

ChemComm

Supporting Information

Relevance of *Cis*- and *Trans*-Dichloride Ru Intermediates in
Grubbs-II Olefin Metathesis Catalysis ($\text{H}_2\text{IMesCl}_2\text{Ru}=\text{CHR}$)

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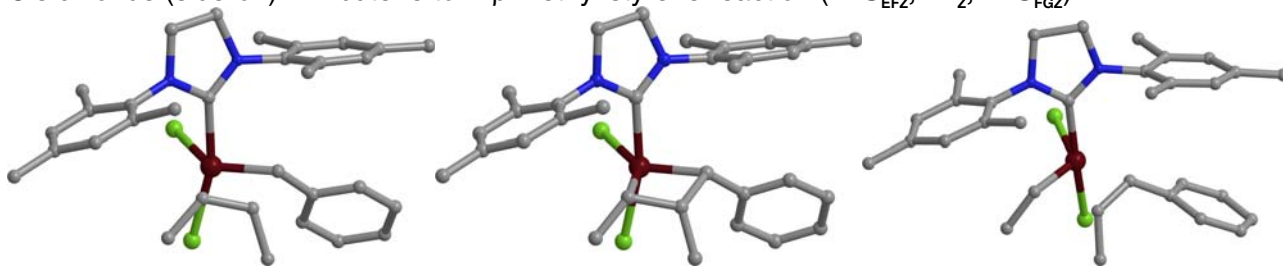
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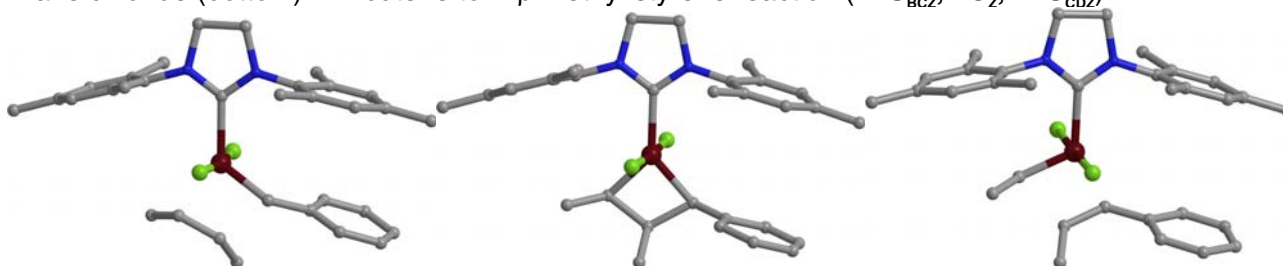
Structure	B3LYP SP Gas Phase LACV3P***+(2f)	M06 SP Gas Phase LACV3P***+(2f)	LACVP** CH ₂ CL ₂	B3LYP LACVP** gas phase			Imaginary Frequency
	E _{SCF} Hartrees	E _{SCF} Hartrees	Vsol kcal/mol	Hvib kcal/mol	ZPE kcal/mol	Svib cal/molK	
A	-2210.501651	-2209.4784726	-14.4491	20.288	334.254	141.775	
X _Z	-157.2725877	-157.12901158	-1.0755	1.676	67.455	9.71	
X _E	-157.2744738	-157.13068597	-1.3264	1.668	67.346	9.161	
1B _Z	-2367.77538	-2366.635777	-12.3489	24.264	403.894	164.587	
1B _E	-2367.776464	-2366.635711	-12.1779	24.272	403.882	165.299	
1TSBC _Z	-2367.766138	-2366.629298	-11.7258	23.135	404.871	154.179	-215.23
1TSBC _E	-2367.767979	-2366.629927	-11.5799	23.187	404.742	154.586	-219.93
1C _Z	-2367.771106	-2366.635655	-11.645	23.153	405.845	153.31	
1C _E	-2367.774845	-2366.637823	-12.0346	23.195	405.804	154.959	
1TSCD _Z	-2367.764	-2366.625282	-11.8471	23.095	404.683	153.155	-178.88
1TSCD _E	-2367.76442	-2366.625765	-12.2616	23.178	404.328	156.382	-179.06
1D _Z	-2367.770416	-2366.627169	-12.1787	24.188	403.671	164.923	
1D _E	-2367.770194	-2366.63484	-12.4149	23.998	403.832	161.538	
2B _Z	-2367.775167	-2366.637863	-12.4149	24.059	404.03	161.284	
2B _E	-2367.775803	-2366.638247	-12.3238	24.125	403.978	162.87	
2TSBC _Z	-2367.766275	-2366.629103	-11.8176	23.091	404.71	152.792	-203.17
2TSBC _E	-2367.766528	-2366.628336	-11.6073	23.169	404.635	154.562	-211.61
2C _Z	-2367.773248	-2366.636734	-11.538	23.194	405.727	153.976	
2C _E	-2367.776972	-2366.639193	-12.0754	23.263	405.609	155.524	
2TSCD _Z	-2367.765017	-2366.626371	-11.878	23.116	404.612	153.471	-204.75
2TSCD _E	-2367.766234	-2366.627922	-12.3263	23.19	404.297	154.892	-185.79
2D _Z	-2367.770799	-2366.628128	-11.9119	24.112	403.74	163.729	
2D _E	-2367.770368	-2366.632067	-12.3071	23.57	403.562	157.237	
1E _Z	-2367.759513	-2366.623000	-16.4351	24.594	404.215	169.641	
1E _E	-2367.748656	-2366.613295	-16.7617	24.005	404.103	162.563	
1TSEF _Z	-2367.744335	-2366.611697	-17.6993	23.127	404.777	154.638	-189.8
1TSEF _E	-2367.736267	-2366.607573	-16.9383	23.451	405.079	158.172	-193.06
1F _Z	-2367.745358	-2366.613684	-16.9819	23.389	405.229	156.252	
1F _E	-2367.736654	-2366.607333	-17.378	23.179	405.638	154.246	
1TSFG _Z	-2367.736413	-2366.602768	-18.9219	23.377	403.796	157.489	-111.16
1TSFG _E	-2367.720777	-2366.589421	-18.9519	23.135	403.964	152.304	-63.13
1G _Z	-2367.744847	-2366.611581	-17.2002	24.716	403.461	171.772	
1G _E	-2367.742415	-2366.610924	-17.3293	24.418	403.771	166.287	
2E _Z	-2367.755892	-2366.621968	-17.3163	23.771	404.488	159.093	
2E _E	-2367.757091	-2366.622108	-17.5471	24.365	404.434	165.452	
2TSEF _Z	-2367.73567	-2366.605609	-17.0482	23.594	404.855	161.344	-190.32
2TSEF _E	-2367.744051	-2366.611031	-17.9688	23.131	404.808	154.839	-193.55
2F _Z	-2367.737456	-2366.607785	-16.5975	23.151	405.507	153.433	
2F _E	-2367.747896	-2366.615866	-18.1219	23.95	405.412	164.611	
2TSFG _Z	-2367.723459	-2366.591647	-18.8776	23.397	403.791	157.598	-113.66
2TSFG _E	-2367.738029	-2366.604047	-20.892	23.936	403.799	163.577	-92.84
2G _Z	-2367.744847	-2366.611581	-17.2002	24.716	403.461	171.772	
2G _E	-2367.742415	-2366.610924	-17.3293	24.418	403.771	166.287	
H	-2018.715647	-2017.8418638	-13.6728	18.444	300.279	126.955	
Y _Z	-349.0553756	-348.7632645	-3.3837	3.206	101.164	18.57	
Y _E	-349.0599028	-348.7662493	-3.5568	3.476	100.78	21.721	

Structures for Z-2-butene

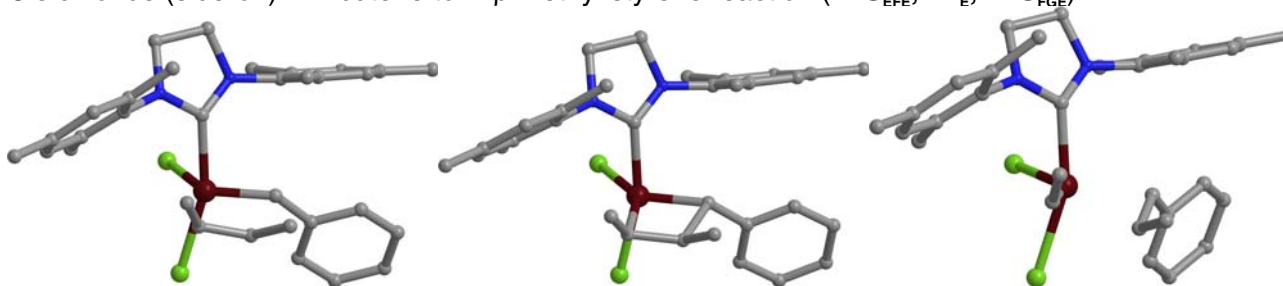
Cis chloride (side-on) Z-2-butene to Z-β-methyl styrene reaction (1TS_{EFZ} , 1F_{Z} , 1TS_{FGZ})



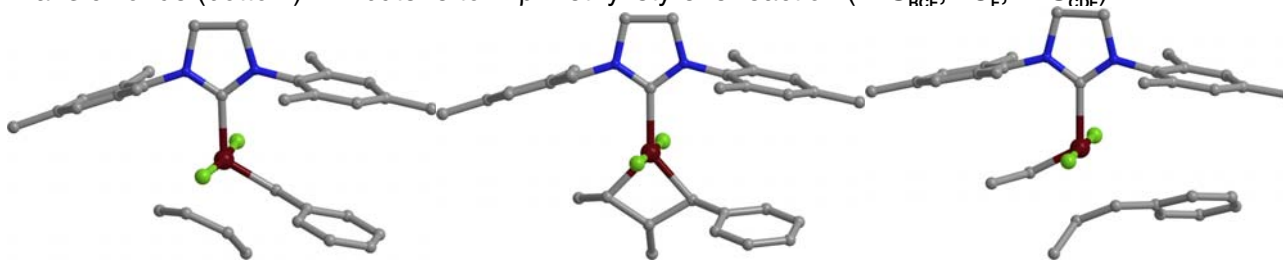
Trans chloride (bottom) Z-2-butene to Z-β-methyl styrene reaction (1TS_{BCZ} , 1C_{Z} , 1TS_{CDZ})



Cis chloride (side-on) Z-2-butene to E-β-methyl styrene reaction (1TS_{EFE} , 1F_{E} , 1TS_{FGE})

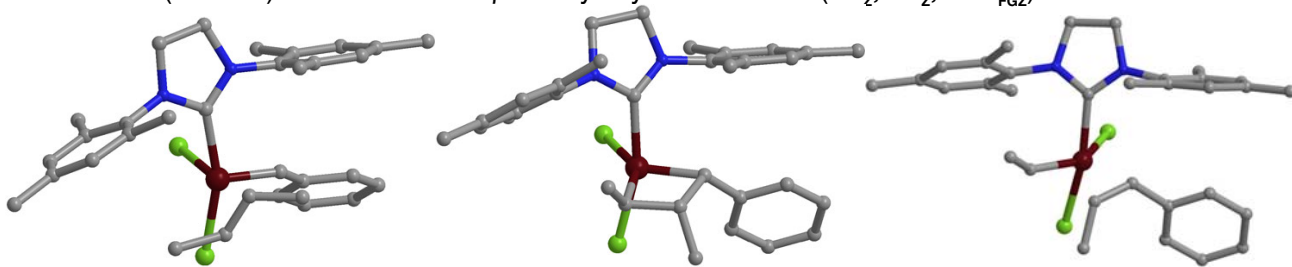


Trans chloride (bottom) Z-2-butene to E-β-methyl styrene reaction (1TS_{RCF} , 1C_{E} , 1TS_{CDF})

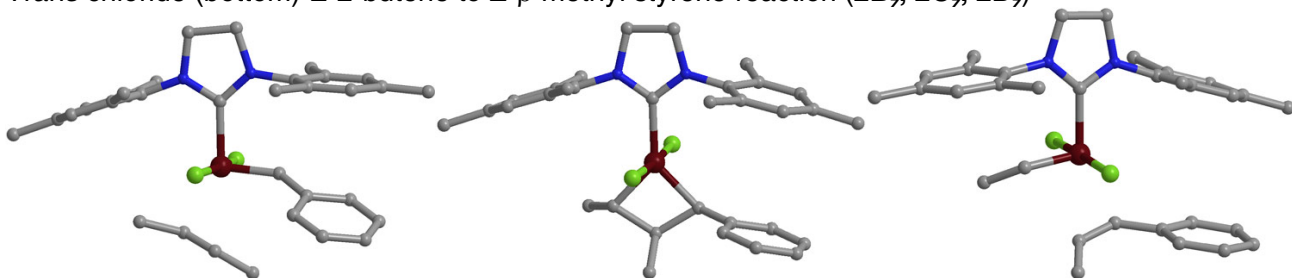


Structures for *E*-2-butene

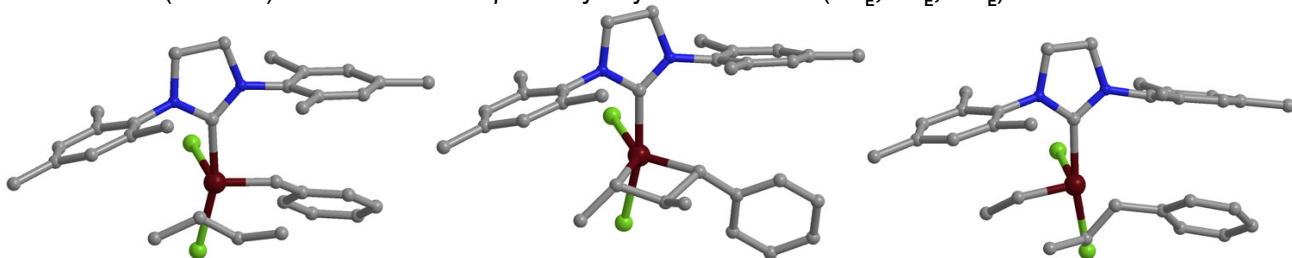
Cis chloride (side-on) *E*-2-butene to *Z*- β -methyl styrene reaction (**2E_Z**, **2F_Z**, **2TS_{FGZ}**)



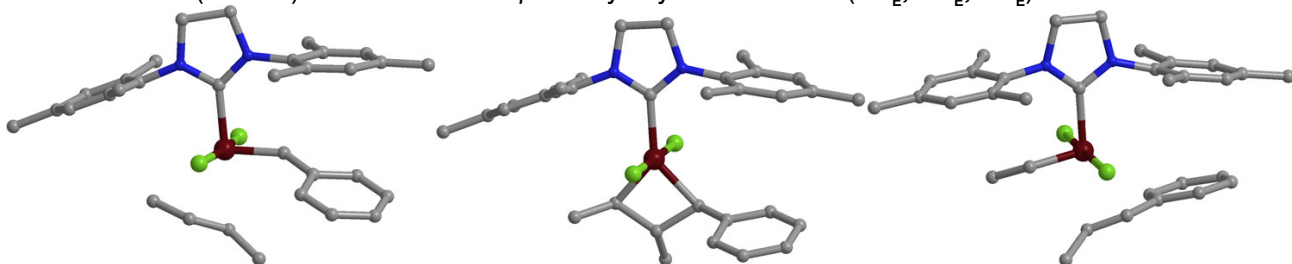
Trans chloride (bottom) *E*-2-butene to *Z*- β -methyl styrene reaction (**2B_Z**, **2C_Z**, **2D_Z**)

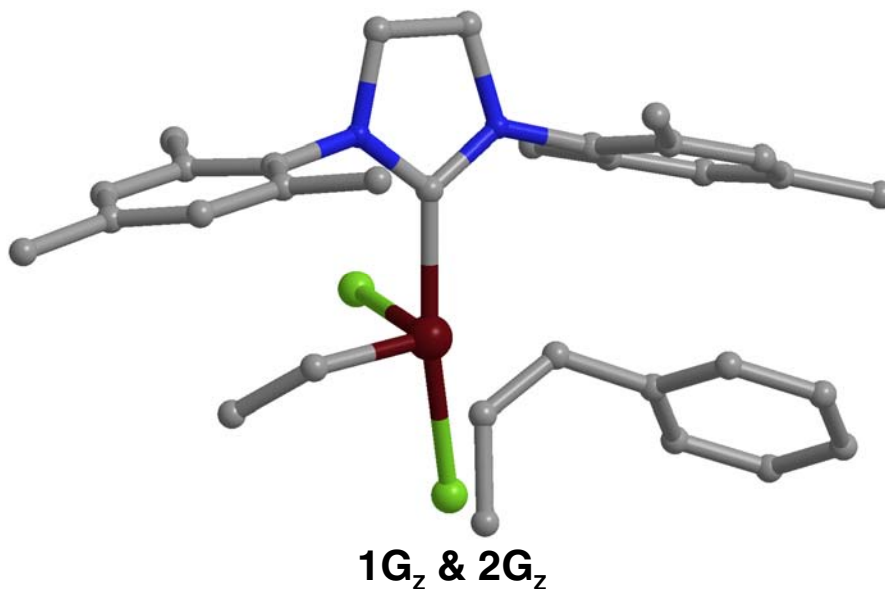
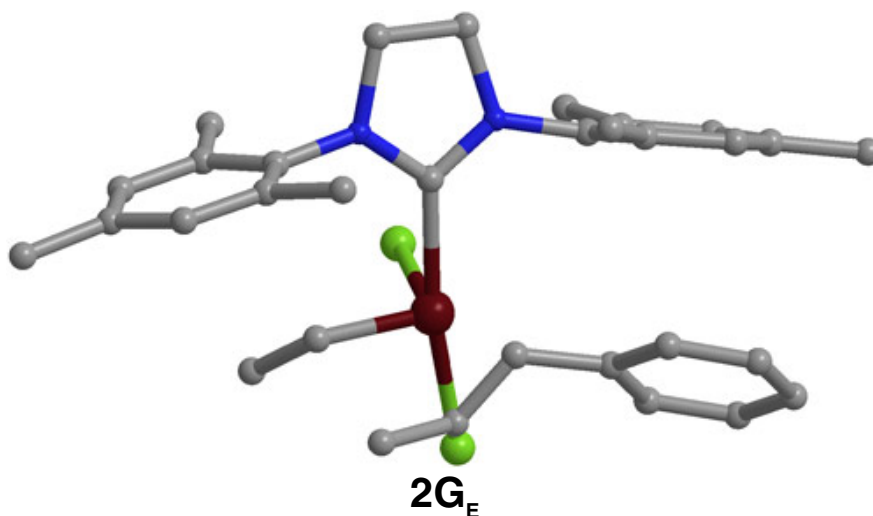


Cis chloride (side-on) *E*-2-butene to *E*- β -methyl styrene reaction (**2E_E**, **2F_E**, **2G_E**)



Trans chloride (bottom) *E*-2-butene to *E*- β -methyl styrene reaction (**2B_E**, **2C_E**, **2D_E**)





A stable intermediate where the alkylidene remains pointing towards the NHC-ligand could not be found. Following from **TSFG_z**, the alkylidene rotates away from the NHC-ligand and leads to the same product (**1G_z** and **2G_z**) that is generated with Z-2-butene as substrate.

The steric hindrance that originates in the positioning of the alkylidene and the coordinated olefin is alleviated by a rotation of the product with respect to the Ru=C alkylidene. This destabilizes the coordinated product **2G_E**.

