H5	13.845209	3.743389	3.397817	1
N-NB	13.231441	1.956718	2.506403	1
C-CB	12.933339	1.694394	1.171476	1
C-CA	12.579378	0.521768	0.458755	1
N-N2	12.510639	-0.705444	0.986109	1
H-H	12.322977	-1.509925	0.394233	1
H-H	12.769368	-0.857478	1.950476	1
N-NC	12.336012	0.627258	-0.858690	1
C-CQ	12.455638	1.807075	-1.467559	1
H-H5	12.234327	1.817565	-2.531510	1
N-NC	12.816997	2.968172	-0.922578	1
C-CB	13.038822	2.841131	0.417648	1
C-CT	14.488532	7.236371	1.970250	1
H-H1	14.567801	7.704087	2.956711	1
C-CT	13.302203	6.275975	1.883156	1
H-HC	13.118944	5.844246	2.863113	1
H-HC	12.398204	6.762322	1.529041	1
O-OS	14.467647	8.224115	0.951547	1
P-P	13.448648	9.473656	0.983979	1
O-O2	13.056162	9.733491	2.384221	1
O-O2	13.999551	10.551741	0.137970	1
O-OS	12.202503	8.814778	0.217689	1
C-CT	12.311937	8.457996	-1.149786	1
H-H1	13.253356	7.932792	-1.321817	1
H-H1	12.298423	9.361384	-1.762596	1
C-CT	11.167222	7.535078	-1.569481	1
H-H1	11.229373	7.385849	-2.650542	1
O-OS	11.255544	6.269435	-0.931473	1
C-CT	9.974831	5.690664	-1.073489	1
H-H2	9.803162	5.387928	-2.116590	1
N-N*	9.847933	4.524061	-0.168543	1
C-CM	10.036731	4.640869	1.193271	1
H-H4	10.263140	5.609915	1.612240	1
C-CM	9.961859	3.562532	2.016452	1
C-CT	10.186773	3.742813	3.510605	1
H-HC	10.532429	2.797864	3.935940	1
H-HC	9.246009	4.018271	3.986877	1
H-HC	10.935818	4.511787	3.696914	1
C-C	9.682488	2.241567	1.461596	1
O-O	9.610162	1.183210	2.078980	1
N-NA	9.512322	2.213937	0.100137	1
H-H	9.349829	1.319155	-0.327149	1
C-C	9.578096	3.286735	-0.750607	1

O-O	9.415849	3.113421	-1.953935	l	
C-CT	9.773270	8.084664	-1.249173	l	
H-H1	9.832772	8.852691	-0.470198	l	
C-CT	9.039794	6.844994	-0.726545	l	
H-HC	8.914106	6.939510	0.349308	l	
H-HC	8.075464	6.700738	-1.204230	l	
O-OS	9.209817	8.600956	-2.442939	l	
P-P	7.796318	9.381839	-2.465378	l	
O-O2	7.522103	9.911116	-1.113428	l	
O-O2	7.768495	10.266961	-3.647096	l	
O-OS	6.816275	8.141298	-2.738168	l	
C-CT	6.919283	7.403741	-3.945692	l	
H-H1	7.969106	7.211717	-4.172498	l	
H-H1	6.483569	7.978586	-4.765198	l	
C-CT	6.210917	6.054343	-3.826572	l	
H-H1	6.296785	5.532760	-4.782641	l	
O-OS	6.783840	5.249178	-2.807014	l	
C-CT	5.859665	4.210584	-2.577743	l	
H-H2	5.938266	3.449131	-3.363510	l	
N-N*	6.066705	3.599511	-1.253913	l	
C-CK	6.405803	4.203878	-0.070018	l	
H-H5	6.574523	5.268860	0.011555	l	
N-NB	6.506931	3.383762	0.939780	l	
C-CB	6.222605	2.135643	0.379566	l	
C-CA	6.181716	0.811532	0.888951	l	
N-N2	6.495671	0.473398	2.142053	l	
H-H	6.549810	-0.508027	2.408605	l	
H-H	6.837322	1.176411	2.777855	l	
N-NC	5.836124	-0.191134	0.059242	l	
C-CQ	5.571562	0.078777	-1.219396	l	
H-H5	5.296921	-0.772130	-1.835698	l	
N-NC	5.608247	1.264875	-1.828599	l	
C-CB	5.943114	2.263258	-0.960548	l	
C-CT	4.728128	6.166248	-3.479238	l	
H-H1	4.554340	7.059212	-2.869887	l	
C-CT	4.506262	4.902816	-2.648345	l	
H-HC	4.159574	5.187250	-1.657577	l	
H-HC	3.802138	4.231457	-3.124478	l	
O-OS	3.956262	6.185760	-4.668671	l	
P-P	2.341627	6.282752	-4.662067	l	
O-O2	1.902775	6.825270	-3.358176	l	
O-O2	1.901533	6.903132	-5.927107	l	
O-OS	1.952754	4.725104	-4.702956	l	
C-CT	2.461303	3.870605	-5.720295	l	
H-H1	3.532620	4.038269	-5.837303	l	
H-H1	1.972729	4.087054	-6.671970	l	
C-CT	2.259338	2.399320	-5.341084	l	
H-H1	2.743139	1.767188	-6.088889	l	
O-OS	2.844882	2.177262	-4.057182	l	
C-CT	1.923741	1.425843	-3.295562	l	H-H
H-H2	2.008180	0.368960	-3.583130	l	
N-N*	2.149267	1.611007	-1.837352	h	
C-CM	2.194493	2.866708	-1.254467	h	
H-H4	1.978409	3.699539	-1.917147	h	
C-CM	2.488216	3.060107	0.047539	h	
C-CT	2.598244	4.409446	0.689229	h	
H-HC	2.208662	5.188400	0.026922	h	

H-HC	3.638940	4.637944	0.931503	h	
H-HC	2.042516	4.419081	1.630418	h	
C-C	2.758907	1.880846	0.872532	h	
O-O	3.054647	1.923828	2.064101	h	
N-NA	2.654143	0.666720	0.217687	h	
H-H	2.850992	-0.208549	0.763993	h	
C-C	2.376506	0.457938	-1.106820	h	
O-O	2.324633	-0.664956	-1.597694	h	
C-CT	0.777557	2.004680	-5.246505	l	
H-H1	0.118883	2.741285	-5.717069	l	
C-CT	0.567964	1.948782	-3.746858	l	
H-HC	0.387986	2.953024	-3.367487	l	
H-HC	-0.235103	1.265691	-3.487977	l	
O-OS	0.544086	0.697883	-5.744090	l	
P-P	0.329794	0.438509	-7.312773	l	
O-O2	-0.816682	1.256387	-7.752939	l	
O-O2	1.640847	0.547186	-7.983593	l	
O-OS	-0.123477	-1.101291	-7.282082	l	
C-CT	0.829305	-2.147730	-7.168941	l	
H-H1	1.516528	-1.928047	-6.349834	l	
H-H1	1.402796	-2.199385	-8.095763	l	
C-CT	0.177166	-3.513955	-6.896403	l	
H-H1	0.890829	-4.296264	-7.163746	l	
O-OS	-0.125054	-3.606063	-5.507283	l	
C-CT	-1.528190	-3.681595	-5.324547	l	H-H
H-H2	-1.834845	-4.694975	-5.030985	l	
N-N*	-1.851612	-2.703793	-4.268854	h	
C-CK	-1.679772	-1.338306	-4.317089	h	
H-H5	-1.253414	-0.856788	-5.186174	h	
N-NB	-2.045629	-0.724810	-3.220972	h	
C-CB	-2.463288	-1.753829	-2.397778	h	
C-CA	-2.941273	-1.753049	-1.078587	h	
N-N2	-3.144863	-0.579389	-0.416579	h	
H-H	-3.543740	-0.632500	0.521848	h	
H-H	-3.489647	0.177631	-0.999218	h	
N-NC	-3.123720	-2.932507	-0.475487	h	
C-CQ	-2.934027	-4.069716	-1.183248	h	
H-H5	-3.124664	-4.986856	-0.631997	h	
N-NC	-2.573666	-4.188662	-2.453524	h	
C-CB	-2.330026	-2.996586	-3.012330	h	
C-CT	-1.120900	-3.753779	-7.676520	l	
H-H1	-1.153678	-3.138829	-8.581509	l	
C-CT	-2.173110	-3.322710	-6.660043	l	
H-HC	-2.332662	-2.251359	-6.749328	l	
H-HC	-3.117380	-3.843558	-6.787026	l	
O-OS	-1.208136	-5.133598	-7.995249	l	
P-P	-2.353832	-5.721802	-8.967149	l	
O-O2	-2.782072	-4.653779	-9.893743	l	
O-O2	-1.906424	-7.032899	-9.478744	l	
O-OS	-3.524478	-5.968506	-7.896700	l	
C-CT	-3.369637	-6.939749	-6.875738	l	
H-H1	-2.388400	-6.834726	-6.410071	l	
H-H1	-3.443002	-7.938773	-7.310428	l	
C-CT	-4.436794	-6.770903	-5.792404	l	
H-H1	-4.336873	-7.599103	-5.086071	l	
O-OS	-4.278375	-5.549818	-5.082772	l	
C-CT	-5.528645	-5.310043	-4.468618	l	

H-H2	-5.691623	-6.017678	-3.643763	1
N-N*	-5.600439	-3.914439	-3.976407	1
C-CM	-5.366820	-2.840505	-4.810565	1
H-H4	-5.163578	-3.021172	-5.855542	1
C-CM	-5.361807	-1.564782	-4.342584	1
C-CT	-5.075418	-0.416741	-5.299185	1
H-HC	-4.691455	0.435274	-4.734407	1
H-HC	-5.999741	-0.119296	-5.794607	1
H-HC	-4.335254	-0.709937	-6.042787	1
C-C	-5.607242	-1.308290	-2.926574	1
O-O	-5.569337	-0.221197	-2.355793	1
N-NA	-5.862869	-2.429516	-2.175581	1
H-H	-6.009590	-2.309619	-1.188390	1
C-C	-5.857729	-3.726134	-2.620437	1
O-O	-6.042197	-4.639744	-1.822752	1
C-CT	-5.872797	-6.782230	-6.329897	1
H-H1	-5.881306	-6.608014	-7.411804	1
C-CT	-6.518825	-5.608703	-5.587057	1
H-HC	-6.601997	-4.764953	-6.268076	1
H-HC	-7.492401	-5.855813	-5.171950	1
O-OS	-6.459430	-8.029259	-5.998968	1
P-P	-7.906875	-8.477429	-6.556989	1
O-O2	-8.190782	-7.729237	-7.798854	1
O-O2	-7.983730	-9.951857	-6.525165	1
O-OS	-8.833448	-7.895639	-5.383483	1
C-CT	-8.728680	-8.415669	-4.068196	1
H-H1	-7.678632	-8.478870	-3.778784	1
H-H1	-9.161492	-9.417646	-4.036422	1
C-CT	-9.444120	-7.517323	-3.059116	1
H-H1	-9.379238	-7.988097	-2.075156	1
O-OS	-8.862154	-6.227690	-2.988335	1
C-CT	-9.796238	-5.434262	-2.292839	1
H-H2	-9.768212	-5.665085	-1.220949	1
N-N*	-9.495347	-4.009862	-2.515235	1
C-CK	-9.071790	-3.390253	-3.664052	1
H-H5	-8.956526	-3.918416	-4.600887	1
N-NB	-8.809429	-2.119907	-3.522601	1
C-CB	-9.066389	-1.879419	-2.170711	1
C-CA	-8.947306	-0.741339	-1.329779	1
N-N2	-8.462233	0.444727	-1.713203	1
H-H	-8.328566	1.196113	-1.042589	1
H-H	-8.094147	0.549917	-2.646159	1
N-NC	-9.311367	-0.854973	-0.039579	1
C-CQ	-9.738428	-2.028902	0.425377	1
H-H5	-10.022860	-2.043802	1.473487	1
N-NC	-9.857238	-3.176562	-0.243773	1
C-CB	-9.502138	-3.029181	-1.553555	1
C-CT	-10.919335	-7.282441	-3.376404	1
H-H1	-11.081778	-7.346248	-4.458166	1
C-CT	-11.139170	-5.847247	-2.884759	1
H-HC	-11.394574	-5.218717	-3.734658	1
H-HC	-11.911058	-5.785808	-2.121041	1
O-OS	-11.688918	-8.240703	-2.672550	1
P-P	-13.282290	-8.390360	-2.880570	1
O-O2	-13.645653	-7.826267	-4.196987	1
O-O2	-13.675133	-9.764561	-2.509339	1
O-OS	-13.797962	-7.390604	-1.737001	1

C-CT	-13.477009	-7.630710	-0.375287	1
H-H1	-12.402659	-7.788896	-0.271612	1
H-H1	-13.998218	-8.523336	-0.023722	1
C-CT	-13.867902	-6.429114	0.484930	1
H-H1	-13.619429	-6.645714	1.527105	1
O-OS	-13.154639	-5.275918	0.068165	1
C-CT	-13.954940	-4.155590	0.378341	1
H-H2	-13.881881	-3.920040	1.448604	1
N-N*	-13.495209	-3.019740	-0.454468	1
C-CM	-13.367799	-3.142129	-1.823464	1
H-H4	-13.688619	-4.057290	-2.301568	1
C-CM	-12.827880	-2.149313	-2.576771	1
C-CT	-12.709811	-2.326731	-4.083779	1
H-HC	-11.846050	-2.945688	-4.316381	1
H-HC	-12.567793	-1.349248	-4.550896	1
H-HC	-13.615825	-2.781821	-4.484605	1
C-C	-12.354891	-0.927672	-1.935066	1
O-O	-11.798036	0.017942	-2.483394	1
N-NA	-12.566318	-0.867476	-0.579575	1
H-H	-12.261766	-0.035356	-0.104134	1
C-C	-13.103455	-1.857067	0.202093	1
O-O	-13.200295	-1.690921	1.412218	1
C-CT	-15.360867	-6.099008	0.407043	1
H-H1	-15.844192	-6.695223	-0.375146	1
C-CT	-15.371340	-4.613160	0.047174	1
H-HC	-15.570510	-4.508911	-1.016856	1
H-HC	-16.100955	-4.050129	0.624895	1
O-OS	-15.922459	-6.348828	1.683652	1
P-P	-17.508478	-6.537562	1.901594	1
O-O2	-18.105744	-7.043912	0.649083	1
O-O2	-17.723578	-7.243797	3.180690	1
O-OS	-17.946197	-5.008903	2.088880	1
C-CT	-17.551444	-4.277633	3.238937	1
H-H1	-16.470947	-4.354966	3.375647	1
H-H1	-18.046827	-4.689608	4.119782	1
C-CT	-17.915202	-2.798800	3.087044	1
H-H1	-17.757608	-2.293648	4.042992	1
O-OS	-17.072744	-2.219432	2.093994	1
C-CT	-17.883458	-1.446118	1.233478	1
H-H2	-18.083678	-0.458089	1.675481	1
N-N*	-17.192907	-1.289643	-0.064042	1
C-CK	-17.326185	-1.986214	-1.243933	1
H-H5	-17.945912	-2.865835	-1.357331	1
N-NB	-16.625220	-1.503561	-2.232989	1
C-CB	-16.007787	-0.380441	-1.682153	1
C-CA	-15.166637	0.637505	-2.201675	1
N-N2	-14.745826	0.725753	-3.468033	1
H-H	-14.124762	1.490624	-3.726439	1
H-H	-15.024673	0.038400	-4.148949	1
N-NC	-14.754173	1.611373	-1.373447	1
C-CQ	-15.146009	1.608524	-0.101615	1
H-H5	-14.788109	2.432894	0.506060	1
N-NC	-15.927415	0.721690	0.507257	1
C-CB	-16.333440	-0.258028	-0.351793	1
C-CT	-19.369869	-2.581348	2.645002	1
H-H1	-19.976727	-3.483118	2.773899	1
C-CT	-19.176887	-2.238709	1.170892	1

H-HC	-19.036072	-3.158060	0.606295	1
H-HC	-19.992835	-1.650335	0.768129	1
O-OS	-19.892525	-1.502331	3.404777	1
P-P	-21.375137	-0.906681	3.186835	1
O-O2	-22.143869	-1.820165	2.315749	1
O-O2	-21.909013	-0.470082	4.492319	1
O-OS	-20.978724	0.392091	2.335369	1
C-CT	-20.249599	1.451969	2.942205	1
H-H1	-19.421108	1.041578	3.520694	1
H-H1	-20.902552	2.012440	3.614219	1
C-CT	-19.668686	2.403026	1.893695	1
H-H1	-19.082503	3.175841	2.396993	1
O-OS	-18.841816	1.699863	0.976451	1
C-CT	-18.892030	2.337080	-0.291341	1
H-H2	-17.904060	2.737378	-0.559497	1
N-N*	-19.325191	1.344033	-1.305852	1
C-CM	-20.304322	0.411127	-1.040025	1
H-H4	-20.782257	0.414782	-0.072837	1
C-CM	-20.664173	-0.521106	-1.959326	1
C-CT	-21.745471	-1.540667	-1.621108	1
H-HC	-22.110307	-1.420789	-0.599510	1
H-HC	-21.346914	-2.548020	-1.749016	1
H-HC	-22.579453	-1.418013	-2.313936	1
C-C	-20.014583	-0.544253	-3.266711	1
O-O	-20.234477	-1.347749	-4.166012	1
N-NA	-19.074412	0.443206	-3.467220	1
H-H	-18.613514	0.458143	-4.356951	1
C-C	-18.697802	1.388608	-2.545265	1
O-O	-17.839842	2.215233	-2.829137	1
C-CT	-20.729040	3.102300	1.054078	1
H-H1	-21.529229	2.397499	0.804164	1
C-CT	-19.906395	3.475411	-0.168210	1
H-HC	-20.521117	3.576554	-1.062193	1
H-HC	-19.368158	4.404245	0.022561	1
O-OH	-21.193352	4.275675	1.690823	1
H-HO	-21.886514	4.685601	1.162050	1
H-HO	-15.086609	8.450311	-7.602299	1
O-OH	-14.709891	9.199217	-8.097997	1
C-CT	-15.478635	10.350736	-7.778693	1
H-H1	-16.492908	10.245868	-8.174332	1
H-H1	-15.023305	11.239599	-8.222090	1
C-CT	-15.568641	10.516640	-6.257204	1
H-H1	-16.128864	11.425182	-6.020159	1
O-OS	-16.247114	9.377802	-5.745309	1
C-CT	-15.549013	8.910265	-4.611195	1
H-H2	-15.846795	9.475686	-3.721780	1
N-N*	-15.805525	7.465647	-4.431350	1
C-CK	-16.156046	6.813801	-3.274297	1
H-H5	-16.254716	7.315970	-2.319568	1
N-NB	-16.377367	5.536918	-3.423645	1
C-CB	-16.109965	5.309061	-4.773137	1
C-CA	-16.115752	4.151428	-5.595115	1
N-N2	-16.459674	2.928232	-5.184921	1
H-H	-16.417621	2.161935	-5.835337	1
H-H	-16.781201	2.775353	-4.227641	1
N-NC	-15.758513	4.268124	-6.889150	1
C-CQ	-15.415034	5.465902	-7.358776	1

