

Supporting information

Dimerization of pentacyclopentacorannulene C₃₀H₁₀ as a strategy to produce C₆₀H₂₀ as precursor for C₆₀

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Content: Coordinates of all structures of C₆₀H₂₀ plotted on Figs. 3 and 4

Fig. 3 a)

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frame 1

H	-2.21433303	4.00755012	-1.66555100
H	0.34548698	4.56590285	-1.66601925
H	-4.22996914	1.73908049	-1.66514650
H	-4.49639099	-0.86713205	-1.66430000
H	-2.96127777	-3.48851090	-1.66393975
H	-0.56241929	-4.54304531	-1.66468250
H	2.40484016	-3.89756939	-1.66546375
H	4.14790242	-1.94187383	-1.66501525
H	4.44658202	1.08272686	-1.66483275
H	3.12665749	3.34496442	-1.66530525
H	0.56414580	4.54372845	1.66555100
H	2.96327520	3.49082085	1.66601925
H	-2.39991105	3.89325915	1.66514650
H	-4.14734415	1.94138775	1.66430000
H	-4.44621930	-1.08166920	1.66393975
H	-3.12534180	-3.34481910	1.66468250
H	-0.34537725	-4.56672945	1.66546375
H	2.21431875	-4.00908480	1.66501525
H	4.23377130	-1.73769090	1.66483275
H	4.49563980	0.86832990	1.66530525
C	1.05118586	0.61554807	-4.77178650
C	-0.26266211	1.19052232	-4.77504900
C	-1.21623556	0.11959919	-4.77485400
C	-0.48918976	-1.11669512	-4.77140425
C	0.91142235	-0.81219479	-4.77482700
C	-0.50421319	2.30809907	-4.00659275

C	-1.75596884	2.50520734	-3.30265450
C	-2.69005354	1.45502252	-3.30359600
C	-2.35618372	0.23325920	-4.00975950
C	-2.92940194	-0.89730168	-3.30419250
C	-2.21694344	-2.10892018	-3.30288225
C	-0.95021198	-2.16606363	-4.00717725
C	-0.05151863	-3.06144335	-3.30341550
C	1.32194753	-2.76283262	-3.30377550
C	1.76513436	-1.57374439	-4.00652175
C	2.89591243	-0.99603548	-3.30249700
C	3.03296793	0.40317820	-3.30208225
C	2.03911510	1.19219218	-4.00497975
C	0.55374304	3.00925680	-3.30308925
C	1.84098167	2.44585057	-3.30327475
C	-1.48306338	3.57248641	-2.34477475
C	-0.13856351	3.86579601	-2.34505475
C	-3.71483546	1.06142561	-2.34405500
C	-3.85575156	-0.30766357	-2.34412750
C	-2.15856470	-3.20714388	-2.34332850
C	-0.89822051	-3.76090279	-2.34371275
C	2.38524124	-3.04810361	-2.34597550
C	3.30134926	-2.02051268	-2.34532000
C	3.63156766	1.32682505	-2.34421800
C	2.93939238	2.51531866	-2.34498675
C	1.21223730	-0.11988270	4.77178650
C	0.48727335	1.11754170	4.77504900
C	-0.91365660	0.81164310	4.77485400
C	-1.05213975	-0.61588680	4.77140425
C	0.25996005	-1.19280000	4.77482700
C	0.94874955	2.16366045	4.00659275
C	0.05191530	3.05888790	3.30265450
C	-1.32105825	2.75831175	3.30359600
C	-1.76908635	1.57364070	4.00975950
C	-2.89735665	0.99592695	3.30419250
C	-3.03313710	-0.40306560	3.30288225
C	-2.04191790	-1.19386170	4.00717725
C	-1.84115070	-2.44647780	3.30341550
C	-0.55447425	-3.01219980	3.30377550
C	0.50299995	-2.31070590	4.00652175
C	1.75738740	-2.50798425	3.30249700
C	2.69070480	-1.45655580	3.30208225
C	2.35043175	-0.23405805	4.00497975
C	2.21678430	2.10905790	3.30308925
C	2.92702035	0.89663280	3.30327475
C	0.90003135	3.76192500	2.34477475
C	2.16015765	3.20894025	2.34505475
C	-2.38147470	3.04223685	2.34405500
C	-3.30020865	2.01744885	2.34412750
C	-3.63142740	-1.32586140	2.34332850
C	-2.93727885	-2.51467350	2.34371275
C	0.13807035	-3.86797725	2.34597550

C	1.48322010	-3.57511350	2.34532000
C	3.71788815	-1.06115790	2.34421800
C	3.85648560	0.30720405	2.34498675

Fig. 3 b)

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frame 1

H	-2.26835040	4.25079210	-1.01593875
H	0.28385220	4.80415920	-1.00660350
H	-4.49735175	1.74907470	-1.01753675
H	-4.75209855	-0.84985860	-1.01219125
H	-3.06203355	-3.72284835	-0.99989450
H	-0.66991605	-4.77454050	-0.98928200
H	2.59323630	-4.07369160	-0.98905200
H	4.33365135	-2.12581035	-0.98603100
H	4.67233590	1.20215460	-0.99541950
H	3.34841940	3.45510930	-0.99630575
H	0.68584065	4.77254925	0.98700275
H	3.07732830	3.72261510	1.00133025
H	-2.59488450	4.06728495	0.98906925
H	-4.33543320	2.11966875	0.99604225
H	-4.66670670	-1.20430170	1.00122775
H	-3.34000200	-3.45466920	0.99641825
H	-0.27756600	-4.80330870	1.00500250
H	2.27488905	-4.25311965	1.02069800
H	4.49662515	-1.76475840	1.02423825
H	4.75595160	0.83409660	1.01282650
C	1.05395595	0.59793225	-3.77451325
C	-0.24902610	1.16063955	-3.75004900
C	-1.19115045	0.10301055	-3.74985400
C	-0.47594025	-1.12206525	-3.77664825
C	0.91142235	-0.81219480	-3.74982700
C	-0.49540695	2.28151680	-3.02262325
C	-1.77734895	2.51878845	-2.39102075
C	-2.72293410	1.46332110	-2.39775525
C	-2.34018255	0.21886905	-3.03322200
C	-2.96011230	-0.92253015	-2.39804825
C	-2.24287095	-2.14425330	-2.40038875
C	-0.94252350	-2.17068120	-3.04174775
C	-0.04847940	-3.10705005	-2.39064625
C	1.33573050	-2.80509255	-2.38354825
C	1.76698215	-1.58010315	-3.02514450
C	2.93493645	-1.01717370	-2.38279175
C	3.08058300	0.39311745	-2.39211175
C	2.04580635	1.17707955	-3.03987375
C	0.56709975	3.02641590	-2.38402825
C	1.86749130	2.46135015	-2.39127850
C	-1.51712700	3.69537885	-1.57019675
C	-0.16613265	3.98808480	-1.56461450
C	-3.86559900	1.06807785	-1.58079575
C	-4.00002735	-0.30737265	-1.57796975