1B _z				C74			
N1	-0.1522398696	0.1932965973	-0.1886693164	H75	-4.2584765166	0.2299783473	1.5788240769
C2	1.3223098073	0.2504847467	-0.2164073806	H76	-6.0092291931	0.3370111953	1.3822509551
H3	1.6605334688	1.2819596408	-0.3558294512	H77	-5.2192150587	-1.2499737929	1.5181492056
C4	1.6695448860	-0.6596158922	-1.4007179139				
N5	0.3558731303	-1.2251439198	-1.7781591850				
H6	2.3616366072	-1.4634905280	-1.1324357821				
C7	-0.8556468539	0.9838080682	0.7880554907	N1	-0.1226235828	0.2012879778	-0.2434205266
C8	0.3479932739	-2.2486743590	-2.7838167925	C2	1.3451006036	0.3352180209	-0.3270449140
C9	0.5741497707	-4.2429993821	-4.7387563736	H3	1.6150735373	1.3513969018	-0.6347498500
C10	0.4870498665	-3.5935367838	-2.3849987277	C4	1.7193307609	-0.7203567966	-1.3754018060
C11	0.3483842063	-1.8810417731	-4.1420950639	N5	0.4026736637	-1.2331022427	-1.8130230108
C12	0.4571948719	-2.8973977562	-5.0983724253	H6	2.3195284016	-1.5383193967	-0.9608501444
C13	0.5927492983	-4.5686791872	-3.3788808287	C7	-0.8306116411	0.9337151733	0.7746185113
C14	0.5157840733	-3.9820628760	-0.9267265545	C8	0.4034927019	-2.2937564659	-2.7796743109
C15	0.2240323495	-0.4378930272	-4.5702764245	C9	0.6245586621	-4.3607546257	-4.6588635606
H16	0.4525438749	-2.6260892692	-6.1519773508	C10	0.4621481939	-3.6294342437	-2.3325246995
H17	0.6902787324	-5.6105348857	-3.0814322425	C11	0.4819933086	-1.9727095510	-4.1476203942
C18	0.6527273880	-5.3273883469	-5.7875190245	C12	0.5867132795	-3.0241027843	-5.0656477021
C19	-2.1201762007	2.5904817303	2.7125126358	C13	0.5673254547	-0.6408308585	-3.2900256861
C20	-1.2766944643	2.2855674807	0.4367830765	C14	0.4060791422	-3.9735412414	-0.8635714048
C21	-0.9674174289	0.51732088148	2.1136040101	C15	0.4394482857	-0.5405582244	-4.6255348219
C22	-1.6209055352	1.3298421495	3.0468993994	H16	0.6405388984	-2.7881012943	-6.1262797158
C23	-1.9193578190	3.0567969453	1.4094761056	H17	0.6040727591	-5.6753680387	-2.9555857768
C24	-1.0005236684	2.8710448709	-0.9264657412	C18	0.6995785576	-5.4825725359	-5.6679597578
C25	-0.3361230318	-0.7732870477	2.5776292035	C19	-2.0937296784	2.4019580476	2.8125001547
H26	-1.7258948411	0.9677132377	4.0674200748	C20	-1.2920426306	2.2396971043	0.5032410998
H27	-2.2538498358	4.0571543727	1.1436883034	C21	-0.9011290468	0.3970693907	2.0779141269
C28	-2.8490666180	3.4330617649	3.7329445167	C22	-1.5534622117	1.1391414943	3.0668733902
H29	1.3504959042	-3.5067467537	-0.3966089551	C23	-1.9334159520	2.9404516362	1.5319072729
H30	-0.4031133905	-3.6837519799	-0.4106635859	C24	-1.0549104046	2.9095138231	-0.8290079760
H31	1.0833796356	0.1595406986	-4.2413310755	C25	-0.2211946717	-0.8971309273	2.4563022890
H32	-0.6747191949	0.0318843933	-4.1554678205	H26	-1.6253954693	0.7198783290	4.0680907111
H33	0.9413694128	-4.9249851236	-6.7628475220	H27	-2.2968455254	3.9451047272	1.3271872000
H34	-0.3192652886	-5.8224448142	-5.9064530338	C28	-2.8184651005	3.1655734249	3.8959062778
H35	1.3764440470	-6.1012207294	-5.5106421316	H29	1.2197939795	-3.4974223285	-0.3029929135
H36	0.6845511477	-0.5857357064	2.9387636290	H30	-0.5336434876	-3.6455377750	-0.4063107255
H37	-0.3016203124	-1.5248662145	1.7903970233	H31	1.3085082597	0.0308798203	-4.2762122103
H38	-1.2777727824	3.9285677257	-0.9476288337	H32	-0.4555388081	-0.0224622650	-4.263287720
H39	-1.5609341643	2.3520338298	-1.7100337060	H33	1.0160137716	-5.1205400540	-6.6503541533
H40	-2.6941181884	4.5017268340	3.5542021055	H34	-0.2798771882	-5.9619055680	-5.7897767823
H41	-2.5184300477	3.2052783921	4.7509847102	H35	1.4009176398	-6.2614440033	-5.3503330156
H42	-3.9300470103	3.2503050206	3.6926112974	H36	0.8214135652	-0.7068351433	2.7473002112
C43	-0.6748390105	-0.6953362634	-1.0757059168	H37	-0.2329773000	-1.6241487852	1.6457510646
Ru44	-2.6802630865	-1.0210974928	-1.1656016643	H38	-1.4749531786	3.9191815415	-0.8263317324
Cl45	-2.5907718966	-2.5162486388	0.7730918413	H39	-1.5048580791	2.3515550585	-1.6552652222
Cl46	-2.9954640082	0.7463451500	-2.8779218839	H40	-2.7572567265	4.2461737858	3.7349522064
C47	-2.6681045130	-2.2238168681	-2.5931161260	H41	-2.4054961078	2.9440448031	4.8851749397
H48	-2.4341149888	-1.7340958082	-3.5440904516	H42	-3.8823552815	2.8981980194	3.9215862626
H49	-0.9012938274	-1.2009300776	3.4094829038	C43	-0.6343549942	-0.6989609316	-1.1236576164
H50	0.0635306256	2.8021182907	-1.1829496996	Ru44	-2.6507862314	-0.9802980463	-1.2613395454
H51	0.1763536002	-0.3655130507	-5.6601896902	Cl45	-2.7046624593	-2.3827609373	0.7519229869
H52	0.6329612411	-5.0638465856	-0.8213351842	Cl46	-2.7583813346	0.7390601594	-3.0387069651
H53	2.1003189758	-0.1102153890	-2.2450289032	C47	-2.6329010721	-2.2521715655	-2.6235728298
H54	1.7311876929	-0.1171758711	0.7310908258	H48	-2.2650311677	-1.8527017679	-3.5739546804
C55	-5.3594827440	-1.2389900780	-1.2493065990	H49	-0.7189751706	-1.3567666558	3.3133625917
C56	-4.9895168421	-0.2425209354	-0.3970110867	H50	0.0183750938	3.0029037469	-1.0382430298
C57	-3.0214716197	-3.6225866345	-2.8018405286	H51	0.4418706685	-0.5018500631	-5.7181805185
C58	-3.7071994971	-6.2829140201	-3.4328093212	H52	0.4970281186	-5.0534749561	-0.7203616431
C59	-3.2717689387	-4.5656350586	-1.7802914478	H53	2.2647916907	-0.3003511404	-2.2255309719
C60	-3.1245670994	-4.0545495966	-4.1468517768	H54	1.8002292812	0.1430618610	0.6490868916
C61	-3.4719106143	-5.3645691020	-4.4591611610	C55	-5.2645264387	-1.2781296936	-1.4331767535
C62	-3.6012071460	-5.8794795502	-2.0986017649	H56	-5.2031735228	-2.3146837586	-1.1096135877
H63	-3.1921111012	-4.2471436953	-0.7471698965	C57	-4.9911231546	-0.3287853097	-0.4942432979
H64	-2.9262766367	-3.3429268569	-4.9435155644	C58	-3.1165255677	-3.6193000752	-2.7776796761
H65	-3.5572640395	-5.6714613208	-5.4981418515	C59	-0.4090044784	-6.2274901682	-3.2980436031
H66	-3.7841702662	-6.5941805781	-1.3006917447	C60	-3.5709951035	-4.4473751749	-1.7268420186
H67	-3.9742970938	-7.3092669470	-3.6718055520	C61	-3.1392829677	-4.1406846814	-4.0942280515
H68	-5.3575924177	-0.9982578160	-2.3104028378	C62	-3.6069220932	-5.4250058737	-4.3525111181
C70	-5.9484575585	-2.5627866570	-0.8555384397	C63	-4.0240042923	-5.7359068991	-1.9897081163
H71	-5.6662323309	-3.3491132801	-1.5602772940	H64	-3.5416275989	-4.0668509111	-0.7117550483
H72	-5.6384736814	-2.8732589942	0.1441687495	H65	-2.7824255146	-3.5192673518	-4.9109903754
H73	-7.0453661543	-2.4950289428	-0.8700431367	H66	-3.6265546573	-5.8015333736	-5.3716212937
H74	-4.7454280752	0.7163185703	-0.8525596622	H67	-4.3634767751	-6.3621532462	-1.1691154891
				H68	-4.4123422150	-7.2328881886	-3.4948513301

C69	-5.8421659368	-1.0341033894	-2.8010134029	H65	0.4284482293	-4.3376912769	-3.1955083004
H70	-5.4909732889	-0.0947653154	-3.2320985038	H66	-3.5887463146	-3.9263876037	-4.6668653972
H71	-5.5792356050	-1.8443140449	-3.4869770203	H67	-3.7151740130	-6.3660444782	-5.0397521333
H72	-6.9388532223	-1.0008821328	-2.7392485438	H68	0.3086456852	-6.7812067198	-3.5744968328
H73	-4.7452655925	-0.6882583168	0.5035464629	H69	-1.7593203106	-7.8082634841	-4.4949508315
C74	-5.2137078394	1.1539640131	-0.6264528769	C70	0.3125380353	-2.4680856402	-5.8590871254
H75	-4.4201805607	1.7181745856	-0.1256019400	H71	1.1179293536	-2.8386738540	-5.2216092135
H76	-5.2616021729	1.4837928532	-1.6644594714	H72	-0.2722679402	-3.3207884131	-6.2102551568
H77	-6.1574426116	1.4189211123	-0.1281025961	H73	0.7657748706	-1.9848756197	-6.7339515187
		1TS _{BCZ}		X74	-0.1934080507#	-0.9703037174#	-4.8552155731#
N1	-0.0812863464	0.1128116628	-0.0411735570	H75	1.8287554129	0.8050392477	-3.9888898189
C2	-0.2789250313	0.0117710297	1.4225523764	H76	2.1579584534	-0.8027084508	-4.6432198679
H3	0.6790811449	-0.1796403510	1.9173462403	H77	1.6795687703	0.5294431869	-5.7271782966
C4	-1.2548152201	-1.1663287574	1.5481317241	H78	-0.5972475091	0.6318797680	-4.6571953793
N5	-1.3399118824	-1.6679697063	0.1570891882				
H6	-2.2471113409	-0.8595365489	1.8956820014	N1	-0.0185350710	0.0836167713	0.0040370770
C7	0.7346429491	1.1752344563	-0.5695896770	C2	-0.0618664420	-0.0970920245	1.4727743915
C8	-2.0992850965	-2.8626740118	-0.1008399775	H3	0.9257962607	-0.3976635975	1.8406431266
C9	-3.5902075970	-5.2155378643	-0.4057701199	C4	-1.1107834083	-1.2030847802	1.6365094330
C10	-3.4906569815	-2.7728462201	-0.2930111603	N5	-1.2837102280	-1.6886803501	0.2478010892
C11	-1.4491633973	-4.1089753894	-0.0038751610	H6	-2.0665120394	-2.8265870874	2.0200682993
C12	-2.2139026213	-5.2664427202	-0.1679618825	C7	0.7284144099	1.1804657564	-0.5590912174
C13	-4.2082038192	-3.9635370631	-0.4536572879	C8	-2.1504975626	-2.8136976115	0.0121956081
C14	-4.2131006658	-1.4470725220	-0.3090851256	C9	-3.8577110339	-5.0142476107	-0.2895788725
C15	0.0292834159	-4.2118270726	0.2854633948	C10	-3.5259256829	-2.5937132332	-0.1995168470
H16	-1.7187696794	-6.2328763464	-0.1041517048	C11	-1.6222666385	-4.1131363908	0.1257787750
H17	-5.2832164616	-3.9059556744	-0.6102126106	C12	-2.4960074595	-5.1941736145	-0.0359768775
C18	-4.3816605806	-6.4843887947	-0.6181518082	C13	-4.3532568914	-3.7088703617	-0.3557103361
C19	2.3224473535	3.2976679215	-1.4909148552	C14	-4.1135677350	-1.2037361197	-0.2504509264
C20	2.1369241787	1.0296032731	-0.5907030458	C15	-0.1610760759	-4.3574142085	0.4177855422
C21	0.1224595547	2.3995365827	-0.9109391361	H16	-2.0969194626	-6.2031329702	0.0426110565
C22	0.9358043873	3.4345762552	-1.3822780661	H17	-5.4148611884	-3.5499903183	-0.5321988664
C23	2.9024562280	2.0968202364	-1.0735025253	C18	-4.7746513933	-6.1955906619	-0.5030309813
C24	2.8275040662	-0.2011050091	-0.0526039868	C19	2.1659571741	3.3608766934	-1.5831652739
C25	-1.3601876261	2.6264442135	-0.7404758719	C20	2.1080242713	1.0391167825	-0.8077623997
H26	0.4702631526	4.3786441212	-1.6563922170	C21	0.0789282329	2.4220108577	-0.7240231901
H27	3.9842291751	1.9872865196	-1.1073791751	C22	0.8145013585	3.4872934272	-1.2497155214
C28	3.1716812327	4.4211559701	-2.0379139045	C23	2.7962441838	2.1388932527	-1.3347293265
H29	-4.1048248461	-0.9142081150	0.6440549026	C24	2.8592561170	-0.2275808810	-0.4762044277
H30	-3.8328395497	-0.7915515165	-1.0987569618	C25	-1.3601815142	2.6288771809	-0.3186907428
H31	0.2934653146	-3.7214654960	1.2307252627	H26	0.3167968002	4.4437660139	-1.3930514347
H32	0.6284099091	-3.7417986489	-0.5010398397	H27	3.8594669123	2.0361445546	-1.5405993949
H33	-4.0356526383	-7.2881063544	0.0402616712	C28	2.9220293231	4.5186528017	-2.1920619917
H34	-4.2719196897	-6.8400776576	-1.6500559015	H29	-3.9044385342	-0.6392576440	0.6665199125
H35	-5.4485985932	-6.3287601360	-0.4331205047	H30	-3.7124131887	-0.6223097599	-1.0866943371
H36	-1.6865981813	2.4034186324	0.2827216241	H31	0.1467202618	-3.9052522985	1.3689451054
H37	-1.9437056892	1.9942959194	-1.4164381073	H32	0.4742536898	-3.9360239660	-0.3677942819
H38	3.8790341027	-0.2096329889	-0.3517932695	H33	-4.3326471664	-7.1217208877	-0.1244264215
H39	2.3699394115	-1.1212562470	-0.4202338255	H34	-4.9809726231	-6.3374898333	-1.5711754666
H40	4.1835113963	4.3986305363	-1.6215936874	H35	-5.7392588226	-6.0505289835	-0.0050340486
H41	2.7328714589	5.3991470545	-1.8169277952	H36	-1.5215751148	2.3833850284	0.7380748611
H42	3.2663010194	4.3463816752	-3.1283703263	H37	-2.0303681198	2.0061631784	-0.9171494811
C43	-0.6778433862	-0.8895840353	-0.7206647860	H38	3.8960572418	-0.1545472991	-0.8159235141
Ru44	-0.5826617958	-1.1820279662	-2.7959520764	H39	2.4111813071	-1.1078851140	-0.9445213399
Cl45	-2.5868408469	0.2596325595	-3.0543099765	H40	3.9952092749	4.4481237202	-1.9913782972
Cl46	1.5565827179	-2.3635180211	-2.4999144136	H41	2.5645922977	5.4781261078	-1.8050950292
C47	-1.6167221098	-2.4881492886	-3.7391316280	H42	2.7935192269	4.5412320458	-3.2815224415
H48	-2.6148809984	-2.1086042903	-3.9683179280	C43	-0.6848152083	-0.8885987210	-0.6574081275
H49	-1.6095253762	3.6712853115	-0.9448147169	Ru44	-0.6878200537	-1.1365980308	-2.7371536849
H50	2.8047104629	-0.2136213529	1.0454628178	Cl45	-2.4225311300	0.6047899531	-2.9685658648
H51	0.3293563741	-5.2601266143	0.3659783708	Cl46	1.2368181892	-2.6776953177	-2.4811485479
H52	-5.2831529023	-1.5992249733	-0.4752985245	C47	-1.5596955490	-2.5974951754	-3.5924725965
H53	-0.8905330363	-1.9556776479	2.2121281582	H48	-0.9018737730	-3.4701650501	-3.6069444156
H54	-0.6851643227	0.9485802909	1.8150171423	H49	-1.6485337953	3.6739309165	-0.4604614091
C55	-0.5565603172	-1.4592312307	-5.1357971306	H50	2.8851976537	-0.3977880325	0.6077605426
H56	-1.5150463802	-1.2511993869	-5.6093129203	H51	0.0394458916	-5.4301750972	0.4864192324
C57	0.0451972535	-0.2441755573	-4.5897891745	H52	-5.2000969505	-1.2550390766	-0.3616889632
C58	1.5167602988	0.0718257442	-4.7392638459	H53	-0.7789700653	-2.0167380193	2.2865524475
C59	-1.5634582038	-3.9493674723	-3.9147588129	H54	-0.3413960998	0.8380700502	1.9651606051
C60	-1.7083024791	-6.7345110706	-4.3337499174	C55	-0.7035640872	-1.4432179673	-5.0842479683
C61	-0.4698955727	-4.7819015609	-3.6063257825	H56	-1.6808505315	-1.1404144546	-5.4518401652
C62	-2.7325025097	-4.5526013824	-4.4294015231	C57	0.0807198590	-0.3380461738	-4.5742706043
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C61	-3.9986208324	-2.0749913278	-4.1939428502	H56	0.8711948031	-2.8285631649	-5.1113936586
C62	-3.1613259320	-4.3456125194	-4.1889455486	C57	0.5774669438	-0.9788549090	-4.1484783608
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H66	-2.3465953490	-5.0475646804	-4.0311430874	C63	-1.5156309662	-5.6549271648	-3.7727885421
H67	-4.5637022779	-5.8810446292	-4.7408147398	C64	-2.5658824953	-6.5517683629	-3.9549257941
H68	-6.0543032921	-1.8447332008	-4.7656567569	C65	-4.0774153222	-4.6963044102	-4.2449668588
C69	-6.4308146199	-4.2768800295	-5.1156353321	H66	-3.2250961293	-2.7334701113	-4.0586681523
H70	-0.0312292416	-2.5561341250	-5.8686532171	H67	-0.5140732157	-6.0346347995	-3.5868800826
H71	0.7852068965	-3.0100167038	-5.3028509797	H68	-2.3758533134	-7.6211418760	-3.9124304993
H72	-0.7464867571	-3.3362613543	-6.1430030141	H69	-5.0802110071	-4.3150655095	-4.4192895963
H73	0.3837407230	-2.1398509666	-6.7954227405	H70	-4.6784611942	-6.7682613129	-4.3399932576
X74	-0.1934080508#	-0.9703037174#	-4.8552155731#	C71	-1.0306766710	-2.1036192261	-5.8917919373
H75	1.9927025353	0.4694773679	-4.0085403720	H72	-0.5512871730	-1.5319722523	-6.6923798351
H76	2.0883360121	-1.1942047213	-4.6001361107	H73	-1.3604809379	-3.0593641865	-6.3076749265
H77	1.8057104538	0.1516067424	-5.7356263868	H74	-1.9105976514	-1.5518270408	-5.5586392430
H78	-0.4334154733	0.6209741070	-4.6188545157	H75	1.6588513829	-1.0788866404	-4.0505130288
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		1C _z		H76	0.5762092728	1.1553211517	-4.1378337083
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N5	-0.7410338883	-2.0373603430	0.4772554134	N1	-0.0627848533	0.0010908290	-0.0377052230
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C10	-2.7224288359	-3.4667577793	0.1826520531	H6	-1.9326983561	-1.1393064913	2.0259829895
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H17	-4.3451544804	-4.8508488636	-0.0239297776	C13	-3.1729349363	-2.778967559	0.0928767482
C18	-3.1224428763	-7.2700612690	0.2376408567	C14	-3.6547210374	-2.4235334613	-0.1791991173
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C20	1.7574553362	1.3928835642	-1.0575242426	H16	-0.3449328289	-6.5410366631	0.9313974813
C21	-0.5929988156	2.1070758001	-1.0140758001	H17	-4.2250069458	-5.0535359587	-0.1199488431
C22	-0.2231768413	3.2777334166	-1.6826189418	C18	-2.8832700556	-7.3738671785	0.3569285058
C23	2.0708111362	2.5784552751	-1.7336744746	C19	1.3019670865	3.5164955903	-1.9854509620
C24	2.8604114058	0.4492966043	-0.6439893043	C20	1.7908653190	1.3625645534	-0.9280248855
C25	-2.0257838805	1.9099187938	-0.5826233101	C21	-0.5254386543	2.1717811594	-1.0752357143
H26	-0.9898381860	4.0175268352	-1.9017804541	C22	-0.0549093993	3.3232704956	-1.7119279169
H27	3.1105695663	2.7706965205	-1.9891646289	C23	2.2068442181	2.5363176129	-1.5686234100
C28	1.4571663847	4.7759803110	-2.8341747056	C24	2.8160641162	0.3664183650	-0.4413820057
H29	-3.4575078215	-1.5213945172	0.8093261099	C25	-1.9940923449	2.0351380377	-0.7546318862
H30	-3.4443960233	-1.7565503983	-0.9378788198	H26	-0.7707937951	4.0924194124	-1.9930308314
H31	1.0835319981	-3.8460556034	1.9430890338	H27	3.2712161332	2.6889912500	-1.7334600983
H32	1.4790207926	-3.8080401333	0.2163637692	C28	1.7734856368	4.7533814340	-2.7140158512
H33	-2.5128342562	-8.0243157758	0.7439860460	H29	-3.6276014286	-1.6755113894	0.6221440374
H34	-3.2237002155	-7.5737356119	-0.8116970894	H30	-3.4208604282	-1.9037941585	-1.1137578444
H35	-4.1245623984	-7.2887686156	0.6787608024	H31	1.0572257991	-3.5656019778	1.9681667103
H36	-2.1036112221	1.7001587397	0.4908140621	H32	1.5200768139	-3.6969653832	0.2641425123
H37	-2.4846440415	1.0770759616	-1.1230924989	H33	-2.1987272634	-8.0750834158	0.8428133935
H38	3.8165686751	0.7740608583	-1.0635854972	H34	-3.0378676630	-7.7193647245	-0.6727255528
H39	2.6723478458	-0.5757443444	-0.9748491205	H35	-3.8515864202	-7.4370237958	0.8650576181
H40	2.5103804000	5.0400360101	-2.7001986607	H36	-2.1628413423	1.8708064959	0.3166273239
H41	0.8482614887	5.6280489109	-2.5152641379	H37	-2.4361608353	1.1949947583	-1.2978125647
H42	1.2872191825	4.6422923495	-3.9100679667	H38	3.8217833887	0.6865831819	-0.7271873305
C43	-0.3689275779	-1.2294735119	-0.5347672980	H39	2.6475002971	-0.6330874957	-0.8531462531
Ru44	-0.3136674923	-1.7489658390	-2.5339481593	H40	2.8118680735	4.9942576405	-2.4672594459
Cl45	-2.4545487678	-0.6490900383	-2.9866379286	H41	1.1539583459	5.6223094435	-2.4702540497
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C47	-0.5068299601	-3.4192245813	-3.6504959502	C43	-0.3989453095	-1.1978803863	-0.5576918041
H48	0.3448477495	-4.0566324071	-3.4235850209	Ru44	-0.2350685546	-1.7017491343	-2.5477822768
H49	-2.6116126730	2.8106456415	-0.7848166027	Cl45	-2.3860055434	-0.6249211763	-3.0407221857
H50	2.9754380434	0.4323217056	0.4477199642	Cl46	1.9547786547	-2.7426945292	-2.0486941714
H51	1.3836225106	-5.3539726663	1.0796750137	C47	-0.5408734799	-3.2973799262	-3.7448700350
H52	-4.6673548220	-2.5642099640	0.0567013169	H48	0.2655401951	-3.5980800346	-3.5289105415
H53	-0.1197349900	-1.9768058955	2.5076854898	H49	-2.5309245982	2.9453394491	-1.0352571757
H54	-0.4498504142	0.8368083675	1.8427935673	H50	2.8016862773	0.2816254959	0.6526742439

