

Supporting Information

Improved cluster-in-molecule approach for electron correlation calculation of large systems

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Cartesian Coordinates:

1. C ₃₀ H ₆₂				
C	-2.60417	-0.48607	0.00636	
H	-2.24749	0.01833	-0.86729	
H	-3.67417	-0.48606	0.00636	
C	-2.09082	0.23989	1.26377	
H	-1.02082	0.23970	1.26387	
H	-2.44766	-0.26440	2.13742	
C	-2.60391	1.69190	1.26363	
H	-2.24607	2.19649	0.39056	
H	-3.67391	1.69244	1.26250	
C	-2.09153	2.41708	2.52187	
H	-1.02154	2.41652	2.52301	
H	-2.44939	1.91251	3.39494	
C	-2.60411	3.86927	2.52192	
H	-3.67411	3.86984	2.52080	
H	-2.24626	4.37384	1.64885	
C	-2.09171	4.59446	3.78015	
H	-1.02171	4.59391	3.78127	
H	-2.44954	4.08989	4.65323	
C	-2.60429	6.04665	3.78021	
H	-3.67429	6.04721	3.77910	
H	-2.24646	6.55122	2.90713	
C	-2.09188	6.77184	5.03844	
H	-1.02188	6.77129	5.03954	
H	-2.44971	6.26727	5.91152	
C	-2.60447	8.22403	5.03849	

H	-3.67447	8.22458	5.03739
H	-2.24664	8.72861	4.16541
C	-2.09206	8.94923	6.29672
H	-1.02206	8.94868	6.29782
H	-2.44989	8.44465	7.16980
C	-2.60465	10.40141	6.29678
H	-3.67465	10.40196	6.29568
H	-2.24683	10.90599	5.42370
C	-2.09224	11.12661	7.55500
H	-1.02224	11.12604	7.55611
H	-2.45008	10.62204	8.42808
C	-2.60481	12.57880	7.55505
H	-3.67481	12.57937	7.55394
H	-2.24697	13.08337	6.68197
C	-2.09240	13.30399	8.81328
H	-1.02240	13.30343	8.81439
H	-2.45024	12.79943	9.68636
C	-2.60497	14.75619	8.81332
H	-3.67497	14.75675	8.81221
H	-2.24713	15.26075	7.94024
C	-2.09256	15.48138	10.07155
H	-1.02256	15.48082	10.07266
H	-2.45040	14.97682	10.94463
C	-2.09085	-1.93800	0.00636
H	-2.44754	-2.44240	0.88001
H	-1.02085	-1.93801	0.00638
C	-2.60418	-2.66395	-1.25105
H	-2.24908	-2.15843	-2.12470
H	-3.67417	-2.66562	-1.25010
C	-2.08858	-4.11508	-1.25245
H	-2.44323	-4.62044	-0.37853
H	-1.01858	-4.11341	-1.25395
C	-2.60255	-4.84125	-2.50947
H	-2.24790	-4.33589	-3.38339
H	-2.24431	-5.84950	-2.51044
H	-3.67255	-4.84292	-2.50797
C	-2.60513	16.93358	10.07160
H	-3.67513	16.93414	10.07049
H	-2.24730	17.43814	9.19852
C	-2.09272	17.65877	11.32982
H	-1.02272	17.65821	11.33093
H	-2.45056	17.15420	12.20290
C	-2.60530	19.11096	11.32987
H	-3.67529	19.11152	11.32876

H	-2.24746	19.61553	10.45679
C	-2.09288	19.83615	12.58810
H	-1.02288	19.83559	12.58920
H	-2.45072	19.33159	13.46118
C	-2.60546	21.28835	12.58815
H	-3.67546	21.28891	12.58704
H	-2.24763	21.79291	11.71507
C	-2.09305	22.01354	13.84637
H	-1.02305	22.01298	13.84747
H	-2.45087	21.50897	14.71945
C	-2.60562	23.46573	13.84642
H	-3.67562	23.46629	13.84532
H	-2.24780	23.97030	12.97334
C	-2.09321	24.19093	15.10464
H	-1.02321	24.19037	15.10574
H	-2.45103	23.68636	15.97773
C	-2.60579	25.64312	15.10470
H	-3.67579	25.64367	15.10360
H	-2.24797	26.14769	14.23161
C	-2.09337	26.36831	16.36292
H	-1.02337	26.36776	16.36401
H	-2.44952	27.37730	16.36296
H	-2.45119	25.86375	17.23600

2. C₃₀H₃₂

C	0.00000	0.00000	0.00000
H	0.03632	-1.06938	0.00000
C	1.14711	0.72159	0.00000
H	1.11079	1.79098	0.00000
C	2.50759	0.00000	0.00000
C	5.01518	0.00000	0.00000
C	7.52277	0.00000	0.00000
C	10.03036	0.00000	0.00000
C	12.53795	0.00000	0.00000
C	15.04555	0.00000	0.00000
C	17.55314	0.00000	0.00000
C	20.06073	0.00000	0.00000
C	22.56832	0.00000	0.00000
H	2.54391	-1.06938	0.00000
H	5.05150	-1.06938	0.00000
H	7.55909	-1.06938	0.00000
H	10.06668	-1.06938	0.00000
H	12.57427	-1.06938	0.00000

H	15.08186	-1.06938	0.00000	3. Mg ₄₀ O ₄₀			
H	17.58945	-1.06938	0.00000				
H	20.09705	-1.06938	0.00000	Mg	0.00000	-2.10560	0.00000
H	22.60464	-1.06938	0.00000	Mg	4.21120	-2.10560	0.00000
C	3.65470	0.72159	0.00000	Mg	0.00000	0.00000	-2.10560
C	6.16229	0.72159	0.00000	Mg	4.21120	0.00000	-2.10560
C	8.66989	0.72159	0.00000	Mg	2.10560	-2.10560	-2.10560
C	11.17748	0.72159	0.00000	Mg	6.31680	-2.10560	-2.10560
C	13.68507	0.72159	0.00000	Mg	2.10560	0.00000	0.00000
C	16.19266	0.72159	0.00000	Mg	6.31680	0.00000	0.00000
C	18.70025	0.72159	0.00000	O	2.10560	0.00000	-2.10560
C	21.20784	0.72159	0.00000	O	6.31680	0.00000	-2.10560
H	3.61839	1.79098	0.00000	O	2.10560	-2.10560	0.00000
H	6.12598	1.79098	0.00000	O	6.31680	-2.10560	0.00000
H	8.63357	1.79098	0.00000	O	0.00000	0.00000	0.00000
H	11.14116	1.79098	0.00000	O	4.21120	0.00000	0.00000
H	13.64875	1.79098	0.00000	O	0.00000	-2.10560	-2.10560
H	16.15634	1.79098	0.00000	O	4.21120	-2.10560	-2.10560
H	18.66393	1.79098	0.00000	Mg	8.42240	-2.10560	0.00000
H	21.17152	1.79098	0.00000	Mg	16.84480	-2.10560	0.00000
H	-0.94527	0.50137	0.00000	Mg	25.26720	-2.10560	0.00000
C	23.71543	0.72159	0.00000	Mg	33.68960	-2.10560	0.00000
H	23.67911	1.79098	0.00000	Mg	12.63360	-2.10560	0.00000
C	25.07591	0.00000	0.00000	Mg	21.05600	-2.10560	0.00000
H	25.11223	-1.06938	0.00000	Mg	29.47840	-2.10560	0.00000
C	26.22729	0.71477	0.00000	Mg	37.90080	-2.10560	0.00000
H	26.19732	1.78435	0.00000	Mg	8.42240	0.00000	-2.10560
C	27.58346	-0.01490	0.00000	Mg	16.84480	0.00000	-2.10560
H	27.61342	-1.08448	0.00000	Mg	25.26720	0.00000	-2.10560
C	28.73906	0.69301	0.00000	Mg	33.68960	0.00000	-2.10560
H	28.71545	1.76275	0.00000	Mg	12.63360	0.00000	-2.10560
C	30.09087	-0.04470	0.00000	Mg	21.05600	0.00000	-2.10560
H	30.11448	-1.11443	0.00000	Mg	29.47840	0.00000	-2.10560
C	31.25066	0.65634	0.00000	Mg	37.90080	0.00000	-2.10560
H	31.23341	1.72620	0.00000	Mg	10.52800	-2.10560	-2.10560
C	32.59806	-0.08939	0.00000	Mg	18.95040	-2.10560	-2.10560
H	32.61531	-1.15925	0.00000	Mg	27.37280	-2.10560	-2.10560
C	33.76200	0.60474	0.00000	Mg	35.79520	-2.10560	-2.10560
H	33.75110	1.67469	0.00000	Mg	14.73920	-2.10560	-2.10560
C	35.10494	-0.14898	0.00000	Mg	23.16160	-2.10560	-2.10560
H	35.11584	-1.21892	0.00000	Mg	31.58400	-2.10560	-2.10560
C	36.27298	0.53823	0.00000	Mg	40.00640	-2.10560	-2.10560
H	36.26845	1.60822	0.00000	Mg	10.52800	0.00000	0.00000
H	37.20294	0.00900	0.00000	Mg	18.95040	0.00000	0.00000