H-H5	-15.139188	5.500486	-8.405581	1
N-NC	-15.372115	6.624325	-6.701981	1
C-CB	-15.741546	6.479996	-5.393849	1
C-CT	-14.198890	10.589357	-5.568830	1
H-H1	-13.401480	10.760526	-6.299514	1
C-CT	-14.095207	9.207766	-4.931763	1
H-HC	-13.711694	8.499351	-5.661404	1
H-HC	-13.489988	9.203776	-4.033620	1
O-OS	-14.241764	11.617954	-4.591422	1
P-P	-12.916597	12.137748	-3.831269	1
O-O2	-11.752127	11.927818	-4.715878	1
O-O2	-13.199058	13.468399	-3.256067	1
O-OS	-12.844381	11.072542	-2.633835	1
C-CT	-13.800828	11.095179	-1.586396	1
H-H1	-14.805442	11.172327	-2.003737	1
H-H1	-13.617145	11.963821	-0.950452	1
C-CT	-13.721967	9.821281	-0.739708	1
H-H1	-14.388676	9.927401	0.119111	1
O-OS	-14.085825	8.663297	-1.477137	1
C-CT	-13.617369	7.549797	-0.735758	1
H-H2	-14.367776	7.256484	0.010715	1
N-N*	-13.337591	6.418941	-1.649800	1
C-CM	-12.698038	6.608280	-2.857137	1
H-H4	-12.319341	7.590819	-3.094139	1
C-CM	-12.557248	5.595348	-3.753578	1
C-CT	-11.878081	5.861400	-5.089813	1
H-HC	-11.075749	6.590430	-4.976378	1
H-HC	-12.612650	6.224248	-5.808288	1
H-HC	-11.458519	4.928045	-5.471880	1
C-C	-13.075642	4.267444	-3.436287	1
O-O	-13.063628	3.275411	-4.160358	1
N-NA	-13.627166	4.155950	-2.185895	1
H-H	-13.967541	3.249118	-1.924657	1
C-C	-13.778854	5.157336	-1.264949	1
O-O	-14.279427	4.914299	-0.171652	1
C-CT	-12.316891	9.535807	-0.221859	1
H-H1	-11.583643	9.794977	-0.992573	1
C-CT	-12.356586	8.023452	-0.017836	1
H-HC	-11.461816	7.577286	-0.446895	1
H-HC	-12.434307	7.769250	1.039241	1
O-OS	-12.081358	10.245203	0.980023	1
P-P	-10.660300	10.190762	1.739619	1
O-O2	-9.626904	9.723471	0.791701	1
O-O2	-10.480235	11.443926	2.498970	1
O-OS	-10.941189	9.006304	2.782015	1
C-CT	-11.995272	9.105930	3.729306	1
H-H1	-12.945421	9.225860	3.206919	1
H-H1	-11.836364	9.978830	4.364990	1
C-CT	-12.075773	7.846640	4.599407	1
H-H1	-12.865691	7.979106	5.341995	1
O-OS	-12.381805	6.734410	3.764805	1
C-CT	-11.365612	5.755172	3.885379	1
H-H2	-11.681220	4.952439	4.567301	1
N-N*	-11.115283	5.227574	2.526393	1
C-CK	-10.457645	5.823221	1.475507	1
H-H5	-10.034609	6.820269	1.530188	1
N-NB	-10.408628	5.100258	0.391713	1

C-CB	-11.081059	3.931476	0.748905	1
C-CA	-11.372244	2.724226	0.064545	1
N-N2	-11.018012	2.465795	-1.197469	1
H-H	-11.276911	1.580834	-1.634426	1
H-H	-10.503311	3.149416	-1.729461	1
N-NC	-12.032961	1.753504	0.721214	1
C-CQ	-12.405537	1.954738	1.985756	1
H-H5	-12.917767	1.125249	2.462795	1
N-NC	-12.211237	3.041581	2.733760	1
C-CB	-11.528148	4.005237	2.047944	1
C-CT	-10.759742	7.564976	5.329284	1
H-H1	-10.124545	8.455810	5.345879	1
C-CT	-10.148713	6.469822	4.467173	1
H-HC	-9.553295	6.938588	3.688797	1
H-HC	-9.539037	5.786116	5.046980	1
O-OS	-11.039981	7.131104	6.649198	1
P-P	-9.873038	6.905604	7.741155	1
O-O2	-8.689384	7.697147	7.345558	1
O-O2	-10.458062	7.039261	9.090630	1
O-OS	-9.563258	5.356719	7.470942	1
C-CT	-10.517278	4.368379	7.821407	1
H-H1	-11.515732	4.699091	7.530016	1
H-H1	-10.498463	4.214873	8.902033	1
C-CT	-10.228826	3.045802	7.110324	1
H-H1	-10.924245	2.286795	7.476303	1
O-OS	-10.347244	3.172198	5.698872	1
C-CT	-9.779759	1.996118	5.149048	1
H-H2	-10.544658	1.210482	5.080191	1
N-N*	-9.179338	2.238868	3.820510	1
C-CM	-8.439427	3.371178	3.559650	1
H-H4	-8.321601	4.106615	4.339541	1
C-CM	-7.856056	3.573886	2.349969	1
C-CT	-7.060497	4.847677	2.108551	1
H-HC	-6.043844	4.706681	2.469021	1
H-HC	-7.525575	5.688659	2.622085	1
H-HC	-7.044962	5.053748	1.035647	1
C-C	-7.990113	2.566471	1.300949	1
O-O	-7.518131	2.610591	0.168600	1
N-NA	-8.714854	1.456964	1.659506	1
H-H	-8.821990	0.722336	0.982154	1
C-C	-9.303638	1.226939	2.874331	1
O-O	-9.892686	0.170985	3.080576	1
C-CT	-8.806070	2.540506	7.303222	1
H-H1	-8.115105	3.379693	7.174879	1
C-CT	-8.693297	1.574903	6.132076	1
H-HC	-7.699480	1.660730	5.698841	1
H-HC	-8.888664	0.550693	6.450922	1
O-OS	-8.596057	1.878448	8.536688	1
P-P	-7.131403	1.336230	8.947818	1
O-O2	-6.112430	2.165868	8.270494	1
O-O2	-7.092572	1.141769	10.411182	1
O-OS	-7.135454	-0.108271	8.243765	1
C-CT	-7.930937	-1.163352	8.764907	1
H-H1	-8.973167	-0.846335	8.819933	1
H-H1	-7.585499	-1.408906	9.771685	1
C-CT	-7.845984	-2.422647	7.896261	1
H-H1	-8.382743	-3.230185	8.398411	1

O-OS	-8.413966	-2.228019	6.605940	l	
C-CT	-7.712812	-3.021080	5.656919	l	
H-H2	-8.388810	-3.711714	5.138892	l	
N-N*	-7.092943	-2.104907	4.677069	l	
C-CK	-6.761648	-0.786562	4.843577	l	
H-H5	-6.804793	-0.311851	5.813605	l	
N-NB	-6.420332	-0.166951	3.746982	l	
C-CB	-6.500183	-1.164572	2.774414	l	
C-CA	-6.276255	-1.193740	1.372141	l	
N-N2	-5.993263	-0.127858	0.614515	l	
H-H	-5.920047	-0.219364	-0.397361	l	
H-H	-5.995803	0.797411	1.019499	l	
N-NC	-6.382059	-2.370164	0.729574	l	
C-CQ	-6.727429	-3.463411	1.410016	l	
H-H5	-6.796741	-4.375561	0.825591	l	
N-NC	-7.010832	-3.562879	2.710234	l	
C-CB	-6.870711	-2.362264	3.344175	l	
C-CT	-6.416480	-2.887099	7.659371	l	
H-H1	-5.796883	-2.024187	7.402697	l	
C-CT	-6.657014	-3.781599	6.450892	l	
H-HC	-5.756112	-3.949209	5.870972	l	
H-HC	-7.067882	-4.736181	6.773660	l	
O-OS	-5.922577	-3.598132	8.779975	l	
P-P	-4.346923	-3.705292	9.078879	l	
O-O2	-3.713652	-2.439189	8.660496	l	
O-O2	-4.145793	-4.218873	10.447197	l	
O-OS	-3.869152	-4.830427	8.053589	l	
C-CT	-4.458583	-6.122649	8.037185	l	
H-H1	-5.544089	-6.027621	8.056894	l	
H-H1	-4.145137	-6.688442	8.915447	l	
C-CT	-4.064996	-6.865027	6.751159	l	
H-H1	-4.592765	-7.820123	6.706122	l	
O-OS	-4.434666	-6.039224	5.647085	l	
C-CT	-3.303736	-5.845934	4.823310	l	H-H
H-H2	-3.294500	-6.625900	4.051336	l	
N-N*	-3.314659	-4.479776	4.231779	h	
C-CM	-3.320863	-3.344373	5.026710	h	
H-H4	-3.382034	-3.507472	6.100129	h	
C-CM	-3.264511	-2.091475	4.531559	h	
C-CT	-3.269430	-0.854482	5.377719	h	
H-HC	-2.368081	-0.266592	5.188328	h	
H-HC	-3.312880	-1.118552	6.439287	h	
H-HC	-4.123127	-0.218219	5.142271	h	
C-C	-3.201786	-1.947845	3.080883	h	
O-O	-3.112857	-0.860874	2.504678	h	
N-NA	-3.251825	-3.122604	2.354677	h	
H-H	-3.229717	-3.043860	1.309225	h	
C-C	-3.247531	-4.408643	2.844721	h	
O-O	-3.181009	-5.392757	2.123885	h	
C-CT	-2.557197	-7.135962	6.671138	l	
H-H1	-2.098022	-7.045527	7.658909	l	
C-CT	-2.103688	-6.031740	5.740202	l	
H-HC	-1.943778	-5.145805	6.342616	l	
H-HC	-1.210508	-6.294601	5.180542	l	
O-OS	-2.290840	-8.402077	6.094970	l	
P-P	-0.868089	-9.144291	6.297094	l	
O-O2	-0.316678	-8.745127	7.609279	l	

O-O2	-1.046981	-10.573144	5.969934	l	
O-OS	0.059173	-8.488288	5.156310	l	
C-CT	-0.239731	-8.665835	3.780631	l	
H-H1	-1.122926	-8.083505	3.518845	l	
H-H1	-0.453540	-9.719265	3.586544	l	
C-CT	0.932222	-8.237259	2.890310	l	
H-H1	0.657271	-8.446730	1.855940	l	
O-OS	1.221571	-6.848635	3.019409	l	
C-CT	2.612993	-6.707259	2.811699	l	H-H
H-H2	2.851067	-6.806507	1.744581	l	
N-N*	3.022034	-5.375109	3.309463	h	
C-CK	3.241435	-4.961764	4.610578	h	
H-H5	3.264691	-5.659902	5.436318	h	
N-NB	3.400863	-3.670334	4.727548	h	
C-CB	3.273167	-3.195915	3.434630	h	
C-CA	3.211188	-1.888509	2.894473	h	
N-N2	3.227057	-0.775713	3.647074	h	
H-H	3.169252	0.149246	3.213630	h	
H-H	3.304839	-0.860741	4.650630	h	
N-NC	3.081893	-1.775814	1.562707	h	
C-CQ	2.976705	-2.883828	0.800535	h	
H-H5	2.937035	-2.703163	-0.271136	h	
N-NC	2.913986	-4.143322	1.204914	h	
C-CB	3.053375	-4.236239	2.535614	h	
C-CT	2.227667	-9.006119	3.182602	l	
H-H1	2.085422	-9.716282	4.004144	l	
C-CT	3.194204	-7.890255	3.571768	l	
H-HC	3.129614	-7.731915	4.645911	l	
H-HC	4.215013	-8.099185	3.257981	l	
O-OS	2.627989	-9.655437	1.985161	l	
P-P	3.763941	-10.799094	1.969481	l	
O-O2	3.808115	-11.430648	3.304137	l	
O-O2	3.559670	-11.620503	0.758752	l	
O-OS	5.110037	-9.932033	1.773337	l	
C-CT	5.578420	-9.534838	0.490469	l	
H-H1	5.680381	-10.419558	-0.141058	l	
H-H1	6.561315	-9.080152	0.607680	l	
C-CT	4.651769	-8.520336	-0.198116	l	
H-H1	3.640658	-8.932690	-0.266773	l	
O-OS	4.679935	-7.306790	0.544627	l	
C-CT	5.084988	-6.235828	-0.290899	l	
H-H2	4.208985	-5.768153	-0.761031	l	
N-N*	5.834537	-5.244704	0.515603	l	
C-CM	6.351993	-5.569373	1.753999	l	
H-H4	6.363644	-6.602234	2.072972	l	
C-CM	6.799448	-4.615181	2.608940	l	
C-CT	7.306101	-5.029506	3.982960	l	
H-HC	6.542163	-5.608168	4.501540	l	
H-HC	7.533364	-4.137385	4.570927	l	
H-HC	8.215306	-5.621352	3.877241	l	
C-C	6.755500	-3.210860	2.216182	l	
O-O	7.064142	-2.246040	2.908093	l	
N-NA	6.301078	-2.982637	0.940177	l	
H-H	6.256627	-2.025775	0.633975	l	
C-C	5.825509	-3.928337	0.067667	l	
O-O	5.368061	-3.585111	-1.016936	l	
C-CT	5.147549	-8.166896	-1.603056	l	

H-H1	5.772408	-8.960335	-2.022340	1
C-CT	5.936147	-6.885556	-1.366316	1
H-HC	6.928234	-7.112032	-0.979361	1
H-HC	5.981581	-6.257450	-2.258264	1
O-OS	4.031557	-7.895936	-2.432269	1
P-P	4.023425	-8.350204	-3.973538	1
O-O2	4.525590	-9.736215	-4.057915	1
O-O2	2.711116	-7.988046	-4.549269	1
O-OS	5.140599	-7.359036	-4.567003	1
C-CT	4.771833	-6.124015	-5.156527	1
H-H1	4.090475	-5.588363	-4.493116	1
H-H1	4.260352	-6.324486	-6.099376	1
C-CT	5.978656	-5.222208	-5.422602	1
H-H1	5.672814	-4.447449	-6.129159	1
O-OS	6.384790	-4.585025	-4.228145	1
C-CT	7.715118	-4.167100	-4.420283	1
H-H2	7.768515	-3.288576	-5.079190	1
N-N*	8.256377	-3.843536	-3.085578	1
C-CK	8.585276	-4.678044	-2.045293	1
H-H5	8.552113	-5.754849	-2.119904	1
N-NB	8.922265	-4.064555	-0.945057	1
C-CB	8.813451	-2.714220	-1.278851	1
C-CA	9.026509	-1.503652	-0.568352	1
N-N2	9.359983	-1.420999	0.723095	1
H-H	9.460990	-0.511887	1.172681	1
H-H	9.444266	-2.256198	1.281589	1
N-NC	8.882562	-0.338823	-1.224799	1
C-CQ	8.511142	-0.346377	-2.504936	1
H-H5	8.426084	0.627398	-2.976511	1
N-NC	8.232745	-1.403141	-3.268560	1
C-CB	8.417190	-2.572758	-2.588580	1
C-CT	7.220412	-5.921383	-5.992815	1
H-H1	7.147229	-7.008681	-5.887170	1
C-CT	8.349786	-5.367854	-5.110377	1
H-HC	8.629766	-6.126060	-4.382619	1
H-HC	9.215378	-5.054303	-5.688616	1
O-OS	7.321895	-5.549965	-7.357313	1
P-P	8.526961	-6.032167	-8.318153	1
O-O2	9.195183	-7.197543	-7.702441	1
O-O2	8.029359	-6.084407	-9.707400	1
O-OS	9.479478	-4.748874	-8.165872	1
C-CT	8.996208	-3.461772	-8.516818	1
H-H1	7.972166	-3.340336	-8.162027	1
H-H1	9.001700	-3.345075	-9.601864	1
C-CT	9.838878	-2.368581	-7.863236	1
H-H1	9.390872	-1.401799	-8.106760	1
O-OS	9.853740	-2.524409	-6.448153	1
C-CT	11.059932	-1.935240	-6.015927	1
H-H2	10.991130	-0.840798	-6.090488	1
N-N*	11.371820	-2.348609	-4.628980	1
C-CM	11.547651	-3.672388	-4.277348	1
H-H4	11.420667	-4.439823	-5.026749	1
C-CM	11.876131	-4.031832	-3.007729	1
C-CT	12.066698	-5.503413	-2.672319	1
H-HC	13.074361	-5.811401	-2.952108	1
H-HC	11.332249	-6.113250	-3.197511	1
H-HC	11.945293	-5.644123	-1.595761	1