H51	1.4575620427	-5.1436726847	1.2880233817	C47	-2.9321791041	-2.2848325788	-2.3935209633
H52	-4.6800633134	-2.7971072999	-0.2443015437	H48	-3.0050863158	-0.2697901510	3.9767263605
H53	-0.4042265778	-1.8952235901	2.5150992251	H49	-0.5663356936	3.1429985640	-0.5573930972
H54	-0.6920525205	0.8991074689	1.7821792902	H50	1.1852768988	0.6287635193	-4.2387534643
C55	-0.0412085871	-2.2045741469	-4.7982018023	H51	0.3700766955	-4.6061539557	-0.0518447913
H56	-0.9212197358	-1.9579634966	-5.3922928716	H52	1.8444376296	0.4083186590	-0.4242715056
C57	0.4339361545	-0.7947018157	-4.2015501697	H53	0.3767460575	0.5902795196	2.1544798452
C60	-1.8125536103	-4.0219194672	-3.9808597264	C54	-5.0091225792	-1.7109011087	-2.1834411826
C61	-4.0996159526	-5.6110918250	-4.4316021497	H55	-5.1218846608	-2.7523557586	-1.8877209819
C62	-2.9426159358	-3.4914685063	-4.6303599995	C56	-5.1890471199	-0.8283520688	-1.0632377493
C63	-1.8608899809	-5.3658840022	-3.5617892565	C57	-5.4730796416	-1.3892892843	-3.5875138597
C64	-2.9902137467	-6.1513768311	-3.7806766914	H58	-4.8815425961	-0.5960738937	-4.0480903443
C65	-4.0677221798	-4.2797328662	-4.8543499705	H59	-5.4221923326	-2.2748560580	-4.2259224058
H66	-2.9520276174	-2.4513039570	-4.9316481478	H60	-6.5176312485	-1.0554006611	-3.5560259025
H67	-0.9968968030	-5.7921776666	-3.0581026925	H61	-5.2933426977	-1.3596455747	-0.1215341142
H68	-2.9987770451	-7.1876753561	-3.4528109791	C62	-7.4473147843	2.8178693679	-0.7417784803
H69	-4.9287155190	-3.8495909595	-5.3589143110	C63	-7.3033299274	1.9397549978	0.3331410259
H70	-4.9813720343	-6.2209292235	-4.6100498509	C64	-6.5328178658	0.7887715373	0.1918536058
C71	1.0581003514	-2.8658944638	-5.6460646680	C65	-5.8947223891	0.4754961917	-1.0257690881
H72	1.3984800953	-2.1890794659	-6.4353274592	C66	-6.0368906408	1.3818077566	-2.0941413454
H73	1.9143146169	-3.1466105416	-5.0291987022	C67	-6.8060595594	2.5340137193	-1.9490644642
H74	0.6603864893	-3.7691283835	-6.1185221334	H68	-8.0490618055	3.7172009826	-0.6389728526
H75	-0.2822397573	-0.0250630323	-4.4931055870	H69	-7.7947466558	2.1463230663	1.2803976896
C75	1.8637031885	-0.3426825831	-4.3888401869	H70	-6.4268364462	0.1074373711	1.0319695152
H76	2.0264343442	0.5626215764	-3.7955703745	H71	-5.5114803654	1.2101560817	-3.0224568085
H77	2.5974076296	-1.0880679660	-4.0859458979	H72	-6.8994677349	3.2197260419	-2.8772291376
H78	2.0352473233	-0.0693424073	-5.4408565378	X73	-5.1693448804#	-0.8562935559#	-1.0759161330#
1TS _{CDZ}				C74	-2.5628471861	-2.3603438281	-3.8403557703
N1	-1.0783834990	0.6943610616	0.6141848781	H75	-3.1541801048	-3.1310481474	-4.3536523495
C2	0.3109587416	0.8576312089	1.0955316282	H76	-2.6372385838	-1.4081793216	-4.3621729105
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C21	-2.7135953446	1.1582047196	2.3962145156	H16	1.5488211404	-1.2992797345	-5.1449735031
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H27	-3.5607063694	4.5585826221	0.7056902804	C22	-3.3331134396	1.4769632406	3.3301812775
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H41	-5.2312348590	3.9139683157	3.9954491816	H36	-0.7105545270	-0.4507635373	3.1306864707
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H60	-5.0168798489	-2.8958273391	-4.1202878251	H55	-5.0565210764	-2.2855377494	-1.5615950356
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H76	-5.8015079229	1.0706607856	0.1992018190	H71	-5.1743943533	1.6584448708	-2.6201021177
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		1D _z		H75	-1.9634837115	-3.0660918426	-4.6285725715
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C43	-0.6718730345	-0.7775004124	-0.9312370106	C39	3.4729767377	-2.1149071212	3.3458303180
Ru44	-2.7191124848	-1.0567715442	-1.1022534445	H40	2.9746695147	-1.5245546528	1.3354586983
Cl45	-2.4830463047	-2.9521599760	0.4780148132	H41	0.0899645526	-0.5373920829	4.3786503673
Cl46	-3.0069521666	0.9545317525	-2.5209921634	H42	1.5298647185	-1.5928046321	6.0956237251
C47	-2.6901357087	-2.2434777512	-2.5096858189	H43	4.4176772874	-2.5661042489	3.0559865954
H48	-1.1184244323	-0.9507607381	3.7606075708	H44	3.7048681891	-2.6019388844	5.4337316801
H49	0.5735808133	2.3864360154	-1.1805258095	C45	2.5029884799	2.2203205094	-3.0033729152
H50	0.2750375308	0.2060934739	-5.2515662966	H46	3.0448267152	1.2879251749	-2.8226016811
H51	0.4601605947	-5.3591894957	-1.4193119661	H47	2.5532337041	2.7812769887	-2.0709801807
H52	2.1937008091	-0.4358165184	-1.9451741171	H48	3.0307655003	2.7773250893	-3.7851742931
H53	1.6673286169	-0.6078985125	1.0116324443	C49	-2.5757846406	2.4587170134	-2.3586561974
C54	-5.2189933619	-1.8159294805	-0.8664738713	H50	-3.4165432617	1.7923030984	-2.5752715567
H55	-5.0557728093	-2.5523851058	-0.0853513351	H51	-2.8948958746	3.4722023086	-2.6353828402
C56	-5.0869221693	-0.4853112056	-0.5793378995	H52	-2.4074114186	2.4532474217	-1.2805831559
H57	-5.3123070426	0.2243168116	-1.3714351455	C53	-0.6113842670	0.8549467921	-6.7014725761
C58	-5.8793771355	-2.3204485010	-2.1188813335	H54	-0.6238721942	-0.2413056952	-6.3727795511
H59	-5.8358574412	-1.5896136113	-2.9304465679	H55	0.1957798119	1.1915221729	-7.3592703828
H60	-5.4532346956	-3.2671988553	-2.4619521702	H56	-1.5605627307	1.2059325324	-7.1180652399
H61	-6.9392290993	-2.5134109404	-1.8995254235	C57	2.5833377582	3.1209946506	2.5144753122
C62	-4.9821279951	1.4173798230	3.2594666511	H58	3.3636281783	3.0706015901	3.2785829993
C63	-4.8810677331	0.0252887909	3.1871269780	H59	2.6173011851	4.1289845090	2.0809532256
C64	-4.8611675979	-0.6179778997	1.9534982388	H60	2.8278487890	2.4115679047	1.7183443643
C65	-4.9430561159	0.1256964776	0.7605576719	C61	-2.4374359533	2.3586226022	2.0761573512
C66	-5.0097623243	1.5284818116	0.8473383630	H62	-2.6869752139	3.3150150167	1.5995340384
C67	-5.0371482408	2.1676944747	2.0846077897	H63	-3.2919630522	2.0706734149	2.6942309874
H68	-5.0141666403	1.9124869314	4.2266801896	H64	-2.3357890239	1.6218988840	1.2742669639
H69	-4.8257637059	-0.5638474555	4.0985525492	C65	-0.2397320964	2.3583591350	6.6228866529
H70	-4.7772568373	-1.6985792184	1.9143232565	H66	0.3217328663	3.1474788151	7.1342072516
H71	-5.0499142464	2.1104897569	-0.0692161720	H67	0.1753178562	1.4003151150	6.9595125041
H72	-5.1050106213	3.2513921976	2.1293924910	H68	-1.2783797036	2.4069533745	6.9621311002
H73	-2.4006487880	-3.2724203377	-2.2569303611	H69	-1.7997635076	0.3401623552	-1.2287879408
C74	-3.1038436251	-2.0694504853	-3.9332312802	C70	-1.5483917100	-2.5951250446	0.6394653006
H75	-2.2645815398	-2.3621120705	-4.5787647633	H71	-0.8761866773	-3.1925512286	0.0241964268
H76	-3.9140495201	-2.7772365175	-4.1603093551	H72	-1.2317592490	-2.6980969246	1.6816417584
H77	-3.4157608432	-1.0547684761	-4.1751039542	H73	-2.5655163131	-3.0060305266	0.5624662137
		1E _z		X74	-1.4261060320#	-0.95904454361#	-0.4890445447#
Ru1	0.6720005545	-0.1043162819	-0.0606670886	C75	-1.2805116781	-1.4955974659	-2.3130588335
Cl2	2.9663012387	0.6461832910	-0.0963732076	H76	-0.6614911623	-0.9825692196	-3.0540650757
C3	0.1999429824	1.9442379780	-0.0977073512	H77	-0.8353234746	-2.4691340209	-2.1161513506
N4	0.1624450295	2.8633322994	0.9055674242	H78	-2.2737084176	-1.6389260869	-2.7643655146
N5	0.1163457687	2.6450029925	-1.2684711425				
C6	0.0276146414	4.2590670581	0.4345541370	Ru1	0.7420105722	1E _E	-0.1068550127
H7	-0.9297660567	4.6777133183	0.7676502890	Cl2	2.9894924188	-0.0305261881	0.0886280305
H8	0.8275771870	4.8788540838	0.8492929849	C3	0.2579563752	1.9910538746	-0.1352889991
C9	0.1164887634	4.1106277500	-1.0854599290	N4	0.2918218758	2.9089662159	0.8717358479
H10	1.0362082935	4.5383071475	-1.5007918518	N5	0.2779589240	2.6958986958	-1.3112050865
H11	-0.7323043542	4.5608355533	-1.6096599224	C6	0.2812105347	4.3053102084	0.3856616410
C12	0.5113696086	-0.3291473438	1.7928171582	H7	-0.7000681365	4.7620049824	0.5725709082
H13	-0.4182124161	-0.0319551251	2.2870924980	H8	1.0383372757	4.8985630816	0.9030600537
Cl14	1.5254147047	-2.2962174842	-0.7351453119	C9	0.5786908262	4.1282938343	-1.1003940136
C15	-1.4408883034	-0.6673343767	-1.0628142356	H10	1.6322126396	4.3197368085	-1.3393008770
C16	-1.5691338856	-1.1499701170	0.2189315389	H11	-0.0403048257	4.7570724687	-1.7433814957
H17	-1.9926621348	-0.4653622165	0.9495605808	C12	0.4720061228	-0.2881469819	1.7181450266
C18	0.0809437812	2.6672094300	2.3263174864	H13	-0.4996472013	-0.0117327864	2.1399640716
C19	-0.1384218689	2.4931463318	5.1214300025	Cl14	1.7560713761	-2.0991261020	-0.9899320004
C20	1.2327994981	2.8319908259	3.1212300622	C15	-1.2428048262	-1.7039339401	0.0178953253
C21	-1.1828101075	2.4618668651	2.9132941459	C16	-1.3704638285	-0.9795078349	-1.1363185231
C22	-1.2667861186	2.3669396716	4.3063520838	H17	-0.7295972493	-1.2705605197	-1.9663832754
C23	1.0950409266	2.7322550845	4.5091043608	C18	0.0944510291	2.7117548144	2.2821972309
H24	-2.2393301797	2.1976951373	4.7638408285	C19	-0.3542324416	2.5026821234	5.0545758654
H25	1.9829517360	2.8431620625	5.1275162066	C20	1.1705565827	2.8888618611	3.1749061146
C26	-0.0378044883	2.1561395388	-2.6154724647	C21	-1.2102363962	2.4849075363	2.7658429370
C27	-0.4125072779	1.3452212412	-5.2866307004	C22	-1.4084450484	2.3733059409	4.1456339104
C28	-1.3457714251	2.0557237014	-3.1446769501	C23	0.9196498746	2.7690537936	4.5462306987

H24	-2.4144619025	2.1899226968	4.5173485552	C20	0.0521222497	2.7149525853	5.0586131823
H25	1.7526266853	2.8882525328	5.2356819438	C21	1.3624297946	3.0673869167	3.0180556640
C26	-0.0273083389	2.2659416945	-2.6558560685	C22	-1.0385606018	2.5936913573	2.8771359769
C27	-0.7023998834	1.6326526324	-5.3211743905	C23	-0.0908799446	2.5364791788	4.2717512865
C28	-1.3277528788	2.5438504121	-3.1436950110	C24	1.2587736012	2.9873405901	4.4127884000
C29	0.9569385510	1.7426817059	-3.5166753020	H25	-2.0476481193	2.3493467477	4.7550710729
C30	0.5839745926	1.4196906032	-4.8302855252	H26	2.1544434704	3.1503475518	5.0079866774
C31	-1.6420097225	2.2134060319	-4.4626365955	C27	-0.0580396302	2.1665238975	-2.6652389754
H32	1.3431185221	1.0069157864	-5.4911189444	C28	-0.4897012628	1.2131873235	-5.2882511185
H33	-2.6449631747	2.4204523414	-4.8304639096	C29	-1.3576689375	1.7674517853	-3.0729360380
C34	1.3383069812	-0.9082674370	2.7041215970	C30	1.0046239833	2.1561996558	-3.5899336341
C35	2.8771715523	-2.1174538342	4.7231309237	C31	0.7639589593	1.6705153948	-4.8820466032
C36	2.5830717495	-1.5058096919	2.3979617679	C32	-1.5427433048	1.2893101284	-4.3716585644
C37	0.8819197491	-0.9484167201	4.0444966564	H33	1.5877924008	1.6649763569	-5.5925885147
C38	1.6444714541	-1.5403581586	5.0434127009	H34	-2.5396698676	0.9781031498	-4.6779676418
C39	3.3371527070	-2.1015500327	3.4037592542	C35	0.9220601466	-1.1234581870	2.7644738787
H40	2.9297252889	-1.5087353713	1.3725179279	C36	1.7654165346	-2.5630156609	5.0353527775
H41	-0.0757791252	-0.4952606616	4.2869800864	C37	2.1085199990	-1.8803890437	2.7338933103
H42	1.2816504527	-1.5598804910	6.0675673386	C38	0.1797171542	-1.0939415515	3.9652434455
H43	4.2895637321	-2.5613797837	3.1556355797	C39	0.5895355710	-1.8113259687	5.0853941195
H44	3.4745039265	-2.5866739051	5.5008186137	C40	2.5199841956	-2.5885996014	3.8613123720
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H46	2.5843749344	0.5238481404	-2.7702503769	H42	-0.7277124566	-0.4972499319	4.0126662742
H47	2.6973667527	2.2019870992	-2.3002104487	H43	-0.0037083232	-1.7814971887	5.9956428583
H48	3.0476130042	1.7287690672	-3.9779090681	H44	3.4413545957	-3.1630362915	3.8203077990
C49	-2.3746104730	3.2259414663	-2.2907232597	H45	2.0944304805	-3.1198973892	5.9089718891
H50	-3.3774034360	3.0330843836	-2.6822154079	C46	2.3747464607	2.7026469280	-3.2725061150
H51	-2.2385092524	4.3152714575	-2.2868928178	H47	3.0855739406	1.8949740122	-3.0774431677
H52	-2.3446214508	2.8896663370	-1.2527465084	H48	2.3767340083	3.3297451362	-2.3809901937
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H54	-1.5018257219	0.2411598763	-6.7687948800	C50	-2.5719352309	1.9160819010	-2.1797921320
H55	-0.2026965393	1.2579221230	-7.3944853001	H51	3.2736846460	1.0905401162	-2.3349880106
H56	-1.8232886041	1.9336417858	-7.1505529591	H52	-3.1139797101	2.8414890860	-2.4147690331
C57	2.5609009371	3.2282184942	2.6974522515	H53	-2.3165598429	1.9468970152	-1.1191453162
H58	3.2947123060	3.0213848761	3.4811438478	C54	-0.7059232611	0.6539383023	-6.6748103370
H59	2.6428499125	4.2964463258	2.4548750779	H55	-0.5251103344	-0.4278187321	-6.6923557599
H60	2.8320897328	2.6537452448	1.8087301667	H56	-0.0252947181	1.1082631098	-7.4011580362
C61	-2.3882178687	2.3706595120	1.8275961813	H57	-1.7319500194	0.8178552578	-7.0187967146
H62	-2.5514734822	3.2992125819	1.2671824958	C58	2.6782906585	3.4491245293	2.3871262041
H63	-3.3058119808	2.1555847900	2.3816966521	H59	3.5011825932	3.2846714057	3.0879192483
H64	-2.2380774125	1.5765726781	1.0906986312	H60	2.6869976225	4.5158371880	2.1246712150
C65	-0.5787810388	2.3539194397	6.5409058906	H61	2.8818146164	2.8773121630	1.4798717343
H66	-0.0679198982	3.1427045121	7.1032328190	C62	-2.3045420024	2.4306074688	2.0708881245
H67	-0.1867150850	1.3959353950	6.9041375261	H63	-2.5217964009	3.2700293288	1.4351790032
H68	-1.6425457215	2.3932043468	6.7923482237	H64	-3.1632327958	2.2553684731	2.7312722538
H69	-0.4854400114	-2.4806616172	0.0362050446	H65	-2.2433079391	1.5343078557	1.4061303105
C70	-2.5927076538	-0.1696837289	-1.4827890106	C66	-0.0148121767	2.5911411454	6.5623449378
H71	-2.9790658721	0.4118545630	-0.6415324638	H67	0.7020704306	3.2564230639	7.0532411218
H72	-2.3997440038	0.5044328749	-2.3149443493	H68	0.2238050818	1.5674705649	6.8765450995
H73	-3.3968960172	-0.8516742648	-1.7954961631	H69	-1.04141432004	2.8260837736	6.9415440062
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C75	-2.2441162843	-1.7211455420	1.1411518395	C74	-0.3151296357	-1.7275812827	-2.1718584161
H76	-1.7794534910	-1.9953682194	2.0922668427	H75	0.4241116085	-2.4983560094	-1.9641404033
H77	-2.7696024011	-0.7710200861	1.2706827879	H76	-1.2833691510	-2.2024656062	-2.3951456348
H78	-3.0040260299	-2.4852533598	0.9241790057	H77	-0.0059532688	-1.0883632560	-3.0722575465
				C78	-0.5821561494	-2.7241780378	0.6551970016
				H79	-0.7918798842	-2.9388805875	1.7056650042
				H80	-1.3341385727	-3.2373910683	0.0440876791
				H81	0.4007943316	-3.1247214620	0.4027432741