Mg	27.37280	0.00000	0.00000	B	2.48775	4.30890	0.00000
Mg	35.79520	0.00000	0.00000	B	0.00000	4.30890	0.00000
Mg	14.73920	0.00000	0.00000	B	-1.24387	2.15445	0.00000
Mg	23.16160	0.00000	0.00000	N	-0.91702	0.90686	-0.71303
Mg	31.58400	0.00000	0.00000	N	1.24387	-0.34074	-0.71303
Mg	40.00640	0.00000	0.00000	N	3.40477	0.90686	-0.71303
O	10.52800	0.00000	-2.10560	N	3.40477	3.40204	-0.71303
O	18.95040	0.00000	-2.10560	N	1.24387	4.64964	-0.71303
O	27.37280	0.00000	-2.10560	N	-0.91702	3.40205	-0.71303
O	35.79520	0.00000	-2.10560	B	-0.86840	0.93493	-2.16693
O	14.73920	0.00000	-2.10560	B	1.24387	-0.28459	-2.16693
O	23.16160	0.00000	-2.10560	B	3.35615	0.93493	-2.16693
O	31.58400	0.00000	-2.10560	B	3.35615	3.37397	-2.16693
O	40.00640	0.00000	-2.10560	B	1.24387	4.59349	-2.16693
O	10.52800	-2.10560	0.00000	B	-0.86840	3.37397	-2.16693
O	18.95040	-2.10560	0.00000	N	-1.26454	2.15445	-2.89017
O	27.37280	-2.10560	0.00000	N	-0.01033	-0.01790	-2.89017
O	35.79520	-2.10560	0.00000	N	2.49808	-0.01790	-2.89017
O	14.73920	-2.10560	0.00000	N	3.75229	2.15445	-2.89017
O	23.16160	-2.10560	0.00000	N	2.49808	4.32680	-2.89017
O	31.58400	-2.10560	0.00000	N	-0.01033	4.32680	-2.89017
O	40.00640	-2.10560	0.00000	B	-1.21110	2.15445	-4.33999
O	8.42240	0.00000	0.00000	B	0.01638	0.02838	-4.33999
O	16.84480	0.00000	0.00000	B	2.47136	0.02838	-4.33999
O	25.26720	0.00000	0.00000	B	3.69885	2.15445	-4.33999
O	33.68960	0.00000	0.00000	B	2.47136	4.28052	-4.33999
O	12.63360	0.00000	0.00000	B	0.01639	4.28052	-4.33999
O	21.05600	0.00000	0.00000	N	-0.93287	3.41119	-5.06139
O	29.47840	0.00000	0.00000	N	-0.93287	0.89771	-5.06139
O	37.90080	0.00000	0.00000	N	1.24387	-0.35903	-5.06139
O	8.42240	-2.10560	-2.10560	N	3.42061	0.89771	-5.06139
O	16.84480	-2.10560	-2.10560	N	3.42061	3.41119	-5.06139
O	25.26720	-2.10560	-2.10560	N	1.24387	4.66793	-5.06139
O	33.68960	-2.10560	-2.10560	B	-0.88244	3.38208	-6.51054
O	12.63360	-2.10560	-2.10560	B	-0.88244	0.92682	-6.51055
O	21.05600	-2.10560	-2.10560	B	1.24387	-0.30080	-6.51055
O	29.47840	-2.10560	-2.10560	B	3.37018	0.92683	-6.51054
O	37.90080	-2.10560	-2.10560	B	3.37018	3.38208	-6.51055
				B	1.24387	4.60970	-6.51055
				N	-0.01285	4.33116	-7.23219
				N	-1.26957	2.15445	-7.23219
				N	-0.01285	-0.02226	-7.23219
				N	2.50059	-0.02225	-7.23219
				N	3.75732	2.15445	-7.23219
4. B ₇₂ N ₇₂ H ₁₂							
B	0.00000	0.00000	0.00000	N	-0.01285	-0.02226	-7.23219
B	2.48774	0.00000	0.00000	N	2.50059	-0.02225	-7.23219
B	3.73162	2.15445	0.00000	N	3.75732	2.15445	-7.23219

N	2.50060	4.33116	-7.23219	N	2.50069	4.33131	-15.91513
B	0.01639	4.28052	-8.68112	N	-0.01294	4.33131	-15.91513
B	-1.21110	2.15445	-8.68112	N	-1.26975	2.15445	-15.91513
B	0.01639	0.02838	-8.68112	N	-0.01294	-0.02241	-15.91513
B	2.47136	0.02838	-8.68112	N	2.50069	-0.02241	-15.91513
B	3.69885	2.15445	-8.68112	B	3.69783	2.15446	-17.36505
B	2.47136	4.28052	-8.68112	B	2.47085	4.27964	-17.36505
N	1.24387	4.66792	-9.40294	B	0.01689	4.27964	-17.36505
N	-0.93286	3.41119	-9.40294	B	-1.21009	2.15445	-17.36505
N	-0.93286	0.89771	-9.40294	B	0.01689	0.02926	-17.36505
N	1.24387	-0.35902	-9.40294	B	2.47085	0.02926	-17.36505
N	3.42061	0.89772	-9.40294	N	3.42094	0.89753	-18.08585
N	3.42061	3.41119	-9.40294	N	3.42094	3.41139	-18.08584
B	1.24387	4.60927	-10.85186	N	1.24387	4.66831	-18.08585
B	-0.88207	3.38186	-10.85186	N	-0.93320	3.41138	-18.08585
B	-0.88207	0.92704	-10.85186	N	-0.93320	0.89752	-18.08585
B	1.24387	-0.30037	-10.85186	N	1.24387	-0.35940	-18.08585
B	3.36981	0.92704	-10.85186	B	3.36833	0.92790	-19.53662
B	3.36981	3.38186	-10.85186	B	3.36833	3.38101	-19.53662
N	2.50064	4.33123	-11.57367	B	1.24387	4.60756	-19.53662
N	-0.01289	4.33123	-11.57367	B	-0.88058	3.38101	-19.53662
N	-1.26965	2.15445	-11.57367	B	-0.88058	0.92789	-19.53662
N	-0.01289	-0.02233	-11.57367	B	1.24387	-0.29865	-19.53663
N	2.50064	-0.02232	-11.57367	N	2.50039	-0.02189	-20.25681
N	3.75740	2.15445	-11.57367	N	3.75690	2.15446	-20.25680
B	2.47119	4.28022	-13.02274	N	2.50039	4.33079	-20.25681
B	0.01656	4.28022	-13.02274	N	-0.01264	4.33080	-20.25681
B	-1.21075	2.15445	-13.02274	N	-1.26915	2.15445	-20.25681
B	0.01656	0.02868	-13.02274	N	-0.01264	-0.02189	-20.25681
B	2.47119	0.02869	-13.02274	B	2.46693	0.03606	-21.70887
B	3.69850	2.15446	-13.02274	B	3.68999	2.15446	-21.70887
N	3.42069	3.41124	-13.74440	B	2.46693	4.27285	-21.70887
N	1.24387	4.66803	-13.74440	B	0.02082	4.27285	-21.70887
N	-0.93295	3.41124	-13.74440	B	-1.20224	2.15445	-21.70887
N	-0.93295	0.89766	-13.74440	B	0.02081	0.03605	-21.70887
N	1.24387	-0.35913	-13.74440	N	1.24387	-0.34939	-22.42862
N	3.42069	0.89767	-13.74440	N	3.41226	0.90254	-22.42862
B	3.36940	3.38162	-15.19379	N	3.41226	3.40637	-22.42862
B	1.24387	4.60879	-15.19379	N	1.24387	4.65829	-22.42862
B	-0.88165	3.38162	-15.19378	N	-0.92452	3.40637	-22.42862
B	-0.88165	0.92728	-15.19379	N	-0.92452	0.90253	-22.42862
B	1.24387	-0.29989	-15.19379	B	1.24387	-0.29671	-23.88613
B	3.36940	0.92729	-15.19378	B	3.36664	0.92888	-23.88613
N	3.75750	2.15446	-15.91513	B	3.36664	3.38003	-23.88613