C-C	12.040529	-3.006702	-1.980605	1
O-O	12.356694	-3.172919	-0.805456	1
N-NA	11.792706	-1.728921	-2.409232	1
H-H	11.878446	-0.988164	-1.737499	1
C-C	11.490293	-1.335868	-3.684155	1
O-O	11.339390	-0.145210	-3.933993	1
C-CT	11.296782	-2.342247	-8.339886	1
H-H1	11.516243	-3.192441	-8.994714	1
C-CT	12.075323	-2.441166	-7.030666	1
H-HC	12.322291	-3.484727	-6.849562	1
H-HC	12.972786	-1.827304	-7.026765	1
O-OS	11.518218	-1.104841	-8.995961	1
P-P	12.915891	-0.742975	-9.715607	1
O-O2	13.679559	-1.990240	-9.926255	1
O-O2	12.639415	0.173300	-10.840160	1
O-OS	13.621465	0.093527	-8.538511	1
C-CT	13.085190	1.340922	-8.121731	1
H-H1	12.068960	1.199631	-7.750715	1
H-H1	13.054620	2.024194	-8.972748	1
C-CT	13.925766	1.973074	-7.009952	1
H-H1	13.563914	2.989323	-6.836356	1
O-OS	13.799322	1.236148	-5.805485	1
C-CT	14.986621	1.431571	-5.071893	1
H-H2	15.001945	2.416189	-4.589383	1
N-N*	15.086467	0.345663	-4.082189	1
C-CK	14.793609	-0.982581	-4.258164	1
H-H5	14.497596	-1.387828	-5.215731	1
N-NB	14.885726	-1.701706	-3.175340	1
C-CB	15.247297	-0.773688	-2.198417	1
C-CA	15.460516	-0.859498	-0.799500	1
N-N2	15.275231	-1.973487	-0.086771	1
H-H	15.343287	-1.953841	0.928856	1
H-H	14.910837	-2.800164	-0.537481	1
N-NC	15.827824	0.251151	-0.128839	1
C-CQ	15.955542	1.401393	-0.795518	1
H-H5	16.254885	2.264421	-0.207935	1
N-NC	15.747392	1.621441	-2.095274	1
C-CB	15.394717	0.477420	-2.749060	1
C-CT	15.421180	2.046731	-7.340647	1
H-H1	15.641402	1.515071	-8.272985	1
C-CT	16.060955	1.342304	-6.143411	1
H-HC	16.242811	0.301134	-6.402135	1
H-HC	16.975023	1.827015	-5.811988	1
O-OS	15.788703	3.413190	-7.424777	1
P-P	17.210150	3.886902	-8.025192	1
O-O2	17.711270	2.844481	-8.944233	1
O-O2	17.085733	5.290146	-8.468597	1
O-OS	18.095865	3.856669	-6.689747	1
C-CT	17.798375	4.732882	-5.615309	1
H-H1	16.736367	4.672057	-5.371570	1
H-H1	18.032763	5.757819	-5.906089	1
C-CT	18.596129	4.354624	-4.367682	1
H-H1	18.431666	5.114219	-3.599056	1
O-OS	18.154968	3.094928	-3.876506	1
C-CT	19.285163	2.512888	-3.263351	1
H-H2	19.542296	3.070237	-2.350027	1
N-N*	19.043642	1.080900	-2.960793	1

C-CM	18.732873	0.159136	-3.940934	l
H-H4	18.684972	0.477107	-4.971281	l
C-CM	18.469452	-1.139970	-3.634885	l
C-CT	18.121010	-2.119321	-4.746270	l
H-HC	17.563352	-1.621693	-5.538118	l
H-HC	17.511035	-2.926060	-4.333026	l
H-HC	19.037321	-2.548910	-5.151384	l
C-C	18.515422	-1.585224	-2.244436	l
O-O	18.268304	-2.709463	-1.816068	l
N-NA	18.856929	-0.609072	-1.344221	l
H-H	18.878263	-0.863917	-0.373038	l
C-C	19.109605	0.706702	-1.622906	l
O-O	19.370674	1.481318	-0.708671	l
C-CT	20.109480	4.225144	-4.614936	l
H-H1	20.383133	4.459890	-5.650554	l
C-CT	20.372608	2.760440	-4.297810	l
H-HC	20.205414	2.158058	-5.188191	l
H-HC	21.367765	2.602860	-3.883396	l
O-OH	20.838043	4.984256	-3.665527	l
H-HO	20.907068	5.902608	-3.950003	l
C-CA	0.365695	-4.156365	-1.248467	h
C-CA	0.062083	-5.132160	-0.257853	h
C-CA	0.084800	-6.505290	-0.619925	h
C-CA	0.434312	-6.885077	-1.892497	h
C-CA	0.763121	-5.909209	-2.868641	h
C-CA	0.725191	-4.576030	-2.554082	h
H-HA	-0.171819	-7.247974	0.128097	h
H-HA	0.476379	-7.935126	-2.162672	h
H-HA	1.043695	-6.223046	-3.868332	h
H-HA	0.977283	-3.820406	-3.294325	h
C-CA	0.281469	-2.782549	-0.926535	h
H-HA	0.491895	-2.051959	-1.700430	h
C-CA	0.011125	-2.397844	0.362421	h
C-CA	-0.123537	-3.372934	1.389048	h
C-CA	-0.190810	-4.708931	1.070396	h
H-HA	-0.403027	-5.457172	1.828052	h
N-NC	-0.110125	-2.825493	2.701346	h
N-NC	-0.114315	-1.059783	0.812723	h
C-CA	-0.416077	-0.114332	-0.013627	h
C-CA	0.179315	-3.565401	3.724127	h
Ni-Ni	-0.098900	-0.897559	2.715683	h
C-CA	-0.586230	1.264651	0.358440	h
H-HA	-0.550259	-0.352696	-1.070497	h
C-CA	-1.021048	2.156355	-0.636423	h
C-CA	-1.137356	3.511571	-0.395966	h
C-CA	-0.827036	3.999965	0.892824	h
C-CA	-0.408363	3.136450	1.889660	h
C-CA	-0.308238	1.728659	1.680325	h
H-HA	-1.288668	1.746167	-1.607039	h
H-HA	-1.456282	4.183176	-1.188124	h
C-CT	-0.940166	5.472506	1.184367	h
H-HA	-0.136782	3.490990	2.881402	h
O-OS	0.029646	0.976798	2.667678	h
H-HA	0.398107	-4.622558	3.562187	h
C-CA	0.195339	-3.117469	5.089027	h
C-CA	-0.089143	-1.762460	5.439009	h
C-CA	-0.341811	-1.505375	6.819767	h

C-CA	-0.245200	-2.494684	7.781053	h
C-CA	0.177446	-3.796265	7.429316	h
C-CA	0.399895	-4.077559	6.096302	h
O-OS	-0.168582	-0.792205	4.599718	h
H-HA	-0.687450	-0.505222	7.069454	h
C-CT	-0.744206	-2.204514	9.173252	h
H-HA	0.244697	-4.583580	8.173939	h
H-HA	0.677735	-5.086604	5.798164	h
N-N3	-2.335454	5.935690	1.629248	h
H-HC	-0.259859	5.766727	1.985258	h
H-HC	-0.695174	6.069280	0.303458	h
H-HC	-1.288541	-3.071210	9.553415	h
H-HC	-1.447347	-1.368753	9.152068	h
N-N3	0.304726	-1.862935	10.227672	h
C-CT	-2.770862	5.189890	2.879009	h
C-CT	-2.240415	7.424801	1.883222	h
C-CT	-3.370974	5.630846	0.560765	h
C-CT	-3.539153	8.078760	2.326107	h
H-HC	-1.460215	7.557570	2.633805	h
H-HC	-1.876179	7.869122	0.955378	h
H-HC	-4.342695	5.841720	1.007644	h
C-CT	-3.217928	6.406332	-0.738625	h
H-HC	-3.314042	4.553993	0.390308	h
H-HC	-3.819515	5.442606	3.036586	h
H-HC	-2.717026	4.129220	2.626199	h
C-CT	-1.970012	5.493831	4.135243	h
H-HC	-0.898222	5.332424	4.012461	h
H-HC	-2.138958	6.505541	4.508198	h
H-HC	-2.310597	4.799115	4.906858	h
H-HC	-4.326477	8.000128	1.573893	h
H-HC	-3.911461	7.675474	3.270081	h
H-HC	-3.342237	9.141111	2.480764	h
H-HC	-3.936462	5.992596	-1.449634	h
H-HC	-3.445170	7.467757	-0.625595	h
H-HC	-2.228590	6.306715	-1.188985	h
C-CT	1.160818	-3.095220	10.467593	h
C-CT	1.196447	-0.736460	9.736624	h
C-CT	-0.426709	-1.436528	11.485616	h
H-HC	0.330844	-1.071356	12.179719	h
H-HC	-1.055928	-0.594371	11.193580	h
C-CT	-1.299669	-2.512344	12.116629	h
H-HC	-0.756828	-3.421065	12.376654	h
H-HC	-1.723002	-2.101654	13.033910	h
H-HC	-2.144767	-2.778248	11.474521	h
C-CT	2.080794	-3.029084	11.677420	h
H-HC	0.460988	-3.928293	10.564186	h
H-HC	1.724353	-3.241557	9.544187	h
H-HC	2.638895	-3.966608	11.705732	h
H-HC	2.809571	-2.220617	11.618086	h
H-HC	1.528330	-2.949161	12.614723	h
C-CT	0.510985	0.616359	9.607053	h
H-HC	2.024745	-0.671434	10.440935	h
H-HC	1.580281	-1.073312	8.772620	h
H-HC	1.177512	1.274430	9.047627	h
H-HC	-0.426299	0.560223	9.047805	h
H-HC	0.313636	1.081018	10.573336	h

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H-HO	21.943690	-1.347192	7.279882	1
O-OH	22.153079	-0.980747	8.151911	1
C-CT	21.428358	0.235523	8.274959	1
H-H1	21.831469	0.986202	7.590321	1
H-H1	21.493631	0.622898	9.297108	1
C-CT	19.964747	-0.024758	7.910636	1
H-H1	19.393889	0.907640	7.950090	1
O-OS	19.906346	-0.552880	6.594497	1
C-CT	18.691082	-1.258712	6.541639	1
H-H2	17.852469	-0.553237	6.613322	1
N-N*	18.590206	-2.061403	5.303653	1
C-CK	18.113365	-3.341277	5.137139	1
H-H5	17.841158	-3.989093	5.959570	1
N-NB	18.016257	-3.723197	3.894971	1
C-CB	18.436104	-2.607355	3.172380	1
C-CA	18.530994	-2.317258	1.786011	1
N-N2	18.216346	-3.165383	0.800815	1
H-H	18.286743	-2.872173	-0.171934	1
H-H	17.878296	-4.089182	1.022393	1
N-NC	18.945601	-1.094424	1.412637	1
C-CQ	19.255114	-0.191384	2.342996	1
H-H5	19.563887	0.783327	1.978370	1
N-NC	19.213781	-0.338268	3.665836	1
C-CB	18.791798	-1.586598	4.024577	1
C-CT	19.288970	-1.071500	8.817128	1
H-H1	20.011867	-1.516898	9.509498	1
C-CT	18.795883	-2.101141	7.804693	1
H-HC	19.557955	-2.867827	7.665967	1
H-HC	17.838254	-2.532512	8.093081	1
O-OS	18.154294	-0.574647	9.507854	1
P-P	18.286132	0.545032	10.660199	1
O-O2	17.106321	0.455870	11.544879	1
O-O2	19.655447	0.498233	11.212609	1
O-OS	18.147632	1.859643	9.747432	1
C-CT	16.883754	2.263369	9.249480	1
H-H1	16.472428	3.027910	9.909467	1
H-H1	16.199215	1.413038	9.211042	1
C-CT	17.050815	2.808099	7.830905	1
H-H1	17.939166	3.445858	7.795420	1
O-OS	17.162620	1.694634	6.936713	1
C-CT	16.359919	1.992859	5.811791	1
H-H2	16.852193	2.754197	5.188623	1
N-N*	16.030305	0.792550	5.012420	1
C-CM	15.485434	-0.338857	5.583766	1
H-H4	15.350918	-0.375688	6.655816	1
C-CM	15.124294	-1.406987	4.824938	1
C-CT	14.536117	-2.636766	5.498783	1
H-HC	15.052510	-2.840968	6.436219	1
H-HC	14.649198	-3.496581	4.833827	1
H-HC	13.474320	-2.475999	5.684511	1
C-C	15.301038	-1.366365	3.375403	1
O-O	15.001206	-2.242515	2.569995	1
N-NA	15.871560	-0.214037	2.896944	1
H-H	16.000763	-0.136605	1.903520	1
C-C	16.229943	0.880774	3.637359	1

O-O	16.689172	1.871426	3.077644	1
C-CT	15.837114	3.623949	7.352447	1
H-H1	15.201921	3.961843	8.175123	1
C-CT	15.133786	2.599662	6.468216	1
H-HC	14.611983	1.863583	7.077897	1
H-HC	14.459358	3.045286	5.743551	1
O-OS	16.317151	4.733072	6.602063	1
P-P	15.337580	5.735526	5.805786	1
O-O2	13.977995	5.637089	6.374604	1
O-O2	15.997273	7.047928	5.657444	1
O-OS	15.316547	5.008042	4.366251	1
C-CT	16.286813	5.275433	3.354757	1
H-H1	16.705586	4.334014	2.991391	1
H-H1	17.110317	5.861767	3.766741	1
C-CT	15.698681	6.011850	2.135715	1
H-H1	16.492590	6.607107	1.679297	1
O-OS	15.245635	5.044370	1.196282	1
C-CT	13.828700	5.004073	1.174848	1
H-H2	13.452840	5.317574	0.190079	1
N-N*	13.466441	3.597423	1.440455	1
C-CK	13.581620	2.876629	2.604486	1
H-H5	13.919807	3.307393	3.534006	1
N-NB	13.266587	1.617512	2.495121	1
C-CB	12.945909	1.481639	1.147166	1
C-CA	12.577914	0.378973	0.338551	1
N-N2	12.511640	-0.887872	0.763011	1
H-H	12.320167	-1.644648	0.112326	1
H-H	12.773772	-1.114581	1.711689	1
N-NC	12.324184	0.600871	-0.962550	1
C-CQ	12.443616	1.829899	-1.467226	1
H-H5	12.222882	1.932989	-2.527665	1
N-NC	12.814172	2.937319	-0.823587	1
C-CB	13.049977	2.690560	0.497882	1
C-CT	14.506467	6.928844	2.433406	1
H-H1	14.557513	7.324864	3.452699	1
C-CT	13.328870	5.972969	2.245195	1
H-HC	13.130257	5.459312	3.181882	1
H-HC	12.428467	6.481458	1.914164	1
O-OS	14.505625	7.985086	1.485355	1
P-P	13.501026	9.241521	1.599125	1
O-O2	13.121398	9.421479	3.015284	1
O-O2	14.060725	10.361879	0.816107	1
O-OS	12.240641	8.647542	0.803686	1
C-CT	12.326851	8.394418	-0.588362	1
H-H1	13.265069	7.884745	-0.815041	1
H-H1	12.302921	9.341362	-1.131169	1
C-CT	11.174720	7.504575	-1.057159	1
H-H1	11.216425	7.439416	-2.147538	1
O-OS	11.274447	6.193704	-0.519621	1
C-CT	9.993126	5.624098	-0.693497	1
H-H2	9.813232	5.403148	-1.755627	1
N-N*	9.870965	4.390458	0.118484	1
C-CM	10.077931	4.397888	1.482704	1
H-H4	10.316064	5.329534	1.973726	1
C-CM	10.005269	3.258161	2.219032	1
C-CT	10.251134	3.317994	3.719568	1
H-HC	10.597356	2.340743	4.063484	1

H-HC	9.318594	3.559209	4.229385	1	
H-HC	11.007089	4.066158	3.956106	1	
C-C	9.708129	1.987092	1.565224	1	
O-O	9.632554	0.883464	2.097625	1	
N-NA	9.521863	2.068811	0.208170	1	
H-H	9.349470	1.211818	-0.286999	1	
C-C	9.581288	3.205458	-0.555410	1	
O-O	9.393751	3.130464	-1.765188	1	
C-CT	9.786622	8.024779	-0.669383	1	
H-H1	9.859875	8.718697	0.175190	1	
C-CT	9.057721	6.744374	-0.249728	1	
H-HC	8.933326	6.748794	0.830495	1	
H-HC	8.093313	6.638462	-0.737093	1	
O-OS	9.202273	8.646921	-1.801155	1	
P-P	7.793245	9.433192	-1.722925	1	
O-O2	7.552173	9.841087	-0.323407	1	
O-O2	7.746659	10.421054	-2.819621	1	
O-OS	6.796707	8.228329	-2.083477	1	
C-CT	6.851893	7.616236	-3.362174	1	
H-H1	7.892369	7.452959	-3.647270	1	
H-H1	6.384303	8.269244	-4.101633	1	
C-CT	6.149060	6.258310	-3.354158	1	
H-H1	6.199484	5.834670	-4.359783	1	
O-OS	6.756979	5.359918	-2.437616	1	
C-CT	5.853626	4.287752	-2.294156	1	
H-H2	5.947787	3.596520	-3.140679	1	
N-N*	6.072474	3.570331	-1.026861	1	
C-CK	6.425117	4.074110	0.199371	1	
H-H5	6.601405	5.127871	0.366216	1	
N-NB	6.528679	3.173349	1.137876	1	
C-CB	6.229563	1.977106	0.480568	1	
C-CA	6.182793	0.616029	0.880374	1	
N-N2	6.509653	0.175457	2.097990	1	
H-H	6.558762	-0.824263	2.285482	1	
H-H	6.865468	0.822923	2.783376	1	
N-NC	5.819953	-0.313348	-0.024611	1	
C-CQ	5.545466	0.062880	-1.274384	1	
H-H5	5.258021	-0.731354	-1.957137	1	
N-NC	5.586661	1.294734	-1.784713	1	
C-CB	5.938848	2.215941	-0.841615	1	
C-CT	4.682145	6.324472	-2.938957	1	
H-H1	4.546292	7.112719	-2.191386	1	
C-CT	4.482949	4.949588	-2.304873	1	
H-HC	4.098714	5.079507	-1.296666	1	
H-HC	3.813510	4.335305	-2.895638	1	
O-OS	3.851793	6.526717	-4.070635	1	
P-P	2.239574	6.616563	-3.963876	1	
O-O2	1.872057	6.946397	-2.569550	1	
O-O2	1.736232	7.426622	-5.090461	1	
O-OS	1.833476	5.084924	-4.224950	1	
C-CT	2.269304	4.397216	-5.391918	1	
H-H1	3.333172	4.582354	-5.545634	1	
H-H1	1.727445	4.760510	-6.266707	1	
C-CT	2.078329	2.882359	-5.237143	1	
H-H1	2.535348	2.375901	-6.089976	1	
O-OS	2.712344	2.475286	-4.023754	1	
C-CT	1.793160	1.674887	-3.309939	1	H-H

