Supplementary Material

Understanding Heterogeneous Growth Mechanisms at Graphene Edges: a Theoretical Study on Acetylene Deposition and Mechanistic Analysis

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Pre-exponential factors A are given in cm3 mol-1 s-1 or s-1 for bimolecular and unimolecular reactions, respectively, and Ea are given in cal mol-1. The pre-exponential factor (A) of the addition/decomposition step (marked with *) are corrected to account for the effect of the hindered rotor treatment found for the analogous gas phase system (see the “Hindered rotor effects” section).

Figure S9: Torsional potential [kcal/mol] related to the torsion in the ethenyl group (R-CH=ĊH) at the zigzag edge (solid line) and in the analogous gas phase molecule (dotted line).

Table S1: Parameters of fitted modified Arrhenius expressions $k = AT^n exp(-E_a/RT)$ for rate constants of individual reactions channels in the armchair PES considering 800-1900 K temperature range. Pre-exponential factors A are given in $cm^3\ mol^{-1}\ s^{-1}$ or s^{-1} for bimolecular and unimolecular reactions, respectively, and E_a are given in cal mol^{-1}.

Reaction	A [cm3, mol, s]	n []	Ea [cal/mol]
A0+C2H2=>A1	2.73E+03	2.63	1496.27
A1=>A2	2.01E+12	0.08	12450.02
A2=>A3	2.75E+12	0.35	19043.65
A3=>A4+H	5.02E+11	0.71	43420.48
A2=>A4+H	1.27E+12	0.72	20087.59
A0+C2H2=>B1	3.70E+03	2.54	268.62
B1=>B2	6.66E+12	0.44	37525.34
B2=>A1	3.59E+12	0.60	53435.97
B2=>C3+H	7.72E+13	0.61	66874.07
A0+C2H2=>C1	1.44E+01	3.14	-2664.67
C2=>C3+H	6.03E+12	0.55	34771.39
B2=>B3	7.84E+11	0.51	21236.56
B3=>B4	1.20E+12	0.01	550.94
B4=>B5	2.03E+11	0.31	24370.70
B5=>B6+H	2.96E+11	0.79	51841.06
B4=>B6+H	1.44E+11	0.69	29810.05
C1=>C2	3.95E+11	0.42	19962.64
B2=>C1	2.91E+12	0.58	53045.68
B1=>C1	1.55E+13	0.06	3236.54
C1=>C3+H	4.14E+12	0.66	37907.59
A1=>A0+C2H2	4.14E+12	0.66	37907.59
A2=>A1	1.03E+14	0.33	56438.07
A3=>A2	6.03E+11	0.35	33350.08
A4+H=>A3	5.15E+08	1.44	12737.32
A4+H=>A2	1.94E+08	1.49	3594.51
B1=>A0+C2H2	8.36E+11	1.03	65733.05
B2=>B1	2.44E+12	0.58	53761.98
A1=>B2	2.01E+12	0.41	35222.98
C3+H=>B2	1.84E+10	1.27	15707.67
C1=>A0+C2H2	2.05E+12	0.66	38108.70
C3+H=>C2	8.68E+08	1.25	1601.58
B3=>B2	3.93E+11	0.47	9018.86
B4=>B3	2.78E+12	-0.14	15145.49
B5=>B4	7.81E+10	0.56	48808.97
B6+H=>B5	1.59E+09	1.40	-247.81
B6+H=>B4	3.92E+08	1.52	2252.70
C2=>C1	4.66E+11	0.43	17582.83
C1=>B2	2.91E+12	0.58	53045.68
C1=>B1	1.18E+13	0.09	3975.61
C3+H=>C1	5.16E+08	1.41	2255.72
B4=>A3	9.25E+11	-0.10	12171.78
A3=>B4	2.98E+12	0.21	49736.14
A1=>B1	1.82E+12	-0.08	42773.04
B1=>A1	6.39E+12	0.01	44652.05

Table S2: Parameters of fitted modified Arrhenius expressions $k = AT^n exp(-E_a/RT)$ for rate constants of individual reactions channels in the zigzag PES considering 800-1900 K temperature range. Pre-exponential factors A are given in $cm^3\ mol^{-1}\ s^{-1}$ or s^{-1} for bimolecular and unimolecular reactions, respectively, and E_a are given in cal mol^{-1}. The pre-exponential factor (A) of the addition/decomposition step (marked with *) are corrected to account for the effect of the hindered rotor treatment found for the analogous gas phase system (see the "**Hindered rotor effects"** section).

Reaction	A [cm^3,mol,s]	n []	Ea [cal/mol]
Z0+C2H2=>Z1*	7.74E+03 (9.67E+03)	2.60	-1810.49
Z1=>Z2	6.30E+13	0.11	3557.38
Z2=>Z3	4.15E+12	0.27	13488.42
Z3=>Z4+H	7.16E+12	0.74	66161.83
Z1=>Y1	1.91E+13	0.12	3050.03
Y1=>Y2	1.40E+13	0.20	20093.89
Y2=>Y3+H	1.10E+13	0.84	69690.18
Y1=>Y3+H*	2.48E+13 (2.48E+13)	0.62	40828.40
Y1=>X1	1.57E+11	0.48	3593.30
X1=>Z3	7.63E+11	0.08	314.38
Z0+C2H2=>Y1*	3.20E+03 (4.00E+03)	2.49	1411.55
Z1=>Z0+C2H2*	4.10E+14 (8.20E+14)	0.22	41525.69
Z2=>Z1	1.02E+15	0.22	60370.99
Z3=>Z2	1.26E+12	0.26	26502.46
Z4+H=>Z3	1.78E+09	1.53	-1153.28
Y1=>Z1	1.51E+13	0.05	5259.19
Y2=>Y1	4.92E+12	0.44	57644.90
Y3+H=>Y2	1.06E+09	1.47	-469.78
Y3+H=>Y1*	1.50E+08 (9.37E+07)	1.47	8254.74
X1=>Y1	7.56E+10	0.61	2882.37
Z3=>X1	1.41E+13	0.09	68765.58
Y1=>Z0+C2H2*	1.43E+14 (2.85E+14)	0.03	46978.36

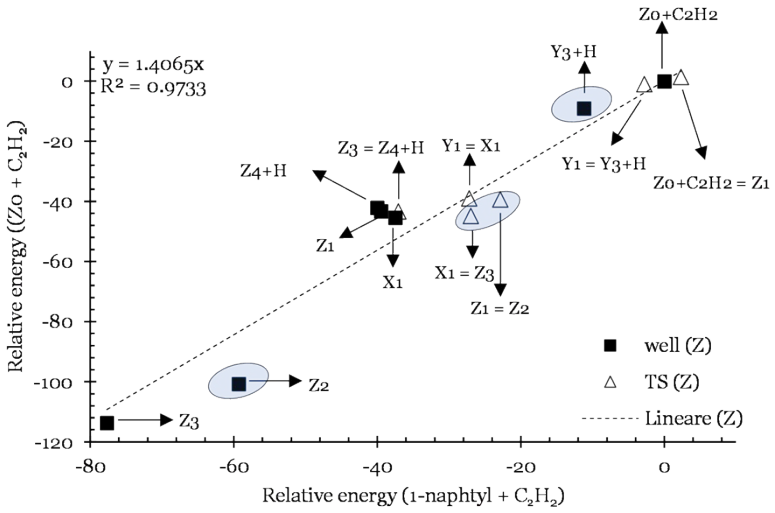

Figure S1: Relative energies of the intermediates (solid squares) and transition states (empty triangles) for the C_2H_2 deposition on zigzag site compared to that observed in the '1-naphtyl+ C_2H_2' PES from [1]. TS with larger deviations from the linear correlations found for are highlighted by circles.