B	1.24387	4.60561	-23.88613	H	3.70499	0.02498	-0.00086
B	-0.87889	3.38003	-23.88613	C	-0.83261	-5.09623	-0.00066
B	-0.87889	0.92887	-23.88613	H	-0.28050	-5.41915	-0.87413
N	-0.03702	-0.06413	-24.56122	H	-0.28000	-5.41906	0.87253
N	2.52477	-0.06412	-24.56122	C	-3.99716	3.26917	-0.00067
N	3.80567	2.15446	-24.56122	H	-4.55286	2.95250	-0.87415
N	2.52477	4.37303	-24.56122	C	4.82977	1.82705	-0.00064
N	-0.03702	4.37303	-24.56122	H	4.83337	2.46665	-0.87412
N	-1.31792	2.15445	-24.56122	H	4.83305	2.46705	0.87254
H	-0.12590	-0.21806	1.15629	H	-4.55306	2.95201	0.87251
H	2.61364	-0.21806	1.15629	C	6.06531	0.91727	-0.00021
H	3.98341	2.15445	1.15629	H	6.03879	0.27865	0.87780
H	2.61364	4.52696	1.15629	H	6.03910	0.27822	-0.87792
H	-0.12590	4.52696	1.15629	C	7.37107	1.73334	-0.00019
H	-1.49567	2.15445	1.15629	H	7.39257	2.37607	-0.87555
H	-0.04669	-0.08086	-25.56572	H	7.39229	2.37649	0.87485
H	2.53443	-0.08085	-25.56572	C	8.62183	0.83410	0.00023
H	3.82499	2.15446	-25.56572	H	8.60071	0.19041	-0.87468
H	2.53443	4.38976	-25.56572	H	8.60042	0.19083	0.87544
H	-0.04668	4.38976	-25.56572	C	9.92962	1.64835	0.00025
H	-1.33724	2.15445	-25.56572	H	9.95050	2.29240	0.87506

5. C₃₃H₅₇N₃O₃

C	-1.17549	-0.71982	-0.00057	H	9.95079	2.29198	-0.87487
C	0.03022	-1.38641	-0.00058	C	11.18147	0.75069	0.00067
C	1.21113	-0.65810	-0.00055	H	11.16124	0.10631	-0.87400
C	1.18555	0.71938	-0.00056	H	11.16095	0.10673	0.87564
C	-0.03563	1.37792	-0.00055	C	12.49069	1.56252	0.00069
C	-1.21578	0.66703	-0.00058	H	12.51203	2.20634	0.87472
H	-2.11858	-1.22343	-0.00051	H	12.51232	2.20592	-0.87364
H	2.11881	-1.22303	-0.00048	C	13.73479	0.65334	0.00112
H	-0.00023	2.44646	-0.00048	H	13.74192	0.01664	-0.87730
C	-2.58637	1.27628	-0.00054	H	14.64686	1.23997	0.00113
C	0.18790	-2.87800	-0.00054	H	13.74163	0.01706	0.87984
C	2.39848	1.60172	-0.00051	C	-3.82703	4.79407	-0.00022
O	2.27314	2.82080	-0.00038	H	-3.26049	5.09091	-0.87792
O	-3.57945	0.55819	-0.00041	H	-3.26072	5.09041	0.87779
O	1.30631	-3.37899	-0.00038	C	-5.18665	5.51686	-0.00021
N	-2.68159	2.61681	-0.00065	H	-5.75425	5.21365	0.87483
H	-1.87413	3.19612	-0.00088	H	-5.75402	5.21413	-0.87557
N	-0.92543	-3.63073	-0.00066	C	-5.03327	7.04967	0.00023
H	-1.83086	-3.22110	-0.00090	H	-4.46525	7.35323	-0.87467
N	3.60702	1.01392	-0.00063	H	-4.46548	7.35276	0.87545
				C	-6.39232	7.77513	0.00024
				H	-6.96054	7.47118	0.87506
				H	-6.96030	7.47165	-0.87488

C	-6.24086	9.30809	0.00068
H	-5.67268	9.61277	-0.87398
H	-5.67291	9.61230	0.87566
C	-7.59853	10.03599	0.00070
H	-8.16677	9.73256	0.87473
H	-8.16654	9.73304	-0.87364
C	-7.43321	11.56801	0.00114
H	-6.88536	11.89254	-0.87727
H	-8.39727	12.06457	0.00115
H	-6.88559	11.89207	0.87987
C	-2.23827	-5.71134	-0.00023
H	-2.77860	-5.36913	-0.87794
H	-2.77808	-5.36907	0.87778
C	-2.18442	-7.25020	-0.00020
H	-1.63855	-7.59020	-0.87555
H	-1.63804	-7.59015	0.87485
C	-3.58856	-7.88377	0.00022
H	-4.13495	-7.54359	0.87543
H	-4.13546	-7.54364	-0.87469
C	-3.53729	-9.42348	0.00025
H	-2.99048	-9.76363	-0.87487
H	-2.98997	-9.76358	0.87507
C	-4.94062	-10.05879	0.00068
H	-5.48805	-9.71902	0.87564
H	-5.48855	-9.71908	-0.87399
C	-4.89216	-11.59851	0.00071
H	-4.34578	-11.93896	-0.87362
H	-4.34527	-11.93890	0.87475
C	-6.30158	-12.22135	0.00114
H	-6.24958	-13.30454	0.00116
H	-6.85605	-11.90912	0.87985
H	-6.85655	-11.90918	-0.87728

6. (C₉N₃H₃)₇

C	1.19532	0.71644	0.00232
C	1.22527	-0.67809	0.00350
C	0.02577	-1.38999	0.00140
C	-1.19690	-0.71866	-0.00182
C	-1.21366	0.67608	-0.00296
C	-0.02094	1.39929	-0.00091
H	2.17622	-1.20608	0.00602
H	-2.12963	-1.27821	-0.00346
H	-0.03917	2.48684	-0.00183

C	-6.32744	-3.79655	-0.01171
C	-6.29679	-5.19074	-0.01115
C	-7.49502	-5.90460	-0.01352
C	-8.71417	-5.22829	-0.01642
C	-8.73694	-3.83430	-0.01695
C	-7.54306	-3.11319	-0.01460
H	-5.34627	-5.71816	-0.00887
H	-9.64420	-5.78619	-0.01825
H	-7.56091	-2.02629	-0.01503
C	8.86546	-3.53958	0.02379
C	8.88933	-4.93355	0.02516
C	7.69349	-5.65027	0.02304
C	6.47205	-4.97689	0.01955
C	6.45605	-3.58245	0.01821
C	7.64813	-2.85880	0.02031
H	9.83750	-5.46003	0.02786
H	5.53970	-5.53580	0.01790
H	7.62962	-1.77192	0.01925
C	1.05105	9.48678	-0.00586
C	1.07862	8.09229	-0.00447
C	-0.12099	7.38119	-0.00635
C	-1.34374	8.05174	-0.00960
C	-1.36285	9.44637	-0.01099
C	-0.16758	10.16405	-0.00912
H	2.02883	7.56432	-0.00192
H	-2.27575	7.49226	-0.01103
H	-0.18573	11.24843	-0.01021
C	-6.45457	4.96342	-0.01754
C	-6.42375	3.56891	-0.01639
C	-7.62373	2.85779	-0.01832
C	-8.84416	3.53191	-0.02136
C	-8.86805	4.92611	-0.02249
C	-7.67201	5.64294	-0.02057
H	-5.47257	3.04075	-0.01405
H	-9.77411	2.97343	-0.02287
H	-7.68962	6.72756	-0.02145
C	1.34141	-8.03231	0.00912
C	1.36784	-9.42630	0.00990
C	0.17239	-10.14410	0.00717
C	-1.04643	-9.46674	0.00366
C	-1.06669	-8.07264	0.00288
C	0.12557	-7.34868	0.00561
H	2.31648	-9.95241	0.01263
H	-1.97692	-10.02431	0.00154