H-H2	1.837674	0.651923	-3.708163	l	
N-N*	2.077378	1.699435	-1.851905	h	
C-CM	2.145108	2.883394	-1.136179	h	
H-H4	1.927345	3.785590	-1.701350	h	
C-CM	2.456933	2.932002	0.174831	h	
C-CT	2.591868	4.202594	0.958179	h	
H-HC	2.178466	5.048209	0.399060	h	
H-HC	3.641074	4.408404	1.183874	h	
H-HC	2.071238	4.108314	1.914187	h	
C-C	2.718830	1.665720	0.860834	h	
O-O	2.995611	1.570140	2.054618	h	
N-NA	2.634751	0.534737	0.068710	h	
H-H	2.811133	-0.398294	0.517086	h	
C-C	2.333750	0.472586	-1.265438	h	
O-O	2.290210	-0.587896	-1.879677	h	
C-CT	0.602819	2.461542	-5.144895	l	
H-H1	-0.077483	3.223080	-5.537901	l	
C-CT	0.433760	2.269540	-3.651762	l	
H-HC	0.289792	3.234799	-3.170482	l	
H-HC	-0.377761	1.582125	-3.432208	l	
O-OS	0.372703	1.193157	-5.735689	l	
P-P	0.124573	1.039245	-7.311729	l	
O-O2	-1.055777	1.851010	-7.665074	l	
O-O2	1.413181	1.229739	-8.007282	l	
O-OS	-0.283808	-0.512683	-7.368327	l	
C-CT	0.699153	-1.537141	-7.323795	l	
H-H1	1.377680	-1.357588	-6.487796	l	
H-H1	1.276699	-1.505384	-8.248974	l	
C-CT	0.086752	-2.938999	-7.156017	l	
H-H1	0.814531	-3.676769	-7.500691	l	
O-OS	-0.191567	-3.161359	-5.775844	l	
C-CT	-1.590763	-3.282135	-5.582532	l	H-H
H-H2	-1.873928	-4.322262	-5.370002	l	
N-N*	-1.913008	-2.399952	-4.445706	h	
C-CK	-1.720558	-1.038614	-4.369707	h	
H-H5	-1.304324	-0.485392	-5.200123	h	
N-NB	-2.059771	-0.523737	-3.215911	h	
C-CB	-2.481314	-1.618672	-2.484815	h	
C-CA	-2.944688	-1.737378	-1.166564	h	
N-N2	-3.121123	-0.627051	-0.390341	h	
H-H	-3.530934	-0.769721	0.531861	h	
H-H	-3.476519	0.179542	-0.896072	h	
N-NC	-3.143233	-2.964104	-0.675474	h	
C-CQ	-2.983087	-4.033605	-1.488903	h	
H-H5	-3.184393	-4.994780	-1.023345	h	
N-NC	-2.639010	-4.036047	-2.769097	h	
C-CB	-2.378008	-2.801130	-3.215017	h	
C-CT	-1.216907	-3.140685	-7.937520	l	
H-H1	-1.276653	-2.447908	-8.782967	l	
C-CT	-2.263320	-2.826209	-6.873698	l	
H-HC	-2.450243	-1.755405	-6.865313	l	
H-HC	-3.195489	-3.359220	-7.034565	l	
O-OS	-1.281011	-4.487655	-8.378450	l	
P-P	-2.407483	-4.998864	-9.414467	l	
O-O2	-2.830960	-3.859199	-10.253743	l	
O-O2	-1.941126	-6.258085	-10.029264	l	
O-OS	-3.592922	-5.344976	-8.389080	l	

C-CT	-3.454257	-6.412689	-7.467051	1
H-H1	-2.478506	-6.358239	-6.981365	1
H-H1	-3.525503	-7.363523	-7.999105	1
C-CT	-4.534297	-6.346298	-6.385527	1
H-H1	-4.453794	-7.245860	-5.769756	1
O-OS	-4.365058	-5.209144	-5.549887	1
C-CT	-5.624285	-4.998148	-4.944320	1
H-H2	-5.828253	-5.782651	-4.202103	1
N-N*	-5.666952	-3.660128	-4.309395	1
C-CM	-5.422646	-2.507196	-5.027734	1
H-H4	-5.235486	-2.575854	-6.088759	1
C-CM	-5.386609	-1.289260	-4.426440	1
C-CT	-5.091879	-0.050051	-5.258696	1
H-HC	-4.685042	0.729824	-4.611710	1
H-HC	-6.017021	0.314022	-5.705607	1
H-HC	-4.367091	-0.273530	-6.040625	1
C-C	-5.607722	-1.181955	-2.987720	1
O-O	-5.538241	-0.163777	-2.304417	1
N-NA	-5.877780	-2.371643	-2.357038	1
H-H	-6.013034	-2.357167	-1.361076	1
C-C	-5.905346	-3.612869	-2.937795	1
O-O	-6.101470	-4.602513	-2.239709	1
C-CT	-5.964389	-6.280103	-6.937174	1
H-H1	-5.957542	-6.023046	-8.002438	1
C-CT	-6.591329	-5.153221	-6.110878	1
H-HC	-6.620775	-4.250158	-6.715710	1
H-HC	-7.586210	-5.397237	-5.747364	1
O-OS	-6.585308	-7.533768	-6.709301	1
P-P	-8.039622	-7.899217	-7.309072	1
O-O2	-8.298888	-7.042845	-8.484663	1
O-O2	-8.150965	-9.368876	-7.401700	1
O-OS	-8.959573	-7.396397	-6.094353	1
C-CT	-8.871783	-8.025909	-4.826744	1
H-H1	-7.824552	-8.136439	-4.541384	1
H-H1	-9.326404	-9.017266	-4.879313	1
C-CT	-9.570568	-7.199390	-3.747310	1
H-H1	-9.516398	-7.752462	-2.806447	1
O-OS	-8.960254	-5.933558	-3.566818	1
C-CT	-9.881969	-5.183377	-2.809793	1
H-H2	-9.875517	-5.513921	-1.763977	1
N-N*	-9.543852	-3.752968	-2.894474	1
C-CK	-9.095714	-3.038573	-3.976949	1
H-H5	-8.986438	-3.478215	-4.959168	1
N-NB	-8.801482	-1.795058	-3.713421	1
C-CB	-9.062136	-1.677986	-2.346038	1
C-CA	-8.916095	-0.630171	-1.399294	1
N-N2	-8.391120	0.570325	-1.666253	1
H-H	-8.224258	1.243825	-0.924030	1
H-H	-8.009959	0.749063	-2.582432	1
N-NC	-9.292354	-0.855725	-0.127355	1
C-CQ	-9.756949	-2.055577	0.220529	1
H-H5	-10.050405	-2.162324	1.260648	1
N-NC	-9.903144	-3.130020	-0.555992	1
C-CB	-9.533812	-2.868519	-1.843784	1
C-CT	-11.041403	-6.908455	-4.041330	1
H-H1	-11.211126	-6.897358	-5.123799	1
C-CT	-11.224962	-5.504079	-3.454344	1

H-HC	-11.437004	-4.808940	-4.263539	1
H-HC	-12.011265	-5.466679	-2.703892	1
O-OS	-11.829644	-7.892983	-3.396620	1
P-P	-13.428959	-7.985545	-3.592863	1
O-O2	-13.792812	-7.315857	-4.858675	1
O-O2	-13.853939	-9.372962	-3.318948	1
O-OS	-13.903214	-7.060480	-2.370758	1
C-CT	-13.564851	-7.405860	-1.036310	1
H-H1	-12.492346	-7.591350	-0.963721	1
H-H1	-14.097688	-8.312423	-0.742618	1
C-CT	-13.917399	-6.265532	-0.081417	1
H-H1	-13.658252	-6.567466	0.936666	1
O-OS	-13.187052	-5.096518	-0.417468	1
C-CT	-13.959873	-3.991910	0.001389	1
H-H2	-13.873560	-3.856259	1.087857	1
N-N*	-13.487230	-2.792615	-0.728462	1
C-CM	-13.360449	-2.796347	-2.102614	1
H-H4	-13.694289	-3.661027	-2.659122	1
C-CM	-12.803962	-1.750093	-2.765770	1
C-CT	-12.684466	-1.800037	-4.282201	1
H-HC	-11.869188	-2.461467	-4.567213	1
H-HC	-12.464782	-0.798646	-4.660305	1
H-HC	-13.619266	-2.146778	-4.723226	1
C-C	-12.313713	-0.596519	-2.019355	1
O-O	-11.738090	0.382618	-2.482572	1
N-NA	-12.529762	-0.649674	-0.663958	1
H-H	-12.211151	0.131727	-0.116845	1
C-C	-13.081367	-1.697137	0.027588	1
O-O	-13.175894	-1.638552	1.247682	1
C-CT	-15.404090	-5.900208	-0.107976	1
H-H1	-15.913764	-6.426238	-0.923085	1
C-CT	-15.387003	-4.391496	-0.355350	1
H-HC	-15.586423	-4.203361	-1.407849	1
H-HC	-16.102027	-3.858187	0.267168	1
O-OS	-15.948516	-6.232741	1.157118	1
P-P	-17.534275	-6.401264	1.391477	1
O-O2	-18.165911	-6.800183	0.117221	1
O-O2	-17.743448	-7.194563	2.619506	1
O-OS	-17.930717	-4.880812	1.698720	1
C-CT	-17.498900	-4.246274	2.892133	1
H-H1	-16.417995	-4.355129	3.001387	1
H-H1	-17.987036	-4.713202	3.749306	1
C-CT	-17.834145	-2.753520	2.858431	1
H-H1	-17.656929	-2.326309	3.848347	1
O-OS	-16.991083	-2.114717	1.903116	1
C-CT	-17.793834	-1.251440	1.124820	1
H-H2	-17.969000	-0.302405	1.654500	1
N-N*	-17.114353	-0.995028	-0.162754	1
C-CK	-17.265550	-1.592314	-1.393726	1
H-H5	-17.897024	-2.452540	-1.571940	1
N-NB	-16.566822	-1.039522	-2.346977	1
C-CB	-15.930420	0.027655	-1.712810	1
C-CA	-15.078512	1.072565	-2.155802	1
N-N2	-14.662867	1.254813	-3.413811	1
H-H	-14.029131	2.026699	-3.613317	1
H-H	-14.953023	0.626501	-4.145202	1
N-NC	-14.646649	1.971286	-1.255563	1

C-CQ	-15.028047	1.870476	0.015443	1
H-H5	-14.651967	2.637249	0.684628	1
N-NC	-15.816830	0.947466	0.557797	1
C-CB	-16.243944	0.046144	-0.373986	1
C-CT	-19.288858	-2.476196	2.451466	1
H-H1	-19.909295	-3.376234	2.508613	1
C-CT	-19.103197	-2.011691	1.010104	1
H-HC	-18.985813	-2.881945	0.367607	1
H-HC	-19.911931	-1.376407	0.668937	1
O-OS	-19.788018	-1.458434	3.305382	1
P-P	-21.265180	-0.828988	3.156299	1
O-O2	-22.052639	-1.651593	2.214262	1
O-O2	-21.782240	-0.505090	4.500791	1
O-OS	-20.859649	0.535815	2.420772	1
C-CT	-20.111359	1.527605	3.113112	1
H-H1	-19.285379	1.056250	3.647000	1
H-H1	-20.751935	2.035804	3.836595	1
C-CT	-19.522880	2.558734	2.148043	1
H-H1	-18.924117	3.277061	2.713352	1
O-OS	-18.709710	1.927593	1.168205	1
C-CT	-18.758018	2.673810	-0.038769	1
H-H2	-17.766239	3.083172	-0.276971	1
N-N*	-19.209090	1.779628	-1.134020	1
C-CM	-20.196492	0.837045	-0.944340	1
H-H4	-20.666966	0.759686	0.023461	1
C-CM	-20.572807	-0.006099	-1.939913	1
C-CT	-21.661006	-1.042202	-1.684213	1
H-HC	-22.060140	-0.968730	-0.671003	1
H-HC	-21.255085	-2.041868	-1.843675	1
H-HC	-22.472080	-0.890067	-2.398304	1
C-C	-19.932593	0.080424	-3.249295	1
O-O	-20.168158	-0.637042	-4.214936	1
N-NA	-18.982484	1.071604	-3.368437	1
H-H	-18.527039	1.160515	-4.256635	1
C-C	-18.589160	1.927314	-2.369133	1
O-O	-17.723493	2.766506	-2.584612	1
C-CT	-20.578055	3.342122	1.379130	1
H-H1	-21.388756	2.672132	1.073532	1
C-CT	-19.756655	3.809914	0.189077	1
H-HC	-20.374492	3.996250	-0.688920	1
H-HC	-19.205564	4.711833	0.456677	1
O-OH	-21.023485	4.461300	2.118671	1
H-HO	-21.714535	4.924139	1.632504	1
H-HO	-14.780323	9.349372	-6.762143	1
O-OH	-14.392637	10.129460	-7.197710	1
C-CT	-15.096235	11.272345	-6.731056	1
H-H1	-16.130022	11.247760	-7.087411	1
H-H1	-14.621590	12.182573	-7.105487	1
C-CT	-15.114158	11.288301	-5.198134	1
H-H1	-15.618877	12.192379	-4.846909	1
O-OS	-15.825745	10.135338	-4.770021	1
C-CT	-15.106459	9.525350	-3.719901	1
H-H2	-15.341768	10.009286	-2.765942	1
N-N*	-15.426662	8.082679	-3.676027	1
C-CK	-15.776317	7.333770	-2.578974	1
H-H5	-15.822596	7.740472	-1.576011	1
N-NB	-16.066505	6.090631	-2.848141	1

C-CB	-15.849582	5.988662	-4.221936	1
C-CA	-15.937599	4.922482	-5.155607	1
N-N2	-16.332849	3.681580	-4.860916	1
H-H	-16.348543	2.986112	-5.587612	1
H-H	-16.642261	3.445860	-3.916538	1
N-NC	-15.611663	5.153503	-6.442528	1
C-CQ	-15.221905	6.375285	-6.800827	1
H-H5	-14.974658	6.503307	-7.847539	1
N-NC	-15.102336	7.457402	-6.032879	1
C-CB	-15.440394	7.198015	-4.734044	1
C-CT	-13.714684	11.230455	-4.570989	1
H-H1	-12.941527	11.433470	-5.319442	1
C-CT	-13.653576	9.790502	-4.072475	1
H-HC	-13.331329	9.140578	-4.881768	1
H-HC	-13.015422	9.673395	-3.205328	1
O-OS	-13.662625	12.161805	-3.501018	1
P-P	-12.281748	12.538874	-2.756021	1
O-O2	-11.165334	12.344976	-3.703978	1
O-O2	-12.464411	13.826306	-2.055736	1
O-OS	-12.227718	11.368605	-1.660198	1
C-CT	-13.143719	11.349938	-0.577251	1
H-H1	-14.156239	11.518725	-0.945695	1
H-H1	-12.887775	12.146964	0.124099	1
C-CT	-13.109621	10.003347	0.151269	1
H-H1	-13.739787	10.068335	1.041165	1
O-OS	-13.564553	8.937704	-0.669949	1
C-CT	-13.135980	7.737267	-0.049636	1
H-H2	-13.883690	7.408871	0.685008	1
N-N*	-12.934126	6.688521	-1.075470	1
C-CM	-12.316375	6.964231	-2.277504	1
H-H4	-11.894061	7.945852	-2.429472	1
C-CM	-12.251753	6.038950	-3.272120	1
C-CT	-11.595964	6.401772	-4.597229	1
H-HC	-10.764533	7.089212	-4.441599	1
H-HC	-12.334283	6.853389	-5.259386	1
H-HC	-11.221247	5.492796	-5.073160	1
C-C	-12.829757	4.713176	-3.069572	1
O-O	-12.889965	3.799185	-3.887901	1
N-NA	-13.351813	4.505278	-1.818739	1
H-H	-13.730076	3.594094	-1.636310	1
C-C	-13.430024	5.418275	-0.801667	1
O-O	-13.916333	5.094857	0.277093	1
C-CT	-11.706866	9.596029	0.586983	1
H-H1	-10.988092	9.869742	-0.192168	1
C-CT	-11.837156	8.077887	0.676523	1
H-HC	-10.978202	7.611925	0.198384	1
H-HC	-11.914459	7.749828	1.713204	1
O-OS	-11.382952	10.194870	1.828060	1
P-P	-9.950448	9.978786	2.536386	1
O-O2	-8.982727	9.497354	1.527978	1
O-O2	-9.650530	11.159524	3.370195	1
O-OS	-10.297563	8.752065	3.507620	1
C-CT	-11.326639	8.864056	4.480847	1
H-H1	-12.270873	9.098712	3.987512	1
H-H1	-11.088936	9.671204	5.175974	1
C-CT	-11.500228	7.553018	5.255814	1
H-H1	-12.276083	7.689545	6.012357	1