C15	-0.5136729656	-1.2822661604	-1.1126935045	H11	-1.4794878801	3.9493772883	-1.2190404710
H16	0.1028741887	-1.9875820791	-1.6664271952	C12	0.2811490941	-0.6247034377	1.8244694045
C17	-0.6652423875	-1.6781201982	0.3116245964	Cl13	2.7589335849	-2.0334210992	-0.1889128902
C18	-0.0012290457	2.6624873234	2.1605849812	C14	-0.2656334529	-1.0159869682	-0.8359549002
C19	-0.3445423044	2.5802359279	4.9546531563	C15	-0.4760213540	-1.5246644839	0.6352040582
C20	1.0943721411	2.9327084402	3.0030056154	C16	0.0732948665	2.5796823571	2.4921410431
C21	-1.2822227873	2.4237488723	2.7038984401	C17	-0.1082256008	2.5311927222	5.2992877087
C22	-1.4272944708	2.3780470388	4.0931258343	C18	1.2095104499	2.8842997504	3.2633390500
C23	0.8979302107	2.8654672904	4.3879051764	C19	-1.1675306241	2.3089575224	3.1098770885
H24	-2.4138865599	2.1889271531	4.5116646692	C20	-1.2331790054	2.2858639434	4.5050157678
H25	1.7487624599	3.0527565353	5.0394598584	C21	1.0936044212	2.8326369008	4.6585459511
C26	-0.3327117958	2.0740143597	-2.7542504234	H22	-2.1877281164	2.0745186315	4.9826721412
C27	-1.1492253402	1.3434558930	-5.3531312114	H23	1.9748453181	3.0492934078	5.2582337237
C28	-1.6860417152	2.2269345473	-3.1407915352	C24	-0.1472493191	1.87472488471	-2.4322469272
C29	0.6242615339	1.6204857864	-3.6808187553	C25	-0.5200810128	0.9172872209	-5.0582504196
C30	0.1842568553	1.2436423857	-4.9588415822	C26	-1.4170607546	1.4025028110	-2.8374372418
C31	-2.0676151245	1.8566430351	-4.4307854704	C27	0.9090554741	1.9585560963	-3.3595034231
H32	0.9233772473	0.8820864344	-5.6703149471	C28	0.6993099072	1.4592972678	-4.6525821182
H33	-3.1108307005	1.9646939984	-4.7204323435	C29	-1.5725566063	0.9166986629	-4.1370668325
C34	0.6509428110	-1.2532009065	2.7290744105	H30	1.5211004182	1.5117724107	-5.3636702465
C35	1.5043563604	-2.5596663579	5.0730243320	H31	-2.5459043516	0.5354447079	-4.4399453345
C36	1.8237050200	-2.0324469917	2.7274108107	C32	0.816504296	-1.3329892301	3.0237813166
C37	-0.0752581232	-1.1366188666	3.9337819182	C33	1.6566926744	-2.5676267809	5.4186538714
C38	0.3430392932	-1.7857584035	5.0925616218	C34	1.9993817973	-2.0929708897	3.0642780162
C39	2.2390766120	-2.6762022630	3.8904878303	C35	0.0739398638	-1.1999852075	4.2153058170
H40	2.3982396971	-2.1236696001	1.8117663983	C36	0.4821570595	-1.8142969345	5.3968305864
H41	-0.9702650530	-0.5210673169	3.9560920354	C37	2.4092504728	-2.6993980190	4.2507122799
H42	-0.2350404511	-1.6872685733	6.0078258081	H38	2.5969690948	-2.1921385742	2.1649149367
H43	3.1480562205	-3.2711826638	3.8731968687	H39	-0.8344527676	-0.6039089709	4.2107327876
H44	1.8378964040	-3.0654001519	5.9755902159	H40	-0.1140684524	-1.7019208738	6.2989593754
C45	2.1001293919	1.5432511429	-3.3829093619	H41	3.3307340141	-3.2753626286	4.2606793285
H46	2.3851796343	0.5600792595	-2.9938244356	H42	1.9856497891	-3.0420794636	6.3397091773
H47	2.4108003839	2.2680800939	-2.6309890049	C43	2.2395687202	2.5973758210	-3.0459752065
H48	2.6736153792	1.7140044374	-4.2991220620	H44	3.0188994083	1.8405788885	-2.9198260475
C49	-2.7330251693	2.7780132168	-2.1984138648	H45	2.2175290638	3.1684442528	-2.1189283135
H50	-3.7376470396	2.5525937502	-2.5673375705	H46	2.5370865874	3.2578378880	-3.8675530376
H51	-2.6648406887	3.8698416416	-2.1013450522	C47	-2.6324527989	1.4534262733	-1.9353754179
H52	-2.6402336766	2.3620747005	-1.1921168714	H48	-3.2768857355	0.5839262574	-2.0986225279
C53	-1.5937142692	0.9035601609	-6.7283655294	H49	-3.2386583563	2.3424293645	-2.1518011081
H54	-1.9038332344	-0.1489610192	-6.7223757717	H50	-2.3706217349	1.4860817318	-0.8765342262
H55	-0.7859467252	0.9993437450	-7.4602189748	C51	-0.7015719302	0.3473661110	-6.4449987563
H56	-2.4467386094	1.4914998855	-7.0818217213	H52	-0.4759674468	-0.7260554075	-6.4589118927
C57	2.4424031750	3.3527085015	2.4706408983	H53	-0.0349176732	0.8288282444	-7.1665888898
H58	3.2308197330	3.1093468868	3.1883778557	H54	-1.7309741618	0.4677559042	-6.7969708290
H59	2.4721951754	4.4409216409	2.3187480152	C55	2.5136996502	3.3206787030	2.6440065198
H60	2.6790659705	2.8669171865	1.5237071291	H56	3.3360477274	3.1929294065	3.3530966218
C61	-2.5008957804	2.2540087526	1.8247534054	H57	2.4774422402	4.3868554177	2.3822928514
H62	-2.7465957037	3.1808286263	1.2922446436	H58	2.7513111234	2.7605608005	1.7386151105
H63	-3.3734055590	1.9814571387	2.4244572623	C59	-2.4203205120	2.0567964214	2.2997995059
H64	-2.3593796156	1.4803484626	1.0645507209	H60	-2.6756690054	2.9096892565	1.6597157841
C65	-0.5103178062	2.4776256736	6.4525585862	H61	-3.2732599844	1.8730748983	2.9586912465
H66	0.1085005880	3.2130054252	6.9765522185	H62	-2.3183066436	1.1875818266	1.6401820559
H67	-0.2072095284	1.4856119340	6.8104733991	C63	-0.1877042513	2.4515439048	6.8053936983
H68	-1.5508254162	2.6324863147	6.7536300487	H64	0.4923286541	3.1642477845	7.2822199437
C69	-1.7056977913	-0.7972483114	-1.8966082279	H65	0.0934593896	1.4504636124	7.1549318068
H70	-2.2375291767	0.0284849376	-1.4199262771	H66	-1.2009633552	2.6528394870	7.1665336369
H71	-1.4074093193	-0.4844139287	-2.8974044149	H67	-0.4411064078	0.1110837374	2.1603926687
H72	-2.4221640493	-1.6252332940	-2.0183081507	H68	-1.0561959128	-0.3256853326	-1.1070531491
H73	-0.0862181303	-2.5719440019	0.5342898162	X69	-0.0307205035#	-1.2535449218#	0.5489314772#
C74	-2.0899170387	-1.7280472078	0.8650452036	H70	-1.4935157836	-1.1881887003	0.8548535489
H75	-2.0930280541	-2.0032412123	1.9228447319	C71	-0.0306433364	-2.0160630313	-1.9456012730
H76	-2.6254554125	-0.7830061806	0.7495554567	H72	0.2128147641	-1.4727510619	-2.8642996149
H77	-2.6478174456	-2.4947118307	0.3142603519	H73	0.7808327540	-2.7071846112	-1.7288076833
				H74	-0.9546612931	-2.5814696609	-2.1422755526
		1F _Z		C75	-0.3334840423	-3.0300268468	0.8392417315
Ru1	1.2461379665	-0.1009519044	0.1642835954	H76	-0.6180623333	-3.2992658128	1.8595069004
Cl2	3.1691897525	1.1987602119	-0.1667145414	H77	-0.9956747578	-3.5589616241	0.1464749433
C3	0.2753374350	1.7971217907	0.0721145692	H78	0.6906459852	-3.3609078483	0.6619423300
N4	0.0947994524	2.7215181054	1.0568479589				
N5	-0.0046890207	2.4269546062	-1.1067593065			1F _E	
C6	-0.1690788620	4.0853523154	0.5418669643	Ru1	1.2725809263	-0.1105475981	0.1433761194
H7	-1.0229788652	4.5318533003	1.0595409496	Cl2	3.1422400883	1.2955443561	-0.0523183339
H8	0.7066008725	4.7201088744	0.7182135079	C3	0.2646102489	1.7822713202	0.0127400700
C9	-0.4237076602	3.8358087541	-0.9435652886	N4	0.1763224648	2.7066394227	1.0137904850
H10	0.1678606654	4.4840966066	-1.5961759877	N5	0.0870597909	2.4664789794	-1.1587226327

C6	-0.0717310493	4.0837206771	0.5292660006	Ru1	1.0909123840	-0.0442823205	-0.1787187955
H7	-1.0819721275	4.4065143209	0.8128042550	Cl2	3.0317791333	1.2567384700	-0.5744196397
H8	0.6443504623	4.7764340871	0.9783229076	C3	0.0876883127	1.8381993210	-0.3434249091
C9	0.1076163856	3.9354816934	-0.9776682078	N4	-0.0429295481	2.7456582540	0.6680709694
H10	1.0698148691	4.3304632481	-1.3247364849	N5	-0.2439182491	2.4957319432	-1.4921237284
H11	-0.6861857460	4.4110592725	-1.5585634998	C6	-0.5128581061	4.0745664442	0.2186156921
C12	0.3101697552	-0.7127728575	1.7667655500	H7	-1.5244376213	4.2617897926	0.6000796030
Cl13	2.9179951677	-1.9504276352	-0.1471908277	H8	0.1444577934	4.8593836512	0.6026412771
C14	0.0523808806	-1.4020592213	-0.8851653143	C9	-0.4673377688	3.9458769695	-1.3031220580
C15	-0.1948525754	-1.7881029169	0.6023570339	H10	0.3608686997	4.5092272814	-1.7474692821
C16	0.0494505918	2.5363110431	2.4406140101	H11	-1.3947750308	4.2584045233	-1.7923965527
C17	-0.3245453442	2.4955744503	5.2323531742	C12	-0.2426329485	-0.7337513747	1.3595383018
C18	1.1227973005	2.8644035605	3.2906572305	H13	-0.9045975115	0.0986220349	1.5632581256
C19	-1.2253679574	2.2453764731	2.9745539933	Cl14	2.6737091651	-1.9309300305	0.1073634637
C20	-1.3856741776	2.2258416646	4.3625636910	C15	0.1504476958	-0.8552536262	-1.6013894417
C21	0.9130785478	2.8145495855	4.6744581961	C16	-0.6808809436	-1.5563153069	0.2580734866
H22	-2.3680569878	2.0016417840	4.7735425491	H17	-1.6176345768	-1.2204400188	-0.1836966810
H23	1.7474545990	3.0494230977	5.3317799164	C18	-0.0054881083	2.5462562333	2.0963827239
C24	-0.2356388096	1.9934454684	-2.4834339404	C19	-0.0050850310	2.3054827044	4.9009471635
C25	-0.9962134471	1.2489376258	-5.0937525613	C20	1.1558580566	2.8809735298	2.8225699438
C26	-1.6053713321	1.9525056235	-2.8371839409	C21	-1.1919279766	2.1849801950	2.7696160751
C27	0.7556412595	1.7382855951	-3.4470287851	C22	-1.1618955795	2.0546551131	4.1611107481
C28	0.3457290101	1.3497256831	-4.7316311342	C23	1.1321881712	2.7350820702	4.2133698989
C29	-1.9594014093	1.5755111702	-4.1324332950	H24	-2.0700044246	1.7503745481	4.6778763779
H30	1.1133871855	1.1410794643	-5.4737503172	H25	2.0328881975	2.9735723700	4.7744545232
H31	-3.0137188846	1.5332971134	-4.3976183706	C26	-0.4459873293	1.9767386978	-2.8184834286
C32	0.8446416544	-1.3346032808	3.0092674060	C27	-0.9518213650	1.0396249894	-5.4207916377
C33	1.6476337569	-2.4874020902	5.4542759593	C28	-1.7213521687	1.4643047431	-3.1432867266
C34	1.9996648196	-2.1352643785	3.0797807452	C29	0.5514729704	2.1024126112	-3.8015974621
C35	0.1094828264	-1.1214858280	4.1926435307	C30	0.2774436362	1.6087719509	-5.0847894989
C36	0.5026019243	-1.6930020207	5.4010933978	C31	-1.9476353165	0.9955410861	-4.4386157633
C37	2.3904535761	-2.7018439352	4.2907754045	H32	1.0540619266	1.6826789257	-5.8430057982
H38	2.5915184639	-2.2934280360	2.1842795830	H33	-2.9245009674	0.5863937272	-4.6872824976
H39	-0.7784194224	-0.4971591275	4.1609513052	C34	0.3141645667	-1.3080911782	2.6379525031
H40	-0.0869111713	-1.5191245058	6.2978016364	C35	1.1244788649	-2.2680706392	5.1608993150
H41	3.2882741412	-3.3129851825	4.3257192330	C36	-0.5642944047	-2.0478216682	3.4483313965
H42	1.9613175106	-2.9331707158	6.3946809520	C37	1.6004580745	-1.0446447556	3.1235376440
C43	2.2327466164	1.8880405006	-3.1847285927	C38	2.0005425094	-1.5225982697	4.3719622058
H44	2.6824422107	0.9435710589	-2.8635265797	C39	-0.1641900068	-2.5294304459	4.6944196021
H45	2.4441433767	2.6066707408	-2.3936221573	H40	-1.5773500520	-2.2414140042	3.1023126377
H46	2.7422302340	2.2065406623	-4.0992756442	H41	2.3033622781	-0.4872954468	2.5156696086
C47	-2.6942384892	2.3076156210	-1.8502373469	H42	3.0074019576	-1.3146673437	4.7234569161
H48	-3.6789377061	2.0838138272	-2.2690362369	H43	-0.8598082674	-3.1058499352	5.2992237981
H49	-2.6859190716	3.3744382129	-1.5938209702	H44	1.4428016328	-2.6434921330	6.1300309173
H50	-2.5939623629	1.7568512067	-0.9110521695	C45	1.8671290829	2.7921845839	-3.5367471007
C51	-1.4028084789	0.7997985500	-6.4775646393	H46	2.2230342140	2.6240552020	-2.5194564528
H52	-1.5860604866	-0.2816376812	-6.5008867328	H47	1.7692968351	3.8741631764	-3.6990609938
H53	-0.6222172577	1.0132611652	-7.2136400450	H48	2.6362763281	2.4331114912	-4.2261652611
H54	-2.3245158217	1.2915540945	-6.8045967235	C49	-2.8355752662	1.4131913108	-2.1212570168
C55	2.4580809621	3.3329483292	2.7677621864	H50	-3.7542995804	1.0280680818	-2.5716980081
H56	3.2491666180	3.1209470277	3.4924375487	H51	-3.0576613830	2.4044163777	-1.7091445557
H57	2.4485479646	4.4209930757	2.6129284300	H52	-2.5871628266	0.7686668276	-1.2703342310
H58	2.7213614448	2.8578085857	1.8230354420	C53	-1.1994341410	0.4759949222	-6.8002283164
C59	-2.4233293519	1.9895495131	2.0884952092	H54	-0.9132744016	-0.5823565958	-6.8474589979
H60	-2.6812928042	2.8689754103	1.4869922128	H55	-0.6162081579	1.0034672496	-7.5606586063
H61	-3.2994064708	1.7362455714	2.6913780859	H56	-2.2566972771	0.5384687592	-7.0754402123
H62	-2.2508200934	1.1668382538	1.3878393901	C57	2.3825313328	3.4518618719	2.1544039607
C63	-0.5087801264	2.4278033278	6.7297604164	H58	3.2296592126	3.4522466165	2.8455693211
H64	0.0862381435	3.1899197946	7.2428456222	H59	2.2104276435	4.4945695187	1.8536648260
H65	-0.1882885999	1.4523995201	7.1160980404	H60	2.6659299139	2.8926285980	1.2610130813
H66	-1.5566694959	2.5661096601	7.0128212031	C61	-2.5108986135	1.9813640861	2.0536592580
H67	-0.5332277837	-0.0756361960	2.0208997838	H62	-3.1348572096	2.8817193068	2.1274690000
H68	0.7214737404	-2.1282736867	-1.3445116669	H63	-3.0788736076	1.1643322747	2.5096712354
C69	-1.1216571089	-1.0851057315	-1.7714633697	H64	-2.3856685209	1.7559446105	0.9932326298
H70	-1.7926795343	-0.3288426698	-1.3641636674	C65	0.0202160657	2.1006509938	6.3968467752
H71	-0.7714224061	-0.7486723766	-2.7485036927	H66	0.7293063885	2.7772902400	6.8837420838
H72	-1.7099517007	-1.9998424240	-1.9427269453	H67	0.3261853507	1.0752667501	6.6371398747
X73	-0.0307205035#	-1.2535449218#	0.5489314772#	H68	-0.9665991366	2.2613796075	6.8423892327
H74	0.4047681690	-2.6750437347	0.8035025743	H69	-0.7715299959	-0.4124487839	-1.9732291865
C75	-1.6822730904	-2.0186678774	0.9237537076	C70	-0.4723299584	-3.0527046797	0.2401568291
H76	-1.7923042961	-2.3274232956	1.9671874266	H71	0.5629219367	-3.3062298904	0.4737623809
H77	-2.2886374432	-1.1238110405	0.7644967158	H72	-1.1217498435	-3.5032200089	1.0005447444
H78	-2.0785696515	-2.8151398737	0.2859942498	H73	-0.7402494051	-3.4893761392	-0.7248660456
				C75	0.6709366602	-1.9279602018	-2.5047406942
				H76	-0.1450080413	-2.5648520268	-2.8733713185