H	0.10736	-6.26085	0.00500	N	3.58917	-6.68977	0.01425
C	8.70335	5.22036	0.01492	N	0.21621	-12.76173	0.00865
C	8.72616	3.82615	0.01634	N	4.16620	-2.31099	0.01168
C	7.52898	3.11154	0.01436	N	7.73934	-8.26838	0.02558
C	6.30587	3.78207	0.01098	N	11.11201	-2.19435	0.02778
C	6.28998	5.17684	0.00957	N	7.57788	0.49382	0.01701
C	7.48398	5.89675	0.01153	N	4.00340	6.45213	0.00317
H	9.67428	3.29912	0.01896	N	10.94835	6.56715	0.01857
H	5.37290	3.22237	0.00943				
H	7.46527	6.98134	0.01042				
C	-2.64042	10.15693	-0.01439				
C	2.30412	10.23971	-0.00391	N	-2.42171	4.10938	-1.73995
C	-0.09651	5.91821	-0.00490	N	-1.15944	4.12220	0.35426
C	-2.49272	1.38625	-0.00636	N	0.00747	4.06728	2.55243
C	-5.20169	5.71738	-0.01555	N	1.16212	4.01521	4.76148
C	-10.14558	5.63547	-0.02570	N	2.31900	3.96184	6.97132
C	-7.60131	1.39572	-0.01715	N	3.47712	3.90769	9.18230
C	-10.01552	-3.12555	-0.01999	N	4.63640	3.85261	11.39486
C	-5.07270	-3.04386	-0.00922	N	5.79657	3.79528	13.60937
C	-7.47161	-7.36629	-0.01294	N	6.94321	3.71780	15.80934
C	0.19685	-11.60516	0.00800	N	-1.43032	6.11691	-3.51415
C	-2.34609	-7.36463	-0.00082	N	-1.10771	6.15149	-1.05143
C	2.59638	-7.28185	0.01199	N	-0.05809	6.14537	1.22000
C	0.05027	-2.85277	0.00262	N	1.08460	6.09816	3.43907
C	5.17683	-2.87215	0.01456	N	2.23956	6.04576	5.65116
C	7.71898	-7.11192	0.02446	N	3.39759	5.99176	7.86174
C	10.11962	-2.78846	0.02602	N	4.55660	5.93677	10.07252
C	7.55553	1.64954	0.01583	N	5.71556	5.88034	12.28339
C	2.44988	1.46904	0.00446	N	6.85918	5.80843	14.47410
C	5.01256	5.88843	0.00600	N	-2.82157	8.50093	-4.23198
C	9.95641	5.97210	0.01697	N	-1.22892	8.30045	-2.34217
N	-3.65115	10.71930	-0.01708	N	-0.10947	8.24710	-0.11644
N	3.29545	10.83561	-0.00236	N	1.00997	8.20913	2.11634
N	-0.07716	4.76240	-0.00375	N	2.16270	8.15852	4.32978
N	-4.21197	6.31457	-0.01399	N	3.32322	8.10444	6.53852
N	-11.15686	6.19701	-0.02825	N	4.48342	8.04957	8.74738
N	-7.58498	0.23990	-0.01623	N	5.64253	7.99398	10.95616
N	-11.02721	-2.56495	-0.02239	N	6.78589	7.92473	13.14400
N	-4.08140	-2.44920	-0.00734	N	-1.93893	10.53404	-6.01666
N	-7.45329	-8.52278	-0.01248	N	-1.45855	10.47114	-3.58046
N	0.06963	-4.00855	0.00354	N	-0.33069	10.40695	-1.35536
N	-3.50332	1.94741	-0.00908	N	0.87912	10.33649	0.82578
N	3.44115	2.06368	0.00618	N	2.06842	10.27697	3.01898
N	-3.35815	-6.80613	-0.00376	N	3.24456	10.21931	5.21819

7. B₆₄N₈₀H₄₈

N	4.41014	10.16344	7.42298	N	3.70940	20.77428	1.00998
N	5.57076	10.10803	9.62975	N	6.05920	20.19159	2.51440
N	6.71452	10.03999	11.81622	N	6.35650	20.62058	5.32648
N	-3.47143	12.87028	-6.56635	B	-1.57010	4.79238	-0.83725
N	-1.78646	12.66718	-4.75470	B	-0.40246	4.75471	1.37506
N	-0.53394	12.56476	-2.59929	B	0.74669	4.70424	3.58688
N	0.69521	12.48243	-0.42946	B	1.90176	4.65150	5.79748
N	1.93453	12.40757	1.73289	B	3.05942	4.59747	8.00830
N	3.15505	12.33803	3.90532	B	4.21847	4.54249	10.22044
N	4.33730	12.27765	6.09939	B	5.37897	4.48620	12.43506
N	5.50108	12.22141	8.30344	B	6.54207	4.42448	14.65706
N	6.64513	12.15354	10.48930	B	-1.27530	6.84954	-2.31247
N	-2.80631	15.06639	-8.25946	B	-0.43367	6.84569	0.01721
N	-2.21333	14.88666	-5.85388	B	0.67863	6.81603	2.25782
N	-0.95084	14.76522	-3.70603	B	1.82890	6.76573	4.47350
N	0.43985	14.64513	-1.63911	B	2.98668	6.71231	6.68458
N	1.77077	14.54716	0.46594	B	4.14598	6.65766	8.89522
N	3.04994	14.46327	2.60337	B	5.30569	6.60220	11.10653
N	4.27338	14.39015	4.77207	B	6.46607	6.54571	13.31971
N	5.43686	14.33346	6.97508	B	-1.82970	9.08038	-3.40707
N	6.57917	14.26520	9.16205	B	-0.55896	8.98496	-1.27295
N	-4.55610	17.30081	-8.56933	B	0.59194	8.92920	0.94008
N	-2.75352	17.12402	-6.86763	B	1.74635	8.88090	3.15495
N	-1.40468	16.97834	-4.77185	B	2.90995	8.82685	5.36268
N	0.06901	16.83171	-2.76764	B	4.07243	8.77195	7.57065
N	1.57759	16.69089	-0.78878	B	5.23308	8.71697	9.77975
N	2.91234	16.59556	1.31765	B	6.39344	8.66269	11.99018
N	4.24580	16.49431	3.42665	B	-1.74935	11.21698	-4.79246
N	5.38988	16.44126	5.63837	B	-0.77582	11.14563	-2.51301
N	6.51967	16.37403	7.83284	B	0.41199	11.07516	-0.31975
N	-4.77407	21.37983	-8.45134	B	1.62621	11.00676	1.85858
N	-3.44253	19.36202	-7.77592	B	2.82219	10.94486	4.04767
N	-2.07853	19.20497	-5.67500	B	3.99730	10.88687	6.24765
N	-0.53999	19.05726	-3.69637	B	5.16141	10.83125	8.45371
N	1.29972	18.85244	-2.00457	B	6.32244	10.77750	10.66258
N	2.83796	18.69696	-0.02711	B	-2.48266	13.46598	-5.74746
N	4.21043	18.58713	2.07132	B	-1.09198	13.33178	-3.68887
N	5.45229	18.52395	4.25220	B	0.19842	13.22992	-1.55636
N	6.45390	18.48198	6.50888	B	1.46528	13.14632	0.58959
N	-4.17416	19.75316	-10.14362	B	2.71235	13.07082	2.74724
N	-2.29471	21.36391	-6.88033	B	3.92156	13.00283	4.92621
N	-1.94353	21.08629	-4.05058	B	5.09262	12.94487	7.12725
N	0.68154	21.07252	-2.92221	B	6.25401	12.89055	9.33540
N	3.22436	20.41830	-1.78290	B	-2.61077	15.68641	-7.00146