O-OS	-11.893113	6.533565	4.342641	1
C-CT	-10.945857	5.480608	4.367429	1
H-H2	-11.317381	4.642837	4.975062	1
N-N*	-10.731495	5.061866	2.964761	1
C-CK	-10.018886	5.694327	1.972523	1
H-H5	-9.518137	6.645567	2.115531	1
N-NB	-10.019420	5.070070	0.828135	1
C-CB	-10.787387	3.932762	1.077469	1
C-CA	-11.168571	2.819981	0.285970	1
N-N2	-10.821874	2.649822	-0.992851	1
H-H	-11.141751	1.829453	-1.508684	1
H-H	-10.247057	3.334727	-1.457313	1
N-NC	-11.911743	1.850338	0.849814	1
C-CQ	-12.276845	1.966412	2.127383	1
H-H5	-12.857151	1.141348	2.527372	1
N-NC	-12.001038	2.961090	2.972097	1
C-CB	-11.237753	3.924939	2.377252	1
C-CT	-10.208836	7.117755	5.953283	1
H-H1	-9.508991	7.954742	6.035156	1
C-CT	-9.681338	6.050966	5.005329	1
H-HC	-9.044526	6.531733	4.268227	1
H-HC	-9.131701	5.277258	5.529019	1
O-OS	-10.518613	6.604031	7.237597	1
P-P	-9.370151	6.204678	8.299606	1
O-O2	-8.129191	6.929641	7.955030	1
O-O2	-9.939595	6.280775	9.660141	1
O-OS	-9.182062	4.661008	7.911478	1
C-CT	-10.212812	3.726943	8.186224	1
H-H1	-11.181629	4.162342	7.935101	1
H-H1	-10.203104	3.478605	9.249153	1
C-CT	-10.037306	2.453133	7.358544	1
H-H1	-10.799695	1.728627	7.654341	1
O-OS	-10.135154	2.719770	5.964707	1
C-CT	-9.664811	1.557737	5.305493	1
H-H2	-10.493363	0.850984	5.160343	1
N-N*	-9.031769	1.873008	4.007647	1
C-CM	-8.189538	2.953205	3.858714	1
H-H4	-8.008688	3.592029	4.708518	1
C-CM	-7.583525	3.220931	2.672805	1
C-CT	-6.671121	4.431734	2.549430	1
H-HC	-5.644899	4.120722	2.736540	1
H-HC	-6.964113	5.208498	3.255307	1
H-HC	-6.751384	4.822744	1.532424	1
C-C	-7.803950	2.339701	1.529648	1
O-O	-7.327729	2.456718	0.404616	1
N-NA	-8.623224	1.267006	1.780001	1
H-H	-8.786615	0.611535	1.035934	1
C-C	-9.234483	0.970419	2.968813	1
O-O	-9.909350	-0.048244	3.074056	1
C-CT	-8.666340	1.807378	7.503409	1
H-H1	-7.902798	2.590386	7.457976	1
C-CT	-8.628683	0.952884	6.245054	1
H-HC	-7.627158	0.992597	5.823000	1
H-HC	-8.916991	-0.075264	6.465211	1
O-OS	-8.524747	1.008225	8.663685	1
P-P	-7.114582	0.304153	9.018126	1
O-O2	-6.024062	1.111274	8.431100	1

O-O2	-7.106270	-0.039275	10.454380	l	
O-OS	-7.224153	-1.058256	8.170976	l	
C-CT	-8.084484	-2.107552	8.592043	l	
H-H1	-9.107583	-1.737176	8.668206	l	
H-H1	-7.764531	-2.458050	9.575997	l	
C-CT	-8.060062	-3.293883	7.621061	l	
H-H1	-8.634472	-4.113270	8.058138	l	
O-OS	-8.619310	-2.970896	6.352245	l	
C-CT	-7.945169	-3.702793	5.335966	l	
H-H2	-8.646158	-4.305180	4.746125	l	
N-N*	-7.265969	-2.726780	4.458016	l	
C-CK	-6.897280	-1.442457	4.755094	l	
H-H5	-6.954795	-1.060849	5.763737	l	
N-NB	-6.501724	-0.735714	3.732466	l	
C-CB	-6.582665	-1.635325	2.670414	l	
C-CA	-6.315784	-1.537534	1.279923	l	
N-N2	-5.978927	-0.411434	0.640848	l	
H-H	-5.885112	-0.400096	-0.373807	l	
H-H	-5.972929	0.469636	1.135131	l	
N-NC	-6.438387	-2.642955	0.524932	l	
C-CQ	-6.839119	-3.783553	1.087686	l	
H-H5	-6.916698	-4.632945	0.416594	l	
N-NC	-7.167933	-3.996726	2.363723	l	
C-CB	-7.009618	-2.867487	3.113517	l	
C-CT	-6.654863	-3.806835	7.340995	l	
H-H1	-5.993833	-2.956902	7.154650	l	
C-CT	-6.938501	-4.585683	6.063676	l	
H-HC	-6.046663	-4.753668	5.470148	l	
H-HC	-7.403055	-5.539207	6.308217	l	
O-OS	-6.195830	-4.635058	8.393260	l	
P-P	-4.630086	-4.775532	8.727327	l	
O-O2	-3.989811	-3.465287	8.497633	l	
O-O2	-4.470080	-5.462969	10.022833	l	
O-OS	-4.114918	-5.758181	7.581200	l	
C-CT	-4.675447	-7.051336	7.403614	l	
H-H1	-5.763298	-6.980210	7.402555	l	
H-H1	-4.370667	-7.706070	8.221095	l	
C-CT	-4.229349	-7.635013	6.055259	l	
H-H1	-4.697198	-8.610319	5.904831	l	
O-OS	-4.644188	-6.720778	5.041181	l	
C-CT	-3.530402	-6.387023	4.241471	l	H-H
H-H2	-3.489751	-7.076221	3.388583	l	
N-N*	-3.596302	-4.965415	3.804368	h	
C-CM	-3.612108	-3.928288	4.722791	h	
H-H4	-3.766501	-4.211131	5.761320	h	
C-CM	-3.442706	-2.631494	4.389518	h	
C-CT	-3.471770	-1.508259	5.383376	h	
H-HC	-2.540848	-0.940112	5.342963	h	
H-HC	-3.610411	-1.901668	6.395581	h	
H-HC	-4.281456	-0.808893	5.172208	h	
C-C	-3.192301	-2.342272	2.982524	h	
O-O	-2.860561	-1.228352	2.550785	h	
N-NA	-3.336828	-3.402540	2.114105	h	
H-H	-3.240113	-3.213086	1.085397	h	
C-C	-3.442151	-4.736684	2.442399	h	
O-O	-3.384945	-5.628532	1.610854	h	
C-CT	-2.706246	-7.802135	5.973967	l	

H-H1	-2.265721	-7.747290	6.972841	l	
C-CT	-2.315181	-6.607977	5.130724	l	
H-HC	-2.181167	-5.771028	5.805803	l	
H-HC	-1.419538	-6.784713	4.541798	l	
O-OS	-2.337898	-9.003491	5.320790	l	
P-P	-0.856119	-9.635150	5.482393	l	
O-O2	-0.307464	-9.210240	6.788060	l	
O-O2	-0.930310	-11.069400	5.139325	l	
O-OS	-0.002252	-8.897135	4.334656	l	
C-CT	-0.334514	-9.051255	2.963834	l	
H-H1	-1.232492	-8.475717	2.740162	l	
H-H1	-0.540324	-10.102843	2.752091	l	
C-CT	0.805740	-8.586740	2.049623	l	
H-H1	0.490720	-8.748632	1.017962	l	
O-OS	1.100504	-7.205885	2.236834	l	
C-CT	2.492091	-7.052148	2.037303	l	H-H
H-H2	2.732648	-7.072497	0.966242	l	
N-N*	2.890197	-5.761386	2.638192	h	
C-CK	3.007320	-5.440311	3.977689	h	
H-H5	3.006351	-6.198869	4.749110	h	
N-NB	3.107073	-4.157700	4.202062	h	
C-CB	3.043687	-3.591055	2.942377	h	
C-CA	2.936219	-2.253527	2.500759	h	
N-N2	2.707894	-1.213248	3.339453	h	
H-H	2.830092	-0.256390	2.991343	h	
H-H	2.849968	-1.373530	4.329526	h	
N-NC	2.945815	-2.035247	1.180275	h	
C-CQ	2.940414	-3.081258	0.328039	h	
H-H5	2.981334	-2.818130	-0.726648	h	
N-NC	2.873462	-4.368572	0.629183	h	
C-CB	2.927403	-4.566158	1.953938	h	
C-CT	2.110107	-9.368586	2.255868	l	
H-H1	1.985980	-10.145529	3.017610	l	
C-CT	3.077456	-8.282217	2.715626	l	
H-HC	3.017431	-8.196997	3.798063	l	
H-HC	4.097412	-8.468477	2.384946	l	
O-OS	2.496818	-9.911275	1.002008	l	
P-P	3.615226	-11.066095	0.876125	l	
O-O2	3.632618	-11.836428	2.136421	l	
O-O2	3.410160	-11.751287	-0.416395	l	
O-OS	4.980454	-10.211086	0.785328	l	
C-CT	5.470819	-9.688539	-0.443466	l	
H-H1	5.547717	-10.499039	-1.170860	l	
H-H1	6.467077	-9.282055	-0.273343	l	
C-CT	4.581865	-8.572443	-1.012803	l	
H-H1	3.555146	-8.936626	-1.114684	l	
O-OS	4.663212	-7.446593	-0.145926	l	
C-CT	5.066655	-6.302590	-0.879540	l	
H-H2	4.189162	-5.790890	-1.298190	l	
N-N*	5.824166	-5.389170	0.008133	l	
C-CM	6.317951	-5.815678	1.225106	l	
H-H4	6.317790	-6.870810	1.460503	l	
C-CM	6.756058	-4.936335	2.161464	l	
C-CT	7.237179	-5.463625	3.505732	l	
H-HC	6.436864	-6.020827	3.992075	l	
H-HC	7.522328	-4.624977	4.144953	l	
H-HC	8.105495	-6.106565	3.361550	l	

C-C	6.724943	-3.504433	1.883185	1
O-O	7.027887	-2.600153	2.654909	1
N-NA	6.292566	-3.170836	0.623041	1
H-H	6.260745	-2.192383	0.393219	1
C-C	5.831712	-4.040680	-0.332066	1
O-O	5.399685	-3.607198	-1.394525	1
C-CT	5.078033	-8.087267	-2.377877	1
H-H1	5.676715	-8.847882	-2.886749	1
C-CT	5.900821	-6.856406	-2.019474	1
H-HC	6.888623	-7.143199	-1.662805	1
H-HC	5.955347	-6.142792	-2.844338	1
O-OS	3.960445	-7.699444	-3.157002	1
P-P	3.905945	-8.013094	-4.731206	1
O-O2	4.339665	-9.407827	-4.947661	1
O-O2	2.602185	-7.540441	-5.243416	1
O-OS	5.059933	-7.024616	-5.255806	1
C-CT	4.736477	-5.738976	-5.757027	1
H-H1	4.052191	-5.238056	-5.069841	1
H-H1	4.243072	-5.852981	-6.723562	1
C-CT	5.969417	-4.849031	-5.922826	1
H-H1	5.695451	-4.008648	-6.564474	1
O-OS	6.364563	-4.328067	-4.669958	1
C-CT	7.698707	-3.904438	-4.811223	1
H-H2	7.762050	-2.972099	-5.390767	1
N-N*	8.233081	-3.699362	-3.450558	1
C-CK	8.576869	-4.619983	-2.490619	1
H-H5	8.550862	-5.686405	-2.658971	1
N-NB	8.920820	-4.102921	-1.343808	1
C-CB	8.799951	-2.729327	-1.556670	1
C-CA	9.014457	-1.584018	-0.745562	1
N-N2	9.363523	-1.610876	0.544104	1
H-H	9.468422	-0.741969	1.066631	1
H-H	9.463778	-2.490427	1.026579	1
N-NC	8.857611	-0.367565	-1.296434	1
C-CQ	8.472213	-0.265457	-2.568310	1
H-H5	8.378679	0.745005	-2.953156	1
N-NC	8.189300	-1.253146	-3.417573	1
C-CB	8.387596	-2.476382	-2.844368	1
C-CT	7.208363	-5.523362	-6.528252	1
H-H1	7.120810	-6.614075	-6.493831	1
C-CT	8.333806	-5.043378	-5.598647	1
H-HC	8.615023	-5.859932	-4.937677	1
H-HC	9.199005	-4.679178	-6.146207	1
O-OS	7.328751	-5.064444	-7.865018	1
P-P	8.562969	-5.454464	-8.832529	1
O-O2	9.254707	-6.636267	-8.276882	1
O-O2	8.089225	-5.435929	-10.230940	1
O-OS	9.477761	-4.156222	-8.587814	1
C-CT	8.957516	-2.863294	-8.855354	1
H-H1	7.921005	-2.805942	-8.520858	1
H-H1	8.982046	-2.666593	-9.928275	1
C-CT	9.736097	-1.787877	-8.098876	1
H-H1	9.236236	-0.829875	-8.263696	1
O-OS	9.741728	-2.075784	-6.701185	1
C-CT	10.981264	-1.599729	-6.225220	1
H-H2	10.972495	-0.500870	-6.215009	1
N-N*	11.294046	-2.127509	-4.878363	1

C-CM	11.503605	-3.470618	-4.634845	1
H-H4	11.380205	-4.182849	-5.436973	1
C-CM	11.865509	-3.919115	-3.402968	1
C-CT	12.091359	-5.407894	-3.186559	1
H-HC	13.091510	-5.676703	-3.526973	1
H-HC	11.345737	-5.989413	-3.727903	1
H-HC	12.013959	-5.631153	-2.119918	1
C-C	12.035887	-2.972203	-2.303791	1
O-O	12.386541	-3.220200	-1.153125	1
N-NA	11.754447	-1.670979	-2.627261	1
H-H	11.858650	-0.975641	-1.910735	1
C-C	11.420488	-1.188275	-3.861947	1
O-O	11.257444	0.016088	-4.021511	1
C-CT	11.198713	-1.635310	-8.545039	1
H-H1	11.435865	-2.273729	-9.402185	1
C-CT	11.954277	-2.066521	-7.294115	1
H-HC	12.049714	-3.150444	-7.291910	1
H-HC	12.924440	-1.584777	-7.193639	1
O-OS	11.412917	-0.261806	-8.834757	1
P-P	12.831373	0.317733	-9.336841	1
O-O2	13.725122	-0.814312	-9.658139	1
O-O2	12.575956	1.379305	-10.330877	1
O-OS	13.352916	1.006658	-7.977698	1
C-CT	12.680499	2.138182	-7.434669	1
H-H1	11.741554	1.825845	-6.975054	1
H-H1	12.454831	2.844155	-8.236113	1
C-CT	13.526054	2.868270	-6.384859	1
H-H1	13.072020	3.842125	-6.188016	1
O-OS	13.549969	2.124260	-5.177379	1
C-CT	14.855233	2.165431	-4.645636	1
H-H2	15.010419	3.060802	-4.031251	1
N-N*	15.017436	0.930295	-3.861807	1
C-CK	14.678917	-0.347508	-4.229035	1
H-H5	14.304973	-0.584740	-5.216414	1
N-NB	14.823907	-1.234174	-3.284563	1
C-CB	15.261725	-0.479855	-2.195900	1
C-CA	15.533748	-0.786454	-0.838943	1
N-N2	15.347473	-1.990522	-0.290746	1
H-H	15.445407	-2.115489	0.714804	1
H-H	14.948315	-2.736183	-0.842371	1
N-NC	15.944497	0.203536	-0.022536	1
C-CQ	16.059786	1.444133	-0.501427	1
H-H5	16.390185	2.203237	0.202173	1
N-NC	15.800131	1.866359	-1.738807	1
C-CB	15.403860	0.842077	-2.547103	1
C-CT	14.976280	3.091471	-6.832113	1
H-H1	15.120728	2.781411	-7.872958	1
C-CT	15.753644	2.194701	-5.871574	1
H-HC	15.834492	1.198729	-6.303619	1
H-HC	16.733310	2.595875	-5.624829	1
O-OS	15.285916	4.464438	-6.662145	1
P-P	16.633837	5.122302	-7.256923	1
O-O2	17.107502	4.300268	-8.389342	1
O-O2	16.415805	6.574501	-7.414596	1
O-OS	17.615847	4.890505	-6.012028	1
C-CT	17.362178	5.536505	-4.776165	1
H-H1	16.325843	5.370030	-4.477498	1

H-H1	17.526163	6.609278	-4.886874	l
C-CT	18.268983	4.988949	-3.675449	l
H-H1	18.128767	5.591932	-2.774317	l
O-OS	17.928041	3.640591	-3.383464	l
C-CT	19.117675	3.059467	-2.893426	l
H-H2	19.381484	3.506066	-1.923083	l
N-N*	18.983258	1.587349	-2.779100	l
C-CM	18.619075	0.796029	-3.849592	l
H-H4	18.468564	1.252563	-4.815953	l
C-CM	18.421501	-0.542171	-3.706675	l
C-CT	18.000723	-1.372574	-4.910413	l
H-HC	17.388342	-0.782327	-5.590837	l
H-HC	17.422703	-2.233187	-4.565773	l
H-HC	18.888415	-1.734801	-5.429051	l
C-C	18.598544	-1.169907	-2.399286	l
O-O	18.409682	-2.348667	-2.110784	l
N-NA	18.998220	-0.314614	-1.404279	l
H-H	19.099591	-0.696177	-0.480476	l
C-C	19.177971	1.037761	-1.516197	l
O-O	19.480698	1.694193	-0.525388	l
C-CT	19.764834	4.989307	-4.036081	l
H-H1	19.947712	5.366982	-5.049221	l
C-CT	20.135216	3.516378	-3.926743	l
H-HC	19.963126	3.022209	-4.880699	l
H-HC	21.157202	3.374742	-3.576693	l
O-OH	20.514383	5.672267	-3.046298	l
H-HO	20.519143	6.619965	-3.222449	l
C-CA	0.286152	-4.029371	-1.504030	h
C-CA	-0.036475	-5.100800	-0.625627	h
C-CA	-0.026241	-6.428003	-1.130884	h
C-CA	0.336330	-6.674384	-2.432173	h
C-CA	0.685453	-5.604236	-3.296613	h
C-CA	0.653520	-4.310332	-2.845067	h
H-HA	-0.300542	-7.241725	-0.467777	h
H-HA	0.371685	-7.690175	-2.812023	h
H-HA	0.975579	-5.815461	-4.320728	h
H-HA	0.914990	-3.483254	-3.501829	h
C-CA	0.220003	-2.699555	-1.031434	h
H-HA	0.456481	-1.895807	-1.721128	h
C-CA	-0.054076	-2.441279	0.289770	h
C-CA	-0.213421	-3.522121	1.208843	h
C-CA	-0.295773	-4.813659	0.737088	h
H-HA	-0.543141	-5.632275	1.406499	h
N-NC	-0.252787	-3.148479	2.576833	h
N-NC	-0.156531	-1.146404	0.850542	h
C-CA	-0.433739	-0.131238	0.105635	h
C-CA	0.056450	-3.990863	3.506955	h
Cu-Cu	-0.304205	-1.131139	2.845062	h
C-CA	-0.599802	1.220495	0.578805	h
H-HA	-0.560960	-0.272241	-0.971060	h
C-CA	-0.982762	2.173890	-0.380211	h
C-CA	-1.082428	3.518254	-0.078927	h
C-CA	-0.800942	3.935202	1.240408	h
C-CA	-0.452236	3.010497	2.209106	h
C-CA	-0.379668	1.608299	1.941417	h
H-HA	-1.213412	1.819151	-1.381573	h
H-HA	-1.352480	4.235576	-0.849252	h