1TS_{FGZ}

H77	1.0849198059	-1.4116820533	-3.3836938916	H72	-2.5737218331	-1.3549392929	-1.9745587217
H78	1.4641159866	-2.5205703184	-2.0513481466	H73	-0.2541712422	-2.7572513248	0.6466170793
				X74	-0.5344255177#	-1.1876216217#	1.3004394919#
		1TS _{FGE}		C75	-2.3135135859	-1.9755885641	0.6853478581
Ru1	0.7002033212	-0.3235991021	-0.1997731896	H76	-2.6145677955	-2.5655892649	-0.1825958011
Cl2	2.8692380684	0.7398488515	-0.2220916574	H77	-2.6697452638	-2.5128929262	1.5754311646
C3	0.1395310886	1.7475022199	-0.2533487090	H78	-2.8283514130	-1.0115799150	0.6596223806
N4	0.2018097318	2.6726353351	0.7472095457				
N5	0.1488067786	2.4604958263	-1.4287163898			1G _z	
C6	0.2290137767	4.0716276166	0.2605410914	Ru1	1.3466001006	0.1361744575	-0.4265395136
H7	-0.7316931581	4.5588481479	0.4760795392	Cl2	2.5426255006	0.9472238126	-2.3740037323
H8	1.0175078947	4.6350378491	0.7640407505	C3	0.4271717670	2.0388295077	-0.4719441898
C9	0.4842811328	3.8869897077	-1.2269911573	N4	0.9911119119	3.1665240151	0.0431391550
H10	1.5356544579	4.0519877957	-1.4923827612	N5	-0.6643400128	2.4342333744	-1.1828397913
H11	-0.1353055509	4.5286494945	-1.8570936705	C6	0.3495901305	4.4105080564	-0.4335191811
C12	-0.2702951806	-0.9067027479	1.7292552905	H7	0.1358049945	5.0766459496	0.4065296537
H13	-0.9506457623	-0.1315412448	2.0694559454	H8	1.0245369407	4.9333379721	-1.1213098078
Cl14	1.9421185581	-2.4337454383	-0.7411529582	C9	-0.9116128473	3.8912724183	-1.1256239030
C15	-0.5521447804	-0.9392142912	-1.4666016555	H10	-1.0441448134	4.2972008539	-2.1316107155
H16	-0.1821204414	-1.8297853286	-1.9906083738	H11	-1.8262863497	4.0963030707	-0.5550236703
C17	-0.8156817091	-1.8432676589	0.8189876749	C12	0.7136559994	-0.0169229819	1.9265073949
C18	-0.0143478554	2.5590490300	2.1654142862	H13	0.1000983521	0.84186749651	1.9797018544
C19	-0.5313991566	2.8117593354	4.9236742490	Cl14	2.9676989989	-1.6966022615	-0.4202666711
C20	1.0476804084	2.8297370843	3.0496331030	C15	0.0759909886	-0.7801635069	-1.4122729192
C21	-1.3356454757	2.4275760134	2.6467182086	H16	-0.9412408966	-0.9394478964	-1.0381372095
C22	-1.5658418371	2.5403368788	4.0207096181	C17	0.1361154424	-1.1132039729	1.3234871874
C23	0.7609000896	2.9495712840	4.4158750532	C18	2.0621295039	3.2986208451	1.0003646645
H24	-2.5832044053	2.4358583546	4.3921434458	C19	4.0771638882	3.6872525480	2.9254498558
H25	1.5814831503	3.1577248935	5.0993336567	C20	3.3933358550	3.4825209894	0.5811395051
C26	-0.1984004354	2.0849270320	-2.7789022220	C21	1.7170238034	3.4186749651	2.3671032421
C27	-0.9730838224	1.5408980557	-5.4382238485	C22	2.7336252111	3.5954447431	3.3038181039
C28	-1.5127787634	2.3848397589	-3.2108557033	C23	4.3778807596	3.6487238414	1.5657525364
C29	0.7547078247	1.5996041323	-3.6958233676	H24	2.4703569890	3.6636175132	4.3568729019
C30	0.3321382539	1.3173607188	-5.0029612004	H25	5.4103514599	3.7714611109	1.2448669533
C31	-1.8770857106	2.0999029563	-4.5285122994	C26	-1.6642012673	1.6231039055	-1.8173055228
H32	1.0663617059	0.9276907106	-5.7048436288	C27	-3.6947740883	0.1333039036	-3.0623248776
H33	-2.8935464328	2.3168475564	-4.8503836456	C28	-2.7314004018	1.1191285089	-1.0449641820
C34	0.7756982682	-1.2300294893	2.7403977331	C29	-1.6299195799	1.4428105078	-3.2130221226
C35	2.5413488428	-1.8299256861	4.8538498910	C30	-2.6517588999	0.6902448690	-3.8062338636
C36	1.7382082203	-2.2477982499	2.6046640124	C31	-3.7233542818	0.3714194115	-1.6835572332
C37	0.7164645967	-0.5272920148	3.9574532464	H32	-2.6240829629	0.5346514203	-4.8824281081
C38	1.5860890816	-0.8249926186	5.003826139	H33	-4.5407051795	-0.0326340649	-1.0898518042
C39	2.6098464896	-2.5363526268	3.6511787411	C34	1.7815405048	-0.0592217348	2.9760663418
H40	1.8344076662	-2.7812712362	1.6657603745	C35	3.5869792338	-0.1377146443	5.1415114986
H41	-0.0315903263	0.2465062748	4.0882716736	C36	3.1088178628	-0.4649177333	2.7838049003
H42	1.5158789611	-0.2699104257	5.9357550979	C37	1.3770794605	0.3063456838	4.2742577422
H43	3.3540654300	-3.3171969505	3.5205884820	C38	2.2646272465	0.2620764666	5.3468458619
H44	3.2274067270	-2.0602018687	5.6649092508	C39	3.9998962074	-0.4983396360	3.8594686276
C45	2.2104260733	1.3981034845	-3.3630207340	H40	3.4407182454	-0.7659703742	1.7958883548
H46	2.4068389482	0.3857490269	-2.9971226826	H41	0.3459959768	0.6075686328	4.4458203935
H47	2.5542947221	2.0705116727	-2.5779140287	H42	1.9232898832	0.5372533433	6.3417206126
H48	2.8193408643	1.5561532384	-4.2583792244	H43	5.0250234389	-0.8157579410	3.6869132378
C49	-2.5364900770	3.0117111712	-2.2902141404	H44	4.2845421508	-0.1723580150	5.9744871097
H50	-3.5451661964	2.8870459065	-2.6942489202	C45	-0.5330689194	2.0386038237	-4.0615298674
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H55	-0.5735807310	1.3170500797	-7.5544697662	H50	-3.6969765830	0.8723124527	0.8659963058
H56	-2.2357240148	1.8060619821	-7.1789437184	H51	-2.9079459268	2.4388780898	0.6718085019
C57	2.4647434914	3.0318906081	2.5702880847	H52	-1.9377073275	1.0022574991	0.9735016133
H58	3.1737965719	2.7258949885	3.3449136989	C53	-4.7531139764	-0.7226151737	-3.7184132292
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H60	2.6751740185	2.4578685657	1.6658202140	H55	-4.8737098422	-0.4721815457	-4.7763555481
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H71	-1.7790399762	-0.1946938552	-3.0105214313	H66	6.0973579252	4.1837518511	3.5287208460

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H73	1.1333120840	-1.0341297346	-3.2788582758	H68	5.3052222117	2.9874669992	4.6140986042
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C75	0.5230053721	-2.5487006074	1.5419278086	C70	-1.1292029042	-2.0193091135	0.9906428747
H76	0.3681302136	-3.1489157940	0.6416256922	H71	-1.8781079127	-1.2348526628	0.8496025334
H77	1.5630379604	-2.6588096724	1.8415909001	H72	-1.1630284523	-2.7017923662	0.1363287407
H78	-0.1210397565	-2.9598342588	2.3335368715	H73	-1.4269554014	-2.6025949369	1.8733257091
				C74	0.2825052234	-1.4992600277	-2.7312253933
		1Ge		H75	0.6923220267	-2.4793308104	-2.4348145335
Ru1	1.2608544523	0.0104073905	-0.3885394857	H76	-0.6187947666	-1.6581613916	-3.3339286175
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C3	0.4351697031	1.9808506551	-0.4175996977				
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C6	0.5170878241	4.3503863787	-0.4906098155	C2	1.3430551108	0.1995922418	-0.1745534856
H7	0.3869863146	5.0890853863	0.3042304064	H3	1.7280449125	1.2182653013	-0.2786871307
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H11	-1.6730363387	4.1630472280	-0.5057881032	C7	-0.7917716492	1.0764244227	0.7775497194
C12	0.4914415619	-0.2734624282	1.8792325932	C8	0.3042575772	-2.2526494708	-2.7508896193
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H16	-1.0545070377	-0.8518850933	-1.1333586293	C12	0.3707954194	-2.8813009964	-5.0724554014
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C20	4.0799311574	3.7091966839	2.9936194589	H16	0.3462797896	-2.6007204427	-6.1233369248
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C27	-1.6764196171	1.6644891192	-1.7678842844	C23	-1.6992888352	3.2465731761	1.3106930302
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H34	-4.6658909333	0.2175955287	-1.0517275884	H30	-0.3883419371	-3.6956618500	-0.3717049075
C35	1.5697065426	-0.0850143039	2.8945552391	H31	1.0247745810	0.1656650806	-4.1976196975
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C37	2.9015778824	-0.5014758901	2.7395496861	H33	0.8002022592	-4.8941324317	-6.7668802333
C38	1.1718561205	0.4249778446	4.1442743506	H34	-0.4307175151	-5.8029796989	-5.8798618308
C39	2.0678004211	0.5111081238	5.2075149030	H35	1.2770372896	-6.0791046800	-5.5382270105
C40	3.8005277549	-0.3962331287	3.8011805101	H36	0.6767952957	-0.4832922477	2.9744385989
H41	3.2310124077	-0.9216030615	1.7939954179	H37	-0.4014334728	-1.4158777997	1.9052337588
H42	0.1384913729	0.7303909708	4.2897782798	H38	-1.0337700349	3.9592519798	-1.0918026981
H43	1.7300054178	0.8918993199	6.1682550883	H39	-1.4480806900	2.3725748022	-1.7704286612
H44	4.8278894294	-0.7207154909	3.6586038247	H40	-2.3610831269	4.8424457856	3.3785945449
H45	4.0958050217	0.1706159623	5.8639069253	H41	-2.2267126013	3.6077946356	4.6439721285
C46	-0.4910504792	1.9576443933	-4.0045450132	H42	-3.6612548450	3.6740298071	3.6182694635
H47	0.4832357234	1.7113162580	-3.5713244007	C43	-0.6834653134	-0.6759695626	-1.0376871619
H48	-0.5375586856	3.0498883801	-4.1098420084	Ru44	-2.7086111457	-1.0076780253	-1.1219627910
H49	-0.5415357664	1.5343015684	-5.0114125731	Cl45	-2.5189404621	-2.5054351138	0.8216673904
C50	-2.9014876212	1.5784411810	0.4686607175	Cl46	-2.9864366168	0.7798974281	-2.8266086824
H51	-3.7457466534	1.0481250583	0.9180916343	C47	-2.6959513510	-2.2237164493	-2.5352379459
H52	-3.0633608638	2.6506074678	0.6373631418	H48	-2.4602738849	-1.7445352976	-3.4912356913
H53	-1.9964006185	1.3027983005	1.0153028683	H49	-0.9318034667	-0.9596974721	3.5179484586
C54	-4.8683534819	-0.5457298473	-3.6610258842	H50	0.2156863226	2.7256336711	-1.2965182389
H55	-4.6749020002	-1.6206045582	-3.5522415064	H51	0.1026362616	-0.3462314435	-5.6115070472
H56	-4.9427982052	-0.3352530020	-4.7317864374	H52	0.6212102803	-5.0850569151	-0.8188009064
H57	-5.8429647567	-0.3456977238	-3.2045826737	H53	2.0704005581	-0.1248799152	-2.2251074991
C58	3.9288049465	3.4443911674	-0.7930611885	H54	1.7224220715	-0.2152470841	0.7663367372
H59	4.5789368067	2.5956504056	-1.0253234737	C55	-5.3610255431	-1.0147104152	-1.3643406422
H60	4.5021386699	4.3641217654	-0.9606244333	C56	-4.9431657251	-0.6286680880	-0.1268818995
H61	3.1068598917	3.3967165281	-1.5037248543	C57	-3.0613039657	-3.6217226526	-2.7247419264

C58	-3.7989822789	-6.2770091568	-3.3140856227	H54	1.7516048135	-0.2314030738	0.8104140302
C59	-3.3349772433	-4.5422602360	-1.6889265465	C55	-5.3037266555	-1.4035776610	-1.0147628344
C60	-3.1674777363	-4.0735786756	-4.0627076096	H56	-5.2603221736	-2.2340756604	-0.3118080015
C61	-3.5404485857	-5.3815165775	-4.3544699242	C58	-4.9709850643	-0.1604260947	-0.5713838494
C62	-3.6899823549	-5.8536074310	-1.9863697357	C61	-3.0929387061	-3.5281237035	-2.8691812778
H63	-3.2547103318	-4.2082897609	-0.6607750517	C62	-3.9370204626	-6.1250360994	-3.5682629175
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H66	-3.8913093652	-6.5508772603	-1.1776037108	C65	-3.5495052279	-5.2288759126	-4.5671239411
H67	-4.0874038842	-7.3011222921	-3.5369282599	C66	-3.9037483077	-5.7311902659	-2.2268834663
H68	-5.3837391836	-0.2733511523	-2.1605602321	H67	-3.4668461063	-4.1410866151	-0.8372059558
H69	-4.9777069670	-1.3624769205	0.6763788083	H68	-2.8142111508	-3.2545619061	-4.9950864589
C70	-6.0075869461	-2.3406891803	-1.6495560127	H69	-3.5788981554	-5.5276520842	-5.6115649489
H71	-5.7038855924	-2.7557374337	-2.6138767059	H70	-4.2048710395	-6.4291938898	-1.4502766146
H72	-5.7906252173	-3.0759207435	-0.8700913950	H71	-4.2671466774	-7.1262584262	-3.8336504713
H73	-7.0972189091	-2.2020988729	-1.6889920562	H72	-5.0786415774	0.6691783925	-1.2680491292
C74	-4.6759610902	0.7954959307	0.2943966755	C72	-4.6993852864	0.2131340672	0.8636930494
H75	-3.7537430155	0.8864020500	0.8812249632	H73	-3.8112346414	0.8479356816	0.9667586292
H76	-4.6184883271	1.4723562492	-0.5603170890	H74	-5.5455059596	0.8084835748	1.2356200285
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				C75	-5.9574427884	-1.6589432363	-2.3456965312
		2B _E		H76	-5.7718690099	-0.8385043643	-3.0439105239
N1	-0.1101451403	0.1395139336	-0.1297771112	H77	-5.6221473565	-2.5943055237	-2.7999759165
C2	1.3662794246	0.1433626175	-0.1437763184	H78	-7.0432535728	-1.7461620792	-2.2002175383
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C4	1.6931494374	-0.7844531657	-1.3179172058			2TS _{BCZ}	
N5	0.3609938671	-1.2782940315	-1.7282338328	N1	-0.0983161059	0.1093165576	-0.0726499848
H6	2.3335695551	-1.6246758203	-1.0331390735	C2	-0.4652050223	0.0689814962	1.3612019764
C7	-0.7733623685	0.9629712806	0.8478269064	H3	0.4279228047	0.1469304687	1.9869968669
C8	0.3341204778	-2.2697171523	-2.7649387682	C4	-1.1716003025	-1.2860186338	1.4806976474
C9	0.5367083450	-4.2046769292	-4.7815730700	N5	-1.3701998767	-1.6697333612	0.0638049358
C10	0.4257719064	-3.6302526600	-2.4089092483	H6	-2.1326949345	-1.2248341822	1.9974584558
C11	0.3719930148	-1.8579286606	-4.1100482842	C7	0.7679152094	1.1546286219	-0.5569411129
C12	0.4665064719	-2.8448761717	-5.0978275577	C8	-2.0655302118	-2.8967238772	-0.2246839750
C13	0.5214472712	-4.5749087868	-3.4330669142	C9	-3.4346221650	-5.3062133148	-0.6381219418
C14	0.4162079005	-4.0683297769	-0.9646680144	C10	-3.4700593846	-2.8830330797	-0.3027756091
C15	0.3004463162	-0.3988811486	-4.4933510343	C11	-1.3364465142	-4.1003891872	-0.2943402157
H16	0.4886543273	-2.5388938629	-6.1417225729	C12	-2.0425794390	-5.2862604876	-0.5103287404
H17	0.5823932567	-5.6284815847	-3.1689618447	C13	-4.1277617670	-4.0994471656	-0.5186655292
C18	0.5982470968	-5.2556217959	-5.8648977101	C14	-4.2655021252	-1.6084063715	-0.1559489652
C19	-1.9320975683	2.6350438193	2.7835530894	C15	0.1646314042	-4.1334590553	-0.1309519802
C20	-1.1163023508	2.2889564923	0.5027989965	H16	-1.4874461928	-6.2192173350	-0.5793438442
C21	-0.9108627091	0.4981511448	2.1718908446	H17	-5.2134261790	-4.0992350775	-0.5912334203
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C25	-0.3627903125	-0.8333897637	2.6252558855	C21	0.2274704628	2.3996081039	-0.9360077513
H26	-1.6363739698	0.9844927595	4.1288617707	C22	1.1103711983	3.3912821168	-1.3784944539
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H30	-0.5038329312	-3.7615904332	-0.4559200995	H26	0.7014706637	4.3517301062	-1.6844947780
H31	1.1663872678	0.1627125514	-4.1217021332	H27	4.0737518424	1.8112918665	-0.9480643635
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H33	0.9061690671	-4.8287967461	-6.8238013394	H29	-4.0968962023	-1.1319837454	0.8179183625
H34	-0.3847789561	-5.7216181952	-6.0087312823	H30	-3.9932092539	-0.8824267117	-0.9283755767
H35	1.2992795223	-6.0565990205	-5.6075294418	H31	0.4773507943	-3.7223336580	0.8370810649
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H39	-1.4037716314	2.3691879156	-1.6423684176	H35	-5.2329633242	-6.5134085911	-0.7031889219
H40	-2.4064739065	4.5748346940	3.6221086200	H36	-1.5806475225	2.6972307476	0.2121273885
H41	-2.2712435993	3.2782541305	4.8238886858	H37	-1.8549614754	1.9685233846	-1.3774438918
H42	-3.6951004415	3.3809858185	3.7869618057	H38	3.8504034050	-0.2619719336	0.0466856910
C43	-0.6581953080	-0.7149115914	-1.0353193898	H39	2.4839820105	-1.1864609048	-0.5962109265
Ru44	-2.6871680251	-0.9883022035	-1.1705526237	H40	4.4122078722	4.1912367971	-1.4965197193
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H48	-2.3547465823	-1.6685727167	-3.5533663087	Ru44	-0.6603085471	-1.0242364799	-2.8805672383
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H17	-5.3730072068	-3.5651558946	-0.5295027452	H17	-4.3173212129	-4.87771630820	-0.1346589278
C18	-4.7377500200	-6.2110753914	-0.5788802048	C18	-3.0676787497	-7.2779770469	0.1639654560
C19	2.027142746	3.4421386519	-1.5949451963	C19	1.2239436561	3.5085936571	-2.0447686634
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C21	0.0094412213	2.4153688446	-0.6738981577	C21	-0.5348468200	2.1356087702	-1.0469019015
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H26	0.1530731607	4.4583969449	-1.3028270332	H26	-0.8585088180	4.0421368490	-1.9698562008
H27	3.7611886206	2.1725164071	-1.6595123506	H27	3.2188938218	2.7246513060	-1.8669748638
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H30	-3.6946856544	-0.6436322147	-1.0584728011	H30	-3.4263830214	-1.7505331269	-0.9959106630
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H32	0.5177154217	-3.9470285768	-0.4227858230	H32	1.4830225085	-3.7648700823	0.2818592766
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H34	-4.9629130781	-6.3146670963	-1.6477254818	H34	-3.1529019845	-7.5724541474	-0.8893314295
H35	-5.6934548419	-6.0834727596	-0.0592595322	H35	-4.0741937957	-7.3171632109	0.5937104540
H36	-1.5414943364	2.2754586585	0.8358218165	H36	-2.1039108838	1.7940783748	0.4124148123
H37	-2.0884541855	1.9354723327	-0.8155409162	H37	-2.4398638143	1.1335966239	-1.1966623465
H38	3.8980535182	-0.0336114410	-0.9907450426	H38	3.8472723267	0.7204615711	-0.9009900328
H39	2.4394229311	-1.0333740012	-1.0414475504	H39	2.6765360162	-0.6088713053	-0.8846301304
H40	3.8043419265	4.5749392652	-2.0975097209	H40	2.6803032380	5.0129100415	-2.6032277907
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H42	2.4991567540	4.7121329083	-3.2793866398				
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Ru44	-0.6735304898	-1.1197938274	-2.7504641402				