B	-1.52414	15.54304	-4.77904	H	-1.81654	21.36458	-3.08163
B	-0.14969	15.41376	-2.70438	H	0.18426	21.67909	-3.56170
B	1.26068	15.29617	-0.65314	H	1.32879	21.55948	-2.31554
B	2.57448	15.20432	1.46371	H	3.15969	20.66721	-2.76563
B	3.85661	15.11894	3.60107	H	4.14758	20.60991	-1.40484
B	5.03414	15.05623	5.79587	H	3.13868	21.35168	0.40227
B	6.19100	15.00130	8.00678	H	4.05933	21.28004	1.81624
B	-3.58335	17.92467	-7.75628	H	6.07387	20.47422	1.53952
B	-2.07716	17.77162	-5.77847	H	6.93259	20.39884	2.98838
B	-0.61391	17.62403	-3.75785	H	5.92994	21.24734	4.65332
B	0.97111	17.46429	-1.84421	H	6.66299	21.10487	6.16503
B	2.44012	17.33214	0.17167	H	2.07918	2.97775	7.07219
B	3.78744	17.22958	2.27228	H	6.92501	18.96877	7.26839
B	5.02567	17.16051	4.44346	H	7.04981	16.84867	8.56057
B	6.13875	17.10757	6.67354	H	7.11131	14.73920	9.88882
B	-4.13219	20.16717	-8.79285	H	7.17621	12.62815	11.21651
B	-2.61521	19.99272	-6.77431	H	7.24478	10.51534	12.54360
B	-1.51003	19.80205	-4.48125	H	7.31565	8.40105	13.87118
B	0.48203	19.67983	-2.87520	H	7.38852	6.28587	15.20051
B	2.44868	19.34644	-1.26795	H	7.47143	4.13601	16.56703
B	3.60505	19.36418	1.00600	H	6.73368	2.73832	15.96666
B	5.23661	19.12371	2.94809	H	5.55470	2.81163	13.70818
B	6.09254	19.22919	5.34729	H	4.39530	2.86863	11.49480
H	-2.93637	4.58645	-2.47171	H	3.23677	2.92365	9.28289
H	-2.84699	3.22324	-1.48376	H	0.92237	3.03117	4.86257
H	-1.33516	6.57105	-4.41697	H	-0.23617	3.08449	2.65566
H	-1.20089	5.12898	-3.55364	H	-1.46032	3.16024	0.49515
H	-3.40458	9.06576	-4.83976				
H	-3.24096	7.60497	-4.00852				
H	-1.92872	11.02815	-6.90278				
H	-1.70483	9.55177	-6.11549	O	0.02750	1.32388	8.27761
H	-4.11438	13.43382	-7.11199	H	0.02749	2.26670	7.94427
H	-3.83460	11.94399	-6.36961	H	-0.78901	0.85248	7.94427
H	-2.85650	15.61541	-9.11147	O	0.02750	3.91664	7.36093
H	-2.50132	14.11350	-8.42949	H	0.02751	3.91665	6.36092
H	-5.22256	17.82855	-9.12117	H	0.84401	4.38805	7.69426
H	-4.80612	16.32427	-8.46875	O	2.27290	5.21302	8.27761
H	-5.31420	21.92472	-9.11602	H	2.27291	6.15584	7.94427
H	-4.93127	21.66328	-7.49044	H	3.08941	4.74162	7.94427
H	-4.58766	20.31400	-10.88174	O	4.51829	1.32388	8.27761
H	-3.61444	18.98561	-10.49843	H	5.33480	0.85248	7.94427
H	-2.56438	21.92728	-7.67831	H	4.51830	2.26670	7.94427
H	-1.60397	21.81139	-6.28953	O	4.51829	3.91664	7.36093
H	-2.78211	21.49702	-4.45134	H	4.51830	3.91665	6.36092

8. (H₂O)₁₆

H	5.33480	4.38805	7.69426	H	2.27291	6.15584	7.94427
O	6.76369	5.21302	8.27761	H	3.08941	4.74162	7.94427
H	7.58020	4.74161	7.94429	O	2.27290	7.80578	7.36093
H	6.76370	5.21302	9.27763	H	1.45640	8.27720	7.69428
O	9.00909	1.32388	8.27761	H	3.08940	8.27720	7.69428
H	9.82560	0.85248	7.94427	O	0.02750	9.10216	8.27761
H	9.00910	2.26670	7.94427	H	0.02749	10.04498	7.94427
O	9.00909	3.91664	7.36093	H	-0.78901	8.63076	7.94427
H	9.00910	3.91665	6.36092	O	0.02750	11.69492	7.36093
H	9.82560	4.38805	7.69426	H	0.84400	12.16634	7.69428
O	0.02750	1.32388	11.02765	H	-0.78900	12.16634	7.69428
H	0.02749	1.32388	10.02764	O	4.51829	1.32388	8.27761
H	-0.78901	0.85247	11.36098	H	5.33480	0.85248	7.94427
O	0.02750	3.91664	11.94433	H	4.51830	2.26670	7.94427
H	0.02751	2.97382	11.61099	O	4.51829	3.91664	7.36093
H	0.84401	4.38804	11.61099	H	4.51830	3.91665	6.36092
O	2.27290	5.21302	11.02765	H	5.33480	4.38805	7.69426
H	2.27290	5.21303	10.02764	O	6.76369	5.21302	8.27761
H	2.27290	6.15585	11.36098	H	7.58020	4.74161	7.94429
O	4.51829	1.32388	11.02765	H	6.76370	5.21302	9.27763
H	4.51830	1.32388	10.02764	O	6.76369	7.80578	7.36093
H	5.33480	0.85247	11.36098	H	6.76368	6.86296	7.69428
O	4.51829	3.91664	11.94433	H	5.94718	8.27718	7.69428
H	3.70178	4.38804	11.61099	O	4.51829	9.10216	8.27761
H	4.51828	2.97382	11.61099	H	4.51829	10.04499	7.94429
O	6.76369	5.21302	11.02765	H	4.51829	9.10217	9.27763
H	5.94719	4.74160	11.36099	O	4.51829	11.69492	7.36093
H	7.58019	4.74160	11.36099	H	3.70179	12.16634	7.69428
O	9.00909	1.32388	11.02765	H	5.33479	12.16634	7.69428
H	9.00909	1.32389	10.02764	O	9.00909	1.32388	8.27761
H	9.00909	2.26671	11.36098	H	9.82560	0.85248	7.94427
O	9.00909	3.91664	11.94433	H	9.00910	2.26670	7.94427
H	9.00910	3.91665	12.94434	O	9.00909	3.91664	7.36093
H	9.82560	4.38805	11.61100	H	9.00910	3.91665	6.36092
				H	9.82560	4.38805	7.69426
				O	9.00909	9.10216	8.27761
9. (H ₂ O) ₃₂				H	8.19257	8.63075	7.94429
O	0.02750	1.32388	8.27761	H	9.00908	9.10216	9.27763
H	0.02749	2.26670	7.94427	O	9.00909	11.69492	7.36093
H	-0.78901	0.85248	7.94427	H	9.00909	11.69491	6.36092
O	0.02750	3.91664	7.36093	H	9.00909	10.75210	7.69426
H	0.02751	3.91665	6.36092	O	0.02750	1.32388	11.02765
H	0.84401	4.38805	7.69426	H	0.02749	1.32388	10.02764
O	2.27290	5.21302	8.27761	H	-0.78901	0.85247	11.36098