C	-2.21781960	-3.33967845	-1.56530725
C	-0.95272380	-3.89479800	-1.55934225
C	2.48495280	-3.15142155	-1.55243900
C	3.40615275	-2.12100015	-1.55138800
C	3.76438815	1.38239925	-1.56326500
C	3.06342420	2.57304150	-1.56196700
C	1.20708165	-0.10899285	3.78186975
C	0.48495675	1.11308340	3.75004900
C	-0.90057030	0.81319350	3.74985400
C	-1.04584830	-0.59856465	3.77595025
C	0.25648290	-1.16195400	3.74982700
C	0.95076795	2.16113160	3.02218075
C	0.05683725	3.09861120	2.37600125
C	-1.32967800	2.80059225	2.37782275
C	-1.75919955	1.57825170	3.02491275
C	-2.93107845	1.01446170	2.38938325
C	-3.07587705	-0.39579315	2.39938125
C	-2.03921925	-1.17866985	3.04449125
C	-1.86145800	-2.46277320	2.39462150
C	-0.56124675	-3.02783940	2.38554950
C	0.50127420	-2.28498660	3.02641250
C	1.78349355	-2.52426645	2.39923025
C	2.73092385	-1.47188340	2.41219675
C	2.35267155	-0.22700700	3.05352275
C	2.25376635	2.13425445	2.39104725
C	2.97098295	0.91210155	2.40509350
C	0.96454875	3.88709565	1.55035225
C	2.23080390	3.33171120	1.55785200
C	-2.48328390	3.14559630	1.55230575
C	-3.40509150	2.11522995	1.55646250
C	-3.76067175	-1.38499065	1.57121700
C	-3.05717565	-2.57474970	1.56625625
C	0.17208255	-3.98966145	1.56649475
C	1.52355030	-3.69809115	1.57437475
C	3.87093255	-1.08170130	1.59084600
C	4.00895250	0.29326470	1.58577075

Fig. 3 c)

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frame 1

H	-2.46985632	4.22781410	-0.99401148
H	-0.06948577	4.90108192	-0.98913652
H	-4.67754597	1.46720710	-0.98177829
H	-4.76111580	-1.07443618	-0.94679944
H	-2.86400106	-3.95161368	-0.93545751
H	-0.44737748	-4.85629036	-0.93474104
H	2.88366067	-3.91979872	-0.94100138
H	4.47707592	-1.94684761	-0.96308875
H	4.63199065	1.57744875	-0.97326501
H	3.24692156	3.67507788	-0.98235816
H	0.48274580	4.88299607	0.97606288

H	2.82747910	4.00987820	0.97290919
H	-2.92790737	3.92880811	0.97696205
H	-4.48086533	1.96307870	0.96718370
H	-4.65183295	-1.53100761	0.96323843
H	-3.21039628	-3.66428588	0.94365387
H	0.01010885	-4.86230795	0.95121239
H	2.48518891	-4.19285613	0.97784515
H	4.65929575	-1.45276945	0.98166547
H	4.77327096	1.06358073	0.97593250
C	1.02312977	0.70165711	-3.55877267
C	-0.32508484	1.20701786	-3.56056537
C	-1.21755437	0.08262807	-3.56055416
C	-0.42280459	-1.11421366	-3.55858852
C	0.96101887	-0.73332890	-3.55511339
C	-0.63237373	2.28967424	-2.72533582
C	-1.86683842	2.37967888	-1.98932923
C	-2.73466581	1.29861668	-2.01193977
C	-2.34126347	0.12198367	-2.74068494
C	-2.84565743	-1.03274804	-2.03335892
C	-2.08180160	-2.20956924	-2.06437642
C	-0.81970167	-2.17361151	-2.76420970
C	0.10906887	-3.02363214	-2.05949997
C	1.45556342	-2.63627555	-2.02060275
C	1.83406684	-1.43568956	-2.72888242
C	2.90711040	-0.80454160	-2.00341584
C	2.96496192	0.58557701	-1.99752456
C	1.96454667	1.32137202	-2.73148784
C	0.37657778	3.01085210	-1.98984157
C	1.67818275	2.53065601	-1.99873628
C	-1.73837409	3.41734858	-0.92425923
C	-0.27370841	3.82910510	-0.92411592
C	-3.74857171	0.90461998	-1.01479350
C	-3.82152960	-0.55242486	-1.07537974
C	-2.00850289	-3.33060060	-1.15758219
C	-0.68119502	-3.82394685	-1.14859431
C	2.50122180	-2.91160529	-1.04641986
C	3.40698361	-1.76410373	-1.00551976
C	3.54870761	1.47383402	-0.96810074
C	2.71914927	2.72197831	-0.95466975
C	1.22437974	-0.01367665	3.56247570
C	0.43070096	1.18553247	3.55529722
C	-0.95504381	0.80321153	3.55677261
C	-1.01611353	-0.63162097	3.56819747
C	0.33021551	-1.13510116	3.56959587
C	0.82736448	2.23808328	2.72206903
C	-0.11535782	3.03199355	1.97797012
C	-1.44923035	2.66032133	1.97643025
C	-1.83979619	1.49289236	2.71992314
C	-2.91093715	0.84192166	2.00412275
C	-2.98895861	-0.55183069	2.05726360
C	-1.95672257	-1.26232746	2.77181030

C	-1.69894213	-2.50386867	2.07622402
C	-0.38046295	-2.99364931	2.07027190
C	0.62767395	-2.22592228	2.76707820
C	1.87070466	-2.35892765	2.05122907
C	2.73300298	-1.26363905	2.01943790
C	2.34774464	-0.07378368	2.73555745
C	2.06875080	2.22680584	1.98835205
C	2.83276301	1.06648152	1.99867889
C	0.60282365	3.79833683	0.91798172
C	2.02116377	3.27563680	0.93592913
C	-2.46586060	2.93938348	0.92082839
C	-3.40934264	1.76830208	0.97169468
C	-3.58404817	-1.50224159	1.12939724
C	-2.80051390	-2.68951519	1.16151378
C	0.32488565	-3.84679947	1.14281890
C	1.70275863	-3.45647675	1.10520600
C	3.72998133	-0.88910635	1.00475608
C	3.79103439	0.59465319	0.97638553

Fig. 3 d)

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frame 1

H	-2.39835116	4.22720500	-1.01536864
H	-0.10339223	4.85968836	-1.01165001
H	-4.65063406	1.41498705	-1.01702887
H	-4.75226112	-0.99805364	-0.99517428
H	-2.82163756	-3.96647457	-0.99898021
H	-0.51570772	-4.83510281	-0.99664942
H	2.90215809	-3.86853583	-0.98642463
H	4.41330430	-1.99504519	-1.00115057
H	4.57634767	1.60028776	-1.00483769
H	3.26971850	3.59736950	-1.00999896
H	0.54143207	4.83512755	0.99675386
H	2.77258051	3.99798694	0.99954884
H	-2.93412761	3.87495793	0.99897428
H	-4.42145241	2.00817726	0.99849918
H	-4.60770390	-1.56103436	1.02221287
H	-3.25586179	-3.60562134	1.00665138
H	0.05570464	-4.84571625	1.01119712
H	2.40780955	-4.20160644	1.02795200
H	4.63456137	-1.40026059	1.01389174
H	4.74893158	0.98894372	1.00596842
C	1.03238976	0.70243315	-3.52975302
C	-0.32603001	1.21457013	-3.53126292
C	-1.23015578	0.08151088	-3.53529206
C	-0.43193718	-1.12762880	-3.54008526
C	0.96561084	-0.74615800	-3.53017318
C	-0.63342271	2.31456638	-2.68150990
C	-1.84821087	2.36636312	-1.90781884
C	-2.70816496	1.29315735	-1.91684110
C	-2.37610098	0.12478090	-2.69229479