C-CT	-0.843855	5.400248	1.585294	h
H-HA	-0.207955	3.309995	3.226039	h
O-OS	-0.116475	0.805319	2.909909	h
H-HA	0.348573	-5.009863	3.228416	h
C-CA	0.012301	-3.717632	4.923276	h
C-CA	-0.315726	-2.431759	5.460595	h
C-CA	-0.596708	-2.390021	6.860756	h
C-CA	-0.491758	-3.503667	7.674050	h
C-CA	-0.033035	-4.730433	7.145577	h
C-CA	0.222535	-4.804857	5.790125	h
O-OS	-0.403814	-1.344161	4.780216	h
H-HA	-0.970044	-1.443774	7.244877	h
C-CT	-1.010924	-3.413270	9.085421	h
H-HA	0.033501	-5.621409	7.762131	h
H-HA	0.530652	-5.755669	5.357965	h
N-N3	-2.214808	5.922735	2.036808	h
H-HC	-0.153088	5.632663	2.397266	h
H-HC	-0.561535	6.011219	0.725253	h
H-HC	-1.605892	-4.299003	9.317238	h
H-HC	-1.672842	-2.549339	9.182933	h
N-N3	0.027228	-3.298251	10.199299	h
C-CT	-2.690635	5.173470	3.269257	h
C-CT	-2.046077	7.399619	2.323181	h
C-CT	-3.257377	5.689941	0.957114	h
C-CT	-3.310217	8.105063	2.785932	h
H-HC	-1.257071	7.477454	3.072453	h
H-HC	-1.664130	7.846148	1.403407	h
H-HC	-4.222769	5.925187	1.406274	h
C-CT	-3.067198	6.496453	-0.318374	h
H-HC	-3.239180	4.617370	0.754061	h
H-HC	-3.724536	5.479659	3.431885	h
H-HC	-2.691864	4.117719	2.991472	h
C-CT	-1.875621	5.406210	4.531633	h
H-HC	-0.813508	5.192496	4.404253	h
H-HC	-1.991539	6.416968	4.926547	h
H-HC	-2.251280	4.713434	5.288263	h
H-HC	-4.107315	8.066660	2.040751	h
H-HC	-3.690283	7.709889	3.730039	h
H-HC	-3.066664	9.156724	2.947152	h
H-HC	-3.788881	6.124679	-1.048922	h
H-HC	-3.263456	7.560515	-0.176460	h
H-HC	-2.075628	6.380317	-0.760251	h
C-CT	0.777126	-4.617176	10.297065	h
C-CT	1.026350	-2.197932	9.882459	h
C-CT	-0.708680	-2.978334	11.484809	h
H-HC	0.051783	-2.803331	12.245998	h
H-HC	-1.232141	-2.038889	11.303037	h
C-CT	-1.717495	-4.031709	11.920926	h
H-HC	-1.290066	-5.028158	12.035823	h
H-HC	-2.124841	-3.727691	12.885560	h
H-HC	-2.561746	-4.092117	11.227740	h
C-CT	1.626209	-4.801478	11.546420	h
H-HC	0.017671	-5.399734	10.233397	h
H-HC	1.384959	-4.671878	9.392525	h
H-HC	2.126978	-5.766626	11.451239	h
H-HC	2.400981	-4.042320	11.655340	h
H-HC	1.023170	-4.833724	12.454750	h

C-CT	0.457296	-0.787026	9.903641	h
H-HC	1.828157	-2.294787	10.613186	h
H-HC	1.419291	-2.442401	8.894250	h
H-HC	1.200876	-0.121883	9.462372	h
H-HC	-0.449717	-0.696553	9.301285	h
H-HC	0.246917	-0.431883	10.912684	h

3/[dodeca(dA-dT)]$_2$

H-HO	21.912501	-1.043702	7.677165	l
O-OH	22.183560	-0.590270	8.488220	l
C-CT	21.541535	0.677129	8.490809	l
H-H1	21.946599	1.307344	7.694823	l
H-H1	21.694852	1.182294	9.449788	l
C-CT	20.043759	0.478527	8.244937	l
H-H1	19.538013	1.446978	8.218380	l
O-OS	19.867750	-0.171366	6.996291	l
C-CT	18.653316	-0.871845	7.107767	l
H-H2	17.820993	-0.158319	7.154743	l
N-N*	18.477118	-1.810440	5.978753	l
C-CK	18.022643	-3.108912	5.992989	l
H-H5	17.802244	-3.655287	6.900488	l
N-NB	17.884030	-3.643503	4.812660	l
C-CB	18.256465	-2.620508	3.941231	l
C-CA	18.312363	-2.511253	2.527744	l
N-N2	18.009639	-3.492915	1.671884	l
H-H	18.073321	-3.335955	0.669960	l
H-H	17.708195	-4.388306	2.024204	l
N-NC	18.685785	-1.338472	1.988059	l
C-CQ	18.998823	-0.316564	2.784763	l
H-H5	19.279220	0.607963	2.289245	l
N-NC	18.994909	-0.292275	4.116142	l
C-CB	18.613847	-1.492552	4.644174	l
C-CT	19.374442	-0.423160	9.301192	l
H-H1	20.105842	-0.782696	10.033030	l
C-CT	18.842191	-1.568305	8.447866	l
H-HC	19.608250	-2.338046	8.354009	l
H-HC	17.909708	-1.971909	8.839814	l
O-OS	18.258628	0.175512	9.941136	l
P-P	18.415217	1.461431	10.900047	l
O-O2	17.290583	1.480070	11.857903	l
O-O2	19.814413	1.541906	11.367678	l
O-OS	18.175554	2.604441	9.800286	l
C-CT	16.871632	2.883129	9.327546	l
H-H1	16.441349	3.678542	9.937253	l
H-H1	16.240786	1.994494	9.396215	l
C-CT	16.946951	3.310165	7.861606	l
H-H1	17.808755	3.970875	7.731764	l
O-OS	17.051043	2.146760	7.035463	l
C-CT	16.279885	2.392966	5.875894	l
H-H2	16.796405	3.102117	5.211912	l
N-N*	15.944807	1.140769	5.162281	l
C-CM	15.465760	0.038202	5.835648	l
H-H4	15.384352	0.075472	6.912938	l
C-CM	15.103247	-1.089511	5.172986	l
C-CT	14.589628	-2.288365	5.956742	l

H-HC	15.050150	-2.330134	6.943423	1
H-HC	14.834760	-3.202749	5.410572	1
H-HC	13.505994	-2.221024	6.053442	1
C-C	15.207826	-1.145555	3.718392	1
O-O	14.915391	-2.100550	3.007908	1
N-NA	15.693425	-0.005028	3.122933	1
H-H	15.791369	-0.001612	2.120808	1
C-C	16.081007	1.139015	3.775526	1
O-O	16.523705	2.088394	3.138816	1
C-CT	15.685004	4.054390	7.400593	1
H-H1	15.028782	4.311892	8.236237	1
C-CT	15.039425	3.043829	6.463935	1
H-HC	14.456525	2.324131	7.036596	1
H-HC	14.428721	3.513739	5.700090	1
O-OS	16.068216	5.216427	6.686346	1
P-P	14.992972	6.323877	6.214516	1
O-O2	13.666543	5.967721	6.760619	1
O-O2	15.563630	7.664090	6.454457	1
O-OS	14.944081	6.068043	4.627787	1
C-CT	16.030055	6.431301	3.781486	1
H-H1	16.755156	5.617115	3.737663	1
H-H1	16.529442	7.314227	4.184133	1
C-CT	15.566974	6.768654	2.355033	1
H-H1	16.367619	7.317995	1.855683	1
O-OS	15.308429	5.573392	1.633204	1
C-CT	13.938972	5.494613	1.285295	1
H-H2	13.799941	5.683268	0.212009	1
N-N*	13.528279	4.122649	1.641608	1
C-CK	13.464516	3.548019	2.886044	1
H-H5	13.651316	4.111857	3.788200	1
N-NB	13.174202	2.276529	2.882917	1
C-CB	13.064139	1.975281	1.525325	1
C-CA	12.804256	0.782257	0.803141	1
N-N2	12.634044	-0.424545	1.354784	1
H-H	12.509797	-1.249071	0.775570	1
H-H	12.705273	-0.532842	2.355020	1
N-NC	12.741027	0.848367	-0.538168	1
C-CQ	12.946990	2.012210	-1.154968	1
H-H5	12.869167	1.992581	-2.237559	1
N-NC	13.235857	3.189383	-0.600266	1
C-CB	13.272338	3.101542	0.760852	1
C-CT	14.293584	7.620135	2.326185	1
H-H1	14.152414	8.143356	3.277634	1
C-CT	13.215280	6.564853	2.097491	1
H-HC	12.893401	6.175174	3.059514	1
H-HC	12.363587	6.956411	1.549590	1
O-OS	14.388085	8.546400	1.257259	1
P-P	13.322602	9.742467	1.056923	1
O-O2	12.707766	10.060694	2.362245	1
O-O2	13.951605	10.799243	0.238676	1
O-OS	12.239253	8.979957	0.154793	1
C-CT	12.572015	8.565390	-1.158505	1
H-H1	13.555849	8.093217	-1.159391	1
H-H1	12.599669	9.434761	-1.818067	1
C-CT	11.555873	7.552563	-1.685495	1
H-H1	11.803224	7.332180	-2.726676	1
O-OS	11.588468	6.342673	-0.942748	1

C-CT	10.378243	5.687768	-1.253866	1
H-H2	10.413596	5.296778	-2.280440	1
N-N*	10.131065	4.593584	-0.287890	1
C-CM	10.147443	4.813260	1.074210	1
H-H4	10.312658	5.815766	1.439624	1
C-CM	9.977379	3.796137	1.959801	1
C-CT	10.012678	4.082397	3.453832	1
H-HC	10.443981	3.222222	3.970409	1
H-HC	8.995577	4.231084	3.816193	1
H-HC	10.615670	4.964373	3.667520	1
C-C	9.775885	2.434780	1.472824	1
O-O	9.628769	1.420704	2.149936	1
N-NA	9.774289	2.309084	0.107046	1
H-H	9.650201	1.386892	-0.269465	1
C-C	9.929569	3.317673	-0.806740	1
O-O	9.898434	3.062542	-2.006163	1
C-CT	10.107105	8.046920	-1.639007	1
H-H1	10.004351	8.856947	-0.908905	1
C-CT	9.343136	6.803522	-1.175040	1
H-HC	9.009545	6.956074	-0.151522	1
H-HC	8.497184	6.571865	-1.816749	1
O-OS	9.725371	8.467913	-2.936700	1
P-P	8.330186	9.230871	-3.214181	1
O-O2	7.874385	9.868935	-1.961991	1
O-O2	8.464465	10.013733	-4.459166	1
O-OS	7.389969	7.964922	-3.513337	1
C-CT	7.627191	7.150052	-4.650563	1
H-H1	8.684540	6.882895	-4.695426	1
H-H1	7.367444	7.704910	-5.554452	1
C-CT	6.809120	5.860007	-4.584940	1
H-H1	6.941632	5.313457	-5.521944	1
O-OS	7.238421	5.039790	-3.510990	1
C-CT	6.190151	4.130640	-3.259751	1
H-H2	6.185051	3.324264	-4.003403	1
N-N*	6.325723	3.579665	-1.899211	1
C-CK	6.650755	4.236552	-0.739207	1
H-H5	6.842344	5.300168	-0.707178	1
N-NB	6.702974	3.470209	0.314849	1
C-CB	6.412378	2.200105	-0.188107	1
C-CA	6.329450	0.907715	0.392345	1
N-N2	6.597434	0.640075	1.673152	1
H-H	6.620774	-0.321628	2.010076	1
H-H	6.937340	1.373695	2.275706	1
N-NC	5.992945	-0.134327	-0.392029	1
C-CQ	5.778772	0.070734	-1.692395	1
H-H5	5.525393	-0.809869	-2.273150	1
N-NC	5.851204	1.221513	-2.363900	1
C-CB	6.173834	2.261340	-1.541146	1
C-CT	5.311524	6.093189	-4.380924	1
H-H1	5.135670	7.077770	-3.934713	1
C-CT	4.936853	4.984256	-3.395330	1
H-HC	4.676385	5.434000	-2.439353	1
H-HC	4.122543	4.371576	-3.766105	1
O-OS	4.659754	5.969812	-5.633436	1
P-P	3.076071	6.230864	-5.823815	1
O-O2	2.586495	7.060734	-4.702512	1
O-O2	2.829698	6.626581	-7.224509	1

O-OS	2.521846	4.738740	-5.620748	l	
C-CT	2.990700	3.672970	-6.437188	l	
H-H1	4.079922	3.694452	-6.484241	l	
H-H1	2.599442	3.777117	-7.451236	l	
C-CT	2.575877	2.323452	-5.849345	l	
H-H1	2.952854	1.522979	-6.488171	l	
O-OS	3.132111	2.190836	-4.542203	l	
C-CT	2.139499	1.584585	-3.745711	l	H-H
H-H2	2.077608	0.520756	-4.010360	l	
N-N*	2.416367	1.758309	-2.295789	h	
C-CM	2.579893	3.008651	-1.725210	h	
H-H4	2.459727	3.847059	-2.402042	h	
C-CM	2.865956	3.193854	-0.420175	h	
C-CT	3.094365	4.533246	0.210638	h	
H-HC	2.867648	5.340718	-0.490705	h	
H-HC	4.133085	4.629837	0.535078	h	
H-HC	2.473845	4.633259	1.104677	h	
C-C	2.985314	2.005793	0.424108	h	
O-O	3.193107	2.032463	1.636527	h	
N-NA	2.843229	0.799929	-0.234670	h	
H-H	2.935336	-0.079809	0.322145	h	
C-C	2.550243	0.595359	-1.556791	h	
O-O	2.410269	-0.529184	-2.024910	h	
C-CT	1.050871	2.179066	-5.712896	l	
H-H1	0.506449	2.970148	-6.237962	l	
C-CT	0.862643	2.271968	-4.209661	l	
H-HC	0.848055	3.318252	-3.908383	l	
H-HC	-0.031584	1.740870	-3.893739	l	
O-OS	0.609371	0.887869	-6.091912	l	
P-P	0.327950	0.523312	-7.626071	l	
O-O2	-0.856269	1.286738	-8.064542	l	
O-O2	1.602300	0.607616	-8.368396	l	
O-OS	-0.080726	-1.017267	-7.453079	l	
C-CT	0.902345	-2.022147	-7.255649	l	
H-H1	1.585183	-1.718396	-6.460431	l	
H-H1	1.473822	-2.138276	-8.177764	l	
C-CT	0.283918	-3.375672	-6.868842	l	
H-H1	1.011104	-4.160112	-7.087648	l	
O-OS	-0.001662	-3.378092	-5.472138	l	
C-CT	-1.399668	-3.492626	-5.271368	l	H-H
H-H2	-1.667993	-4.497884	-4.918912	l	
N-N*	-1.748804	-2.468711	-4.268079	h	
C-CK	-1.544383	-1.110385	-4.359983	h	
H-H5	-1.101907	-0.673121	-5.244382	h	
N-NB	-1.913818	-0.451235	-3.290650	h	
C-CB	-2.372165	-1.442853	-2.440740	h	
C-CA	-2.853871	-1.397404	-1.120606	h	
N-N2	-3.012554	-0.220790	-0.464170	h	
H-H	-3.360366	-0.237621	0.493674	h	
H-H	-3.211883	0.593800	-1.031651	h	
N-NC	-3.087639	-2.559019	-0.497953	h	
C-CQ	-2.929552	-3.717931	-1.174997	h	
H-H5	-3.168187	-4.613493	-0.607602	h	
N-NC	-2.545887	-3.879078	-2.432561	h	
C-CB	-2.259517	-2.707629	-3.014274	h	
C-CT	-1.014552	-3.689175	-7.621792	l	
H-H1	-1.074246	-3.115440	-8.551859	l	