O	0.02750	3.91664	11.94433	H	9.82560	12.16632	11.61099
H	0.02751	2.97382	11.61099				
H	0.84401	4.38804	11.61099				
O	2.27290	5.21302	11.02765	10. (H ₂ O) ₆₄			
H	2.27290	5.21303	10.02764	O	0.02750	1.32388	0.94418
H	2.27290	6.15585	11.36098	H	-0.78901	0.85247	0.61085
O	2.27290	7.80578	11.94433	H	0.02749	1.32388	1.94419
H	2.27291	7.80579	12.94434	O	0.02750	3.91664	0.02750
H	3.08941	8.27719	11.61100	H	0.02750	2.97382	0.36083
O	0.02750	9.10216	11.02765	H	0.02750	3.91663	-0.97251
H	0.02751	9.10216	10.02764	O	2.27290	5.21302	0.94418
H	0.84401	8.63075	11.36098	H	1.45639	4.74161	0.61085
O	0.02750	11.69492	11.94433	H	2.27289	5.21302	1.94419
H	0.02751	10.75210	11.61099	O	2.27290	7.80578	0.02750
H	0.84401	12.16632	11.61099	H	2.27289	6.86296	0.36084
O	4.51829	1.32388	11.02765	H	1.45639	8.27718	0.36084
H	4.51830	1.32388	10.02764	O	0.02750	9.10216	0.94418
H	5.33480	0.85247	11.36098	H	-0.78901	8.63075	0.61085
O	4.51829	3.91664	11.94433	H	0.02749	9.10216	1.94419
H	3.70178	4.38804	11.61099	O	0.02750	11.69492	0.02750
H	4.51828	2.97382	11.61099	H	0.02750	10.75210	0.36083
O	6.76369	5.21302	11.02765	H	0.02750	11.69491	-0.97251
H	5.94719	4.74160	11.36099	O	4.51829	1.32388	0.94418
H	7.58019	4.74160	11.36099	H	3.70178	0.85248	0.61084
O	6.76369	7.80578	11.94433	H	4.51828	2.26670	0.61084
H	6.76369	7.80577	12.94434	O	4.51829	3.91664	0.02750
H	6.76369	6.86296	11.61100	H	3.70178	4.38805	0.36083
O	4.51829	9.10216	11.02765	H	4.51828	3.91665	-0.97251
H	5.33480	8.63076	11.36099	O	6.76369	5.21302	0.94418
H	4.51830	10.04498	11.36099	H	5.94718	4.74162	0.61084
O	4.51829	11.69492	11.94433	H	6.76368	6.15584	0.61084
H	4.51830	11.69493	12.94434	O	6.76369	7.80578	0.02750
H	5.33480	12.16633	11.61100	H	5.94719	8.27720	0.36084
O	9.00909	1.32388	11.02765	H	7.58019	8.27720	0.36084
H	9.00909	1.32389	10.02764	O	4.51829	9.10216	0.94418
H	9.00909	2.26671	11.36098	H	3.70178	8.63075	0.61085
O	9.00909	3.91664	11.94433	H	4.51828	9.10216	1.94419
H	9.00910	3.91665	12.94434	O	4.51829	11.69492	0.02750
H	9.82560	4.38805	11.61100	H	3.70178	12.16632	0.36084
O	9.00909	9.10216	11.02765	H	4.51828	10.75210	0.36084
H	8.19258	8.63074	11.36099	O	9.00909	1.32388	0.94418
H	9.82559	8.63074	11.36099	H	8.19257	0.85247	0.61085
O	9.00909	11.69492	11.94433	H	9.00908	1.32388	1.94419
H	9.00910	10.75210	11.61099	O	9.00909	3.91664	0.02750

H	8.19257	4.38804	0.36084	O	9.00909	1.32388	3.69422
H	9.00908	2.97382	0.36084	H	8.19257	0.85248	4.02756
O	9.00909	9.10216	0.94418	H	9.00908	2.26670	4.02756
H	9.82560	8.63076	0.61084	O	9.00909	3.91664	4.61090
H	9.00910	10.04498	0.61084	H	8.19258	4.38806	4.27755
O	9.00909	11.69492	0.02750	H	9.82559	4.38806	4.27755
H	9.82560	12.16633	0.36083	O	9.00909	9.10216	3.69422
H	9.00910	11.69493	-0.97251	H	9.00908	9.10216	2.69420
O	0.02750	1.32388	3.69422	H	8.19257	8.63075	4.02755
H	0.84400	0.85246	4.02756	O	9.00909	11.69492	4.61090
H	-0.78900	0.85246	4.02756	H	8.19257	12.16632	4.27755
O	0.02750	3.91664	4.61090	H	9.00908	10.75210	4.27755
H	0.02749	2.97382	4.27755	O	0.02750	1.32388	8.27761
H	-0.78901	4.38804	4.27755	H	0.02749	2.26670	7.94427
O	2.27290	5.21302	3.69422	H	-0.78901	0.85248	7.94427
H	1.45639	4.74162	4.02756	O	0.02750	3.91664	7.36093
H	2.27289	6.15584	4.02756	H	0.02751	3.91665	6.36092
O	2.27290	7.80578	4.61090	H	0.84401	4.38805	7.69426
H	3.08941	8.27719	4.27757	O	2.27290	5.21302	8.27761
H	2.27291	7.80579	5.61091	H	2.27291	6.15584	7.94427
O	0.02750	9.10216	3.69422	H	3.08941	4.74162	7.94427
H	0.84401	8.63076	4.02756	O	2.27290	7.80578	7.36093
H	0.02751	10.04498	4.02756	H	1.45640	8.27720	7.69428
O	0.02750	11.69492	4.61090	H	3.08940	8.27720	7.69428
H	0.84401	12.16633	4.27757	O	0.02750	9.10216	8.27761
H	0.02751	11.69493	5.61091	H	0.02749	10.04498	7.94427
O	4.51829	1.32388	3.69422	H	-0.78901	8.63076	7.94427
H	4.51828	1.32388	2.69420	O	0.02750	11.69492	7.36093
H	3.70178	0.85247	4.02755	H	0.84400	12.16634	7.69428
O	4.51829	3.91664	4.61090	H	-0.78900	12.16634	7.69428
H	3.70178	4.38804	4.27755	O	4.51829	1.32388	8.27761
H	4.51828	2.97382	4.27755	H	5.33480	0.85248	7.94427
O	6.76369	5.21302	3.69422	H	4.51830	2.26670	7.94427
H	6.76368	5.21302	2.69420	O	4.51829	3.91664	7.36093
H	5.94718	4.74161	4.02755	H	4.51830	3.91665	6.36092
O	6.76369	7.80578	4.61090	H	5.33480	4.38805	7.69426
H	6.76369	6.86296	4.27757	O	6.76369	5.21302	8.27761
H	6.76369	7.80577	5.61091	H	7.58020	4.74161	7.94429
O	4.51829	9.10216	3.69422	H	6.76370	5.21302	9.27763
H	5.33480	8.63076	4.02756	O	6.76369	7.80578	7.36093
H	4.51830	10.04498	4.02756	H	6.76368	6.86296	7.69428
O	4.51829	11.69492	4.61090	H	5.94718	8.27718	7.69428
H	5.33480	12.16633	4.27757	O	4.51829	9.10216	8.27761
H	4.51830	11.69493	5.61091	H	4.51829	10.04499	7.94429

H	-26.63901	-40.12493	1.96707	O	-16.19628	-28.83268	0.32836
H	-27.01407	-38.94859	0.68909	N	-16.88277	-26.77407	-0.30927
H	-27.97044	-40.43915	0.82491	H	-17.63250	-26.13752	-0.55588
C	-24.58072	-40.25344	0.15288	C	-15.57363	-26.17116	-0.18263
O	-23.70668	-40.95241	0.65359	H	-15.13721	-26.47626	0.77631
N	-24.36194	-38.99235	-0.26412	C	-14.63766	-26.59709	-1.31918
H	-25.09470	-38.40589	-0.64712	H	-15.04724	-26.27315	-2.27949
C	-23.07552	-38.35348	-0.09465	H	-13.64334	-26.16008	-1.19668
H	-22.71672	-38.55115	0.92283	H	-14.54668	-27.68432	-1.31247
C	-22.04290	-38.87530	-1.10041	C	-15.79366	-24.65640	-0.18938
H	-22.37801	-38.66645	-2.11974	O	-16.87506	-24.16974	-0.50184
H	-21.06874	-38.40362	-0.94772	N	-14.71929	-23.91637	0.13792
H	-21.93632	-39.95321	-0.96857	H	-13.81758	-24.32477	0.35868
C	-23.30806	-36.85197	-0.27560	C	-14.74638	-22.47104	0.08130
O	-24.35821	-36.41780	-0.73635	H	-15.21512	-22.16406	-0.86174
N	-22.27589	-36.06364	0.07603	C	-15.53065	-21.86839	1.25201
H	-21.39715	-36.43286	0.42222	H	-15.05522	-22.14032	2.19799
C	-22.30720	-34.63231	-0.13067	H	-15.57164	-20.77846	1.18055
H	-22.67942	-34.43015	-1.14261	H	-16.54899	-22.25973	1.23328
C	-23.21151	-33.92859	0.88721	C	-13.28546	-22.01305	0.10262
H	-22.83011	-34.09078	1.89867	O	-12.37613	-22.79318	0.36451
H	-23.25792	-32.85306	0.69801	N	-13.08527	-20.70804	-0.15316
H	-24.21793	-34.34248	0.80895	H	-13.84468	-20.06170	-0.33708
C	-20.85961	-34.14886	-0.00883	C	-11.76905	-20.11225	-0.07676
O	-19.97461	-34.88479	0.41431	H	-11.28476	-20.44447	0.84976
N	-20.64403	-32.86995	-0.36540	C	-10.89341	-20.50771	-1.27112
H	-21.38557	-32.25511	-0.68188	H	-11.34839	-20.15404	-2.19997
C	-19.34509	-32.25085	-0.21498	H	-9.89178	-20.07861	-1.18564
H	-18.94868	-32.50231	0.77636	H	-10.80813	-21.59499	-1.30100
C	-18.35844	-32.72787	-1.28661	C	-11.98445	-18.59743	-0.02847
H	-18.73105	-32.46296	-2.27953	O	-13.08161	-18.10069	-0.25965
H	-17.37453	-32.27240	-1.14824	N	-10.89043	-17.86719	0.25245
H	-18.25706	-33.81193	-1.21550	H	-9.97844	-18.28135	0.41110
C	-19.57216	-30.74032	-0.31090	C	-10.92014	-16.42078	0.23783
O	-20.63771	-30.27832	-0.70467	H	-11.45037	-16.08940	-0.66330
N	-18.51989	-29.97711	0.03483	C	-11.62493	-15.85109	1.47385
H	-17.62933	-30.36842	0.32195	H	-11.08785	-16.14776	2.37850
C	-18.54860	-28.53682	-0.09783	H	-11.66926	-14.75968	1.43431
H	-18.96123	-28.28141	-1.08168	H	-12.64259	-16.24282	1.51240
C	-19.40410	-27.88098	0.99159	C	-9.46129	-15.96090	0.17655
H	-18.98218	-28.09619	1.97676	O	-8.53719	-16.74340	0.37023
H	-19.45064	-26.79699	0.85928	N	-9.27911	-14.65123	-0.06913
H	-20.41608	-28.28480	0.93507	H	-10.04978	-14.00624	-0.20467
C	-17.09295	-28.06916	-0.01387	C	-7.96183	-14.05298	-0.06961