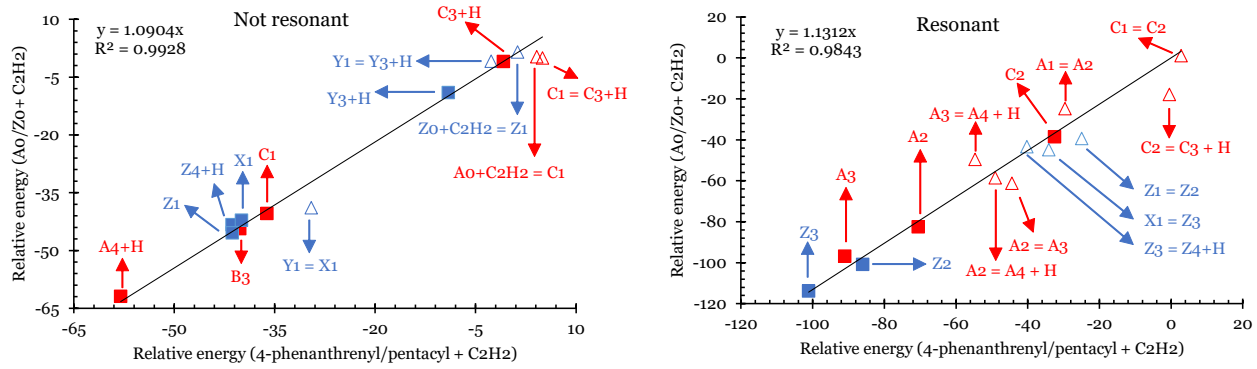

Figure S2: Relative energies of the intermediates (solid squares) and transition states (empty triangles) related to compared to that observed in PESs of analogous gas phase prototypes from [1, 2] for the C_2H_2 deposition on armchair and zigzag sites: a resonant intermediates and their associated transition states; b. non-resonant intermediates and reactions not involving resonant radical intermediates.

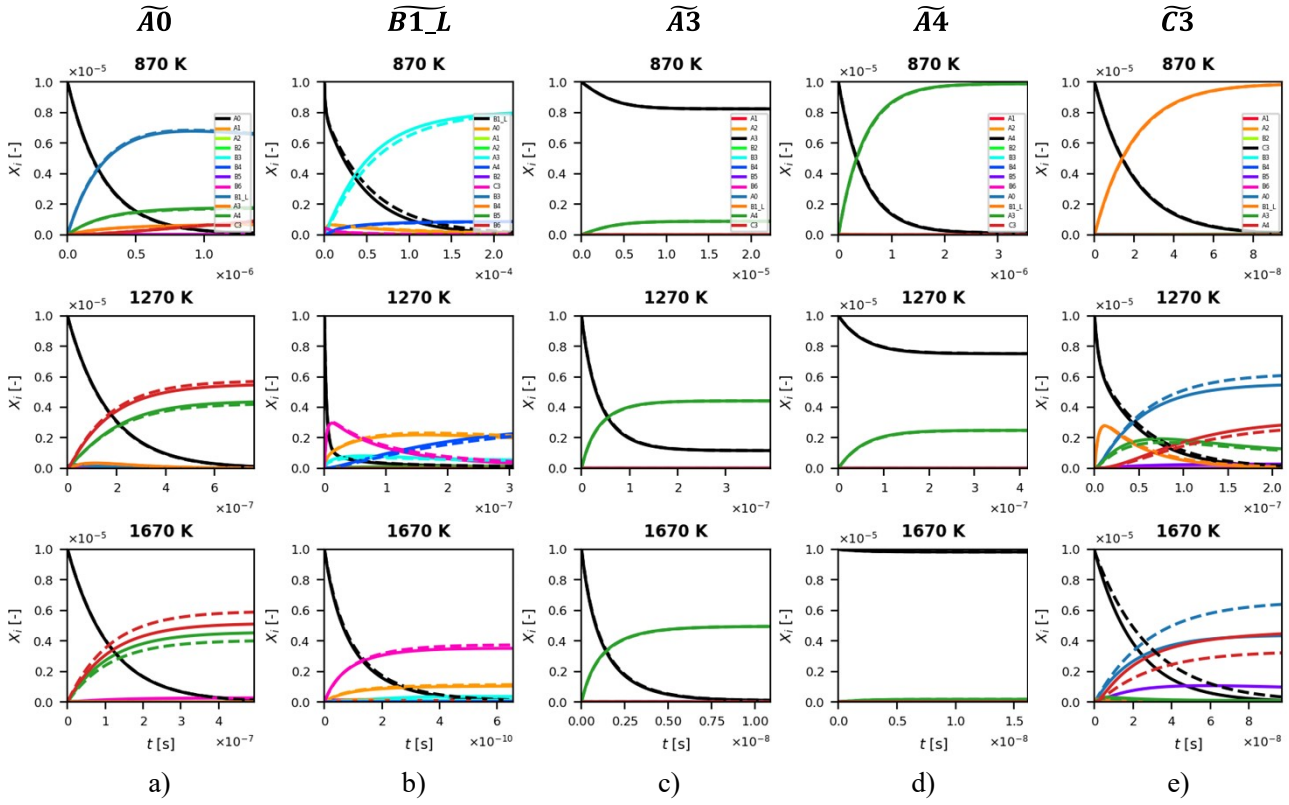

Figure S3: Comparison between the performances of the detailed (solid lines) and lumped with MEL [3] (dashed lines) mechanisms of armchair graphene edge growth in the 800–1900 K range of the reactivity of pseudospecies $\tilde{A}0$ a), $B\tilde{1}\_L$ b), $\tilde{A}3$ c), $\tilde{A}4$ d) and $\tilde{C}3$ e).

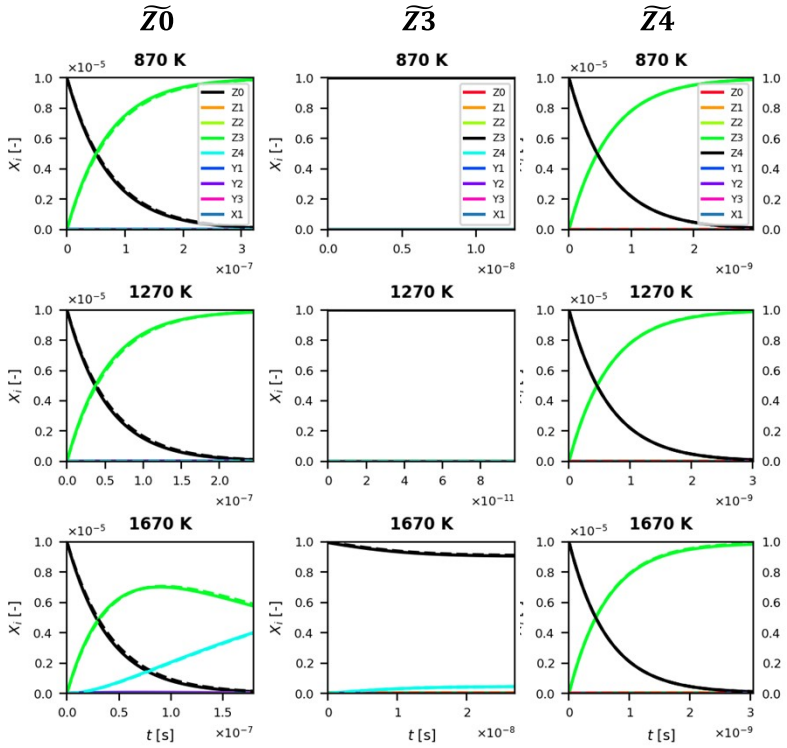

Figure S4: Comparison between the performances of the detailed (solid lines) and lumped with MEL [3] (dashed lines) mechanisms of zigzag graphene edge growth in the 800–1900 K range of the reactivity of pseudospecies $\tilde{Z}0$ a), $\tilde{Z}3$ b), $\tilde{Z}4$ c).