C	-2.82017826	-1.02100163	-1.93545010
C	-2.06868223	-2.17718159	-1.95840102
C	-0.84164982	-2.21102803	-2.71881759
C	0.10114644	-2.99414691	-1.95401596
C	1.42735683	-2.61730272	-1.92335616
C	1.85562565	-1.46734855	-2.68243340
C	2.87417331	-0.80629978	-1.90672090
C	2.93496150	0.56800054	-1.90470119
C	1.98825382	1.32887546	-2.68154314
C	0.38123239	2.98510412	-1.90765674
C	1.66911784	2.50325079	-1.90909212
C	-1.75465797	3.36814255	-0.74301795
C	-0.21294731	3.79134674	-0.74157587
C	-3.66967337	0.96738522	-0.76068980
C	-3.73843146	-0.62024387	-0.76772327
C	-2.05282490	-3.19665817	-0.81536404
C	-0.58325230	-3.74938618	-0.81034458
C	2.38088577	-2.92140230	-0.75149846
C	3.38178261	-1.68186530	-0.74598499
C	3.52298390	1.38377680	-0.74049205
C	2.65035587	2.71925281	-0.74258747
C	1.23669451	-0.01970916	3.53522492
C	0.44017362	1.19256485	3.52627644
C	-0.95964079	0.81008603	3.52995179
C	-1.02567139	-0.63815324	3.54809780
C	0.33068687	-1.14937528	3.54800525
C	0.84370754	2.25650934	2.67318881
C	-0.10549868	3.00972688	1.89380679
C	-1.43113033	2.64499317	1.89394303
C	-1.85782505	1.51366327	2.67675508
C	-2.88040970	0.83958032	1.91561575
C	-2.94922582	-0.53546332	1.94716943
C	-1.98769508	-1.28048100	2.72295298
C	-1.68169891	-2.47361563	1.96945945
C	-0.38831350	-2.95776593	1.96520362
C	0.63093956	-2.26538490	2.71947112
C	1.84625321	-2.33962343	1.94610262
C	2.70323100	-1.26239682	1.92390947
C	2.37818737	-0.08377885	2.68688125
C	2.05846111	2.19680839	1.90022614
C	2.81169820	1.04712072	1.90669441
C	0.55938921	3.76071426	0.72987142
C	2.05291176	3.20012835	0.73219521
C	-2.39602042	2.94376859	0.73158297
C	-3.39156973	1.69496367	0.73954289
C	-3.53969013	-1.37429162	0.80414304
C	-2.67223246	-2.68896010	0.81912099
C	0.21182626	-3.77186045	0.81077862
C	1.73527601	-3.35376174	0.79664329
C	3.65470929	-0.95421258	0.75206050
C	3.73150253	0.63928952	0.74413995

Fig. 3 e)

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frame 72

H	-2.542433	4.216431	-1.028246
H	-0.429600	4.902193	-1.035513
H	-4.782054	1.132850	-1.011745
H	-4.779193	-1.087147	-1.005910
H	-2.545085	-4.171473	-1.001605
H	-0.431939	-4.863298	-1.004526
H	3.191799	-3.680686	-1.014908
H	4.496104	-1.884773	-1.028900
H	4.500705	1.927724	-1.038896
H	3.196555	3.727677	-1.041297
H	0.410750	4.907807	1.000977
H	2.521195	4.224581	0.999822
H	-3.209527	3.730338	1.018119
H	-4.516503	1.935805	1.026126
H	-4.515840	-1.873622	1.037200
H	-3.215723	-3.671856	1.041397
H	0.409424	-4.852515	1.036599
H	2.522651	-4.168461	1.029413
H	4.765308	-1.082398	1.011668
H	4.764072	1.137866	1.004196
C	0.969012	0.731085	-3.274740
C	-0.393750	1.174027	-3.272273
C	-1.235605	0.013740	-3.267267
C	-0.394189	-1.146410	-3.265813
C	0.968402	-0.702791	-3.269773
C	-0.743200	2.262117	-2.465765
C	-1.967206	2.290074	-1.735503
C	-2.774634	1.180106	-1.730231
C	-2.374108	0.017009	-2.454520
C	-2.772505	-1.138764	-1.720575
C	-1.967847	-2.249857	-1.720357
C	-0.745087	-2.230336	-2.453124
C	0.233614	-2.968459	-1.724659
C	1.538470	-2.543659	-1.727748
C	1.892653	-1.371226	-2.459902
C	2.896725	-0.666687	-1.733090
C	2.900873	0.706248	-1.740070
C	1.893746	1.405174	-2.468856
C	0.235798	3.004469	-1.742052
C	1.540901	2.580868	-1.743602
C	-1.942232	3.364298	-0.677752
C	-0.410689	3.858144	-0.682900
C	-3.780266	0.830537	-0.665384
C	-3.780406	-0.778997	-0.659278
C	-1.944027	-3.316805	-0.656041
C	-0.412072	-3.817093	-0.658684
C	2.562971	-2.845775	-0.667299

C	3.510137	-1.544108	-0.673459
C	3.515399	1.590449	-0.684929
C	2.567345	2.894921	-0.687639
C	1.219408	0.034231	3.268557
C	0.377389	1.193814	3.264676
C	-0.985757	0.751874	3.270682
C	-0.986791	-0.680859	3.275530
C	0.376156	-1.124593	3.273553
C	0.729419	2.277798	2.451961
C	-0.250448	3.016274	1.723449
C	-1.555027	2.591271	1.727033
C	-1.909727	1.420838	2.460511
C	-2.917718	0.719013	1.736964
C	-2.918385	-0.653544	1.741918
C	-1.911760	-1.354019	2.469991
C	-1.559130	-2.530776	1.744409
C	-0.254809	-2.956477	1.742472
C	0.724692	-2.212802	2.466023
C	1.949584	-2.238356	1.734559
C	2.757614	-1.127788	1.729235
C	2.357929	0.031651	2.455586
C	1.953374	2.300116	1.719812
C	2.758506	1.187762	1.721169
C	0.391443	3.860846	0.656564
C	1.923898	3.366646	0.654797
C	-2.582674	2.895940	0.667720
C	-3.530504	1.594669	0.674194
C	-3.530385	-1.535128	0.684709
C	-2.586028	-2.840446	0.686957
C	0.390511	-3.811654	0.682914
C	1.921315	-3.313369	0.678390
C	3.764611	-0.778345	0.664504
C	3.764319	0.832495	0.658413

Fig. 4 a)

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frame 1

H	-2.24442540	4.01600880	-0.80239150
H	0.31457385	4.55372175	-0.70335925
H	-4.52943900	1.77906060	-1.19314800
H	-4.82548800	-0.82563975	-1.25432025
H	-3.04834830	-3.51497415	-0.87621650
H	-0.64675020	-4.55086845	-0.75600825
H	2.39897355	-3.91916220	-0.67997400
H	4.16227620	-1.98436785	-0.66269350
H	4.49465610	1.09041975	-0.66851550
H	3.17002020	3.34706565	-0.68197025
H	-1.79915580	4.54898400	4.93589375
H	-0.58440105	3.49489860	7.00039050
H	-3.41336355	3.93052035	2.33506200
H	-4.31897595	1.98187470	0.84697000