C-CT	-2.071560	-3.237680	-6.617731	1
H-HC	-2.276449	-2.178387	-6.762041	1
H-HC	-2.993738	-3.805264	-6.702929	1
O-OS	-1.059959	-5.083941	-7.881312	1
P-P	-2.170973	-5.743432	-8.847328	1
O-O2	-2.595686	-4.734993	-9.840278	1
O-O2	-1.687211	-7.070802	-9.277543	1
O-OS	-3.360483	-5.956199	-7.792369	1
C-CT	-3.211462	-6.875041	-6.723130	1
H-H1	-2.237936	-6.737602	-6.250100	1
H-H1	-3.271201	-7.894685	-7.108789	1
C-CT	-4.291347	-6.664149	-5.661154	1
H-H1	-4.191038	-7.454801	-4.913554	1
O-OS	-4.153322	-5.409742	-5.009923	1
C-CT	-5.397030	-5.187462	-4.379961	1
H-H2	-5.514675	-5.866615	-3.524613	1
N-N*	-5.511046	-3.776650	-3.943747	1
C-CM	-5.267962	-2.732668	-4.812025	1
H-H4	-5.035964	-2.954646	-5.843037	1
C-CM	-5.286448	-1.440359	-4.391651	1
C-CT	-4.983168	-0.325008	-5.381423	1
H-HC	-4.458825	0.481757	-4.866468	1
H-HC	-5.920017	0.067817	-5.777434	1
H-HC	-4.360766	-0.687159	-6.199375	1
C-C	-5.572706	-1.133145	-2.992983	1
O-O	-5.561152	-0.024482	-2.463791	1
N-NA	-5.835776	-2.228915	-2.207344	1
H-H	-6.027453	-2.073613	-1.233090	1
C-C	-5.807359	-3.541254	-2.603164	1
O-O	-5.999598	-4.427232	-1.776490	1
C-CT	-5.721574	-6.712044	-6.209740	1
H-H1	-5.723154	-6.520643	-7.288038	1
C-CT	-6.403104	-5.563145	-5.459437	1
H-HC	-6.559083	-4.735089	-6.146559	1
H-HC	-7.343496	-5.858777	-5.003410	1
O-OS	-6.279321	-7.979693	-5.906616	1
P-P	-7.717339	-8.446794	-6.472461	1
O-O2	-8.012786	-7.689068	-7.705935	1
O-O2	-7.769395	-9.922795	-6.458346	1
O-OS	-8.659454	-7.895548	-5.294021	1
C-CT	-8.547039	-8.420637	-3.979874	1
H-H1	-7.497458	-8.447178	-3.682511	1
H-H1	-8.942536	-9.438629	-3.958329	1
C-CT	-9.303943	-7.555482	-2.971472	1
H-H1	-9.239400	-8.028873	-1.988519	1
O-OS	-8.761747	-6.250458	-2.890187	1
C-CT	-9.726063	-5.476699	-2.214473	1
H-H2	-9.698502	-5.686127	-1.138408	1
N-N*	-9.463890	-4.049523	-2.464250	1
C-CK	-9.031051	-3.447257	-3.618678	1
H-H5	-8.882613	-3.995668	-4.539013	1
N-NB	-8.804504	-2.167525	-3.503664	1
C-CB	-9.091247	-1.902437	-2.162276	1
C-CA	-9.012054	-0.743469	-1.346571	1
N-N2	-8.552431	0.443911	-1.753653	1
H-H	-8.477449	1.217626	-1.104292	1
H-H	-8.194065	0.541811	-2.691329	1

N-NC	-9.391057	-0.833719	-0.058538	1
C-CQ	-9.802173	-2.006332	0.424495	1
H-H5	-10.102128	-2.007335	1.467877	1
N-NC	-9.885844	-3.171143	-0.219737	1
C-CB	-9.511884	-3.047153	-1.526189	1
C-CT	-10.779765	-7.362965	-3.309274	1
H-H1	-10.921521	-7.422865	-4.394330	1
C-CT	-11.051135	-5.939559	-2.809342	1
H-HC	-11.333529	-5.315207	-3.653415	1
H-HC	-11.822536	-5.912250	-2.043363	1
O-OS	-11.528010	-8.351689	-2.624538	1
P-P	-13.109786	-8.561854	-2.868602	1
O-O2	-13.457441	-8.041547	-4.207259	1
O-O2	-13.463481	-9.941297	-2.476882	1
O-OS	-13.694011	-7.556226	-1.762680	1
C-CT	-13.423814	-7.762495	-0.383334	1
H-H1	-12.351860	-7.897845	-0.233546	1
H-H1	-13.943181	-8.656856	-0.033028	1
C-CT	-13.869687	-6.551085	0.436101	1
H-H1	-13.660695	-6.738864	1.492168	1
O-OS	-13.163038	-5.393831	0.025145	1
C-CT	-13.960744	-4.279278	0.356314	1
H-H2	-13.864144	-4.046871	1.425190	1
N-N*	-13.525049	-3.138533	-0.482333	1
C-CM	-13.363122	-3.281795	-1.845182	1
H-H4	-13.638189	-4.220387	-2.306319	1
C-CM	-12.847210	-2.282818	-2.607023	1
C-CT	-12.687851	-2.482768	-4.107271	1
H-HC	-11.772346	-3.034717	-4.308660	1
H-HC	-12.611318	-1.506889	-4.592750	1
H-HC	-13.546022	-3.016751	-4.515435	1
C-C	-12.435374	-1.031505	-1.980946	1
O-O	-11.907827	-0.076068	-2.541052	1
N-NA	-12.675943	-0.954209	-0.630230	1
H-H	-12.416095	-0.099825	-0.167255	1
C-C	-13.198364	-1.946909	0.159365	1
O-O	-13.347837	-1.756116	1.360946	1
C-CT	-15.361240	-6.245325	0.289366	1
H-H1	-15.772032	-6.781116	-0.573113	1
C-CT	-15.383727	-4.734877	0.047500	1
H-HC	-15.626758	-4.549461	-0.996025	1
H-HC	-16.092650	-4.223248	0.694404	1
O-OS	-16.004646	-6.618226	1.495416	1
P-P	-17.602037	-6.810993	1.593231	1
O-O2	-18.120637	-7.182282	0.260690	1
O-O2	-17.900042	-7.641951	2.777256	1
O-OS	-18.054815	-5.306507	1.908566	1
C-CT	-17.710765	-4.684537	3.137372	1
H-H1	-16.633561	-4.757818	3.300087	1
H-H1	-18.223481	-5.188916	3.958554	1
C-CT	-18.098436	-3.203182	3.114819	1
H-H1	-17.948867	-2.777399	4.110052	1
O-OS	-17.264268	-2.533232	2.173710	1
C-CT	-18.082422	-1.736126	1.343457	1
H-H2	-18.282638	-0.767400	1.822811	1
N-N*	-17.394337	-1.533934	0.050777	1
C-CK	-17.473083	-2.242324	-1.126775	1

H-H5	-18.052177	-3.148526	-1.246547	1
N-NB	-16.768734	-1.740361	-2.103490	1
C-CB	-16.203160	-0.594750	-1.544882	1
C-CA	-15.384149	0.445724	-2.053937	1
N-N2	-14.938465	0.535471	-3.311888	1
H-H	-14.331483	1.314856	-3.567949	1
H-H	-15.166917	-0.173443	-3.988971	1
N-NC	-15.029017	1.441513	-1.225918	1
C-CQ	-15.452715	1.436622	0.035621	1
H-H5	-15.138941	2.279298	0.641654	1
N-NC	-16.218359	0.529020	0.634656	1
C-CB	-16.567265	-0.472641	-0.224037	1
C-CT	-19.556317	-2.974046	2.693398	1
H-H1	-20.148855	-3.891994	2.760249	1
C-CT	-19.375429	-2.526862	1.247230	1
H-HC	-19.244467	-3.406144	0.621241	1
H-HC	-20.195211	-1.912074	0.895542	1
O-OS	-20.096431	-1.959734	3.525362	1
P-P	-21.592354	-1.383432	3.346961	1
O-O2	-22.365449	-2.302352	2.485475	1
O-O2	-22.103136	-0.970315	4.669410	1
O-OS	-21.242623	-0.066906	2.500723	1
C-CT	-20.528634	1.004216	3.106954	1
H-H1	-19.666255	0.611733	3.646985	1
H-H1	-21.175868	1.529826	3.812387	1
C-CT	-20.021247	1.996004	2.059587	1
H-H1	-19.452192	2.786025	2.555509	1
O-OS	-19.198846	1.344764	1.103591	1
C-CT	-19.287121	2.026805	-0.135616	1
H-H2	-18.325738	2.502523	-0.374376	1
N-N*	-19.645561	1.036931	-1.181738	1
C-CM	-20.604907	0.071312	-0.964828	1
H-H4	-21.130894	0.054010	-0.021870	1
C-CM	-20.887998	-0.871653	-1.899772	1
C-CT	-21.954492	-1.922376	-1.612094	1
H-HC	-22.150108	-2.012198	-0.542714	1
H-HC	-21.629428	-2.889156	-2.002105	1
H-HC	-22.877982	-1.645084	-2.122021	1
C-C	-20.174736	-0.870424	-3.173639	1
O-O	-20.316559	-1.681153	-4.081656	1
N-NA	-19.262467	0.150196	-3.329700	1
H-H	-18.765145	0.182134	-4.199737	1
C-C	-18.962277	1.107605	-2.390830	1
O-O	-18.120312	1.963196	-2.635276	1
C-CT	-21.140801	2.651843	1.264628	1
H-H1	-21.908441	1.905844	1.028457	1
C-CT	-20.376151	3.090304	0.026356	1
H-HC	-21.020142	3.159170	-0.849939	1
H-HC	-19.898514	4.052464	0.215448	1
O-OH	-21.645744	3.788478	1.936018	1
H-HO	-22.342686	4.199698	1.413353	1
H-HO	-15.512931	8.121924	-7.711383	1
O-OH	-15.123065	8.841710	-8.238814	1
C-CT	-15.866644	10.017455	-7.953451	1
H-H1	-16.883335	9.920847	-8.344402	1
H-H1	-15.393682	10.883487	-8.422326	1
C-CT	-15.949258	10.226550	-6.436919	1

H-H1	-16.512083	11.139430	-6.224958	1
O-OS	-16.619272	9.099898	-5.885926	1
C-CT	-15.913241	8.675240	-4.740297	1
H-H2	-16.205041	9.272455	-3.869574	1
N-N*	-16.159423	7.237148	-4.503601	1
C-CK	-16.480922	6.626841	-3.315744	1
H-H5	-16.571380	7.165435	-2.380096	1
N-NB	-16.678799	5.340837	-3.408926	1
C-CB	-16.434244	5.064084	-4.753329	1
C-CA	-16.432183	3.873932	-5.526844	1
N-N2	-16.733181	2.661283	-5.056909	1
H-H	-16.680616	1.871975	-5.678531	1
H-H	-17.010027	2.540069	-4.085048	1
N-NC	-16.107664	3.944169	-6.832577	1
C-CQ	-15.799954	5.128581	-7.358073	1
H-H5	-15.549246	5.126738	-8.411737	1
N-NC	-15.763500	6.313033	-6.748929	1
C-CB	-16.102396	6.215656	-5.428462	1
C-CT	-14.575796	10.326814	-5.758666	1
H-H1	-13.782969	10.483644	-6.496605	1
C-CT	-14.463847	8.963115	-5.086498	1
H-HC	-14.093079	8.235142	-5.803253	1
H-HC	-13.846674	8.982190	-4.197133	1
O-OS	-14.619008	11.380743	-4.809120	1
P-P	-13.297275	11.917357	-4.053531	1
O-O2	-12.126520	11.684293	-4.924447	1
O-O2	-13.581263	13.263489	-3.516157	1
O-OS	-13.229217	10.886840	-2.825821	1
C-CT	-14.193538	10.934888	-1.787095	1
H-H1	-15.195517	10.990571	-2.213938	1
H-H1	-14.022007	11.823755	-1.176250	1
C-CT	-14.110493	9.687486	-0.901586	1
H-H1	-14.795999	9.809322	-0.059646	1
O-OS	-14.439364	8.500213	-1.608383	1
C-CT	-13.976752	7.420671	-0.816103	1
H-H2	-14.737202	7.154875	-0.070349	1
N-N*	-13.674469	6.257451	-1.680853	1
C-CM	-13.057155	6.413142	-2.903881	1
H-H4	-12.708832	7.395282	-3.184432	1
C-CM	-12.905707	5.369560	-3.762339	1
C-CT	-12.258158	5.595358	-5.121525	1
H-HC	-11.573571	6.442988	-5.092495	1
H-HC	-13.032571	5.766506	-5.869476	1
H-HC	-11.704146	4.698106	-5.405777	1
C-C	-13.385727	4.043675	-3.384330	1
O-O	-13.364314	3.026371	-4.072009	1
N-NA	-13.911662	3.967210	-2.120168	1
H-H	-14.213710	3.060776	-1.813454	1
C-C	-14.080915	5.002471	-1.239706	1
O-O	-14.566247	4.793685	-0.132644	1
C-CT	-12.711983	9.440997	-0.347416	1
H-H1	-11.967414	9.688463	-1.110841	1
C-CT	-12.732311	7.934349	-0.098956	1
H-HC	-11.826859	7.489191	-0.505317	1
H-HC	-12.820981	7.708114	0.963453	1
O-OS	-12.513191	10.193832	0.834699	1
P-P	-11.115230	10.176083	1.639988	1

O-O2	-10.044684	9.715657	0.730302	1
O-O2	-10.981598	11.444386	2.383955	1
O-OS	-11.404906	9.002266	2.693256	1
C-CT	-12.494693	9.092942	3.600179	1
H-H1	-13.424237	9.214847	3.042493	1
H-H1	-12.363122	9.961510	4.247833	1
C-CT	-12.609552	7.826643	4.456477	1
H-H1	-13.447639	7.944202	5.146689	1
O-OS	-12.843801	6.712029	3.601435	1
C-CT	-11.828889	5.744658	3.798167	1
H-H2	-12.179273	4.950743	4.471305	1
N-N*	-11.491711	5.199389	2.466842	1
C-CK	-10.800597	5.797349	1.439847	1
H-H5	-10.404629	6.804839	1.501495	1
N-NB	-10.686772	5.063145	0.368612	1
C-CB	-11.346654	3.882885	0.711577	1
C-CA	-11.580148	2.661586	0.030402	1
N-N2	-11.169661	2.397681	-1.213403	1
H-H	-11.398317	1.505232	-1.650518	1
H-H	-10.654164	3.088323	-1.735706	1
N-NC	-12.242061	1.682354	0.671881	1
C-CQ	-12.669347	1.886804	1.918034	1
H-H5	-13.179518	1.048699	2.381612	1
N-NC	-12.534560	2.986507	2.660136	1
C-CB	-11.849515	3.959855	1.989957	1
C-CT	-11.340856	7.557785	5.270176	1
H-H1	-10.722667	8.457630	5.340479	1
C-CT	-10.657086	6.479672	4.441479	1
H-HC	-10.034026	6.962619	3.693760	1
H-HC	-10.063722	5.806353	5.050522	1
O-OS	-11.709512	7.104325	6.561548	1
P-P	-10.625324	6.892764	7.737362	1
O-O2	-9.439549	7.726744	7.450959	1
O-O2	-11.318671	6.980916	9.038454	1
O-OS	-10.250163	5.358980	7.462991	1
C-CT	-11.201709	4.337172	7.708055	1
H-H1	-12.175065	4.639583	7.317599	1
H-H1	-11.288522	4.176927	8.784368	1
C-CT	-10.797411	3.029638	7.025620	1
H-H1	-11.495481	2.243740	7.323848	1
O-OS	-10.789030	3.159257	5.610608	1
C-CT	-10.126804	2.009642	5.116056	1
H-H2	-10.841381	1.179467	5.026947	1
N-N*	-9.480813	2.267258	3.811709	1
C-CM	-8.772982	3.425091	3.577004	1
H-H4	-8.712796	4.163391	4.361952	1
C-CM	-8.154708	3.647202	2.388128	1
C-CT	-7.393839	4.946529	2.166408	1
H-HC	-6.326974	4.760963	2.286593	1
H-HC	-7.718163	5.712477	2.870722	1
H-HC	-7.580078	5.295462	1.148445	1
C-C	-8.221509	2.639118	1.333551	1
O-O	-7.709196	2.710057	0.220152	1
N-NA	-8.928140	1.507250	1.662193	1
H-H	-9.008920	0.780098	0.972193	1
C-C	-9.547157	1.256448	2.858626	1
O-O	-10.115022	0.185467	3.044549	1

C-CT	-9.382765	2.574507	7.358943	l	
H-H1	-8.720392	3.446369	7.359844	l	
C-CT	-9.073128	1.676748	6.167210	l	
H-HC	-8.066499	1.893846	5.815256	l	
H-HC	-9.166273	0.623690	6.430910	l	
O-OS	-9.308278	1.861982	8.579851	l	
P-P	-7.887036	1.388015	9.185151	l	
O-O2	-6.838519	2.324483	8.729077	l	
O-O2	-8.063119	1.096247	10.622316	l	
O-OS	-7.688293	-0.003885	8.407313	l	
C-CT	-8.465904	-1.137715	8.758346	l	
H-H1	-9.524397	-0.873936	8.753654	l	
H-H1	-8.190015	-1.463918	9.763250	l	
C-CT	-8.248429	-2.297661	7.783436	l	
H-H1	-8.785963	-3.171546	8.156697	l	
O-OS	-8.714036	-1.992271	6.474904	l	
C-CT	-7.956272	-2.737500	5.530703	l	
H-H2	-8.592685	-3.438883	4.980543	l	
N-N*	-7.319891	-1.804136	4.579582	l	
C-CK	-6.965375	-0.494214	4.766479	l	
H-H5	-7.037623	-0.015930	5.732544	l	
N-NB	-6.553216	0.114298	3.687571	l	
C-CB	-6.592943	-0.886491	2.714963	l	
C-CA	-6.283747	-0.929580	1.329626	l	
N-N2	-5.935943	0.126010	0.585791	l	
H-H	-5.814651	0.022200	-0.418118	l	
H-H	-5.934677	1.049942	0.991660	l	
N-NC	-6.371322	-2.107623	0.686944	l	
C-CQ	-6.778467	-3.189600	1.350365	l	
H-H5	-6.833000	-4.104392	0.769296	l	
N-NC	-7.143931	-3.274707	2.630008	l	
C-CB	-7.021033	-2.072866	3.265257	l	
C-CT	-6.784871	-2.679303	7.618057	l	
H-H1	-6.191206	-1.773430	7.465291	l	
C-CT	-6.899068	-3.486294	6.333582	l	
H-HC	-5.956627	-3.543901	5.803283	l	
H-HC	-7.257544	-4.488921	6.552404	l	
O-OS	-6.329818	-3.458715	8.711305	l	
P-P	-4.761852	-3.586751	9.063525	l	
O-O2	-4.114460	-2.292314	8.768212	l	
O-O2	-4.620724	-4.200965	10.398834	l	
O-OS	-4.247679	-4.644278	7.975809	l	
C-CT	-4.820138	-5.940909	7.866766	l	
H-H1	-5.906215	-5.856653	7.847358	l	
H-H1	-4.538296	-6.547259	8.728798	l	
C-CT	-4.367823	-6.620402	6.565261	l	
H-H1	-4.880613	-7.578317	6.455877	l	
O-OS	-4.704441	-5.753476	5.483308	l	
C-CT	-3.551218	-5.531809	4.698769	l	H-H
H-H2	-3.516604	-6.294048	3.910378	l	
N-N*	-3.531185	-4.152582	4.133903	h	
C-CM	-3.554877	-3.033327	4.949857	h	
H-H4	-3.720943	-3.221206	6.007167	h	
C-CM	-3.397945	-1.773642	4.492798	h	
C-CT	-3.461570	-0.556908	5.366926	h	
H-HC	-2.545976	0.029599	5.269097	h	
H-HC	-3.600382	-0.848996	6.412200	h	