Table S1: Total energies and zero-point energy corrections of gas molecules, solid species and transition states. ZPE corrections are estimates by vibrating the six atoms mainly involved.

gas species	**Total Energy [eV]**	**ZPE [kcal/mol]**			
C2H2	-531.338	16.58			
H	-13.600				
zigzag edge					
species	**Total Energy [eV]**	**ZPE [kcal/mol]**	**TS**	**Total Energy [eV]**	**ZPE [kcal/mol]**
Z0	-12153.359	10.33	Z0+C2H2=>Z1	-12684.631	26.91
Z1	-12686.573	29.24	Z1=>Z2	-12686.401	27.65
Z2	-12689.066	31.55	Z2=>Z3	-12688.407	29.04
Z3	-12689.629	31.06	Z3=>Z4+H	-12686.573	24.61
Z4	-12672.925	24.38	Y1=>X1	-12686.383	26.41
Y1	-12686.651	28.71	X1=>Z3	-12686.639	29.89
Y2	-12688.331	29.93	Z1=>Y1	-12686.423	27.91
Y3	-12671.489	22.67	Y1=>Y2	-12685.719	26.52
X1	-12686.641	30.19	Y1=>Y3+H	-12684.734	23.75
			Y2=>Y3+H	-12685.127	23.55
			Z0+C2H2=>Y1	-12684.630	27.06
armchair edge					
species	Total Energy [eV]	ZPE [kcal/mol]	TS	Total Energy [eV]	ZPE [kcal/mol]
A0	-12153.028	10.56	A0+C2H2=A1	-12684.279	27.26
A1	-12685.993	29.15	A1=A2	-12685.440	28.23

A2	-12687.941	31.73	A2=A3	-12687.021	28.67
A3	-12688.561	31.27	A3=A4+H	-12686.515	26.24
A4	-12673.450	25.21	A2=A4+H	-12686.900	26.20
B1	-12686.086	29.47	A0+C2H2=B1	-12684.341	27.24
B2	-12686.811	29.75	B1=B2	-12684.348	25.58
B3	-12686.289	30.23	A1=B2	-12684.355	25.41
B4	-12686.880	29.04	B2=B3	-12685.758	26.43
B5	-12687.982	30.37	B3=B4	-12686.255	29.70
B6	-12671.920	23.89	B4=B5	-12685.747	27.19
C1	-12686.118	29.33	B5=B6+H	-12685.544	24.38
C2	-12686.033	29.96	B4=B6+H	-12685.420	24.45
C3	-12670.808	23.18	B4=A3	-12686.373	25.44
			B2=C1	-12684.375	25.44
			B2=C3+H	-12683.758	23.73
			B1=C1	-12685.935	28.34
			A0+C2H2=C1	-12684.355	27.28
			C2=C3+H	-12684.317	24.05
			C1=C3+H	-12684.368	23.80
			C1=C2	-12685.140	26.45
			A1=B1	-12685.042	29.15

Table S4: Cartesian atomic coordinates (Angstrom) of the unit cell of acetylene and solid structures (i.e., reactants, intermediates, and products) with armchair and zigzag edges.

C2H2				A0				A1			
H	0.0008	4.6403	6.9244	C	0.0140	21.2590	8.0009	C	0.0357	21.2541	8.0029
C	-0.0013	4.7294	7.9911	C	0.7335	22.4665	8.0002	C	0.7547	22.4620	8.0034
C	-0.0011	4.8373	9.1935	C	2.1063	22.4663	8.0001	C	2.1277	22.4635	8.0018
H	0.0005	4.9420	10.2590	C	2.8261	21.2589	8.0009	C	2.8475	21.2559	8.0027
				C	4.2736	21.2585	8.0008	C	4.2951	21.2545	8.0055
				C	4.9934	22.4658	8.0002	C	5.0144	22.4617	8.0055
				C	6.3665	22.4657	8.0003	C	6.3873	22.4632	8.0058
				C	7.0865	21.2584	8.0009	C	7.1083	21.2560	8.0042
				C	0.0014	18.7873	8.0010	C	0.0240	18.7822	7.9944
				C	0.7065	20.0302	8.0011	C	0.7288	20.0254	7.9986
				C	2.1340	20.0301	8.0011	C	2.1565	20.0262	8.0009
				C	2.8396	18.7873	8.0010	C	2.8619	18.7833	8.0015
				C	4.2608	18.7865	8.0009	C	4.2831	18.7834	8.0011
				C	4.9665	20.0295	8.0010	C	4.9881	20.0263	8.0030
				C	6.3941	20.0294	8.0010	C	6.4162	20.0269	8.0006
				C	7.1002	18.7865	8.0008	C	7.1225	18.7840	7.9957
				C	0.0036	16.3288	8.0007	C	0.0253	16.3221	8.0031
				C	0.7019	17.5569	8.0009	C	0.7243	17.5505	7.9953
				C	2.1396	17.5569	8.0009	C	2.1619	17.5517	7.9991
				C	2.8384	16.3290	8.0008	C	2.8600	16.3236	8.0010
				C	4.2632	16.3277	8.0007	C	4.2851	16.3246	8.0012
				C	4.9617	17.5558	8.0008	C	4.9837	17.5529	7.9996
				C	6.3997	17.5556	8.0008	C	6.4217	17.5535	7.9979
				C	7.0988	16.3274	8.0007	C	7.1202	16.3251	8.0048
				C	0.0096	13.8611	8.0007	C	0.0323	13.8512	8.0646