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H49	-2.5477409340	2.8777940614	-0.9093135193	Ru44	-0.2753463246	-1.6732907372	-2.5456294473
H50	2.9284791817	0.3764162165	0.5636216974	Cl45	-2.4589036779	-0.6694274118	-2.9973326720
H51	1.3755888708	-5.2972731579	1.1666648542	Cl46	1.9452189889	-2.6720334450	-2.0700190213
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H53	-0.2156744639	-1.9350420677	2.5236842308	H48	0.2864220187	-3.9603521231	-3.5641506782
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C55	-0.0032132417	-2.3563032878	-4.7375374652	H50	2.8735878288	0.3800160252	0.5565540326
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C57	0.4181405256	-0.9115407926	-4.1849395419	H52	-4.6600025587	-2.7566864552	-0.0710339927
H58	-0.3005564694	-0.1620144698	-4.5236414489	H53	-0.2610922517	-1.9288403488	2.5109847477
C60	-1.7272563146	-4.2463652053	-3.8333201964	H54	-0.5822864556	0.8735631443	1.8178677974
C61	-3.8851318037	-6.0274335530	-4.2256917256	C55	-0.0300042978	-2.1525158506	-4.7980386533
C62	-3.0256799846	-3.7640949241	-4.0856841978	H56	-0.8929747897	-1.8289292203	-5.3804531479
C63	-1.5475162470	-5.6430393776	-3.7639677221	C57	0.5831132893	-0.8312345984	-4.1397743510
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H70	-4.7172963044	-6.7092868215	-4.3812558606	C65	-4.0194529376	-4.2659563454	-4.9687956184
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H72	-0.4376940532	-1.6165430397	-6.7178717310	H67	-1.0118769903	-5.7388855706	-3.0374345731
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Xpi	0.0122773985#	-2.2673624027#	-4.1138885685#	H70	-4.9534598245	-6.1926869535	-4.6897562946
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H77	1.9924223551	-0.2826044709	-5.4959729484	H73	1.9164832282	-3.0948682938	-5.0828472505
H78	2.0527056652	0.4451153159	-3.8874945584	H74	0.6609464582	-3.6592139898	-6.2097828756
		2C _E		Xpi	0.0333782153#	-2.1131020488#	-4.1654759612#
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C12	-0.9848872523	-5.7253059108	0.6621413203	C7	-2.1001011693	1.5496365319	1.1408476621
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C19	1.1763406207	3.5463869594	-2.0197366420	C14	0.3788144305	-3.4478845471	0.1045149933
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H48	-2.1181212321	-2.0073334400	-3.7484144724	Ru44	-2.6580677972	-0.9852517588	-1.1175268993
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H50	0.7130646102	2.4736379399	-1.6583597124	Cl46	-2.9370793821	0.9153072053	-2.6730192520
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H53	2.4069257761	-0.4722418265	-2.0445685711	H49	-0.8703393715	-0.8039658742	3.6957629897
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H56	-5.0248690742	-2.3873843244	-1.6096609980	H52	0.7465421101	-5.1869476728	-1.0157936293
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C58	-5.7292160120	-0.9802000868	-3.1728983452	H54	1.7768491243	-0.3744779272	0.8305962791
H59	-4.9924030497	-0.4598739441	-3.7937643950	C55	-5.2560870517	-1.4785260328	-1.1512706346
H60	-6.0451326909	-1.8839755278	-3.7018688935	H56	-2.2647452952	-2.4056899597	-0.5832178409
H61	-6.5985484548	-0.3198855526	-3.0726255301	C57	-5.0400745524	-0.2926784972	-0.5061560914
C62	-2.8707700503	-3.7486131347	-2.6785390147	H58	-5.0971143922	0.6062209463	-1.1166205536
H63	-3.1447101572	-4.0762941243	-1.6764702255	C59	-5.8037554632	-1.5231776076	-2.5543665486
H64	-3.7228455771	-3.8846352818	-3.3631753038	H60	-5.5035556172	-0.6406509123	-3.1249360636
H65	-2.0665548559	-4.3857812475	-3.0715661685	H61	-5.4991199948	-2.4203779722	-3.0981248734
H66	-4.7465078526	-1.0047072138	0.1880316826	H62	-6.9016753242	-1.5430041942	-2.5043162311
C67	-6.0879114933	3.5922730739	-0.0968369761	C63	-2.9287509216	-3.5911074915	-2.6501067291
C68	-5.9578561751	2.6939844475	0.9639670674	H64	-3.0557451703	-4.0673859745	-1.6796378225
C69	-5.5672104863	1.3807834909	0.7177331665	H65	-3.8196483153	-3.7620702536	-3.2731918237
C70	-5.3207106572	0.9257077459	-0.5924385209	H66	-2.0979617353	-4.0642465510	-3.1907181153
C71	-5.4389650302	1.8481052681	-1.6496111839	C67	-5.1523492424	0.6506520805	3.6717133790
C72	-5.8171507604	3.1652773926	-1.3980950041	C68	-5.1743585738	-0.690368705	3.2768452413
H73	-6.3888989329	4.6198333284	0.0900047128	C69	-5.1017437286	-1.0318432116	1.9308464106
H74	-6.1597406188	3.0155973932	1.9823374577	C70	-4.9962568527	-0.0317810058	0.9459917857
H75	-5.4616519239	0.6845427258	1.5460153315	C71	-4.9572784340	1.3124772350	1.3587712257
H76	-5.1839048472	1.5509849458	-2.6579445431	C72	-5.0424231719	1.6516353627	2.7073066670
H77	-5.8928185780	3.8653510609	-2.2257744634	H73	-5.2226323172	0.9105659148	4.7247339767
		2D _E		H74	-5.2547288043	-1.4751284696	4.0240648754
N1	-0.0526953244	0.1467890655	-0.1042871302	H75	-5.1121286856	-2.0762621813	1.6426692329
C2	1.4247261793	0.0798290280	-0.1024548297	H76	-4.8729256728	2.0934611676	0.6074851794
H3	1.8487774400	1.0851693168	-0.1733736526	H77	-5.0292488559	2.6974106447	3.0016729723
C4	1.7199624235	-0.7858089376	-1.3266789340			2E _Z	
N5	0.3806673810	-1.2973090499	-1.6881596264	Ru1	0.6396784404	-0.1244112494	-0.0832932600
H6	2.3984748351	-1.6158023183	-1.1122792560	Cl2	2.9117125657	0.7370376677	-0.2046832408
C7	-0.6555683884	1.0777547406	0.8155308099	C3	0.1994942285	1.9600643224	-0.1217676378
C8	0.3257566181	-2.2483613057	-2.7603094097	N4	0.2062521531	2.8597281956	0.8980497466
C9	0.4810162613	-4.0992889998	-4.8614645446	N5	0.1468467742	2.6785830757	-1.2807886605
C10	0.5145604882	-3.6126313016	-2.4642261337	C6	0.3149104270	4.2631616095	0.4408804986
C11	0.2525227581	-1.7886014987	-4.0909388021	H7	-0.4332589476	4.8872577027	0.9382696397
C12	0.3181888969	-2.7350774196	-5.1191786819	H8	1.3076945249	4.6552017619	0.6874677762
C13	0.5865737906	-4.5153497971	-3.5298560242	C9	0.0929664153	4.1406724241	-1.0672572877
C14	0.6167841435	-4.1016649111	-1.0398633576	H10	0.8682512259	4.6380395751	-1.6569945144
C15	0.1141301469	-0.3210595586	-4.4173407713	H11	-0.8804636519	4.5317633550	-1.3880795239
H16	0.2525747113	-2.3915942720	-6.1492376865	C12	0.5398824091	-0.3950307624	1.7588541617
H17	0.7287426364	-5.5716098317	-3.3117289115	H13	-0.4006317205	-0.1378510430	2.2506755127
C18	0.5257221997	-5.1008855618	-5.9919113325	Cl14	1.7111435913	-2.2998219403	-0.5969259611

C15	-1.0982115665	-1.4426123666	-0.8588577145	H10	1.3105633949	4.4591626118	-1.6385507965
H16	-0.9343470407	-2.4061327083	-0.3838178134	H11	-0.4477132844	4.5957620952	-1.8148987364
C18	-1.7540004974	-0.4763965056	-0.1192313750	C12	0.4631635396	-0.2026858014	1.7920225076
H20	-2.1328012134	0.3969664526	-0.6392899576	H13	-0.4919233703	0.1552110673	2.1828845109
C21	0.0639503462	2.6467470210	2.3136808767	Cl14	1.6662608453	-2.3596341314	-0.4081099886
C22	-0.2942791098	2.3904052377	5.0895329040	C15	-1.2351277131	-0.6819750382	-1.1403393239
C23	1.1905475876	2.6530273968	3.1584769932	H17	-1.8505640748	0.2099422036	-1.2187296385
C24	-1.2407058673	2.5960502516	2.8474513397	C18	-1.3321274550	-1.4128662742	0.0252778975
C25	-1.3949970007	2.4504149346	4.2293580287	H19	-0.8633509431	-2.3931345276	0.0429573788
C26	0.9817316713	2.5097973223	4.5347501648	C21	0.1854230034	2.7835804460	2.2055812728
H27	-2.3996031049	2.3967110834	4.6434826191	C22	-0.0983733525	2.6793413324	5.0004545183
H28	1.8501014132	2.4902486357	5.1895896229	C23	1.3268449539	2.9131111278	3.0228524603
C29	-0.0793813858	2.2160969694	-2.6272634735	C24	-1.1004554752	2.6761969025	2.7729467632
C30	-0.5691401980	1.4541693389	-5.2958542508	C25	-1.2166405623	2.6114303915	4.1652428641
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C32	1.0064056642	2.0482752589	-3.5138038522	H27	-2.2066926831	2.5096168154	4.6051966378
C33	0.7319859684	1.6467938180	-4.8268793542	H28	2.0368666903	2.9224918895	5.0432203529
C34	-1.6251583736	1.7150001014	-4.4203031403	C29	0.0607947363	2.1335074941	-2.7197782735
H35	1.5687220254	1.4991330716	-5.5061955986	C30	-0.3987003054	1.3152260948	-5.3747782730
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C37	1.4861463706	-0.9687034432	2.6964142850	C32	1.1575746362	1.8585217855	-3.5598152228
C38	3.1565526009	-2.1139080502	4.6514185749	C33	0.8963111558	1.4377917348	-4.8716145511
C39	2.7986064026	-1.3824025146	2.3698702881	C34	-1.4640508425	1.6612049930	-4.5369517357
C40	1.0379047212	-1.1498949009	4.0295281748	H35	1.7416208504	1.2128121003	-5.5185624980
C41	1.8593995584	-1.7182770524	4.9941100381	H36	-2.4817239547	1.6072682626	-4.9186689604
C42	3.6184916561	-1.9423936843	3.3447206172	C37	1.2771785242	-0.8004899844	2.8319511871
H43	3.1502925546	-1.2616951773	1.3548211648	C38	2.6682340546	-2.0239910659	4.9487418880
H44	0.0312406777	-0.8347708631	4.2926619734	C39	2.5686933622	-1.3392788827	2.6271278270
H45	1.4958362425	-1.8560498582	6.0088311164	C40	0.7068630927	-0.8913197981	4.1267928852
H46	4.6244526671	-2.2554166124	3.0798094556	C41	1.3906131026	-1.4997506281	5.1712987563
H47	3.8041853824	-2.5588205730	5.4029079500	C42	3.2506064747	-1.9378716482	3.6818980961
C48	2.4397537685	2.3081673630	-3.1244450721	H43	3.0122306857	-1.2861272846	1.6419748665
H49	2.9287464966	1.3984533170	-2.7654457581	H44	-0.2831585573	-0.4756839846	4.2957193396
H50	2.5228795219	3.0299631838	-2.3101082367	H45	0.9338554736	-1.5714841993	6.1548444247
H51	2.9957944054	2.6854261696	-3.9884302231	H46	4.2407499499	-2.3508268723	3.5112684285
C52	-2.6134499097	2.4479957826	-2.2472444599	H47	3.2066221889	-2.5032914900	5.7627260657
H53	-3.3890256291	1.6808353361	-2.3432225843	C48	2.5944155001	2.0230378681	-3.1295220468
H54	-3.0615861114	3.3938203075	-2.5770814419	H49	3.0419800931	1.0604817701	-2.8649744157
H55	-2.3688359938	2.5501417997	-1.1901775193	H50	2.6981192950	2.6511543482	-2.2451342878
C56	-0.8236268413	0.9803321325	-6.7074294525	H51	3.1793858811	2.4575692744	-3.9468568275
H57	-0.7400987407	-0.1116681937	-6.7736009212	C52	-2.4534455227	2.5339265049	-2.4075616980
H58	-0.0971960251	1.4024892356	-7.4090370377	H53	-3.3559812658	1.9931799404	-2.7080091002
H59	-1.8265932108	1.2535589843	-7.0486158865	H54	-2.6555135280	3.6021496511	-2.5643108387
C60	2.5903434867	2.8494684641	2.6326682901	H55	-2.3091981349	2.3878068962	-1.3357408273
H61	3.3256225243	2.4985908010	3.3618347026	C56	-0.6473052449	0.8195777141	-6.7798797502
H62	2.7910285011	3.9157675934	2.4607962656	H57	-0.7756305209	-0.2698037811	-6.7927015285
H63	2.7577190230	2.3164022440	1.6942069397	H58	0.1906155978	1.056584876	-7.4455886174
C64	-2.4636983887	2.7572628475	1.9723245613	H59	-1.5547777072	1.2588153047	-7.2060791694
H65	-2.5433980007	3.7817437830	1.5857619191	C60	2.7005336348	3.1431266519	2.4442833703
H66	-3.3754442568	2.5545000909	2.5411021276	H61	3.4611819835	3.0671332924	3.2260096276
H67	-2.4486095366	2.0892229886	1.1090952946	H62	2.7828946374	4.1473211987	2.0069235643
C68	-0.4738723511	2.1937638211	6.5765515867	H63	2.9348814586	2.4210280778	1.6575250548
H69	0.1815082022	2.8575362721	7.1501336190	C64	-2.3482466322	2.6565003530	1.9199319500
H70	-0.2245326651	1.1660438020	6.8684193813	H65	-2.6065782185	3.6623378930	1.5633491672
H71	-1.5054689620	2.3842512117	6.8860741207	H66	-3.2044692180	2.2893523528	2.4929064438
Xpi	-1.4805250000#	-0.8123280000#	-0.4244325000#	H67	-2.2305974082	2.0227757786	1.0381008613
C72	-0.9910973478	-1.4584161641	-2.3636928045	C68	-0.2333134462	2.5545079642	6.4996487187
H73	-1.0052339701	-0.4575790248	-2.7993854717	H69	0.3990744932	3.2803041876	7.0214752771
H74	-0.0847930621	-1.9788778444	-2.6790889187	H70	0.0779295450	1.5573018103	6.8352306478
H75	-1.8536109534	-2.0073719725	-2.7699994240	H71	-1.2662911525	2.7065995146	6.8257174000
C75	-2.4525751464	-0.8187675390	1.1750446968	Xpi	-1.4805250000#	-0.8123280000#	-0.4244325000#
H76	-2.0434633225	-1.7301359714	1.6204517187	C72	-2.3560432279	-1.1598543045	1.0976692598
H77	-2.4140118642	-0.0237890942	1.9248913472	H73	-2.7016219163	-0.1229355667	1.1176224333
H78	-3.5148818024	-1.0022736957	0.9625577700	H74	-3.2297559449	-1.7936168668	0.8909640133
		2E _E		H75	-1.9999064303	-1.4338174806	2.0950789266
Ru1	0.7552427249	-0.0986722685	-0.0502219832	C75	-0.7844833726	-1.2863403071	-2.4542133642
Cl2	3.0524794452	0.6518774771	-0.0759868260	H76	-2.2602676399	-2.2286469927	-2.2954357428
C3	0.3100314958	1.9689919789	-0.1957907812	H77	-1.6755958053	-1.4689655562	-3.0718930670
N4	0.3077054935	2.9227992798	0.7796592499	H78	-0.1339204173	-0.6222282179	-3.0287059797
N5	0.2587354766	2.6388698593	-1.3858729624				
C6	0.2184262064	4.3057385057	0.2628837104	Ru1	0.8943876159	-0.1617895888	-0.1321541912
H7	-0.7400894304	4.7541134497	0.5518746255	Cl2	2.9589705326	0.9986469413	-0.2341854144
H8	1.0187834469	4.9205199780	0.6837668238	C3	0.1273618484	1.8266047275	-0.2318859809
C9	0.3491307909	4.1074216754	-1.2463204586	N4	0.0944215411	2.7620736367	0.7620736367

N5	0.0341139028	2.5173833078	-1.4121484105	Ru1	1.1716604407	0.0704445715	-0.0772577921
C6	-0.0515152944	4.1493515502	0.2659469715	Cl2	3.2254077040	1.2059015049	-0.3825635701
H7	-1.0498374210	4.5339886282	0.5130996035	C3	0.3666203813	2.0311111943	-0.1704887286
H8	0.6892182631	4.8004300060	0.7363702771	N4	0.2865178396	2.9730625838	0.8133985644
C9	0.1680195085	3.9804568855	-1.2326388254	N5	0.1238287546	2.6812175533	-1.3464279120
H10	1.1705085319	4.2949787718	-1.5467623624	C6	0.1464336600	4.3524694046	0.2938121430
H11	-0.5653844108	4.5155026393	-1.8399108790	H7	-0.6418351919	4.8876490032	0.8309937809
C12	0.1713888543	-0.5160512684	1.6211266825	H8	1.0873940977	4.8962609122	0.4356610488
H13	-0.5873807466	0.1648790693	1.9941258156	C9	-0.1770729370	4.1190776658	-1.1805890286
Cl14	2.2579935783	-2.1746022104	-0.6747133100	H10	0.4407359123	4.7165094851	-1.8568668964
C15	-0.6599605247	-1.2816548665	-1.0085520715	H11	-1.2296328568	4.3147224585	-1.4204791103
H16	-0.1502492856	-2.0968660676	-1.5202457768	C12	0.3231864914	-0.3129102251	1.6071299464
C17	-0.8560304932	-1.5501084069	0.4424203284	H13	-0.5041895823	0.3313430891	1.8960762262
H18	-1.7883570528	-1.0903921874	0.7739857307	Cl14	2.4992587038	-2.0039632737	-0.4122006760
C19	-0.0602301067	2.6098023991	2.1867483599	C15	-0.4579299699	-0.8062005579	-1.1044515893
C20	-0.4539886795	2.5695746176	4.9739813209	H16	-1.2322962681	-0.0729766785	-1.3114174138
C21	1.0268512369	2.8625880866	3.0445767480	C17	-0.5827385635	-1.4008193445	0.2294548282
C22	-1.3519034852	2.3844643344	2.7090204105	H18	-0.0706231724	-2.3538693338	0.3443216115
C23	-1.5223977682	2.3623401379	4.0960315679	C19	0.2855189431	2.8323387420	2.2480422515
C24	0.8046522516	2.8207945625	4.4263443245	C20	0.1646962048	2.7505049015	5.0580385520
H25	-2.5174687817	2.1853451520	4.4992129088	C21	1.4580493029	3.0425855103	2.9963396358
H26	1.6472107222	2.99930489207	5.0909142572	C22	-0.9589739054	2.6600463677	2.8925120709
C27	-0.2948795246	2.0690147277	-2.7458641596	C23	-0.9947694402	2.6131966997	4.2877725174
C28	-1.0426311075	1.3736618097	-5.3759770287	C24	1.3704603063	2.9747804620	4.3932048697
C29	-1.6443865800	2.1898062790	-3.1549112726	H25	-1.9528036512	2.4754280756	4.7851079931
C30	0.6946376415	1.6865208871	-3.6717737456	H26	2.2789203040	3.1158215783	4.9745507302
C31	0.2885216435	1.3253995625	-4.9644317371	C27	-0.0892797055	2.1342758235	-2.6629719555
C32	-1.9927587039	1.8320894171	-4.4583463392	C28	-0.5863483588	1.2099374216	-5.2764606984
H33	1.0529764797	1.0168258674	-5.6742441815	C29	-1.4024048400	1.7771316504	-3.0453957725
H34	-3.0346305460	1.9100012320	-4.7622594712	C30	0.9579004280	2.1187344861	-3.6044663935
C35	0.8006145936	-1.2299824834	2.7532223938	C31	0.6839401100	1.6396631141	-4.8925923438
C36	1.8796559495	-2.4526491324	5.0478558099	C32	-1.6206378972	1.3031043528	-4.3400990938
C37	1.9987106762	-1.9651913616	2.6754444191	H33	1.4944403355	1.6179280726	-5.6180321574
C38	0.1639006406	-1.1147424452	4.0073966950	H34	-2.6285491454	1.0101872973	-4.6278917595
C39	0.6926532581	-1.7235718200	5.1419136512	C35	0.7658566689	-1.1012317527	2.7718281621
C40	2.5269316780	-2.5665885831	3.8155694756	C36	1.4455529057	-2.5145814039	5.1124574094
H41	2.5054572500	-2.0553197122	1.7207542922	C37	1.9353234516	-1.8860584407	2.8220099083
H42	-0.7515368690	-0.5342827171	4.0856256952	C38	-0.0406002779	-1.0289248219	3.9306232576
H43	0.1826335458	-1.6273518466	6.0969525078	C39	0.2896506685	-1.7319438869	5.0853501928
H44	3.4553095597	-3.1258803854	3.7399550965	C40	2.2632049247	-2.5833278912	3.9821509658
H45	2.3004831368	-2.9250856398	5.9317803602	H41	2.5703379227	-1.9431925048	1.9453651113
C46	2.1704345652	1.6830345481	-3.3636709382	H42	-0.9284049600	-0.4026664284	3.9197474865
H47	2.5116933722	0.7007754966	-3.0230841743	H43	-0.3498963401	-1.6671967937	5.9617581158
H48	2.4311984188	2.3849631214	-2.5722665298	H44	3.1690765709	-3.1827439795	4.0038473543
H49	2.7359898105	1.9385058266	-4.2648996251	H45	1.7116416103	-3.0619731109	6.0131355409
C50	-2.7233133334	2.7151338664	-2.2342236625	C46	2.3459149233	2.6288508775	-3.3049061248
H51	-3.7065010667	2.3480445083	-2.5428664565	H47	3.0244462271	1.8073690180	-3.0586897797
H52	-2.7710712135	3.8123676649	-2.2587827349	H48	2.3651945067	3.3021678102	-2.4473865051
H53	-2.5619468043	2.4219340103	-1.1953472721	H49	2.7460553952	3.1540106221	-4.1781340929
C54	-1.4464384280	0.9423983269	-6.7663982429	C50	-2.5925332186	1.9549756103	-2.1248012760
H55	-1.6630215637	-0.1330303231	-6.7965239356	H51	-3.3367109813	1.1632361861	-2.3016953787
H56	-0.6493836133	1.1322695142	-7.4917519298	H52	-3.0926223517	2.9063528408	-2.3074721109
H57	-2.3468027116	1.4653188429	-7.1034337436	H53	-2.3154274560	1.9180058146	-1.0695878265
C58	2.3960357705	3.2232643015	2.5241421955	C54	-0.8405715689	0.6599254425	-6.6601697308
H59	3.1589991639	3.0163917425	3.2796300966	H55	-0.7249126271	-0.4308325506	-6.6746217317
H60	2.4527648793	4.2966016119	2.2965491413	H56	-0.1373524788	1.0710445535	-7.3905242457
H61	2.6482657664	2.6710349236	1.6175890874	H57	-1.8566281210	0.8832762553	-7.0007181972
C62	-2.5500543564	2.1765762002	1.8101139865	C58	2.7740806623	3.4025667183	2.3535608803
H63	-2.7624163593	3.0638617382	1.2021672874	H59	3.6043335359	3.1879066138	3.0320970099
H64	-3.4435059256	1.9650528053	2.4033953590	H60	2.8096595385	4.4781401868	2.1314832951
H65	-2.4050384186	1.3434882005	1.1146301087	H61	2.9437507954	2.8588336478	1.4232181639
C66	-0.6507980426	2.5046041720	6.4702946717	C62	-2.2484421276	2.5607267061	2.1094145037
H67	-0.0718987628	3.2782805810	6.9849860972	H63	-2.4652160714	3.4878526788	1.5647939710
H68	-0.3191563629	1.5366488428	6.8662857921	H64	-3.0919131236	2.3689678367	2.7778172073
H69	-1.7028572667	2.6297366347	6.7429456963	H65	-2.2214060151	1.7585296441	1.3658689642
C71	-1.8351256875	-0.7434896847	-1.7845351733	C66	0.1119161437	2.6448696566	6.5636849834
H72	-2.3163279387	0.1024907519	-1.2866718548	H67	0.8815422619	3.2618287839	7.0374162448
H73	-1.5469142663	-0.4408353784	-2.7915314522	H68	0.2803042640	1.6096412248	6.8852475212
H74	-2.5891979135	-1.5394466912	-1.8887828379	H69	-0.8623673500	2.9548165618	6.9545335715
C75	-0.7085495772	-3.0053246738	0.8766921313	C70	-1.9761759060	-1.3674463110	0.8526845002
H76	0.2761526187	-3.3908457516	0.6071369176	H71	-2.4477586887	-0.3845976962	0.7613114850
H77	-0.8612520816	-3.1272040751	1.9516566759	H72	-2.6014185522	-2.0830470823	0.3043327834
H78	-1.4673115949	-3.5975532640	0.3514652895	H73	-1.9746237010	-1.6634845655	1.9049341568
				C74	-0.1355072117	-1.6515344720	-2.3215205614
				H75	0.6048964530	-2.4192937975	-2.1029479339