H	-7.41838	-14.39441	0.81992	C	26.32186	11.95628	-4.03714
C	-7.16336	-14.43073	-1.32246	H	27.36813	11.68046	-4.17839
H	-7.68037	-14.07081	-2.21579	H	26.10853	12.85285	-4.62494
H	-6.16092	-13.99558	-1.29767	C	25.36139	10.87177	-4.45883
H	-7.07373	-15.51709	-1.36943	O	24.18385	10.87199	-4.12290
C	-8.17702	-12.53967	0.00874	N	25.86832	9.87207	-5.24031
O	-9.28478	-12.04242	-0.16275	H	26.79993	9.97852	-5.61680
N	-7.07190	-11.80982	0.24457	C	24.96219	8.95829	-5.92195
H	-6.15257	-12.22372	0.35295	H	24.20856	9.52899	-6.47588
C	-7.10765	-10.36352	0.24841	C	25.73708	8.04770	-6.86992
H	-7.68073	-10.02428	-0.62307	H	26.48905	7.47142	-6.32277
C	-7.75735	-9.81197	1.52233	H	25.04475	7.35243	-7.34662
H	-7.17772	-10.11550	2.39793	H	26.23311	8.63172	-7.64938
H	-7.81039	-8.72051	1.49780	C	24.14988	8.10353	-4.95152
H	-8.76970	-10.21098	1.60279	O	23.07970	7.62473	-5.30923
C	-5.65604	-9.89508	0.12314	N	24.67720	7.87778	-3.72885
O	-4.71921	-10.67438	0.25723	H	25.55317	8.31638	-3.48304
N	-5.49253	-8.58004	-0.11045	C	23.95263	7.08946	-2.74889
H	-6.27257	-7.93774	-0.19377	H	23.71440	6.11348	-3.18368
C	-4.17911	-7.97617	-0.16678	C	24.78083	6.91391	-1.48108
H	-3.58923	-8.33347	0.68622	H	25.01138	7.88641	-1.03464
C	-3.44528	-8.32436	-1.46684	H	24.20876	6.33076	-0.75840
H	-4.01072	-7.95138	-2.32478	H	25.71415	6.38904	-1.69799
H	-2.44498	-7.88394	-1.48729	C	22.59028	7.69313	-2.39274
H	-3.35227	-9.40905	-1.53925	O	21.73351	6.97624	-1.88061
C	-4.39400	-6.46642	-0.04535	N	22.39708	9.00183	-2.64391
O	-5.50892	-5.96727	-0.15066	H	23.11048	9.55933	-3.10680
N	-3.28024	-5.73626	0.15180	C	21.10155	9.60587	-2.39006
H	-2.35403	-6.14678	0.19196	H	20.82856	9.45344	-1.34113
C	-3.32702	-4.29181	0.18434	C	21.14405	11.09438	-2.72226
H	-3.95171	-3.94340	-0.64793	H	21.41970	11.24260	-3.77009
C	-3.91190	-3.77102	1.50227	H	20.16070	11.53242	-2.54561
H	-3.28166	-4.08092	2.33951	H	21.88194	11.60371	-2.09854
H	-3.98319	-2.68025	1.50354	C	19.97729	8.93305	-3.18241
H	-4.91256	-4.18684	1.62896	O	18.81478	9.03348	-2.79552
C	-1.88978	-3.80583	-0.01486	N	20.31775	8.26516	-4.30301
O	-0.94389	-4.57365	0.02392	H	21.29108	8.17675	-4.58363
N	-1.75395	-2.47181	-0.20031	C	19.30589	7.56253	-5.06811
H	-2.54548	-1.85672	-0.28498	H	18.51420	8.26212	-5.35528
H	-0.82547	-2.10142	-0.32898	C	19.93262	6.92623	-6.30539
				H	20.72058	6.22606	-6.01394
				H	19.16429	6.38965	-6.86373
				H	20.37501	7.69278	-6.94558
				C	18.58841	6.48781	-4.24716
12. 3_{10} -helix (Ala) ₁₄							
H	26.14049	12.19659	-2.98944				

O	17.48090	6.08880	-4.60402	H	10.51929	4.58347	0.85356
N	19.22294	6.00347	-3.16203	C	10.79165	6.66374	0.30597
H	20.12286	6.37876	-2.87183	H	10.92504	7.26134	-0.59991
C	18.56545	5.03486	-2.30621	H	9.89193	6.99308	0.82814
H	18.27720	4.15985	-2.89737	H	11.66192	6.82162	0.94687
C	19.49445	4.62956	-1.16556	C	9.37061	4.96798	-0.85315
H	19.78038	5.50759	-0.57982	O	8.28814	4.90708	-0.27100
H	18.98277	3.91522	-0.51891	N	9.48442	4.87397	-2.19260
H	20.40441	4.17231	-1.56062	H	10.39781	4.88800	-2.64375
C	17.24861	5.56153	-1.73140	C	8.31448	4.60086	-3.00343
O	16.39197	4.76917	-1.34039	H	7.55176	5.36356	-2.81604
N	17.09171	6.89733	-1.65526	C	8.69692	4.57743	-4.48073
H	17.80217	7.53189	-2.01495	H	9.46423	3.81946	-4.66046
C	15.84381	7.45331	-1.17102	H	7.81325	4.34772	-5.07815
H	15.63143	7.05999	-0.17153	H	9.10007	5.54590	-4.78512
C	15.92552	8.97684	-1.14122	C	7.63424	3.28066	-2.63174
H	16.13847	9.36540	-2.14087	O	6.45318	3.09863	-2.92428
H	14.97550	9.38282	-0.79038	N	8.38328	2.34856	-2.01120
H	16.72635	9.30124	-0.47302	H	9.34684	2.54072	-1.74336
C	14.64255	7.01968	-2.01488	C	7.78103	1.10160	-1.58337
O	13.51072	7.05803	-1.53247	H	7.30679	0.61230	-2.44037
N	14.88064	6.62682	-3.28124	C	8.83987	0.19284	-0.96615
H	15.83076	6.56823	-3.64334	H	9.31093	0.68639	-0.11176
C	13.79252	6.14458	-4.10839	H	8.36953	-0.73461	-0.63587
H	13.01032	6.90843	-4.16694	H	9.61875	-0.03399	-1.69771
C	14.30692	5.79727	-5.50252	C	6.63991	1.30836	-0.58412
H	15.08385	5.03061	-5.43980	O	5.80398	0.42162	-0.41976
H	13.48010	5.42578	-6.10988	N	6.61295	2.46803	0.10269
H	14.73848	6.68028	-5.97907	H	7.29428	3.20252	-0.07834
C	13.09283	4.92495	-3.50330	C	5.51430	2.74071	1.00819
O	11.94233	4.64816	-3.84251	H	5.43290	1.92787	1.73687
N	13.79197	4.18098	-2.62406	C	5.73815	4.07527	1.71293
H	14.72838	4.45505	-2.33168	H	5.82002	4.88138	0.97863
C	13.16573	3.05022	-1.96950	H	4.89703	4.27683	2.37830
H	12.77591	2.36016	-2.72498	H	6.66343	4.05022	2.29322
C	14.17111	2.34104	-1.06676	C	4.15413	2.75693	0.30140
H	14.55877	3.03237	-0.31378	O	3.12758	2.57364	0.95127
H	13.68044	1.50254	-0.57026	N	4.14982	3.01022	-1.02273
H	15.01463	1.97201	-1.65446	H	5.02252	3.10150	-1.53827
C	11.93634	3.45045	-1.15100	C	2.90470	2.98907	-1.76581
O	11.09365	2.60042	-0.86268	H	2.17288	3.61462	-1.24484
N	11.83606	4.73553	-0.76094	C	3.13343	3.50366	-3.18314
H	12.53206	5.42523	-1.04040	H	3.88983	2.89654	-3.68857
C	10.65600	5.18618	-0.05035	H	2.19466	3.44581	-3.73553