				C	0.7088	15.0880	8.0006	C	0.7308	15.0799	8.0217
				C	2.1336	15.0880	8.0006	C	2.1551	15.0820	8.0113
				C	2.8330	13.8608	8.0008	C	2.8542	13.8545	8.0310
				C	4.2706	13.8574	8.0007	C	4.2914	13.8565	8.0420
				C	4.9687	15.0856	8.0007	C	4.9903	15.0840	8.0156
				C	6.3936	15.0848	8.0006	C	6.4154	15.0843	8.0251
				C	7.0923	13.8563	8.0006	C	7.1155	13.8580	8.0683
				C	0.0025	11.3941	8.0011	C	0.0295	11.3713	8.1229
				C	0.7116	12.6327	8.0010	C	0.7333	12.6195	8.0992
				C	2.1335	12.6319	8.0010	C	2.1539	12.6251	8.0789
				C	2.8427	11.3913	8.0013	C	2.8580	11.3881	8.1876
				C	4.2689	11.3824	8.0010	C	4.2864	11.3942	8.2290
				C	4.9723	12.6259	8.0008	C	4.9924	12.6303	8.1179
				C	6.3919	12.6243	8.0006	C	6.4155	12.6301	8.1238
				C	7.0948	11.3778	8.0006	C	7.1204	11.3912	8.1592
				C	-0.0391	9.0089	8.0011	C	-0.0119	8.9350	7.8609
				C	0.7125	10.1707	8.0013	C	0.7255	10.1378	8.0927
				C	2.1525	10.1669	8.0015	C	2.1641	10.1613	8.2949
				C	2.8477	8.9475	8.0010	C	2.8814	9.0130	8.6928
				C	4.2225	8.9383	8.0003	C	4.2595	9.0156	8.7263
				C	4.9526	10.1444	8.0007	C	4.9824	10.1774	8.3918
				C	6.4017	10.1444	8.0006	C	6.4232	10.1667	8.2348
				C	7.1304	8.9239	8.0011	C	7.1261	8.9718	8.0253
				H	2.2758	8.0182	8.0002	H	2.3411	8.1093	8.9608
				H	4.7397	7.9815	7.9982	H	4.7897	8.1106	9.0246
				H	6.6220	7.9611	8.0016	H	6.5672	8.0452	7.8886
				H	0.2151	23.4219	7.9985	H	0.2348	23.4165	8.0005
				H	2.6247	23.4217	7.9981	H	2.6448	23.4193	8.0003
				H	4.4749	23.4211	7.9981	H	4.4946	23.4158	8.0003
				H	6.8848	23.4211	7.9985	H	6.9047	23.4191	8.0016
								H	-0.1573	6.8169	7.4270
								C	0.5170	7.6745	7.2838
								C	1.5776	7.4811	6.5242
								H	2.4356	8.0106	6.1243
A2				A3				A4			
C	0.0015	21.2875	8.0064	C	0.0384	21.2841	8.0069	C	0.0237	21.2720	8.0180
C	0.7244	22.4984	8.0049	C	0.7626	22.4944	8.0066	C	0.7466	22.4816	8.0237
C	2.0935	22.4988	8.0047	C	2.1325	22.4944	8.0068	C	2.1172	22.4813	8.0229
C	2.8183	21.2872	8.0083	C	2.8553	21.2851	8.0074	C	2.8384	21.2714	8.0171
C	4.2603	21.2873	8.0076	C	4.2979	21.2843	8.0075	C	4.2833	21.2719	8.0170
C	4.9845	22.4970	8.0045	C	5.0213	22.4941	8.0074	C	5.0056	22.4811	8.0200
C	6.3545	22.4974	8.0038	C	6.3917	22.4943	8.0073	C	6.3769	22.4809	8.0196
C	7.0798	21.2872	8.0059	C	7.1152	21.2853	8.0070	C	7.0988	21.2718	8.0174
C	-0.0080	18.8184	8.0028	C	0.0236	18.8151	8.0082	C	0.0087	18.8018	8.0134
C	0.6963	20.0574	8.0069	C	0.7314	20.0563	8.0072	C	0.7160	20.0436	8.0149
C	2.1257	20.0590	8.0090	C	2.1605	20.0552	8.0075	C	2.1449	20.0435	8.0148
C	2.8333	18.8176	8.0061	C	2.8645	18.8159	8.0076	C	2.8497	18.8014	8.0135
C	4.2519	18.8178	8.0029	C	4.2833	18.8149	8.0075	C	4.2682	18.8016	8.0132
C	4.9568	20.0575	8.0055	C	4.9909	20.0559	8.0074	C	4.9757	20.0431	8.0147

C	6.3862	20.0585	8.0040	C	6.4196	20.0558	8.0071	C	6.4045	20.0433	8.0152
C	7.0937	18.8177	7.9998	C	7.1242	18.8160	8.0081	C	7.1100	18.8016	8.0135
C	0.0009	16.3560	7.9962	C	0.0217	16.3545	8.0134	C	0.0101	16.3422	8.0101
C	0.6985	17.5818	8.0002	C	0.7253	17.5833	8.0099	C	0.7100	17.5684	8.0118
C	2.1309	17.5844	8.0015	C	2.1587	17.5811	8.0081	C	2.1462	17.5684	8.0117
C	2.8341	16.3547	7.9977	C	2.8551	16.3547	8.0072	C	2.8431	16.3417	8.0099
C	4.2614	16.3535	7.9986	C	4.2829	16.3513	8.0074	C	4.2700	16.3405	8.0100
C	4.9596	17.5825	7.9981	C	4.9853	17.5828	8.0082	C	4.9702	17.5682	8.0117
C	6.3898	17.5842	7.9978	C	6.4170	17.5825	8.0100	C	6.4050	17.5687	8.0119
C	7.0920	16.3517	7.9980	C	7.1153	16.3547	8.0134	C	7.1029	16.3410	8.0104
C	0.0085	13.8870	7.9912	C	0.0166	13.8858	8.0161	C	0.0114	13.8716	8.0100
C	0.7085	15.1158	7.9944	C	0.7238	15.1166	8.0143	C	0.7140	15.1006	8.0098
C	2.1321	15.1184	7.9952	C	2.1475	15.1138	8.0092	C	2.1367	15.1006	8.0098
C	2.8408	13.8856	8.0023	C	2.8452	13.8847	8.0061	C	2.8366	13.8712	8.0098
C	4.2675	13.8814	8.0100	C	4.2790	13.8781	8.0020	C	4.2724	13.8663	8.0096
C	4.9690	15.1130	8.0028	C	4.9841	15.1164	8.0079	C	4.9754	15.1006	8.0092
C	6.3905	15.1172	8.0000	C	6.4072	15.1142	8.0129	C	6.3949	15.1012	8.0092
C	7.0970	13.8754	7.9919	C	7.1077	13.8854	8.0132	C	7.0957	13.8668	8.0097
C	0.0178	11.4241	7.9567	C	0.0076	11.4137	7.9973	C	0.0019	11.4047	8.0171
C	0.7167	12.6565	7.9914	C	0.7165	12.6552	8.0141	C	0.7106	12.6434	8.0111
C	2.1400	12.6573	8.0126	C	2.1376	12.6538	8.0100	C	2.1348	12.6435	8.0121
C	2.8480	11.4184	8.0850	C	2.8392	11.4167	8.0084	C	2.8413	11.4045	8.0270
C	4.2767	11.4152	8.0583	C	4.2627	11.4121	7.9865	C	4.2623	11.3960	8.0278
C	4.9708	12.6387	8.0132	C	4.9735	12.6538	7.9910	C	4.9703	12.6397	8.0134
C	6.4036	12.6498	7.9813	C	6.4034	12.6459	7.9978	C	6.3955	12.6404	8.0138
C	7.1128	11.4073	7.9314	C	7.0997	11.4204	7.9764	C	7.1008	11.3961	8.0207
C	0.0391	8.9611	7.8533	C	-0.0048	8.9331	7.9061	C	0.0091	8.9418	8.0601
C	0.7395	10.1988	7.9964	C	0.7067	10.1938	7.9971	C	0.7078	10.1785	8.0385
C	2.1364	10.2099	8.1484	C	2.1298	10.1864	8.0273	C	2.1339	10.1785	8.0524
C	2.8464	8.9300	8.4849	C	2.8373	8.9576	8.0608	C	2.8306	8.9417	8.1044
C	4.2942	8.9690	8.1434	C	4.2145	8.9804	8.0179	C	4.2317	8.9637	8.1098
C	4.9786	10.1418	8.0044	C	4.9445	10.1781	7.9626	C	4.9488	10.1543	8.0555
C	6.4340	10.1671	7.8756	C	6.3986	10.1670	7.9111	C	6.4117	10.1550	8.0365
C	7.1785	8.9790	7.7644	C	7.0979	8.9864	7.8177	C	7.1281	8.9633	8.0441
H	2.8237	8.8697	9.6085	H	2.2752	7.2488	9.2166	H	4.7487	8.0065	8.1555
H	4.8086	8.0084	8.1313	H	4.7382	8.0252	8.0496	H	6.6109	8.0051	8.0494
H	6.6689	8.0251	7.6262	H	6.5775	8.0357	7.7178	H	0.2285	23.4372	8.0311
H	0.2044	23.4529	8.0006	H	0.2426	23.4489	8.0062	H	2.6377	23.4355	8.0305
H	2.6135	23.4532	7.9988	H	2.6506	23.4502	8.0059	H	4.4876	23.4368	8.0244
H	4.4647	23.4519	8.0004	H	4.5016	23.4487	8.0068	H	6.8967	23.4356	8.0252
H	6.8736	23.4521	8.0020	H	6.9098	23.4500	8.0071	H	0.1719	6.7767	8.1304
H	0.2607	6.8161	7.4939	H	0.0784	6.8027	7.8759	C	0.7366	7.7112	8.1104
C	0.7976	7.7276	7.7666	C	0.6542	7.7279	7.9460	C	2.1012	7.7109	8.1356
C	2.1161	7.6958	8.0285	C	2.1135	7.6410	8.1884	H	2.6631	6.7754	8.1810
H	2.6814	6.7627	7.9836	H	2.5843	6.8796	7.5410				
		B1				B2				B3	
C	0.0388	21.2564	8.0037	C	0.0529	21.2891	8.0130	C	0.0404	21.2618	8.0142
C	0.7587	22.4646	8.0015	C	0.7768	22.4992	8.0125	C	0.7610	22.4694	8.0152
C	2.1310	22.4646	8.0013	C	2.1471	22.4990	8.0119	C	2.1335	22.4696	8.0153