H	-4.51645245	-1.13247510	0.58443850
H	-3.85863420	-3.40213335	1.70386150
H	-2.28300810	-4.56737775	4.09415650
H	-0.97077255	-4.02295830	6.29367100
H	0.05427705	-1.77308100	8.09741450
H	0.19742475	0.82881405	8.32243100
C	1.12285365	0.60850440	-3.79534875
C	-0.18415290	1.18949175	-3.82824075
C	-1.13514030	0.12428265	-3.86361850
C	-0.42471750	-1.11435630	-3.83444300
C	0.97345485	-0.81721680	-3.79872700
C	-0.45607875	2.29994100	-3.06414550
C	-1.74298530	2.50832175	-2.42479425
C	-2.70087795	1.47524160	-2.50364050
C	-2.30566500	0.24523440	-3.16174600
C	-2.94956325	-0.88560765	-2.52687375
C	-2.22722295	-2.09448255	-2.45055175
C	-0.91899585	-2.14746090	-3.07538475
C	-0.04953750	-3.04356915	-2.34161450
C	1.32894165	-2.76042870	-2.31279750
C	1.80099240	-1.57975515	-3.01056975
C	2.92842765	-1.01039100	-2.29684600
C	3.07831455	0.39035430	-2.29723050
C	2.09004090	1.18237110	-3.00673725
C	0.58203810	2.99844840	-2.33170725
C	1.87548090	2.43742605	-2.30924700
C	-1.49419890	3.57417540	-1.45676075
C	-0.14552175	3.85625835	-1.40158175
C	-3.87215985	1.09091385	-1.72121850
C	-4.02174240	-0.27921345	-1.74241250
C	-2.20953555	-3.20632125	-1.49899800
C	-0.94567530	-3.75228375	-1.43334850
C	2.38463790	-3.06208800	-1.35169225
C	3.31335600	-2.04514485	-1.34195600
C	3.67480725	1.32357975	-1.34576175
C	2.97714975	2.51209710	-1.35355975
C	-4.13928165	-0.13480065	7.04598675
C	-4.50192690	1.10531985	6.42728775
C	-5.21984295	0.80327775	5.22638750
C	-5.30103660	-0.62047710	5.10604125
C	-4.62837330	-1.20177825	6.22674725
C	-3.60296820	2.14617375	6.42882300
C	-3.46025835	3.04486980	5.29970725
C	-4.17508590	2.75349240	4.12148525
C	-5.00098965	1.56205860	4.10054925
C	-5.00920935	0.99188400	2.76759200
C	-5.09746395	-0.41060805	2.64875850
C	-5.16953385	-1.19786730	3.86663075
C	-4.48481100	-2.46140955	3.67202275
C	-3.80257245	-3.02116425	4.76703850
C	-3.85231020	-2.32213665	6.03723575

C	-2.60962905	-2.52613710	6.75316250
C	-2.13311310	-1.48399875	7.56874175
C	-2.90308755	-0.25679490	7.63407475
C	-2.35822755	2.09038725	7.17109900
C	-2.00309310	0.87221295	7.77920725
C	-2.21252340	3.75747570	5.55923025
C	-1.57071090	3.20119890	6.64413950
C	-3.95156550	3.06197520	2.71252800
C	-4.43481795	2.03923035	1.92617200
C	-4.64533125	-1.35958245	1.63804175
C	-4.28803470	-2.54990100	2.23015650
C	-2.62182270	-3.87376425	4.86240975
C	-1.93071105	-3.58818720	6.01907525
C	-0.78997680	-1.09510770	7.98718250
C	-0.71385225	0.27432555	8.10478775

Fig. 4 b)

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frame 1

H	-2.20805888	4.22516234	-0.89549005
H	0.35410261	4.73205991	-0.83455985
H	-4.73665863	1.62649654	-1.94060716
H	-4.95935897	-0.70870606	-2.10282875
H	-2.94918537	-3.89946312	-1.13090829
H	-0.51147490	-4.79845810	-1.01169327
H	2.50812214	-3.89907664	-0.72677259
H	4.21935786	-1.91887538	-0.67566026
H	4.50966934	1.12959625	-0.67325569
H	3.18432160	3.38774810	-0.68252179
H	-1.67647141	4.44481353	3.43718815
H	-0.52081813	3.43837175	5.57381480
H	-3.03573821	3.60323574	0.91867391
H	-5.07739790	2.43987253	-0.34435398
H	-5.55000076	-1.53664517	-0.59807100
H	-3.75585983	-3.27338839	0.38118168
H	-2.29535704	-4.48382563	2.68271383
H	-0.98325694	-3.95704816	4.89583718
H	0.03646374	-1.76553168	6.70008951
H	0.19657086	0.84691956	6.93473821
C	1.12678055	0.64158613	-3.78052327
C	-0.19042662	1.19447984	-3.75503792
C	-1.11600601	0.11389274	-3.74178182
C	-0.38871583	-1.10657095	-3.78588093
C	1.00385005	-0.78409313	-3.79282818
C	-0.45164484	2.29602917	-2.98225958
C	-1.71467026	2.50773644	-2.30590972
C	-2.61429116	1.42267647	-2.26862410
C	-2.21763718	0.19591014	-2.92202597
C	-2.83420097	-0.96223793	-2.32093871
C	-2.14100287	-2.18297458	-2.39872657
C	-0.84395432	-2.16692118	-3.04805387

C	0.05586774	-3.09193734	-2.39455301
C	1.42104245	-2.75375477	-2.35454568
C	1.85721500	-1.54444122	-3.02788542
C	2.97303009	-0.96188923	-2.31386039
C	3.10264451	0.43976453	-2.30968737
C	2.10470556	1.22346905	-3.00856321
C	0.60052945	3.03274680	-2.31605965
C	1.89361225	2.47599237	-2.31101861
C	-1.45792280	3.67223777	-1.45607610
C	-0.11014527	3.95883471	-1.44344278
C	-3.87687450	1.05168514	-1.60454932
C	-4.02936529	-0.38677549	-1.63820549
C	-2.10231191	-3.42096250	-1.61326955
C	-0.82243302	-3.92495617	-1.58105925
C	2.48015898	-3.03668739	-1.39103182
C	3.38275287	-1.99675316	-1.36738960
C	3.69507183	1.36985623	-1.35451485
C	2.99798638	2.55611629	-1.35926902
C	-4.15984155	-0.09106388	5.65409575
C	-4.49553844	1.13564949	5.01168697
C	-5.25676478	0.84605189	3.82629799
C	-5.36591172	-0.57267468	3.71983064
C	-4.65597118	-1.14589891	4.83419513
C	-3.57080145	2.16049559	4.99908678
C	-3.36809460	3.00755892	3.85029952
C	-4.04493424	2.65589407	2.65860958
C	-5.01082735	1.57092476	2.68346657
C	-5.12402134	1.00431922	1.35896037
C	-5.24333156	-0.37922334	1.25368562
C	-5.23283275	-1.14716973	2.47753119
C	-4.47013536	-2.36812807	2.26915314
C	-3.80862187	-2.95892009	3.37851302
C	-3.87347450	-2.26726817	4.64087642
C	-2.63069363	-2.47565595	5.36298774
C	-2.15826381	-1.44099009	6.18899591
C	-2.92421795	-0.22198958	6.27431610
C	-2.33660043	2.09872000	5.75936769
C	-2.01285047	0.88794667	6.39419432
C	-2.11288427	3.68736439	4.08624419
C	-1.50666625	3.15886701	5.20831183
C	-3.75225126	2.87340410	1.28596739
C	-4.51277430	2.00377760	0.46233970
C	-4.84340516	-1.32916540	0.18822950
C	-4.27539703	-2.45684630	0.86972497
C	-2.63457866	-3.80097459	3.46045057
C	-1.94191237	-3.51914212	4.62305380
C	-0.79418009	-1.07132506	6.58440774
C	-0.70980119	0.28830564	6.70669712