H-HC	-4.290701	0.088413	5.073476	h	
C-C	-3.158645	-1.610544	3.061766	h	
O-O	-2.866267	-0.534081	2.525813	h	
N-NA	-3.288038	-2.755238	2.301480	h	
H-H	-3.200453	-2.661498	1.258145	h	
C-C	-3.396875	-4.049897	2.754328	h	
O-O	-3.358539	-5.017997	2.009253	h	
C-CT	-2.855477	-6.873321	6.533618	l	
H-H1	-2.433845	-6.801707	7.539313	l	
C-CT	-2.381679	-5.740346	5.649576	l	
H-HC	-2.253218	-4.870338	6.283830	l	
H-HC	-1.467653	-5.982916	5.113804	l	
O-OS	-2.554734	-8.122459	5.936882	l	
P-P	-1.131022	-8.855357	6.167724	l	
O-O2	-0.602643	-8.450007	7.487342	l	
O-O2	-1.297722	-10.286437	5.843493	l	
O-OS	-0.184763	-8.203797	5.040369	l	
C-CT	-0.442494	-8.417381	3.662424	l	
H-H1	-1.315086	-7.837603	3.361500	l	
H-H1	-0.655085	-9.474796	3.489511	l	
C-CT	0.756599	-8.018631	2.793098	l	
H-H1	0.514192	-8.272332	1.760813	l	
O-OS	1.027910	-6.623949	2.863101	l	
C-CT	2.419031	-6.473509	2.666223	l	H-H
H-H2	2.674378	-6.610740	1.608371	l	
N-N*	2.800775	-5.117808	3.115808	h	
C-CK	2.845792	-4.625389	4.405348	h	
H-H5	2.799614	-5.282818	5.262868	h	
N-NB	2.936704	-3.324361	4.472996	h	
C-CB	2.947799	-2.923055	3.149056	h	
C-CA	2.833749	-1.673274	2.521713	h	
N-N2	2.427770	-0.515798	3.185875	h	
H-H	2.757043	0.358089	2.744879	h	
H-H	2.618942	-0.540507	4.186282	h	
N-NC	2.951411	-1.619988	1.198931	h	
C-CQ	3.004366	-2.763355	0.484199	h	
H-H5	3.115906	-2.638094	-0.590523	h	
N-NC	2.900462	-3.997599	0.952387	h	
C-CB	2.889719	-4.023288	2.286736	h	
C-CT	2.053308	-8.758898	3.150698	l	
H-H1	1.904441	-9.415953	4.013757	l	
C-CT	3.009716	-7.614167	3.483027	l	
H-HC	2.948267	-7.401958	4.548460	l	
H-HC	4.033981	-7.827287	3.181532	l	
O-OS	2.466121	-9.478665	1.997944	l	
P-P	3.571728	-10.648170	2.065495	l	
O-O2	3.540046	-11.242078	3.417616	l	
O-O2	3.394613	-11.498867	0.870940	l	
O-OS	4.952577	-9.832023	1.898587	l	
C-CT	5.484115	-9.486916	0.624652	l	
H-H1	5.572929	-10.389970	0.017373	l	
H-H1	6.479790	-9.069481	0.770229	l	
C-CT	4.629367	-8.450389	-0.121689	l	
H-H1	3.603748	-8.817610	-0.222897	l	
O-OS	4.681470	-7.226907	0.601715	l	
C-CT	5.111011	-6.184190	-0.254932	l	
H-H2	4.250128	-5.748322	-0.779224	l	

N-N*	5.823076	-5.143220	0.521649	1
C-CM	6.267824	-5.380038	1.807004	1
H-H4	6.254268	-6.386375	2.200993	1
C-CM	6.676163	-4.367777	2.613438	1
C-CT	7.107208	-4.682937	4.038536	1
H-HC	6.399596	-5.369622	4.502585	1
H-HC	7.139964	-3.758930	4.619686	1
H-HC	8.103687	-5.124332	4.027710	1
C-C	6.668311	-2.995320	2.117606	1
O-O	6.949935	-1.984513	2.752641	1
N-NA	6.281730	-2.855259	0.806597	1
H-H	6.281773	-1.926025	0.421290	1
C-C	5.844122	-3.860928	-0.018026	1
O-O	5.423930	-3.593332	-1.138540	1
C-CT	5.192521	-8.139002	-1.513205	1
H-H1	5.807710	-8.958134	-1.896650	1
C-CT	6.004921	-6.873672	-1.267606	1
H-HC	6.968369	-7.111704	-0.820289	1
H-HC	6.111977	-6.264276	-2.167166	1
O-OS	4.117362	-7.845583	-2.388623	1
P-P	4.171451	-8.261139	-3.942412	1
O-O2	4.666604	-9.649472	-4.031548	1
O-O2	2.882420	-7.880695	-4.559673	1
O-OS	5.322279	-7.271808	-4.482358	1
C-CT	4.992748	-6.024556	-5.072528	1
H-H1	4.305838	-5.479099	-4.422310	1
H-H1	4.501376	-6.206957	-6.029629	1
C-CT	6.219505	-5.139178	-5.304253	1
H-H1	5.939591	-4.351974	-6.007995	1
O-OS	6.602983	-4.520871	-4.093484	1
C-CT	7.941044	-4.117761	-4.253251	1
H-H2	8.018355	-3.250846	-4.922367	1
N-N*	8.458133	-3.778999	-2.914370	1
C-CK	8.680493	-4.590656	-1.829411	1
H-H5	8.576294	-5.664548	-1.867250	1
N-NB	9.006568	-3.956172	-0.737552	1
C-CB	8.994040	-2.614828	-1.123439	1
C-CA	9.229329	-1.390250	-0.444379	1
N-N2	9.481954	-1.271204	0.862851	1
H-H	9.574623	-0.349425	1.286110	1
H-H	9.472939	-2.087285	1.454829	1
N-NC	9.188091	-0.247327	-1.150964	1
C-CQ	8.891848	-0.283722	-2.449456	1
H-H5	8.884222	0.674822	-2.958212	1
N-NC	8.600679	-1.352876	-3.189765	1
C-CB	8.679528	-2.502704	-2.458281	1
C-CT	7.471984	-5.839787	-5.852044	1
H-H1	7.378002	-6.927920	-5.788979	1
C-CT	8.575417	-5.335071	-4.909123	1
H-HC	8.782081	-6.101546	-4.166117	1
H-HC	9.484701	-5.052430	-5.433845	1
O-OS	7.638160	-5.422206	-7.197129	1
P-P	8.860762	-5.917713	-8.128156	1
O-O2	9.447893	-7.140818	-7.542514	1
O-O2	8.421277	-5.882501	-9.537273	1
O-OS	9.866381	-4.690497	-7.880488	1
C-CT	9.476269	-3.372263	-8.232363	1

H-H1	8.452663	-3.190550	-7.902162	1
H-H1	9.517210	-3.250485	-9.316618	1
C-CT	10.371861	-2.337346	-7.554047	1
H-H1	10.012605	-1.341517	-7.826037	1
O-OS	10.322688	-2.468613	-6.142036	1
C-CT	11.477019	-1.815329	-5.664902	1
H-H2	11.355928	-0.726640	-5.751113	1
N-N*	11.748328	-2.202120	-4.263550	1
C-CM	11.806559	-3.524521	-3.876647	1
H-H4	11.653523	-4.293104	-4.620449	1
C-CM	12.044318	-3.875822	-2.585383	1
C-CT	12.104709	-5.347979	-2.204402	1
H-HC	13.128270	-5.707337	-2.314418	1
H-HC	11.435038	-5.935499	-2.831512	1
H-HC	11.807275	-5.457967	-1.158901	1
C-C	12.230944	-2.840676	-1.573113	1
O-O	12.439181	-3.009752	-0.375430	1
N-NA	12.141567	-1.555257	-2.045073	1
H-H	12.242668	-0.804948	-1.385071	1
C-C	11.925461	-1.175414	-3.342705	1
O-O	11.892732	0.015596	-3.632609	1
C-CT	11.846271	-2.430194	-7.956675	1
H-H1	12.057329	-3.405647	-8.409750	1
C-CT	12.570132	-2.284301	-6.616031	1
H-HC	12.954379	-3.256906	-6.315982	1
H-HC	13.373907	-1.552877	-6.646117	1
O-OS	12.127784	-1.361029	-8.844215	1
P-P	13.539394	-1.223155	-9.616421	1
O-O2	14.150963	-2.563632	-9.727713	1
O-O2	13.331823	-0.385386	-10.814522	1
O-OS	14.370283	-0.368748	-8.540459	1
C-CT	13.975346	0.954459	-8.213549	1
H-H1	12.917903	0.969637	-7.945306	1
H-H1	14.127099	1.603099	-9.078453	1
C-CT	14.777466	1.494755	-7.027576	1
H-H1	14.509633	2.543878	-6.881476	1
O-OS	14.482094	0.782547	-5.834902	1
C-CT	15.595195	0.951611	-4.984151	1
H-H2	15.617165	1.958588	-4.549904	1
N-N*	15.548115	-0.077926	-3.930204	1
C-CK	15.239571	-1.408251	-4.058183	1
H-H5	15.028420	-1.865613	-5.014329	1
N-NB	15.214475	-2.066092	-2.933413	1
C-CB	15.519578	-1.093162	-1.980178	1
C-CA	15.630127	-1.108562	-0.566167	1
N-N2	15.387398	-2.182643	0.187988	1
H-H	15.409857	-2.118431	1.202793	1
H-H	15.057906	-3.034050	-0.240387	1
N-NC	15.978729	0.025470	0.073302	1
C-CQ	16.185121	1.134338	-0.641466	1
H-H5	16.469740	2.016887	-0.077042	1
N-NC	16.077826	1.290544	-1.963405	1
C-CB	15.742816	0.121965	-2.582976	1
C-CT	16.294247	1.418606	-7.229467	1
H-H1	16.542906	0.796880	-8.096556	1
C-CT	16.768139	0.759016	-5.932965	1
H-HC	16.929247	-0.300845	-6.117329	1

H-HC	17.665179	1.223724	-5.533533	l
O-OS	16.783576	2.739743	-7.382244	l
P-P	18.294422	3.047603	-7.858592	l
O-O2	18.805448	1.878951	-8.603809	l
O-O2	18.330246	4.398875	-8.453719	l
O-OS	19.029498	3.103916	-6.435871	l
C-CT	18.660091	4.083873	-5.479760	l
H-H1	17.577092	4.079380	-5.346458	l
H-H1	18.966198	5.070165	-5.830850	l
C-CT	19.306505	3.791098	-4.125684	l
H-H1	19.091014	4.616697	-3.443413	l
O-OS	18.759938	2.592568	-3.590255	l
C-CT	19.802522	1.982137	-2.862160	l
H-H2	20.003045	2.560843	-1.948499	l
N-N*	19.458312	0.575308	-2.538847	l
C-CM	19.218955	-0.369507	-3.516728	l
H-H4	19.297561	-0.089469	-4.556593	l
C-CM	18.873939	-1.646481	-3.201369	l
C-CT	18.624088	-2.646699	-4.321935	l
H-HC	17.895487	-2.249182	-5.025856	l
H-HC	18.235147	-3.577848	-3.903939	l
H-HC	19.559287	-2.858531	-4.840597	l
C-C	18.744208	-2.041565	-1.800459	l
O-O	18.407187	-3.140773	-1.368274	l
N-NA	19.019498	-1.044434	-0.899094	l
H-H	18.917097	-1.259275	0.077266	l
C-C	19.360091	0.249151	-1.190677	l
O-O	19.558207	1.045642	-0.279523	l
C-CT	20.830350	3.592895	-4.203503	l
H-H1	21.219311	3.767475	-5.213660	l
C-CT	20.991360	2.135241	-3.800479	l
H-HC	20.877497	1.504137	-4.679108	l
H-HC	21.936431	1.951180	-3.290678	l
O-OH	21.491687	4.370195	-3.220145	l
H-HO	21.549602	5.288935	-3.503509	l
C-CA	0.318340	-3.904772	-1.138427	h
C-CA	-0.081772	-4.831197	-0.137535	h
C-CA	-0.161468	-6.209295	-0.469325	h
C-CA	0.205869	-6.647230	-1.717828	h
C-CA	0.659344	-5.724771	-2.697785	h
C-CA	0.702586	-4.382608	-2.418059	h
H-HA	-0.516065	-6.902590	0.285754	h
H-HA	0.161749	-7.702543	-1.964164	h
H-HA	0.967256	-6.086183	-3.673880	h
H-HA	1.034407	-3.664709	-3.166113	h
C-CA	0.314330	-2.524418	-0.839535	h
H-HA	0.611892	-1.828413	-1.618767	h
C-CA	0.031869	-2.078333	0.431270	h
C-CA	-0.191683	-3.022146	1.484557	h
C-CA	-0.335742	-4.357710	1.171715	h
H-HA	-0.632143	-5.074433	1.932219	h
N-NC	-0.235829	-2.485172	2.795378	h
N-NC	0.017270	-0.714196	0.801474	h
C-CA	-0.245034	0.181572	-0.087839	h
C-CA	-0.029713	-3.232174	3.826613	h
Zn-Zn	0.046346	-0.342221	2.863711	h
C-CA	-0.316534	1.606615	0.145884	h

H-HA	-0.426918	-0.123684	-1.122584	h
C-CA	-0.639172	2.387598	-0.977959	h
C-CA	-0.639633	3.769091	-0.940793	h
C-CA	-0.323841	4.407619	0.277255	h
C-CA	-0.054746	3.659550	1.410740	h
C-CA	-0.075027	2.229967	1.415104	h
H-HA	-0.890607	1.861699	-1.896568	h
H-HA	-0.852602	4.340623	-1.839991	h
C-CT	-0.219577	5.908974	0.332823	h
H-HA	0.215449	4.128665	2.354524	h
O-OS	0.135252	1.609778	2.521594	h
H-HA	0.182619	-4.300497	3.688848	h
C-CA	-0.077850	-2.786225	5.204846	h
C-CA	-0.333915	-1.432398	5.597589	h
C-CA	-0.630348	-1.224047	6.978433	h
C-CA	-0.580156	-2.241743	7.914851	h
C-CA	-0.176519	-3.537134	7.530630	h
C-CA	0.076324	-3.774124	6.192333	h
O-OS	-0.349533	-0.416899	4.804764	h
H-HA	-0.951687	-0.220890	7.249287	h
C-CT	-1.076953	-1.980068	9.313036	h
H-HA	-0.133565	-4.350180	8.249318	h
H-HA	0.351400	-4.777934	5.872860	h
N-N3	-1.534367	6.650893	0.602915	h
H-HC	0.467329	6.222408	1.120582	h
H-HC	0.157576	6.307549	-0.611231	h
H-HC	-1.601772	-2.860254	9.687590	h
H-HC	-1.784391	-1.148090	9.313942	h
N-N3	-0.017140	-1.645599	10.361602	h
C-CT	-2.133306	6.198738	1.923545	h
C-CT	-1.203500	8.127863	0.621115	h
C-CT	-2.557327	6.333162	-0.473836	h
C-CT	-2.390313	9.042388	0.875060	h
H-HC	-0.435670	8.260975	1.384491	h
H-HC	-0.741168	8.347008	-0.343061	h
H-HC	-3.505140	6.750188	-0.131640	h
C-CT	-2.225610	6.859598	-1.861920	h
H-HC	-2.655076	5.245973	-0.476184	h
H-HC	-3.136568	6.624458	1.967369	h
H-HC	-2.229958	5.114038	1.845125	h
C-CT	-1.342231	6.587140	3.162663	h
H-HC	-0.306936	6.243351	3.134651	h
H-HC	-1.354976	7.661957	3.351325	h
H-HC	-1.816401	6.097653	4.016015	h
H-HC	-3.156762	8.957279	0.102312	h
H-HC	-2.850206	8.871693	1.850259	h
H-HC	-2.026626	10.071483	0.860470	h
H-HC	-2.960958	6.444292	-2.554419	h
H-HC	-2.292158	7.946905	-1.928665	h
H-HC	-1.241532	6.548602	-2.218837	h
C-CT	0.871860	-2.863240	10.547770	h
C-CT	0.841901	-0.484753	9.892160	h
C-CT	-0.730508	-1.272459	11.646310	h
H-HC	0.034888	-0.900838	12.329147	h
H-HC	-1.388634	-0.440686	11.390895	h
C-CT	-1.549202	-2.389287	12.279042	h
H-HC	-0.962453	-3.277656	12.514033	h

H-HC	-1.960664	-2.006543	13.214141	h
H-HC	-2.399187	-2.680911	11.656805	h
C-CT	1.818933	-2.808522	11.737478	h
H-HC	0.196543	-3.717139	10.635074	h
H-HC	1.418803	-2.970893	9.608923	h
H-HC	2.393644	-3.736581	11.731805	h
H-HC	2.533844	-1.987552	11.678201	h
H-HC	1.290710	-2.756983	12.690439	h
C-CT	0.129458	0.858311	9.816163	h
H-HC	1.680350	-0.423381	10.585097	h
H-HC	1.219723	-0.781691	8.912544	h
H-HC	0.783012	1.546785	9.277516	h
H-HC	-0.808921	0.809086	9.259096	h
H-HC	-0.067395	1.286270	10.799407	h