C	2.8514	21.2570	8.0044	C	2.8702	21.2901	8.0113	C	2.8533	21.2619	8.0144
C	4.2982	21.2568	8.0063	C	4.3135	21.2898	8.0122	C	4.3003	21.2614	8.0143
C	5.0179	22.4646	8.0051	C	5.0364	22.4998	8.0136	C	5.0198	22.4690	8.0159
C	6.3902	22.4647	8.0061	C	6.4067	22.4994	8.0132	C	6.3924	22.4692	8.0159
C	7.1119	21.2575	8.0060	C	7.1296	21.2901	8.0125	C	7.1132	21.2618	8.0141
C	0.0275	18.7854	8.0032	C	0.0392	18.8191	8.0085	C	0.0276	18.7905	8.0144
C	0.7323	20.0279	8.0035	C	0.7465	20.0610	8.0107	C	0.7332	20.0332	8.0141
C	2.1601	20.0282	8.0052	C	2.1755	20.0605	8.0092	C	2.1611	20.0333	8.0142
C	2.8665	18.7858	8.0057	C	2.8806	18.8208	8.0059	C	2.8669	18.7909	8.0144
C	4.2867	18.7867	8.0045	C	4.2996	18.8199	8.0036	C	4.2876	18.7901	8.0140
C	4.9916	20.0291	8.0058	C	5.0062	20.0611	8.0079	C	4.9928	20.0327	8.0137
C	6.4198	20.0290	8.0036	C	6.4349	20.0605	8.0092	C	6.4206	20.0328	8.0135
C	7.1270	18.7870	8.0011	C	7.1399	18.8203	8.0083	C	7.1267	18.7902	8.0139
C	0.0314	16.3260	7.9996	C	0.0392	16.3569	8.0011	C	0.0302	16.3319	8.0179
C	0.7297	17.5537	8.0026	C	0.7416	17.5867	8.0039	C	0.7289	17.5598	8.0158
C	2.1668	17.5541	8.0013	C	2.1754	17.5858	8.0030	C	2.1666	17.5602	8.0154
C	2.8658	16.3268	7.9904	C	2.8721	16.3592	7.9952	C	2.8654	16.3330	8.0154
C	4.2911	16.3284	7.9876	C	4.3001	16.3566	7.9944	C	4.2905	16.3307	8.0150
C	4.9888	17.5560	7.9971	C	5.0018	17.5876	8.0002	C	4.9885	17.5590	8.0144
C	6.4260	17.5563	7.9985	C	6.4344	17.5865	8.0041	C	6.4259	17.5590	8.0148
C	7.1260	16.3291	7.9980	C	7.1324	16.3586	8.0006	C	7.1249	16.3312	8.0175
C	0.0386	13.8547	8.0148	C	0.0344	13.8841	8.0130	C	0.0365	13.8625	8.0226
C	0.7376	15.0841	7.9998	C	0.7410	15.1173	8.0025	C	0.7359	15.0908	8.0194
C	2.1614	15.0849	7.9893	C	2.1646	15.1174	7.9942	C	2.1606	15.0923	8.0157
C	2.8614	13.8573	7.9888	C	2.8629	13.8882	7.9993	C	2.8606	13.8659	8.0134
C	4.2987	13.8595	7.9924	C	4.2967	13.8830	8.0024	C	4.2979	13.8595	8.0170
C	4.9974	15.0885	7.9868	C	5.0018	15.1205	7.9940	C	4.9960	15.0889	8.0169
C	6.4208	15.0891	7.9976	C	6.4245	15.1181	7.9978	C	6.4200	15.0892	8.0202
C	7.1217	13.8609	8.0159	C	7.1247	13.8881	8.0081	C	7.1191	13.8607	8.0253
C	0.0366	11.3772	8.0353	C	0.0287	11.4050	8.0361	C	0.0281	11.3910	7.9950
C	0.7404	12.6240	8.0258	C	0.7342	12.6526	8.0295	C	0.7372	12.6335	8.0139
C	2.1617	12.6276	8.0132	C	2.1561	12.6576	8.0315	C	2.1596	12.6382	8.0102
C	2.8666	11.3891	8.0995	C	2.8550	11.4258	8.1326	C	2.8700	11.4020	8.0218
C	4.2932	11.3950	8.1207	C	4.2800	11.4214	8.1422	C	4.2968	11.3820	8.0420
C	4.9994	12.6338	8.0335	C	4.9917	12.6588	8.0400	C	4.9985	12.6288	8.0268
C	6.4225	12.6340	8.0432	C	6.4219	12.6511	8.0344	C	6.4187	12.6299	8.0306
C	7.1302	11.3943	8.0639	C	7.1205	11.4237	8.0592	C	7.1225	11.3867	8.0199
C	0.0000	8.9351	7.8162	C	-0.0079	8.9298	7.8844	C	0.0354	8.9326	7.8572
C	0.7327	10.1407	8.0173	C	0.7321	10.1788	8.0577	C	0.7230	10.1682	7.9469
C	2.1738	10.1588	8.2009	C	2.1495	10.1950	8.2388	C	2.1609	10.1779	8.0177
C	2.8998	9.0039	8.5607	C	2.8711	9.0301	8.5773	C	2.9017	9.0139	8.1226
C	4.2796	9.0086	8.5729	C	4.2448	9.0334	8.6004	C	4.2574	8.9327	8.1625
C	4.9909	10.1767	8.2524	C	4.9682	10.1998	8.2831	C	4.9885	10.1472	8.0785
C	6.4328	10.1690	8.1053	C	6.4110	10.1789	8.1367	C	6.4416	10.1472	8.0218
C	7.1320	8.9740	7.9061	C	7.0856	8.9878	8.0096	C	7.1680	8.9476	7.9132
H	2.3695	8.0969	8.8388	H	2.3280	8.1254	8.8393	H	1.1027	5.6173	8.0583
H	4.8163	8.1012	8.8496	H	4.7739	8.1245	8.8843	H	4.7684	7.9758	8.2640
H	6.5792	8.0504	7.7373	H	6.5463	8.0444	7.9519	H	6.6468	7.9971	7.8155
H	0.2396	23.4193	7.9988	H	0.2583	23.4547	8.0078	H	0.2423	23.4247	8.0175