Fig. 4 c)

frame 1

H	-2.17762230	4.32954615	-0.96074175
H	0.36765375	4.80183060	-0.89712025
H	-4.67652675	1.48079280	-2.30919975
H	-4.84269105	-0.59408235	-2.47265525
H	-2.88471900	-4.07919090	-1.25989725
H	-0.45213345	-4.89388425	-1.12981500
H	2.55576720	-3.89322390	-0.74746275
H	4.23955635	-1.89202725	-0.68336875
H	4.51584150	1.14359370	-0.67591000
H	3.19181295	3.40192530	-0.68565525
H	-1.62859335	4.40399550	2.80085175
H	-0.49882590	3.41635635	4.96620825
H	-2.86346895	3.39817425	0.33859600
H	-5.30473335	2.56825365	-0.65512550
H	-5.82174975	-1.64067270	-0.94582375
H	-3.69328665	-3.18275505	-0.17256750
H	-2.30007720	-4.45257645	2.07820125
H	-0.98877795	-3.93360510	4.29990475
H	0.03186660	-1.76178285	6.10793625
H	0.19932285	0.85722300	6.34676450
C	1.12073445	0.64946745	-3.76865425
C	-0.20381100	1.18980000	-3.71661075
C	-1.13048310	0.11239215	-3.67131625
C	-0.38921550	-1.09730205	-3.74941800
C	1.00426890	-0.77412150	-3.78334400
C	-0.45457455	2.28279795	-2.93646150
C	-1.71294585	2.49809685	-2.25377875
C	-2.62190220	1.42067025	-2.19319800
C	-2.24436060	0.18601050	-2.84457850
C	-2.83773495	-1.00119450	-2.26452175
C	-2.12107695	-2.21396730	-2.37123550
C	-0.82223130	-2.16376410	-3.01586500
C	0.09758850	-3.09999540	-2.40567600
C	1.45889775	-2.75283330	-2.37205775
C	1.87568370	-1.53146760	-3.03590150
C	2.99289990	-0.94691205	-2.32738675
C	3.11339070	0.45580740	-2.31813125
C	2.10717915	1.23403350	-3.00970775
C	0.60700890	3.03820815	-2.30630525
C	1.89994245	2.48904675	-2.31205650
C	-1.44014280	3.71399385	-1.46604975
C	-0.09605160	3.99706470	-1.46471125
C	-3.97257015	1.14011175	-1.53038125
C	-4.14063930	-0.49973595	-1.62638150
C	-2.05617675	-3.51561855	-1.67406825
C	-0.76629615	-3.98911395	-1.64710225
C	2.52446985	-3.03388710	-1.41547325
C	3.40958010	-1.98088710	-1.38253225
C	3.70546290	1.38610620	-1.36175525
C	3.00850695	2.57185140	-1.36534775

C	-4.16844570	-0.07235640	5.05260000
C	-4.48588635	1.14154725	4.39229725
C	-5.28548850	0.86369235	3.21574650
C	-5.40699075	-0.55220130	3.12240725
C	-4.65738975	-1.11794640	4.23008600
C	-3.54990705	2.16036030	4.36368375
C	-3.34385370	3.00946755	3.22570300
C	-4.04413335	2.65268865	2.00587775
C	-5.04820620	1.58824980	2.06515075
C	-5.16688470	0.99189750	0.77172750
C	-5.31282075	-0.36840885	0.68220400
C	-5.30253300	-1.14145530	1.88367550
C	-4.52174190	-2.35793055	1.65539175
C	-3.82085460	-2.94679440	2.78055125
C	-3.87353235	-2.24185515	4.02861500
C	-2.63404455	-2.45622420	4.76187850
C	-2.17021425	-1.41863910	5.59650700
C	-2.93238945	-0.20854425	5.69989450
C	-2.32528110	2.10083055	5.14728950
C	-2.02177350	0.89281590	5.80523050
C	-2.08552920	3.66384225	3.45593725
C	-1.48251690	3.13527645	4.59426900
C	-3.68026230	2.77484205	0.67777800
C	-4.51820835	1.89669870	-0.25025625
C	-4.89850395	-1.25061795	-0.46709150
C	-4.28677695	-2.41557495	0.29662900
C	-2.64758355	-3.77432955	2.85640825
C	-1.94655570	-3.49346700	4.02693050
C	-0.79068600	-1.05805680	5.99307475
C	-0.70365435	0.29471820	6.11525000

Fig. 4 d)

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frame 1

H	-2.25406105	4.39495589	-1.29908248
H	0.26069784	4.50280498	-0.59329325
H	-4.78685592	1.51980397	-2.31612206
H	-4.98190791	-0.64077799	-2.40363788
H	-2.98423232	-4.01763982	-1.55763475
H	-0.54525703	-4.52479929	-0.74491013
H	2.47457059	-3.82905106	-0.60769802
H	4.25528964	-1.89205818	-0.63405452
H	4.52880297	1.11111818	-0.61404859
H	3.12107136	3.33379404	-0.53624121
H	-0.41378773	4.51546283	1.80828469
H	1.31997899	3.50773732	3.50940785
H	-3.30063986	4.01645342	0.01437276
H	-5.12061790	2.45089801	-0.41512332
H	-5.50624957	-1.63667297	-0.57027921
H	-4.07728358	-3.53561116	-0.25219612
H	-1.21857402	-4.65856428	1.42568040

H	0.66114032	-4.08770400	3.16980093
H	2.19258658	-1.77105112	4.34563931
H	2.42790267	0.84804203	4.46725269
C	1.14350141	0.64449542	-3.75521450
C	-0.17793587	1.19337181	-3.78241216
C	-1.12309469	0.12657816	-3.85359243
C	-0.37413451	-1.08662749	-3.82085161
C	1.02157131	-0.76781621	-3.77068319
C	-0.46196386	2.25734118	-2.96650514
C	-1.76400329	2.47267188	-2.39395670
C	-2.68909931	1.42926446	-2.46150642
C	-2.30962891	0.21653456	-3.13368176
C	-2.90361441	-0.93866646	-2.52268738
C	-2.17394954	-2.12674134	-2.49275734
C	-0.84681777	-2.11427160	-3.04343729
C	0.02520460	-2.96619560	-2.25366192
C	1.41073945	-2.68470883	-2.25243351
C	1.86447669	-1.52945170	-2.97618357
C	2.99186714	-0.94990803	-2.27085082
C	3.11579565	0.44466005	-2.26129855
C	2.10979841	1.22785205	-2.95139726
C	0.55150961	2.92544958	-2.16978090
C	1.86645333	2.42512959	-2.19559292
C	-1.54804073	3.60106955	-1.47370138
C	-0.18114964	3.78579671	-1.28279839
C	-3.95601419	1.16175334	-1.68661517
C	-4.11184408	-0.49008768	-1.74365409
C	-2.18034311	-3.30003692	-1.59905969
C	-0.85026131	-3.71586129	-1.40534904
C	2.46511950	-2.97475825	-1.28240028
C	3.39617084	-1.96731509	-1.29699909
C	3.69414034	1.35215092	-1.26898023
C	2.95990902	2.50814236	-1.22655265
C	-2.10609267	-0.08343447	4.63274001
C	-2.60747995	1.13232667	4.09195468
C	-3.66894168	0.82590766	3.17888666
C	-3.79246343	-0.58860013	3.12165043
C	-2.80862887	-1.14684864	3.99885214
C	-1.74003038	2.16064130	3.77991214
C	-1.90103133	3.02844915	2.63611021
C	-2.91663855	2.67655225	1.68076609
C	-3.74184974	1.52913809	1.99903868
C	-4.26284360	0.94363713	0.81951065
C	-4.38783636	-0.41833060	0.76646094
C	-3.98947963	-1.18109065	1.89262842
C	-3.37393769	-2.42321899	1.47714599
C	-2.43637220	-3.01174096	2.38332932
C	-2.13133316	-2.27821794	3.59385609
C	-0.74380321	-2.49714717	3.95733754
C	-0.04833476	-1.43607539	4.57065756
C	-0.74074296	-0.20998648	4.86005268