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H76	-1.0611995068	-2.1280791185	-2.6791093832	H72	-0.8001014337	-3.7526002960	0.2962452387
H77	0.2397992439	-1.0258847639	-3.1370775609	H73	0.8584521595	-3.4528443653	0.8523114514
X78	-0.8399851012#	-0.7962469217#	-0.4672036374#	H74	-0.4927486090	-3.3829570711	2.0072900214
		2F _z		Xpi	-0.0760662611#	-1.0472814464#	0.4539861360#
Ru1	1.2362938659	-0.1386754762	0.1469350590	C75	-1.2137937036	-1.0730025248	-1.7201895626
Cl2	3.1287627115	1.2426933570	-0.0129394145	H76	-1.8510383547	-0.2831918921	-1.3181545836
C3	0.2471546305	1.7629183065	0.0185324540	H77	-0.8911828674	-0.7900750951	-2.7243225514
N4	0.1430623722	2.6881432424	1.0163402317	H78	-1.8276926011	-1.9814742557	-1.8238812375
N5	0.0768245358	2.4443440235	-1.1563811235			2F _E	
C6	-0.1261705259	4.0595657257	0.5277020594	Ru1	1.3279742989	-0.0458463597	0.1948414861
H7	-1.1493753948	4.3582140807	0.7913694898	Cl2	3.2070372949	1.3084182226	-0.1100840923
H8	0.5645090133	4.7689767940	0.9898051319	C3	0.3129999498	1.8285491104	0.0808163069
C9	0.0852059928	3.9136937611	-0.9747610561	N4	0.1621859212	2.7628035319	1.0622493369
H10	1.0525514399	4.3139719230	-1.3014729583	N5	0.0171580649	2.4535238534	-1.0966819004
H11	-0.6988946341	4.3850266815	-1.5716748746	C6	-0.0683034163	4.1285418160	0.5375814895
Cl2	0.3116791315	-0.7111863687	1.8161106179	H7	-0.8839581716	4.6163473136	1.0787145523
Cl13	2.8610720121	-1.9916886713	-0.2028988605	H8	0.8392061609	4.7288118656	0.6710364697
C14	-0.0304176647	-1.3794829992	-0.8415151144	C9	-0.3859939125	3.8670945572	-0.9330666010
C15	-0.3734229772	-1.6699653976	0.6721989281	H10	0.1822871738	4.5040506322	-1.6166030873
C16	0.0205348534	2.5140063998	2.4420759993	H11	-1.4518296789	3.9853103177	-1.1646910408
C17	-0.3347777980	2.4183952099	5.2328598849	Cl2	0.2350702564	-0.7016040134	1.7653973702
C18	1.0871539510	2.8674824578	3.2895163672	Cl13	2.9027914270	-1.9410874884	-0.0225150780
C19	-1.2404761533	2.1711367543	2.9768817766	C14	-0.0654983653	-1.0193198152	-0.9010189471
C20	-1.3912070017	2.1240338048	4.3650744796	C15	-0.2830900425	-1.6119813299	0.5411617395
C21	0.8865618362	2.7936780400	4.6737040284	C16	0.1486040180	2.6294516398	2.4983818307
H22	-2.3612861900	1.8553628943	4.7783779825	C17	-0.0246294393	2.6096456406	5.3088913776
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C24	-0.2205806827	1.9693854741	-2.4869036199	C19	-1.0952246590	2.3859845405	3.1245492260
C25	-0.9285027905	1.2153392360	-5.1096655029	C20	-1.1570786333	2.3790083839	4.5196360814
C26	-1.5826188348	1.9373559207	-2.8712163317	C21	1.1768021611	2.8930929982	4.6613472911
C27	0.7902726788	1.7050890425	-3.4285481951	H22	-2.1145544179	2.1929180412	5.0020131383
C28	0.4060000962	1.3107830296	-4.7190405933	H23	2.0627853722	3.1073243284	5.2551401269
C29	-1.9101983486	1.5551297812	-4.1723055702	C24	-0.1813118688	1.8858662720	-2.4076190796
H30	1.1885722272	1.0944260671	-5.4432890922	C25	-0.6615393334	0.8932736495	-4.9994686020
H31	-2.9585683013	1.5186503411	-4.4605158334	C26	-1.4729101345	1.4296419765	-2.7589608898
C32	0.9243295283	-1.3318408594	3.0288086788	C27	0.8471217704	1.9271448653	-3.3672734478
C33	1.8939707852	-2.4120486862	5.4481975549	C28	0.5827441714	1.4140311927	-4.6449665249
C34	2.1667479979	-1.9883604732	3.0744394340	C29	-1.6825286281	0.9267754896	-4.0441075540
C35	0.1876446838	-1.2220137471	4.2254163420	H30	1.3809332401	1.4338931165	-5.3839111296
C36	0.6599058730	-1.7613324196	5.4195659323	H31	-2.6713506214	0.5561077153	-4.3069822308
C37	2.6411098331	-2.5182797932	4.2738597665	C32	0.6732650409	-1.4237375942	2.9918095426
H38	2.7593230283	-2.0684459155	2.1697739611	C33	1.2622877707	-2.7674233234	5.4043038250
H39	-0.7672712928	-0.7042965240	4.2146939257	C34	1.6339617794	-2.4523767601	3.0276064872
H40	0.0664252031	-1.6708447259	6.3259357014	C35	0.0235123197	-1.0847924588	4.1959551953
H41	3.6077586746	-3.0147746519	4.2883797974	C36	0.3127050829	-1.7462128083	5.3877977415
H42	2.2725300909	-2.8275406578	6.3786675301	C37	1.9179116137	-3.1132616599	4.2201921718
C43	2.2623655292	1.8581801524	-3.1402257443	H38	2.1733825094	-2.7058036084	2.1213840374
H44	2.7097273091	0.9155384360	-2.8102221328	H39	-0.7188073062	-0.2927968018	4.1927060107
H45	2.4578414093	2.5795941517	-2.3474260669	H40	-0.2091060010	-1.4675601785	6.3000169230
H46	2.7861304712	2.1770512936	-4.0466787354	H41	2.6652487378	-3.9022621493	4.2248460980
C47	-2.6924412150	2.3128390641	-1.9145804972	H42	1.4919884098	-3.2876717398	6.3306634858
H48	-3.6639294927	2.0161658067	-2.3190254978	C43	2.2080120317	2.5184093318	-3.0949450337
H49	-2.7335570782	3.3959576641	-1.7402475366	H44	2.9282933118	1.7410163945	-2.8238184212
H50	-2.5736933056	1.8390012901	-0.9368597853	H45	2.1964307466	3.2228026937	-2.2625629652
C51	-1.3044431798	0.7577141211	-6.4993785425	H46	2.5787108845	3.0302772957	-3.9884594446
H52	-1.4503966396	-0.3292873253	-6.5280661039	C47	-2.6461068675	1.5031834886	-1.8052674277
H53	-0.5223065944	0.9990138633	-7.2254642193	H48	-3.3650770962	0.7047594186	-2.0119425539
H54	-2.2377669235	1.2197283421	-6.8359677948	H49	-3.1855049061	2.4531686001	-1.9166151482
C55	2.4057319564	3.3764077043	2.7607286156	H50	-2.3420085421	1.4237940218	-0.7598390013
H56	3.2011076922	3.2113504895	3.4926902756	C51	-0.9027793393	0.3013179590	-6.3681691593
H57	2.3568731447	4.4592011174	2.5793962424	H52	-0.7528259733	-0.7853718344	-6.3554011803
H58	2.6900128637	2.8884280490	1.8280020195	H53	-0.2160502818	0.7158913056	-7.1118260768
C59	-2.4291146753	1.8727008558	2.0898866796	H54	-1.9269426095	0.4827161321	-6.7096343440
H60	-2.6992564277	2.7325189486	1.4659961488	C55	2.5884212547	3.3926463180	2.6508995124
H61	-3.3039669143	1.6171423808	2.6937322921	H56	3.4361282692	3.0651906681	3.2597531607
H62	-2.2390298579	1.0359832934	1.4089823640	H57	2.6242176479	4.4902252866	2.6137030750
C63	-0.5037955185	2.3107844163	6.7299923855	H58	2.7326618605	3.0062712186	1.6428032237
H64	0.0754479341	3.0761461105	7.2560969381	C59	-2.3595150303	2.1685816295	2.3234695169
H65	-0.1539970582	1.3349824331	7.0898567853	H60	-2.5840724782	3.0215240862	1.6722012852
H66	-1.5523414353	2.4138965341	7.0253730855	H61	-3.2158692694	2.0272153451	2.9883430104
H67	-0.4513771016	-0.0114267960	2.1381624694	H62	-2.2936916432	1.2872232056	1.6771243725
H68	-1.4178482028	-1.3619763865	0.7605309786	C63	-0.1017923456	2.5405716340	6.8157985151
H69	0.5791012187	-2.1856095286	-1.2496298354	H64	0.6099135585	3.2255600686	7.2866943113
C71	-0.1848629058	-3.1605362188	0.9817144789	H65	0.1364593094	1.5300816471	7.1708373553

H66	-1.1044169336	2.7871841343	7.1788412340	H61	2.6573823693	2.5069059582	1.6518840301
H67	-0.5415262443	0.0090742751	2.0362768620	C62	-2.5402761327	2.1672879459	1.8069378270
H68	0.2381604785	-2.5665319758	0.6024766393	H63	-2.7158031983	3.0201409213	1.1406066530
H70	-0.9078591205	-0.3932479775	-1.1829099034	H64	-3.4482289243	2.0180866552	2.3971289168
X71	-0.0738597041#	-1.1097588880#	0.4462769003#	H65	-2.4060710471	1.2875724474	1.1693026152
C72	-1.8026238021	-1.7891855867	0.7608116506	C66	-0.7069815548	2.7842233624	6.4655973372
H73	-2.2058913295	-2.4749137566	0.0086922015	H67	-0.0402757887	3.5092008495	6.9432831756
H74	-1.9899266613	-2.2107062148	1.7532809886	H68	-0.5136053679	1.8098325299	6.9320372099
H75	-2.3399966924	-0.8399007511	0.6795276442	H69	-1.7383105416	3.0606768767	6.7058139218
C75	0.2641086622	-2.0067059073	-1.9991044072	C70	-1.9814140408	-0.6608371852	-1.7832566908
H76	1.0971505297	-2.6566034035	-1.7345991213	H71	-2.4682078988	0.0903950476	-1.1578407608
H77	-0.6241036063	-2.6179057466	-2.2244044346	H72	-2.1124523338	-0.3946204788	-2.8377559478
H78	0.5185160206	-1.4645820508	-2.9156458563	H73	-2.5018799237	-1.6226134268	-1.6484080840
		2TS _{FGZ}		C74	-0.8621419092	-3.0866711450	0.7385081518
				H75	0.1399810802	-3.4636357981	0.5406090333
Ru1	0.7357538524	-0.2893737038	-0.2316360532	H76	-1.2252589841	-3.5223481220	1.6796922962
Cl2	2.8943823617	0.8174086420	-0.1907367366	H77	-1.5163765725	-3.4362935787	-0.0657521229
C3	0.1117204855	1.7565428309	-0.2306156340	Xpi	-0.4942870064#	-1.1963116814#	1.2357167533#
N4	0.1226521471	2.6872574560	0.7664534244				
N5	0.0505039672	2.4571895422	-1.4088345378			2TS _{FGZ}	
C6	0.0488810047	4.0824807563	0.2738077981	Ru1	1.2643440057	0.1105579255	-0.0909633786
H7	-0.9240177044	4.5186260367	0.5356752839	Cl2	3.2996568752	2.1992890523	-0.3978400908
H8	0.8289985926	4.6897722587	0.7386064604	C3	0.3735599703	2.0409408971	-0.3645477950
C9	0.2416847566	3.9116548435	-1.2279600375	N4	0.3119118420	3.0045917653	0.6019007218
H10	1.2501751620	4.1910699286	-1.5556820889	N5	0.0996720825	2.6781112422	-1.5450516382
H11	-0.4805265761	4.4764857653	-1.8225609484	C6	0.1598315160	4.3755312137	0.0669508511
C12	-0.1582756353	-0.7924978740	1.7495709672	H7	-0.6121414574	4.9188284033	0.6196031634
H13	-0.6532925651	0.1119555676	2.0759478704	H8	1.1047336340	4.9207197020	0.1697601452
Cl14	2.0220475688	-2.3468129845	-0.8219750962	C9	-0.2081063395	4.1165474098	-1.3904332677
C15	-0.5367856822	-0.8770765343	-1.4888414987	H10	0.3817696598	4.7087734300	-2.0954704636
H16	-0.0796915097	-1.6016337413	-2.1761761973	H11	-1.2699679433	4.2993246982	-1.5983890995
C17	-0.9105754001	-1.5827453695	0.8513080166	C12	-0.1729457062	-0.7001264540	1.3842372656
H18	-1.8750254222	-1.1494860288	0.6068646857	H13	-0.8353693694	0.1205079441	1.6419480657
C19	-0.0470807522	2.5659758465	2.1926821105	Cl14	2.6971027809	-1.8733840901	0.3130946313
C20	-0.4823775243	2.7274756555	4.9719858585	C15	0.4797622842	-0.6255125866	-1.6272808225
C21	1.0352648141	2.8406004209	3.0505489329	H16	-0.4264630897	-0.1812780694	-2.0376418241
C22	-1.3506156354	2.3990128162	2.7104577598	C17	-0.5172733998	-1.4303085081	0.2129009226
C23	-1.5410048997	2.4726848066	4.0932438116	H18	-0.0262664624	-2.3937466025	0.0994292804
C24	0.7900266811	2.9066875570	4.4281772131	C19	0.3252524245	2.8849497201	2.0362911458
H25	-2.5445393686	2.3398767346	4.4919910534	C20	0.2146003021	2.8896206090	4.8494259494
H26	1.6273923624	3.1111401284	5.0919129942	C21	1.4726306231	3.2344809845	2.7732556158
C27	-0.2536668614	2.0197780210	-2.7506921432	C22	-0.8995236529	2.6226924841	2.6928485976
C28	-0.9500785868	1.3386351070	-5.3985707424	C23	-0.9263011208	2.6116226331	4.0878788396
C29	-1.5905713011	2.1622276118	-3.1904997461	C24	1.3911569098	3.2116451943	4.1733412668
C30	0.7538220837	1.6317475679	-3.6577033023	H25	-1.8644278219	2.3940480204	4.5938785973
C31	0.3719110893	1.2772792318	-4.9590213724	H26	2.2817457552	3.4625641725	4.7454133002
C32	-1.9148354584	1.8093748287	-4.5024326313	C27	-0.1677846192	2.1325022214	-2.8496649892
H33	1.1480281471	0.9613276154	-5.6527082337	C28	-0.7449693706	1.1804813981	-5.4348812149
H34	-2.9477767128	1.9051834752	-4.8311859373	C29	-1.4896203148	1.7733813051	-3.1848589266
C35	0.8245023325	-1.2734810027	2.7586025838	C30	0.8547483588	2.0955761624	-3.8197455788
C36	2.4742880462	-2.1216722526	4.8840770462	C31	0.5425848939	1.6041775866	-5.0919194856
C37	1.7829052866	-2.2844271235	2.5648832386	C32	-1.7492232050	1.2883966165	-4.4710767870
C38	0.7251602939	-0.6895567475	4.0367301605	H33	1.3317429889	1.5622048806	-5.8393731898
C39	1.5329826477	-1.1125475178	5.0888482992	H34	-2.7657684235	0.9926928118	-4.7234580226
C40	2.5951072582	-2.6979254175	3.6191160367	C35	0.4767090641	-1.3234765538	2.5723038638
H41	1.9344411922	-2.7043181624	1.5777189728	C36	1.5758999229	-2.4465149621	4.9103914211
H42	-0.0058251279	0.0943040543	4.2063456951	C37	0.4460230561	-2.7106548601	2.7889046086
H43	1.4300901953	-0.6496037379	6.0670439472	C38	1.0514769654	-0.5103750784	3.5611466759
H44	3.3383742145	-3.4704473139	3.4421066037	C39	1.6030156062	-1.0657471205	4.7131722379
H45	3.1148030394	-2.4478818130	5.6994459264	C40	0.9899851044	-3.2652972295	3.9439613165
C46	2.2208669083	1.6100649071	-3.3143915555	H41	-0.0089950481	-3.3643511428	2.0519358770
H47	2.5383472246	0.6240844098	-2.9613674914	H42	1.0853700642	0.5625614133	3.4164203134
H48	2.4727643500	2.3075062307	-2.5157959487	H43	2.0598742856	-0.4167248187	5.4557905365
H49	2.8115894045	1.8572702268	-4.2020096123	H44	0.9565207154	-4.3417668157	4.0891540831
C50	-2.6783018231	2.7109994295	-2.2941494920	H45	2.0047865019	-2.8814145943	5.8092186151
H51	-3.6631245514	2.3689310194	-2.6257897507	C46	2.2458544251	2.5989824970	-3.5288965670
H52	-2.6983979227	3.8088714958	-2.3201503955	H47	2.6991923645	2.0840424019	-2.6783392315
H53	-2.5468915811	2.4156701003	-1.2516136072	H48	2.2354898937	3.6680580329	-3.2817593277
C54	-1.3269662423	0.9093427920	-6.7970258700	H49	2.8895352330	2.4691100577	-4.4028948178
H55	-1.5215119769	-0.1699569659	-6.8372431254	C50	-2.6417026440	1.9224278685	-2.2165443846
H56	-0.5237666310	1.1190887367	-7.5099774411	H51	-3.3776711763	1.1254799408	-2.3594995877
H57	-2.2324893225	1.4169347741	-7.1430998311	H52	-3.1676911114	2.8726029064	-2.3774550279
C58	2.4264753645	3.1084076683	2.5330706127	H53	-2.3142690382	1.9022960639	-1.1763214412
H59	3.1682851610	2.8902038386	3.3061708139	C54	-1.0375572573	0.6166211994	-6.8055341507
H60	2.5458618753	4.1670832197	2.2653873515	H55	-0.8158896303	-0.4571818203	-6.8441829139