H	2.6495	23.4195	7.9981	H	2.6656	23.4543	8.0087	H	2.6515	23.4252	8.0176
H	4.4983	23.4190	7.9970	H	4.5176	23.4549	8.0094	H	4.5013	23.4243	8.0189
H	6.9086	23.4197	7.9979	H	6.9251	23.4550	8.0089	H	6.9105	23.4248	8.0188
H	1.5127	7.7467	6.7591	H	0.8508	6.2192	6.1350	H	1.4516	7.6619	6.7812
C	0.6388	7.6555	7.4185	C	0.5058	7.7218	7.5594	C	0.7703	7.6735	7.6388
C	0.2309	6.4519	7.7729	C	0.8252	6.5123	7.1914	C	0.5714	6.5312	8.3244
H	-0.5281	6.0012	8.4069	H	1.1084	5.7355	7.9125	H	-0.0965	6.4912	9.1865
		B4				B5				B6	
C	0.0088	21.2352	8.0143	C	0.0562	21.2706	8.0110	C	0.0276	21.2774	8.0121
C	0.7294	22.4437	8.0115	C	0.7759	22.4762	8.0113	C	0.7482	22.4852	8.0136
C	2.1017	22.4431	8.0133	C	2.1505	22.4761	8.0112	C	2.1206	22.4852	8.0135
C	2.8216	21.2350	8.0158	C	2.8690	21.2701	8.0110	C	2.8409	21.2773	8.0122
C	4.2685	21.2331	8.0167	C	4.3171	21.2679	8.0111	C	4.2876	21.2748	8.0120
C	4.9894	22.4410	8.0161	C	5.0355	22.4742	8.0113	C	5.0075	22.4825	8.0128
C	6.3619	22.4403	8.0138	C	6.4092	22.4742	8.0114	C	6.3797	22.4826	8.0129
C	7.0820	21.2324	8.0152	C	7.1280	21.2679	8.0111	C	7.1008	21.2751	8.0119
C	-0.0055	18.7635	8.0217	C	0.0425	18.8001	8.0101	C	0.0149	18.8078	8.0097
C	0.7007	20.0066	8.0177	C	0.7485	20.0413	8.0106	C	0.7207	20.0495	8.0111
C	2.1290	20.0064	8.0157	C	2.1764	20.0412	8.0106	C	2.1488	20.0494	8.0113
C	2.8346	18.7636	8.0138	C	2.8814	18.7999	8.0102	C	2.8554	18.8079	8.0102
C	4.2551	18.7594	8.0142	C	4.3047	18.7946	8.0104	C	4.2757	18.8031	8.0102
C	4.9609	20.0031	8.0167	C	5.0087	20.0379	8.0110	C	4.9806	20.0459	8.0111
C	6.3891	20.0028	8.0190	C	6.4355	20.0380	8.0109	C	6.4083	20.0459	8.0108
C	7.0940	18.7591	8.0224	C	7.1391	18.7946	8.0103	C	7.1144	18.8032	8.0096
C	-0.0045	16.3072	8.0168	C	0.0423	16.3450	8.0100	C	0.0180	16.3525	8.0064
C	0.6952	17.5336	8.0192	C	0.7429	17.5726	8.0096	C	0.7172	17.5789	8.0081
C	2.1330	17.5337	8.0147	C	2.1808	17.5725	8.0095	C	2.1548	17.5788	8.0084
C	2.8330	16.3074	8.0108	C	2.8804	16.3445	8.0092	C	2.8551	16.3526	8.0068
C	4.2582	16.2970	8.0108	C	4.3058	16.3310	8.0095	C	4.2804	16.3410	8.0074
C	4.9560	17.5260	8.0145	C	5.0028	17.5629	8.0097	C	4.9769	17.5702	8.0086
C	6.3929	17.5257	8.0193	C	6.4398	17.5631	8.0097	C	6.4141	17.5701	8.0083
C	7.0900	16.2967	8.0166	C	7.1365	16.3312	8.0102	C	7.1124	16.3412	8.0069
C	0.0004	13.8454	8.0057	C	0.0455	13.8873	8.0205	C	0.0246	13.8905	8.0100
C	0.7019	15.0712	8.0113	C	0.7477	15.1115	8.0122	C	0.7254	15.1165	8.0055
C	2.1264	15.0711	8.0096	C	2.1748	15.1110	8.0111	C	2.1497	15.1163	8.0056
C	2.8284	13.8453	8.0038	C	2.8760	13.8863	8.0172	C	2.8520	13.8906	8.0098
C	4.2660	13.8174	8.0013	C	4.3110	13.8529	8.0198	C	4.2896	13.8612	8.0144
C	4.9631	15.0500	8.0081	C	5.0062	15.0834	8.0129	C	4.9854	15.0935	8.0089
C	6.3855	15.0495	8.0102	C	6.4351	15.0838	8.0140	C	6.4087	15.0934	8.0088
C	7.0826	13.8169	8.0032	C	7.1302	13.8535	8.0234	C	7.1068	13.8615	8.0146
C	-0.0297	11.3982	7.9611	C	0.0186	11.4437	8.0591	C	-0.0044	11.4446	8.0499
C	0.6988	12.6262	7.9915	C	0.7467	12.6711	8.0322	C	0.7242	12.6724	8.0193
C	2.1299	12.6258	7.9909	C	2.1749	12.6699	8.0295	C	2.1547	12.6720	8.0191
C	2.8585	11.3977	7.9629	C	2.9019	11.4413	8.0536	C	2.8849	11.4446	8.0494
C	4.2799	11.3179	7.9588	C	4.3281	11.3539	8.0617	C	4.3064	11.3612	8.0618
C	4.9682	12.5770	7.9867	C	5.0099	12.6029	8.0384	C	4.9924	12.6203	8.0328
C	6.3807	12.5766	7.9862	C	6.4301	12.6036	8.0416	C	6.4054	12.6202	8.0331
C	7.0688	11.3175	7.9572	C	7.1122	11.3554	8.0677	C	7.0940	11.3617	8.0626
C	0.1658	8.9427	7.8837	C	0.2557	8.9707	8.1229	C	0.2053	8.9861	8.1525