C	-0.33924094	2.11088747	4.15783264
C	0.15981384	0.89841509	4.67388520
C	-0.63569742	3.72767361	2.52534105
C	0.28078855	3.19587742	3.41725229
C	-3.22687121	2.98709547	0.32748834
C	-4.15892812	1.91720513	-0.30291962
C	-4.46348262	-1.30026871	-0.42920055
C	-3.72946687	-2.57080852	0.09061074
C	-1.30254050	-3.89959705	2.20041049
C	-0.31094261	-3.59958629	3.11934761
C	1.37655502	-1.06787293	4.50010528
C	1.49898330	0.29012077	4.56472833

Fig. 4 e)

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frame 40

H	-2.13718095	4.37006715	-1.61408275
H	0.25927740	4.24075605	-0.41588475
H	-4.82610270	1.53945750	-2.11052700
H	-5.02437960	-0.66558210	-2.15983300
H	-2.86919760	-3.95801565	-1.78808925
H	-0.49839600	-4.27520595	-0.56626775
H	2.44269045	-3.79348575	-0.58392525
H	4.25610480	-1.87673340	-0.63548950
H	4.52989710	1.10075775	-0.60917925
H	3.07567110	3.30024450	-0.49769675
H	0.39550215	4.68779205	1.30076000
H	2.41199415	3.58617060	2.52205725
H	-3.20098050	3.96549780	0.19465425
H	-4.72402290	2.42947620	-0.10378400
H	-5.09836395	-1.64221530	-0.19064175
H	-3.88258125	-3.44692485	0.02955600
H	-0.50165685	-4.86984795	1.11661250
H	1.67678655	-4.21785015	2.38613600
H	3.46084725	-1.77985155	3.14829400
H	3.70794600	0.82993740	3.18727825
C	1.09446270	0.64275540	-3.76125350
C	-0.22912800	1.20830490	-3.82135475
C	-1.17693855	0.14126640	-3.93472475
C	-0.42996780	-1.07436840	-3.84871325
C	0.96935790	-0.74792415	-3.77604975
C	-0.52752675	2.25770730	-2.97255800
C	-1.80947970	2.40597315	-2.37649900
C	-2.74460475	1.41015060	-2.53388250
C	-2.38930185	0.23227515	-3.25230875
C	-2.94995610	-0.89315385	-2.57992800
C	-2.20641615	-2.04348180	-2.46036500
C	-0.90954300	-2.08777470	-3.04136400
C	-0.03550500	-2.92730610	-2.21854750
C	1.39045290	-2.65491330	-2.25443500
C	1.82113380	-1.52827740	-2.97079650

C	2.96245725	-0.93743970	-2.26336475
C	3.09088935	0.44258145	-2.25235250
C	2.07083805	1.24119450	-2.94002800
C	0.47868315	2.90708070	-2.12942500
C	1.83861645	2.40278325	-2.18813725
C	-1.71625065	3.40824720	-1.25239750
C	-0.20896995	3.60596250	-1.15548875
C	-3.91178745	1.15414500	-1.63090400
C	-4.05876900	-0.47220960	-1.66547925
C	-2.29878960	-3.09723885	-1.38147600
C	-0.84591345	-3.54473340	-1.28361900
C	2.44443630	-2.93976945	-1.25986925
C	3.38165820	-1.94803320	-1.27813675
C	3.67755105	1.33709610	-1.24163175
C	2.92767330	2.47585140	-1.19310425
C	-0.71960970	-0.08322405	4.16005850
C	-1.32511065	1.13644050	3.72930500
C	-2.52664740	0.83076870	3.03050075
C	-2.65808850	-0.59850720	3.00018450
C	-1.53848475	-1.15025610	3.68275450
C	-0.52639455	2.14769865	3.25405375
C	-0.90505410	3.01593075	2.14925150
C	-2.04619680	2.66588580	1.40326875
C	-2.83377240	1.56025395	1.89128000
C	-3.57565425	0.93845190	0.84804450
C	-3.70130175	-0.42930570	0.81951550
C	-3.09275445	-1.21688340	1.83545650
C	-2.52425115	-2.43359355	1.30309200
C	-1.46831505	-3.01536885	2.02851525
C	-0.94117470	-2.27371290	3.16511175
C	0.48256665	-2.50779180	3.28430075
C	1.29109755	-1.45201065	3.73864700
C	0.65112585	-0.21160875	4.11282500
C	0.91780395	2.09957025	3.36374100
C	1.51347270	0.89678055	3.77516450
C	0.32325120	3.78905220	1.90557325
C	1.38213270	3.23829540	2.58087175
C	-2.62583595	3.04396815	0.00936400
C	-3.77198280	1.89792285	-0.27079275
C	-4.06335735	-1.28988240	-0.33797300
C	-3.14702535	-2.63851170	-0.10799400
C	-0.40635120	-3.99900000	1.75812350
C	0.73021935	-3.68521005	2.45912700
C	2.67780705	-1.08302670	3.44380100
C	2.80728855	0.28288890	3.46167025

Fig. 4 f)

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frame 1

H	-2.11064967	4.39196696	-1.65858811
H	0.16053038	4.70519178	-0.90812518

H	-4.79410466	1.53626363	-2.11476990
H	-4.99123344	-0.67181415	-2.14894539
H	-2.83284616	-3.96496899	-1.77521940
H	-0.65431088	-4.67999976	-1.04209859
H	2.67462357	-3.90238254	-0.77290764
H	4.42605335	-1.94314019	-0.86617367
H	4.70038851	1.18404778	-0.85009190
H	3.30601450	3.41188176	-0.72332555
H	0.33463680	4.84390664	0.98815080
H	2.58167302	3.57770240	1.48502450
H	-3.23711852	4.00121562	0.16413998
H	-4.73967804	2.40183149	-0.07391905
H	-5.09999473	-1.59051178	-0.13225214
H	-3.90582938	-3.44143609	0.04715595
H	-0.56155979	-4.93594186	0.85618327
H	1.87433102	-4.12645667	1.39941701
H	3.83640359	-1.75363112	2.12797483
H	4.08020095	0.87496253	2.15227230
C	1.12613458	0.65544359	-3.72922007
C	-0.18919988	1.20636752	-3.77097547
C	-1.13091671	0.12644004	-3.87557950
C	-0.38240447	-1.09518203	-3.78914780
C	1.00558975	-0.77195645	-3.73830622
C	-0.46773253	2.24986169	-2.89566912
C	-1.76253831	2.40056916	-2.32353329
C	-2.70024465	1.40900692	-2.49095652
C	-2.33920321	0.22042604	-3.19816668
C	-2.90508179	-0.90491059	-2.52181811
C	-2.14824288	-2.04336258	-2.37665861
C	-0.83954215	-2.09179385	-2.93538629
C	0.03912520	-2.91638287	-2.12340363
C	1.43604647	-2.69305515	-2.22593106
C	1.86224375	-1.51813447	-2.96798350
C	3.03414381	-0.94767352	-2.34100621
C	3.15896979	0.46401876	-2.33621640
C	2.09963720	1.23443541	-2.95307264
C	0.54102298	2.89971430	-2.07469768
C	1.88222398	2.45167764	-2.19147700
C	-1.70782079	3.44768069	-1.24745303
C	-0.17824568	3.69169929	-1.08253389
C	-3.88937370	1.15612326	-1.61394557
C	-4.03663863	-0.47172665	-1.63701541
C	-2.28212683	-3.11445286	-1.33200678
C	-0.81417684	-3.61607292	-1.16359732
C	2.56890415	-3.00707570	-1.37921983
C	3.50419917	-1.98435908	-1.44446183
C	3.79934660	1.39112436	-1.42580784
C	3.05059292	2.55544814	-1.34157337
C	-0.17939544	-0.07631798	3.63520969
C	-0.86334045	1.15113172	3.36895743
C	-2.17164621	0.83921144	2.90370849