H	3.48450	4.53828	-3.16407	O	18.38288	3.96478	0.77837
C	2.24545	1.60119	-1.83008	N	19.52189	5.85246	0.26011
O	1.09062	1.50637	-2.21857	H	20.31443	6.23527	-0.24208
N	3.02108	0.54935	-1.47817	C	18.33587	6.68200	0.39895
H	3.97759	0.69627	-1.16909	H	17.85559	6.44437	1.35197
C	2.50947	-0.80265	-1.42607	C	18.71080	8.15920	0.33211
H	1.58330	-0.81032	-2.00977	H	19.21876	8.38236	-0.61058
C	3.51911	-1.78764	-2.00853	H	17.80857	8.76985	0.40023
H	4.48321	-1.67437	-1.50275	H	19.37066	8.41908	1.16315
H	3.15624	-2.80498	-1.85982	C	17.29460	6.34015	-0.66913
H	3.66174	-1.59534	-3.07436	O	16.09978	6.29518	-0.39350
C	2.11080	-1.24835	-0.00866	N	17.76093	6.11903	-1.91540
O	1.82066	-2.41641	0.20705	H	18.75663	6.15473	-2.10666
N	2.08230	-0.28663	0.93785	C	16.83433	5.72053	-2.96102
H	2.35260	0.67548	0.77354	H	16.04183	6.47029	-3.04867
H	1.80330	-0.56957	1.86296	C	17.57619	5.55234	-4.28269

13. α -helix (Ala)₁₄

H	22.65512	8.71619	-1.20723	H	18.35237	4.78810	-4.18068
C	22.93167	8.23359	-2.14502	H	16.87636	5.24591	-5.06235
H	23.99365	7.98382	-2.13395	H	18.03735	6.49809	-4.58027
H	22.74241	8.94549	-2.95279	C	16.11474	4.42211	-2.57872
C	22.04701	7.03148	-2.35190	O	14.91751	4.27275	-2.80551
O	20.84564	7.04658	-2.09117	N	16.87762	3.46339	-2.01984
N	22.63458	5.90542	-2.84128	H	17.87023	3.61766	-1.87371
H	23.58206	5.95916	-3.18885	C	16.27602	2.20775	-1.61099
C	21.79666	4.80149	-3.28814	H	15.75850	1.75362	-2.46227
H	21.07846	5.15858	-4.03493	C	17.35301	1.27684	-1.06241
C	22.65311	3.68007	-3.86795	H	17.83369	1.73732	-0.19372
H	23.35988	3.30366	-3.12284	H	16.90555	0.32802	-0.76057
H	22.01007	2.85670	-4.18296	H	18.10845	1.08290	-1.82886
H	23.20974	4.03170	-4.74042	C	15.18646	2.44480	-0.56081
C	20.93211	4.26267	-2.15101	O	14.12413	1.82911	-0.60228
O	19.80542	3.83958	-2.38027	N	15.48042	3.33147	0.40737
N	21.47416	4.22756	-0.91403	H	16.38169	3.80016	0.41996
H	22.41174	4.57377	-0.76602	C	14.49716	3.64047	1.42804
C	20.69242	3.69550	0.19147	H	14.18772	2.71976	1.93367
H	20.34651	2.68983	-0.06651	C	15.08447	4.64092	2.41907
C	21.52274	3.66627	1.46976	H	15.35978	5.56140	1.89531
H	21.85261	4.67398	1.73962	H	14.34871	4.87388	3.19112
H	20.91614	3.27454	2.28788	H	15.97524	4.22062	2.89371
H	22.39660	3.02168	1.34751	C	13.21818	4.19951	0.79754
C	19.41570	4.51420	0.41304	O	12.11036	3.85784	1.20545
				N	13.38796	5.09836	-0.18922
				H	14.32243	5.36066	-0.49047
				C	12.23164	5.66204	-0.85889

H	11.56308	6.11523	-0.11976	H	7.63132	4.37419	-3.52101
C	12.68634	6.68917	-1.89125	C	5.74985	1.97719	-1.86715
H	13.33314	6.20881	-2.63175	O	4.53853	1.87958	-2.03684
H	11.81804	7.11647	-2.39654	N	6.52789	0.92089	-1.55056
H	13.24216	7.49309	-1.40127	H	7.52835	1.04122	-1.41740
C	11.39909	4.56308	-1.52566	C	5.91896	-0.37573	-1.32994
O	10.17105	4.58724	-1.48653	H	5.32812	-0.65872	-2.20671
N	12.09030	3.60778	-2.17356	C	7.00405	-1.40929	-1.04267
H	13.10655	3.63095	-2.18883	H	7.56220	-1.11901	-0.14729
C	11.38394	2.50823	-2.80147	H	6.54733	-2.38808	-0.88145
H	10.64199	2.90140	-3.50418	H	7.69732	-1.47218	-1.88626
C	12.38116	1.59581	-3.50897	C	4.90602	-0.33887	-0.17753
H	13.09785	1.19896	-2.78363	O	3.87140	-0.99925	-0.22394
H	11.85302	0.76656	-3.98377	N	5.24973	0.41963	0.88030
H	12.92452	2.15594	-4.27479	H	6.12643	0.93276	0.87347
C	10.57385	1.71774	-1.76868	C	4.36962	0.54400	2.02379
O	9.44601	1.30439	-2.02923	H	4.08107	-0.45551	2.36591
N	11.18544	1.48027	-0.59417	C	5.07741	1.31154	3.13633
H	12.12519	1.82877	-0.42312	H	5.33510	2.31288	2.77786
C	10.48066	0.76909	0.45425	H	4.40933	1.39417	3.99526
H	10.12168	-0.19091	0.06886	H	5.99401	0.79359	3.43267
C	11.40619	0.57143	1.65067	C	3.03777	1.23691	1.69805
H	11.73551	1.54478	2.02669	O	2.08999	1.11434	2.46080
H	10.87777	0.03950	2.44432	N	3.01983	1.98607	0.57441
H	12.28387	-0.00980	1.35518	H	3.86437	2.09125	0.02274
C	9.21460	1.52421	0.87318	C	1.82662	2.65872	0.11631
O	8.16862	0.92278	1.10684	H	1.20606	2.86324	0.99504
N	9.33462	2.85839	0.99577	C	2.19482	3.95614	-0.59821
H	10.22428	3.31257	0.80676	H	2.85735	3.73149	-1.44034
C	8.17583	3.65713	1.34672	H	1.28735	4.43072	-0.97350
H	7.74409	3.28540	2.28193	H	2.71668	4.62852	0.08715
C	8.58283	5.12198	1.47256	C	0.94960	1.80327	-0.81289
H	8.98580	5.47689	0.51909	O	-0.07884	2.27650	-1.27863
H	7.71323	5.72492	1.74164	N	1.37447	0.54862	-1.06061
H	9.34833	5.23564	2.24516	H	2.25141	0.17253	-0.71913
C	7.06302	3.49724	0.30403	H	0.80823	-0.00690	-1.68038
O	5.88633	3.39656	0.63595				
N	7.45969	3.50490	-0.98526				
H	8.44287	3.59701	-1.22498				
C	6.47516	3.31782	-2.03204				
H	5.68832	4.07344	-1.93702				
C	7.15409	3.39810	-3.39578				
H	7.91774	2.61850	-3.47672				
H	6.41368	3.26022	-4.18652				