C	0.7036	10.2258	7.9254	C	0.7576	10.2904	8.0852	C	0.7303	10.2782	8.0899
C	2.1248	10.2252	7.9286	C	2.1625	10.2877	8.0828	C	2.1513	10.2779	8.0897
C	2.6657	8.9441	7.8843	C	2.6602	8.9647	8.1215	C	2.6764	8.9857	8.1513
C	4.0781	8.8516	7.8873	C	4.1064	8.8814	8.1274	C	4.0971	8.8944	8.1568
C	4.9168	10.0271	7.9214	C	4.9534	10.0414	8.0984	C	4.9405	10.0664	8.1112
C	6.4321	10.0265	7.9209	C	6.4851	10.0430	8.1006	C	6.4612	10.0668	8.1121
C	7.2721	8.8514	7.8861	C	7.3318	8.8845	8.1275	C	7.3048	8.8949	8.1596
H	1.8942	5.9966	8.8343	H	2.3588	6.1776	7.8488	H	4.5809	7.9160	8.2006
H	4.5632	7.8739	7.8620	H	4.5913	7.9020	8.1583	H	6.8203	7.9170	8.2062
H	6.7911	7.8715	7.8611	H	6.8482	7.9042	8.1530	H	0.2297	23.4406	8.0158
H	0.2119	23.3994	8.0111	H	0.2588	23.4324	8.0124	H	2.6384	23.4409	8.0154
H	2.6221	23.3972	8.0135	H	2.6684	23.4318	8.0120	H	4.4887	23.4377	8.0144
H	4.4719	23.3968	8.0158	H	4.5177	23.4298	8.0117	H	6.8977	23.4383	8.0147
H	6.8827	23.3941	8.0135	H	6.9277	23.4295	8.0121	H	0.5109	6.1698	8.3808
H	1.4198	7.4274	6.8785	H	0.5859	6.2005	7.6709	C	1.4404	8.0768	8.2115
C	1.4029	7.9566	7.8470	C	1.4544	8.1107	8.1465	C	1.4409	6.7369	8.3278
C	1.4228	6.9712	8.9576	C	1.4315	6.6232	8.2344	H	2.3721	6.1714	8.3781
H	1.1338	7.2851	9.9603	H	1.3156	6.2838	9.2794				
		C1				C2				C3	
C	0.0689	21.2549	8.0091	C	0.0310	21.2560	8.0131	C	0.0660	21.2454	8.0147
C	0.7896	22.4630	8.0135	C	0.7548	22.4669	8.0154	C	0.7865	22.4534	8.0175
C	2.1619	22.4632	8.0144	C	2.1238	22.4666	8.0157	C	2.1590	22.4536	8.0181
C	2.8824	21.2552	8.0105	C	2.8486	21.2551	8.0135	C	2.8794	21.2458	8.0149
C	4.3290	21.2556	8.0113	C	4.2907	21.2563	8.0133	C	4.3263	21.2462	8.0151
C	5.0498	22.4633	8.0154	C	5.0139	22.4668	8.0152	C	5.0464	22.4542	8.0190
C	6.4218	22.4637	8.0155	C	6.3838	22.4666	8.0148	C	6.4187	22.4542	8.0185
C	7.1423	21.2557	8.0105	C	7.1094	21.2558	8.0127	C	7.1389	21.2462	8.0150
C	0.0558	18.7831	8.0029	C	0.0223	18.7852	8.0111	C	0.0528	18.7732	8.0114
C	0.7617	20.0260	8.0055	C	0.7265	20.0253	8.0122	C	0.7586	20.0164	8.0128
C	2.1898	20.0264	8.0058	C	2.1562	20.0263	8.0121	C	2.1868	20.0166	8.0124
C	2.8958	18.7836	8.0015	C	2.8635	18.7842	8.0098	C	2.8927	18.7738	8.0099
C	4.3161	18.7844	8.0019	C	4.2822	18.7859	8.0093	C	4.3133	18.7744	8.0098
C	5.0216	20.0270	8.0071	C	4.9864	20.0263	8.0112	C	5.0186	20.0174	8.0125
C	6.4497	20.0272	8.0063	C	6.4159	20.0268	8.0116	C	6.4466	20.0173	8.0129
C	7.1554	18.7846	8.0026	C	7.1236	18.7851	8.0109	C	7.1521	18.7743	8.0113
C	0.0582	16.3230	8.0092	C	0.0324	16.3202	8.0078	C	0.0551	16.3133	8.0143
C	0.7571	17.5510	8.0015	C	0.7291	17.5472	8.0091	C	0.7539	17.5416	8.0099
C	2.1944	17.5515	7.9984	C	2.1614	17.5499	8.0081	C	2.1914	17.5422	8.0083
C	2.8930	16.3239	7.9959	C	2.8648	16.3204	8.0046	C	2.8899	16.3148	8.0061
C	4.3187	16.3251	7.9963	C	4.2918	16.3220	8.0067	C	4.3154	16.3157	8.0058
C	5.0172	17.5530	7.9989	C	4.9896	17.5504	8.0085	C	5.0141	17.5433	8.0078
C	6.4542	17.5531	8.0019	C	6.4199	17.5517	8.0094	C	6.4513	17.5433	8.0096
C	7.1527	16.3255	8.0105	C	7.1232	16.3194	8.0091	C	7.1499	16.3158	8.0142
C	0.0643	13.8515	8.0673	C	0.0424	13.8466	8.0072	C	0.0610	13.8409	8.0572
C	0.7637	15.0807	8.0223	C	0.7410	15.0782	8.0041	C	0.7602	15.0708	8.0245
C	2.1873	15.0820	8.0060	C	2.1641	15.0827	8.0001	C	2.1841	15.0730	8.0127
C	2.8867	13.8535	8.0197	C	2.8729	13.8501	8.0063	C	2.8829	13.8451	8.0226
C	4.3244	13.8557	8.0306	C	4.2993	13.8522	8.0141	C	4.3210	13.8472	8.0247
C	5.0243	15.0849	8.0112	C	5.0002	15.0828	8.0079	C	5.0208	15.0756	8.0132