C	-2.30111560	-0.59321871	2.88375280
C	-1.07412380	-1.15181965	3.34012181
C	-0.15435220	2.16431875	2.76160538
C	-0.73928540	3.02971062	1.77707990
C	-1.99111481	2.69879152	1.27516538
C	-2.68145109	1.57708870	1.84044228
C	-3.50947224	0.95463423	0.86212364
C	-3.63433373	-0.41307259	0.84434989
C	-2.93485588	-1.19997452	1.80501360
C	-2.46030033	-2.41444881	1.21059729
C	-1.29087709	-2.98286338	1.69998277
C	-0.56005832	-2.26136210	2.70425034
C	0.86947650	-2.48034314	2.52979808
C	1.76379706	-1.43310564	2.92438898
C	1.16325272	-0.19508761	3.37141681
C	1.29155579	2.12393539	2.58494111
C	1.97926161	0.92465478	2.95085950
C	0.38558119	3.77800546	1.19349587
C	1.58481194	3.20580092	1.70927869
C	-2.65561575	3.08689317	-0.03196057
C	-3.77213786	1.90723362	-0.25923036
C	-4.05889458	-1.27153958	-0.30353668
C	-3.17337484	-2.63491211	-0.11130647
C	-0.31740859	-3.90185737	1.08859620
C	0.96379306	-3.57746130	1.62873597
C	3.07984336	-1.06167746	2.49253714
C	3.20746065	0.33092561	2.50577979

Fig. 4 g)

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frame 312

H	-2.10462210	4.40861040	-1.70266575
H	0.03805140	4.82579910	-1.34984775
H	-4.75998060	1.53538365	-2.09669650
H	-4.95088815	-0.68297235	-2.11770000
H	-2.82210000	-3.96703845	-1.76894825
H	-0.77868165	-4.74459990	-1.43715700
H	2.93534280	-3.99600270	-1.03651475
H	4.62204990	-2.00915775	-1.10395775
H	4.89687135	1.26155475	-1.09614675
H	3.56177415	3.50437530	-1.02575350
H	0.35190900	4.85323410	0.79981625
H	2.65535790	3.57184080	0.54256525
H	-3.24987180	4.02158055	0.16314650
H	-4.73317335	2.37261705	-0.02433725
H	-5.07901260	-1.54313595	-0.05901000
H	-3.90450795	-3.42932760	0.09497475
H	-0.51544830	-4.88782950	0.72388150
H	1.98061395	-4.03877505	0.50026675
H	4.16150505	-1.72615005	1.19463800
H	4.39736055	0.90037515	1.20475350

C	1.13952945	0.64793445	-3.73287525
C	-0.16662930	1.20141000	-3.73810700
C	-1.10422710	0.11618610	-3.82519175
C	-0.35629635	-1.10681880	-3.74437100
C	1.02197790	-0.77197800	-3.73465750
C	-0.42001605	2.26143870	-2.86533775
C	-1.71688635	2.40448650	-2.28704050
C	-2.65554825	1.40895645	-2.44030350
C	-2.29279455	0.21147540	-3.12872850
C	-2.85359490	-0.91434300	-2.45416325
C	-2.09254650	-2.05156440	-2.31135275
C	-0.78466170	-2.11525995	-2.87936475
C	0.11282580	-2.91573840	-2.08515000
C	1.49638710	-2.67941235	-2.22672225
C	1.89349710	-1.50934425	-2.97445450
C	3.09059700	-0.93591915	-2.39447375
C	3.21019845	0.46400820	-2.39526775
C	2.12542545	1.22935110	-2.97504600
C	0.60217275	2.89655235	-2.06976650
C	1.92875730	2.44573485	-2.22249100
C	-1.70576085	3.48382290	-1.25288875
C	-0.10534920	3.78389760	-1.02216550
C	-3.86313930	1.15557315	-1.58034950
C	-4.00467795	-0.47119125	-1.59318375
C	-2.27519160	-3.13211310	-1.29885425
C	-0.74958540	-3.70557285	-1.07160400
C	2.73020070	-3.03554880	-1.49757700
C	3.64208595	-2.01132315	-1.57535825
C	3.93341895	1.43022285	-1.57217400
C	3.20425200	2.59144020	-1.49139725
C	0.31417305	-0.07030110	3.08583350
C	-0.40958820	1.16339700	2.97726450
C	-1.77928440	0.84304560	2.74208025
C	-1.90760280	-0.58923825	2.73157225
C	-0.61836480	-1.15277010	2.96035925
C	0.18914595	2.17413675	2.25127375
C	-0.56606550	3.01141695	1.39621425
C	-1.88808615	2.71272210	1.15676675
C	-2.48247030	1.58499960	1.79304300
C	-3.41272725	0.96771720	0.89852575
C	-3.53926065	-0.40025205	0.88931000
C	-2.73321165	-1.18329840	1.77560475
C	-2.34520785	-2.38855440	1.12262025
C	-1.09512570	-2.92000635	1.35316325
C	-0.20503995	-2.24261940	2.21826350
C	1.18517370	-2.46880230	1.81172225
C	2.15616570	-1.42639950	2.12436675
C	1.59174900	-0.17961150	2.60913625
C	1.59504510	2.15661210	1.83763425
C	2.36771595	0.95376990	2.13548900

C	0.37067340	3.78434280	0.51244050
C	1.71574335	3.19424985	0.92090950
C	-2.66022915	3.11825505	-0.06257825
C	-3.75359625	1.90953570	-0.22523925
C	-4.03331250	-1.25282415	-0.25045275
C	-3.16875330	-2.63371035	-0.10612000
C	-0.30208905	-3.83376960	0.46174150
C	1.12452330	-3.49939290	0.88146175
C	3.41674290	-1.05308280	1.61264950
C	3.54498270	0.36721800	1.61950375

Fig. 4 h)

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frame 1

H	-2.15225380	4.42588465	-1.73917182
H	0.00419630	4.88195644	-1.47109952
H	-4.75191584	1.53062313	-2.03385830
H	-4.93834393	-0.68557828	-2.04627043
H	-2.87249415	-3.98061483	-1.78489849
H	-0.82300836	-4.80122754	-1.52386718
H	2.84539761	-4.09836822	-1.17888186
H	4.48137424	-2.06200134	-0.98725982
H	4.75267142	1.30346057	-0.95804041
H	3.48511273	3.58128972	-1.16106180
H	0.51139455	4.83333536	0.66841379
H	2.73232064	3.87390470	0.66883596
H	-3.18224478	4.01568981	0.19351279
H	-4.65949348	2.35745789	0.03617810
H	-4.99470508	-1.52931972	0.01862532
H	-3.82492648	-3.42205370	0.15246559
H	-0.35601602	-4.88311392	0.62216214
H	2.03071181	-4.29376401	0.58449260
H	4.37206318	-1.73196714	0.98862278
H	4.60588283	0.89800507	0.99422444
C	1.12649641	0.64673457	-3.72749566
C	-0.18078589	1.20067679	-3.78518380
C	-1.11389279	0.11184426	-3.85473309
C	-0.37308168	-1.11460384	-3.79057624
C	1.00642040	-0.77792955	-3.73065480
C	-0.46372967	2.28966374	-2.95718737
C	-1.74683303	2.42722564	-2.35032187
C	-2.66385470	1.40772821	-2.45740091
C	-2.30285748	0.20892473	-3.14595545
C	-2.85956839	-0.91595796	-2.46701842
C	-2.12432518	-2.07478052	-2.36787427
C	-0.83423876	-2.14964767	-2.97033931
C	0.04842687	-2.97108554	-2.19832268
C	1.41999072	-2.70990058	-2.25468661
C	1.85037187	-1.51811841	-2.93617345
C	3.00451866	-0.95539655	-2.25511604
C	3.11828866	0.47292335	-2.23524981