H56	-0.4283915578	1.0997112005	-7.5758540742	H52	-1.9377073275	1.0022574991	0.9735016133
H57	-2.0905742094	0.7422199386	-7.0749030442	C53	-4.7531139764	-0.7226151737	-3.7184132292
C58	2.7527516422	3.6953959703	2.1197396576	H54	-4.4868861723	-1.7859569449	-3.6629824257
H59	3.6122546916	3.4665141633	2.7560745376	H55	-4.8737098422	-0.4721815457	-4.7763555481
H60	2.7380921023	4.7851635408	1.9793424537	H56	-5.7243063065	-0.6070250956	-3.2268718544
H61	2.9171821872	3.2205767136	1.1517285621	C57	3.8094712791	3.5936281474	-0.8654505683
C62	-2.1882595085	2.4339694666	1.9243093604	H58	4.4823155239	2.7791047267	-1.1473963628
H63	-2.4801995641	3.3565575978	1.4067498065	H59	4.3417462324	4.5400522820	-1.0194917290
H64	-3.0036583428	2.1655329791	2.6010517837	H60	2.9662532371	3.5402946554	-1.5502969537
H65	-2.1158948576	1.6547511648	1.1614127515	C61	0.2804923057	3.4529715667	2.8410176154
C66	0.1679762757	2.8265879101	6.3576254447	H62	-0.0714136627	4.4896090544	2.9284085311
H67	0.9820573760	3.4007844369	6.8089856117	H63	0.1877345723	3.0009056436	3.8321395352
H68	0.2613803624	1.7902812433	6.7056811551	H64	-0.4037928446	2.9380466581	2.1642766917
H69	-0.7796070834	3.2137266321	6.7464857581	C65	5.1605264477	3.8287228262	3.9675595380
C70	-1.9152452648	-1.3318033716	-0.3622102997	H66	6.0973579252	4.1837518511	3.5287208460
H71	-2.2975387388	-0.3084523027	-0.3395516357	H67	5.3606260073	2.8628996076	4.4470317826
H72	-1.9888687504	-1.7097592352	-1.3858893841	H68	4.8675790308	4.5282690939	4.7580382971
H73	-2.5803238668	-1.9464004639	0.2590931391	H69	-0.8658895078	-0.9650390019	0.9307310070
C74	1.0349506259	-1.7056839958	-2.4977967574	C70	0.3710985286	-1.5220093435	-2.6698284506
H75	1.8434005526	-2.2608344348	-2.0247766765	H71	0.8059830552	-2.4872156938	-2.3592107235
H76	0.2336101354	-2.3805590338	-2.8343452156	H72	-0.5408122169	-1.7190752551	-3.2456264682
H77	1.4189020531	-1.2113160107	-3.4027484052	H73	1.1333120840	-1.0341297346	-3.2788582758
				X74	0.3721871241#	-0.8768727114#	1.5634465598#
		2G _Z		C75	0.5230053721	-2.5487006074	1.5419278086
Ru1	1.3466001006	0.1361744575	-0.4265395136	H76	0.3681302136	-3.1489157940	0.6416256922
Cl2	2.5426255006	0.9472238126	-2.3740037323	H77	1.5630379604	-2.6588096724	1.8415909001
C3	0.4271717670	2.0388295077	-0.4719441898	H78	-0.1210397565	-2.9598342588	2.3335368715
N4	0.9911119119	3.1665240151	0.0431391550				
N5	-0.6643400128	2.4342333744	-1.1828397913			2G _E	
C6	0.3495901305	4.4105080564	-0.4335191811	Ru1	1.2608544523	0.0104073905	-0.3885394857
H7	0.1358049945	5.0766459496	0.4065296537	Cl2	2.5464096580	0.8604826611	-2.2673344995
H8	1.0245369407	4.9333379721	-1.1213098078	C3	0.4351697031	1.9808506551	-0.4175996977
C9	-0.9116128473	3.8912724183	-1.1256239030	N4	1.0685905901	3.0899830876	0.0560238899
H10	-1.0441448134	4.2972008539	-2.1316107155	N5	-0.6342341164	2.4227940020	-1.138053762
H11	-1.8262863497	4.0963030707	-0.5550236703	C6	0.5170878241	4.3503863787	-0.4906098155
C12	0.7136559994	-0.0169229819	1.9265073949	H7	0.3869863146	5.0890853863	0.3042304064
H13	0.1000983521	0.8752456833	1.9797018544	H8	1.2116907529	4.7629086517	-1.2320169642
Cl14	2.9676989989	-1.6966022615	-0.4202666711	C9	-0.7988623949	3.8921735515	-1.1118905422
C15	0.0759909886	-0.7801635069	-1.4122729192	H10	-0.9535503898	4.2781973131	-2.1222410829
H16	-0.9412408966	-0.9394478964	-1.0381372095	H11	-1.6730363387	4.1630472280	-0.5057881032
C17	0.1361154424	-1.1132039729	1.3234871874	C12	0.4914415619	-0.2734624282	1.8792325932
C18	2.0621295039	3.2986208451	1.0003646645	H13	-0.3695439141	0.3732215362	2.0330465749
C19	4.0771638882	3.6872525480	2.9254498558	Cl14	2.8109926352	-1.9083770957	-0.4712809385
C20	3.3933358550	3.4825209894	0.5811395051	C15	-0.0168276192	-0.7750322910	-1.4651400591
C21	1.7170238034	3.4186749651	2.3671032421	H16	-1.0545070377	-0.8518850933	-1.1333586293
C22	2.7336252111	3.5954447431	3.3038181039	C17	0.2529326863	-1.4802829947	1.2476605265
C23	4.3778807596	3.6487238414	1.5657525364	H18	1.0366593557	-2.2302483287	1.2825454335
H24	2.4703569890	3.6636175132	4.3568729019	C19	2.1246636801	3.2218394187	1.0310221654
H25	5.4103514599	3.7714611109	1.2448669533	C20	4.0799311574	3.7091966839	2.9936194589
C26	-1.6642012673	1.6231039055	-1.8173055228	C21	3.4640854899	3.3960633835	0.6418965791
C27	-3.6947740883	0.1333039036	-3.0623248776	C22	1.7399305643	3.3906845802	2.3822687814
C28	-2.7314004018	1.1191285089	-1.0449641820	C23	2.7255096535	3.6202830206	3.3387408113
C29	-1.6299195799	1.4428105078	-3.2130221226	C24	4.4192992571	3.6106741903	1.6476795487
C30	-2.6517588999	0.6902448690	-3.8062338636	H25	2.4317951371	3.7357547986	4.3792138195
C31	-3.7233542818	0.3714194115	-1.6835572332	H26	5.4597393423	3.7270719259	1.3509911337
H32	-2.6240829629	0.5346514203	-4.8824281081	C27	-1.6764196171	1.6644891192	-1.7678842844
H33	-4.5407051795	-0.0326340649	-1.0898518042	C28	-3.7737584396	0.2674871766	-3.0102233569
C34	1.7815405048	-0.0592217348	2.9760663418	C29	-2.7898842917	1.2569494082	-1.0039260063
C35	3.5869792338	-0.1377146443	5.1415114986	C30	-1.6307598029	1.4445946146	-3.1578417885
C36	3.1088178628	-0.4649177333	2.7838049003	C31	-2.6866544922	0.7391824954	-3.7496377533
C37	1.3770794605	0.3063456838	4.2742577422	C32	-3.8134591669	0.5508734742	-1.6400856070
C38	2.2646272465	0.2620764666	5.3468458619	H33	-2.6503956931	0.5520669077	-4.8205393981
C39	3.9998962074	-0.4983396360	3.8594686276	H34	-4.6658909333	0.2175955287	-1.0517275884
H40	3.4407182454	-0.7659703742	1.7958883548	C35	1.5697065426	-0.0850143039	2.8945552391
H41	0.3459959768	0.6075686328	4.4458203935	C36	3.3921869549	0.1046675786	5.0380137119
H42	1.9232898832	0.5372533433	6.3417206126	C37	2.9015778824	-0.5014758901	2.7395496861
H43	5.0250234389	-0.8157579410	3.6869132378	C38	1.1718561205	0.4249778446	4.1442743506
H44	4.2845421508	-0.1723580150	5.9744871097	C39	2.0678004211	0.5111081238	5.2075149030
C45	-0.5330689194	2.0386038237	-4.0615298674	C40	3.8005277549	-0.3962331287	3.8011805101
H46	0.4588409921	1.8003951648	-3.6645767070	H41	3.2310124077	-0.9216030615	1.7939954179
H47	-0.6152319632	3.1324961899	-4.1085932933	H42	0.1384913729	0.7303909708	4.2897782798
H48	-0.5971443701	1.6651019535	-5.0870830898	H43	1.7300054178	0.8918993199	6.1682550883
C49	-2.8206317135	1.3701185671	0.4428075546	H44	4.8278894294	-0.7207154909	3.6586038247
H50	-3.6969765830	0.8723124527	0.8659963058	H45	4.0958050217	0.1706159623	5.8639069253
H51	-2.9079459268	2.4388780898	0.6718085019	C46	-0.4910504792	1.9576443933	-4.0045450132

H47	0.4832357234	1.7113162580	-3.5713244007	H43	2.4024743482	-0.8073861281	2.7669628796
H48	-0.5375586856	3.0498883801	-4.1098420084	H44	4.0087454879	-1.4392257166	2.3635390975
H49	-0.5415357664	1.5343015684	-5.0114125731	H45	3.0773819095	-2.1637428756	3.6784023385
C50	-2.9014876212	1.5784411810	0.4686607175	C46	1.8875711493	-3.2048845123	-2.0634439925
H51	-3.7457466534	1.0481250583	0.9180916343	H47	1.1200688278	-3.7971117900	-2.5676320922
H52	-3.0633608638	2.6506074678	0.6373631418	H48	2.8630455832	-3.5480006884	-2.4357412165
H53	-1.9964006185	1.3027983005	1.0153028683	H49	1.7427648630	-2.1678061624	-2.3626453809
C54	-4.8683534819	-0.5457298473	-3.6610258842	C50	0.9135025462	-6.2329620268	1.8430145153
H55	-4.6749020002	-1.6206045582	-3.5522415064	H51	-0.1183584911	-6.1395039657	2.2036977711
H56	-4.9427982052	-0.3352530020	-4.7317864374	H52	1.5193809520	-6.5827286865	2.6853539670
H57	-5.8429647567	-0.3456977238	-3.2045826737	H53	0.9218156910	-7.0081993168	1.0713019522
C58	3.9288049465	3.4443911674	-0.7930611885	C54	2.8295115866	2.9167481128	1.3786080937
H59	4.5789368067	2.5956504056	-1.0253234737	H55	2.8378323188	3.8016403550	2.0202721972
H60	4.5021386699	4.3641217654	-0.9606244333	H56	3.7896111426	2.4044747941	1.5100650307
H61	3.1068598917	3.3967165281	-1.5037248543	H57	2.0493967146	2.2397815913	1.7440073428
C62	0.2849462144	3.4069314614	2.7919545167	C58	2.1520281657	1.6457807855	-3.4998361537
H63	-0.2233495875	4.3092529690	2.4261765558	H59	3.0753571679	1.0616125419	-3.5909463474
H64	0.1925650142	3.4021868183	3.8806812338	H60	1.9594013892	2.1138823372	-4.4686209034
H65	-0.2684150286	2.5506084860	2.4009469692	H61	1.3410792263	0.9380686708	-3.2944201360
C66	5.1301411667	3.9168591598	4.0585427244	C62	1.8543258046	6.4871095728	-2.0586931607
H67	6.0844433203	4.2321221888	3.6270112425	H63	2.7265036707	7.1008850427	-1.8051187800
H68	5.3052222117	2.9874669992	4.6140986042	H64	1.0045316569	6.8914763744	-1.4963883124
H69	4.8187498418	4.6745242902	4.7863215372	H65	1.6467914977	6.6237218274	-3.1236190514
C70	-1.1292029042	-2.0193091135	0.9906428747				
H71	-1.8781079127	-1.2348526628	0.8496025334				
H72	-1.1630284523	-2.7017923662	0.1363287407	Ru1	-0.0202058559	0.0394450632	-0.0355682157
H73	-1.4269554014	-2.6025949369	1.8733257091	Cl2	-0.0755530866	-0.0310087915	2.3466757646
C74	0.2825052234	-1.4992600277	-2.7312253933	C3	1.9358910343	-0.0048117443	-0.3225283902
H75	0.6923220267	-2.4793308104	-2.4348145335	N4	2.7947522728	0.9595854028	-0.7441591840
H76	-0.6187947666	-1.6581613916	-3.3339286175	N5	2.6531157525	-1.1538689654	-0.1700949120
H77	1.0735197638	-1.0174366331	-3.3091069965	C6	4.1958074809	0.4920847813	-0.8025591535
				H7	4.6526015325	0.7773201295	-1.7541614593
				H8	4.7793390553	0.9495064885	0.0060196901
				C9	4.0466488280	-1.0232077930	-0.6359638528
				H10	4.7379288139	-1.4453260296	0.0984589048
				H11	4.1775185954	-1.5634474453	-1.5815095967
				Cl2	-0.4816119843	1.7811880397	-0.2575266390
				H13	0.1962600879	2.6067708844	-0.4715930653
				Cl14	-0.6157181682	-0.7944303025	-2.1887423468
				C15	2.5408686025	2.3486678316	-0.9934541660
				C16	2.1853157985	5.0774790743	-1.5187126330
				C17	2.6325316907	3.2705947670	0.0684523054
				C18	2.2791465054	2.7647619360	-2.3095646434
				C19	2.1033121060	4.1338379484	-2.5453978705
				C20	2.4491050699	4.6254576843	-0.2194969627
				H21	1.8946182207	4.4669780384	-3.5593836966
				H22	2.5112125923	5.3462284044	0.5932273262
				C23	2.1849212479	-2.4379876595	0.2872155837
				C24	1.3793598705	-4.9616852277	1.2089949437
				C25	1.7637763741	-3.4080642236	-0.6416365437
				C26	2.3079658868	-2.7469331843	1.6602489670
				C27	1.8872778174	-4.0041024126	2.0941167280
				C28	1.3455779220	-4.6517237354	-0.1507332566
				H29	1.9674718659	-4.2451840371	3.1516069265
				H30	1.0000072876	-5.4002911347	-0.8603354429
				C31	2.9204816582	-1.7765417523	2.6410617521
				H32	2.2965739521	-0.8874241651	2.7589375660
				H33	3.9168643797	-1.4515830778	2.3178393944
				H34	3.0292440380	-2.2465884995	3.6221393866
				C35	1.8375086162	-3.1940204646	-2.1347912576
				H36	1.0509585944	-3.7559892848	-2.6445608682
				H37	2.8004996916	-3.5575456118	-2.5197175455
				H38	1.7194291246	-2.1483139266	-2.4148098434
				C39	0.8904148554	-6.2968385253	1.7190227357
				H40	-0.1371756391	-6.2193943763	2.0956248678
				H41	1.5101862808	-6.6606366614	2.5451343829
				H42	0.8946635394	-7.0545682141	0.9300978512
				C43	2.8741598877	2.8145142922	1.4886051357
				H44	2.9112811457	3.6717474985	2.1657515706
				H45	3.8213025643	2.2725262182	1.5913814650
				H46	2.0801709801	2.1428993324	1.8335889836
				C47	2.1567165315	1.7687392720	-3.4378291358
				H48	3.0735819964	1.1806437835	-3.5634862311
				H49	1.9607705246	2.2812948900	-4.3831187475
				H50	1.3414459703	1.0598041414	-3.2561677881

C51	1.9909857180	6.5511934525	-1.7922401961	H17	-3.6555470025	0.9281557420	0.2365315535
H52	2.8593484781	7.1341418127	-1.4643844303	H18	-0.1061534513	3.3139818276	-0.1817889959
H53	1.1201312959	6.9434478615	-1.2538893548	H19	-1.4779121635	5.3462790810	-0.2074653399
H54	1.8395646141	6.7444897249	-2.8577007476				
C55	-1.9337694635	2.1172035282	-0.1173354695				
H56	-2.5645668996	1.2459935229	0.0917817837				
H57	-2.0687541033	2.8384393275	0.7014125241				
H58	-2.2983083556	2.5884212117	-1.0410581995				

1Z

H1	-0.0006076762	0.0079556680	0.0011924010
C2	-0.0017341799	0.0043026873	1.0920835025
H3	1.0414117584	0.0099416115	1.4282164234
H4	-0.4384011192	0.9512010699	1.4296543966
C5	-0.7443638026	-1.1637732033	1.6790791980
H6	-0.7622599617	-1.1958300197	2.7677878265
C7	-1.3742158020	-2.1492302271	1.0287890261
H8	-1.8599209494	-2.9131983074	1.6345382345
C9	-1.5011793565	-2.3432841603	-0.4566667947
H10	-2.5550333514	-2.3609740929	-0.7572047807
H11	-1.0792328135	-3.3083139214	-0.7597055339
H12	-1.0024859528	-1.5647243788	-1.0356607769

1E

H1	-1.1722991223	0.0001957084	2.0240476673
C2	-0.0804702498	-0.0001388298	1.9639439927
H3	0.2891447820	-0.8780823801	2.5068622448
H4	0.2896403519	0.8775813021	2.5068860942
C5	0.3952360745	-0.0002006108	0.5379652521
H6	1.4765891163	-0.0005930509	0.3935230544
C7	-0.3952360745	0.0002006108	-0.5379652521
H8	-1.4765891163	0.0005930509	-0.3935230544
C9	0.0804702498	0.0001388298	-1.9639439927
H10	-0.2891447820	0.8780823801	-2.5068622448
H11	-0.2896403519	-0.8775813021	-2.5068860942
H12	1.1722991223	-0.0001957084	-2.0240476673

2Z

C1	0.3370253597	0.6159732533	-0.1206861753
C2	-0.9823290005	0.8013937560	-0.2740797387
H3	-1.5684132961	-0.0836560975	-0.5200081409
C4	-3.4599610541	4.2757722619	0.1340620056
C5	-3.9842057827	2.9921428488	0.2758539086
C6	-3.1593085096	1.8827568163	0.1371124690
C7	-1.7883995555	2.0219350195	-0.1364120131
C8	-1.2783375221	3.3216717773	-0.2970468777
C9	-2.1056275226	4.4331734901	-0.1589559602
H10	-4.1043888936	5.1424717097	0.2396828294
H11	-5.0398270104	2.8554286326	0.4938109316
H12	-3.5739825949	0.8853578523	0.2444211409
H13	-0.2341523489	3.4670348732	-0.5658392997
H14	-1.6888163480	5.4264263153	-0.2918711513
H15	0.6954171579	-0.3963924979	-0.2844853456
C16	1.3987330059	1.6022747691	0.2753353852
H17	2.2129739861	1.0858488614	0.8006587142
H18	1.8561637359	2.0990606222	-0.6075305795
H19	1.0080152438	2.3828944543	0.9242263069

2E

C1	0.3168691466	0.5512442863	-0.0462109304
C2	-1.0096816918	0.7011064619	0.0502045225
H3	-1.6163284642	-0.1973157784	0.1569124703
H4	0.9508914315	1.4287850835	-0.1541063152
C5	1.0311915427	-0.7664624854	-0.0179288413
H6	1.7469408071	-0.8105182365	0.8116068620
H7	0.3340734186	-1.6009843620	0.0900898223
H8	1.6094587116	-0.9224940588	-0.9363723738
C9	-3.3483481820	4.2992949046	-0.0005057020
C10	-3.9527603562	3.0510181908	0.1243150630
C11	-3.1742431290	1.8964005890	0.1388313560
C12	-1.7760721111	1.9566664092	0.0293225471
C13	-1.1831869731	3.2252102063	-0.0954850643
C14	-1.9583579956	4.3784915509	-0.1101521856
H15	-3.9502414590	5.2012279523	-0.0123361100
H16	-5.0313628324	2.9744855044	0.2105200222