C	2.07953413	1.22847933	-2.91995365
C	0.54100923	2.93941414	-2.17484162
C	1.84541313	2.45694377	-2.21898632
C	-1.71625751	3.50786668	-1.31163309
C	-0.11961304	3.83743703	-1.14487542
C	-3.83721616	1.15027170	-1.55091845
C	-3.97324108	-0.47091441	-1.55886020
C	-2.28529553	-3.15772930	-1.34449166
C	-0.76780852	-3.75665100	-1.17964307
C	2.54768254	-3.07453228	-1.38165828
C	3.48595259	-2.01594879	-1.41686262
C	3.75184990	1.41661417	-1.36306070
C	2.98139470	2.62429515	-1.28967322
C	0.54040533	-0.07034686	2.93650359
C	-0.17912407	1.15518127	2.83154158
C	-1.56419029	0.84099303	2.67032927
C	-1.69128649	-0.59053678	2.66451730
C	-0.38582227	-1.14789055	2.82458715
C	0.39857210	2.15740246	2.05947413
C	-0.40113374	2.99154039	1.23991974
C	-1.74379816	2.70843890	1.08553858
C	-2.31026900	1.58438056	1.75667451
C	-3.29075241	0.96766201	0.91405399
C	-3.40633317	-0.40265691	0.90463925
C	-2.55223043	-1.18554994	1.74312666
C	-2.19180972	-2.38632231	1.06502172
C	-0.92704726	-2.90985932	1.22534556
C	0.00324885	-2.23115917	2.04942842
C	1.36367143	-2.43799563	1.57529837
C	2.32284887	-1.41512095	1.85581287
C	1.79804853	-0.18130949	2.40091985
C	1.76881339	2.11367444	1.57778519
C	2.52754273	0.94391922	1.85540980
C	0.48501952	3.78367328	0.32090419
C	1.90193955	3.17607770	0.58857568
C	-2.59764586	3.12144268	-0.07857804
C	-3.68182834	1.90575179	-0.19858873
C	-3.95376948	-1.25200358	-0.21436021
C	-3.09529156	-2.63736371	-0.10675305
C	-0.18741629	-3.83804188	0.30321381
C	1.29278060	-3.49946155	0.60895374
C	3.59625356	-1.04196157	1.29894026
C	3.71857897	0.35397877	1.29462421

Fig. 4 i)

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frame 290

H	-2.17723665	4.43297490	-1.77817600
H	-0.01064730	4.93521180	-1.62177025
H	-4.69078350	1.53489585	-1.95191950
H	-4.88228430	-0.68562900	-1.95939975

H	-2.90902110	-3.97365975	-1.80508675
H	-0.86062335	-4.84258140	-1.65215125
H	2.86407510	-3.98389770	-1.38375600
H	4.32871050	-2.30380755	-1.28240550
H	4.66264815	1.52422290	-1.26666800
H	3.51637155	3.43323825	-1.35924500
H	0.67844250	4.86556350	0.49666000
H	2.72673360	3.99469680	0.64777350
H	-3.05143860	4.00530855	0.22463000
H	-4.51432245	2.32610760	0.12280675
H	-4.84806255	-1.50403575	0.11099800
H	-3.69801750	-3.41375880	0.20366250
H	-0.17575095	-4.90593645	0.46752825
H	1.99176855	-4.40736900	0.61830400
H	4.50817335	-1.51753500	0.79431175
H	4.69785120	0.70423575	0.80278350
C	1.18691040	0.63121260	-3.72709775
C	-0.12802050	1.18980000	-3.82233375
C	-1.06389345	0.10857675	-3.88115525
C	-0.33001455	-1.11788280	-3.82632225
C	1.06111410	-0.79540515	-3.72984200
C	-0.44525055	2.30692140	-3.04518025
C	-1.72008405	2.44600860	-2.41901775
C	-2.62210200	1.40718570	-2.47940400
C	-2.25970530	0.20944935	-3.16465450
C	-2.82367185	-0.91142040	-2.48663800
C	-2.11587870	-2.08975515	-2.43197300
C	-0.83565900	-2.16769365	-3.05639475
C	0.02085735	-2.99973870	-2.27665075
C	1.35992130	-2.69073225	-2.18312575
C	1.86671070	-1.54451490	-2.86742750
C	2.88936390	-0.93542970	-2.07909625
C	3.00762240	0.43728825	-2.07450550
C	2.10720765	1.22184840	-2.85781700
C	0.54348615	2.97204090	-2.25911475
C	1.80702540	2.43290520	-2.16510125
C	-1.68592140	3.53153970	-1.37660950
C	-0.10747260	3.89747040	-1.26380075
C	-3.75426195	1.14757680	-1.51785400
C	-3.89353830	-0.46733880	-1.52310750
C	-2.27003100	-3.17361750	-1.39694850
C	-0.77852955	-3.80566455	-1.28736150
C	2.28764010	-3.09872670	-1.06860000
C	3.35426505	-1.87605570	-0.99493225
C	3.62816595	1.27011690	-0.98315700
C	2.79374250	2.66117925	-1.04829650
C	0.88009245	-0.08406270	2.72508800
C	0.14670195	1.14263295	2.66999125
C	-1.24527435	0.82420995	2.57246750
C	-1.37208915	-0.60180180	2.56921975
C	-0.05772705	-1.16112180	2.66381000

C	0.65213295	2.18993880	1.89780350
C	-0.20482005	3.02159205	1.11783400
C	-1.54479795	2.71624065	1.02461825
C	-2.05285170	1.57251720	1.71117025
C	-3.07544370	0.95947605	0.92460275
C	-3.19470120	-0.41260860	0.92016575
C	-2.29262655	-1.19565300	1.70221900
C	-1.99159440	-2.40485805	1.00715075
C	-0.72688800	-2.93900205	1.09780550
C	0.26019570	-2.27690880	1.88634375
C	1.53566580	-2.42242200	1.26375025
C	2.44024350	-1.38718500	1.32672000
C	2.07669930	-0.18797715	2.01042775
C	1.93202535	2.11158630	1.27275300
C	2.63908005	0.93210660	1.32929150
C	0.59453955	3.83002260	0.12906900
C	2.08655175	3.19614750	0.23894675
C	-2.47328505	3.12118710	-0.09063075
C	-3.54009405	1.89599160	-0.16225675
C	-3.81372810	-1.24828665	-0.17207825
C	-2.97781080	-2.63954505	-0.10779225
C	-0.07765320	-3.86947110	0.10581300
C	1.50012525	-3.50528460	0.21852125
C	3.57065850	-1.13036835	0.36267575
C	3.70907505	0.48589650	0.36691675