C	6.4475	15.0853	8.0288	C	6.4223	15.0864	8.0102	C	6.4447	15.0758	8.0247
C	7.1476	13.8574	8.0751	C	7.1313	13.8460	8.0139	C	7.1443	13.8481	8.0575
C	0.0592	11.3741	8.1196	C	0.0589	11.3701	7.9913	C	0.0575	11.3588	8.1149
C	0.7646	12.6205	8.0931	C	0.7519	12.6118	8.0060	C	0.7609	12.6084	8.0867
C	2.1859	12.6244	8.0625	C	2.1725	12.6196	8.0213	C	2.1815	12.6156	8.0652
C	2.8902	11.3857	8.1567	C	2.8748	11.3783	8.1070	C	2.8851	11.3771	8.1493
C	4.3166	11.3919	8.1935	C	4.3042	11.3942	8.1134	C	4.3116	11.3833	8.1568
C	5.0243	12.6307	8.1013	C	5.0029	12.6120	8.0439	C	5.0208	12.6209	8.0734
C	6.4477	12.6310	8.1207	C	6.4400	12.6231	8.0324	C	6.4445	12.6209	8.0910
C	7.1541	11.3910	8.1531	C	7.1554	11.3845	8.0212	C	7.1509	11.3808	8.1212
C	0.0207	8.9320	7.8820	C	0.0262	8.9034	7.8689	C	0.0141	8.9061	8.0020
C	0.7530	10.1369	8.0913	C	0.7753	10.1253	8.0025	C	0.7527	10.1219	8.1370
C	2.1947	10.1569	8.2677	C	2.1795	10.1553	8.1659	C	2.1954	10.1481	8.2754
C	2.9172	9.0043	8.6410	C	2.9022	8.8904	8.4983	C	2.9238	8.9897	8.6014
C	4.2980	9.0083	8.6648	C	4.3659	8.9888	8.5036	C	4.2998	8.9937	8.5947
C	5.0131	10.1746	8.3455	C	5.0218	10.1419	8.2108	C	5.0070	10.1659	8.2869
C	6.4570	10.1643	8.2048	C	6.4622	10.1592	8.0463	C	6.4482	10.1592	8.1594
C	7.1525	8.9703	7.9970	C	7.1589	8.9646	7.8830	C	7.1407	8.9568	8.0318
H	2.3811	8.1030	8.9298	H	2.5282	8.4920	9.4627	H	2.4005	8.0775	8.8666
H	4.8341	8.1025	8.9475	H	4.9173	8.0748	8.7203	H	4.8341	8.0808	8.8529
H	6.6030	8.0422	7.8374	H	6.6169	8.0304	7.7523	H	6.5985	8.0190	7.9326
H	0.2717	23.4185	8.0211	H	0.2347	23.4216	8.0202	H	0.2677	23.4086	8.0221
H	2.6807	23.4182	8.0211	H	2.6421	23.4218	8.0203	H	2.6776	23.4088	8.0240
H	4.5320	23.4188	8.0200	H	4.4947	23.4218	8.0186	H	4.5279	23.4095	8.0255
H	6.9405	23.4187	8.0201	H	6.9014	23.4222	8.0183	H	6.9373	23.4093	8.0239
H	1.5908	7.7992	6.8613	H	2.6261	8.0911	7.7890	C	0.5498	7.6013	7.7977
C	0.6466	7.6792	7.4195	C	0.5298	7.5839	7.6804	C	0.8396	6.4347	7.6149
C	0.1648	6.4567	7.5446	C	0.7603	6.3976	7.5328	H	1.1446	5.4197	7.4701
H	0.4367	5.4494	7.2449	H	1.0335	5.3712	7.4084				
		Z0				Z1				Z2	
C	-0.0009	-5.7352	0.0000	C	0.0184	-5.7358	0.1707	C	-0.0108	-5.7572	-0.0071
C	1.2293	-5.0519	0.0000	C	1.2483	-5.0533	0.1383	C	1.2197	-5.0751	-0.0108
C	2.4590	-5.7357	0.0002	C	2.4781	-5.7358	0.1703	C	2.4500	-5.7579	-0.0079
C	3.6888	-5.0519	0.0002	C	3.7080	-5.0529	0.1375	C	3.6794	-5.0740	-0.0091
C	4.9192	-5.7350	0.0003	C	4.9384	-5.7352	0.1702	C	4.9085	-5.7583	-0.0080
C	6.1495	-5.0519	0.0002	C	6.1683	-5.0529	0.1380	C	6.1389	-5.0763	-0.0085
C	7.3793	-5.7357	0.0002	C	7.3981	-5.7357	0.1704	C	7.3691	-5.7585	-0.0079
C	8.6090	-5.0519	0.0000	C	8.6282	-5.0532	0.1387	C	8.5983	-5.0749	-0.0096
C	1.2293	-3.6114	0.0000	C	1.2479	-3.6149	0.0722	C	1.2184	-3.6353	-0.0139
C	2.4592	-2.9045	0.0000	C	2.4772	-2.9086	0.0429	C	2.4485	-2.9277	-0.0102
C	3.6888	-3.6116	0.0001	C	3.7075	-3.6144	0.0707	C	3.6790	-3.6338	-0.0073
C	4.9192	-2.9049	0.0001	C	4.9378	-2.9086	0.0416	C	4.9088	-2.9281	0.0017
C	6.1495	-3.6116	0.0001	C	6.1681	-3.6146	0.0710	C	6.1378	-3.6367	-0.0038
C	7.3791	-2.9045	0.0000	C	7.3979	-2.9089	0.0430	C	7.3662	-2.9295	-0.0005
C	8.6090	-3.6114	0.0000	C	8.6280	-3.6147	0.0727	C	8.5965	-3.6355	-0.0091
C	-0.0009	-2.9044	-0.0001	C	0.0181	-2.9086	0.0442	C	-0.0126	-2.9299	-0.0095
C	-0.0009	-1.4727	-0.0001	C	0.0178	-1.4781	-0.0061	C	-0.0135	-1.4992	-0.0038
C	1.2294	-0.7638	0.0000	C	1.2469	-0.7689	-0.0243	C	1.2176	-0.7900	-0.0167
C	2.4591	-1.4729	0.0000	C	2.4762	-1.4782	-0.0061	C	2.4489	-1.4978	-0.0094

C	3.6892	-0.7640	0.0000	C	3.7062	-0.7705	-0.0250	C	3.6800	-0.7887	0.0056
C	4.9191	-1.4730	0.0000	C	4.9374	-1.4781	-0.0079	C	4.9089	-1.4962	0.0165
C	6.1491	-0.7640	0.0000	C	6.1683	-0.7710	-0.0269	C	6.1372	-0.7838	0.0303
C	7.3792	-1.4728	0.0000	C	7.3982	-1.4787	-0.0079	C	7.3647	-1.4980	0.0180
C	8.6089	-0.7638	0.0000	C	8.6279	-0.7695	-0.0268	C	8.5942	-0.7923	0.0156
C	1.2294	0.6668	0.0001	C	1.2460	0.6613	-0.0472	C	1.2185	0.6373	-0.0359
C	2.4595	1.3748	0.0001	C	2.4747	1.3699	-0.0507	C	2.4548	1.3455	-0.0525
C	3.6894	0.6664	0.0000	C	3.7051	0.6588	-0.0465	C	3.6832	0.6402	-0.0041
C	4.9191	1.3759	-0.0001	C	4.9374	1.3627	-0.0530	C	4.9068	1.3608	0.0269
C	6.1489	0.6664	0.0000	C	6.1693	0.6580	-0.0502	C	6.1374	0.6494	0.0441
C	7.3788	1.3748	0.0001	C	7.3990	1.3687	-0.0580	C	7.3687	1.3570	0.0483
C	8.6089	0.6668	0.0001	C	8.6285	0.6608	-0.0521	C	8.5922	0.6353	0.0257
C	-0.0009	1.3762	0.0001	C	0.0174	1.3726	-0.0558	C	-0.0188	1.3379	-0.0103
C	-0.0009	2.8087	0.0000	C	0.0171	2.8058	-0.0606	C	-0.0255	2.7603	-0.0260
C	1.2326	3.5104	-0.0002	C	1.2444	3.5170	-0.0482	C	1.2086	3.4387	-0.1392
C	2.4615	2.8067	0.0000	C	2.4732	2.8017	-0.0497	C	2.4583	2.7679	-0.1107
C	3.6901	3.5160	-0.0004	C	3.7081	3.4974	-0.0449	C	3.6759	3.5121	-0.0490
C	4.9191	2.8081	-0.0004	C	4.9370	2.7906	-0.0526	C	4.9047	2.7970	0.0328
C	6.1482	3.5160	-0.0004	C	6.1657	3.4983	-0.0575	C	6.1401	3.5010	0.0856
C	7.3768	2.8067	0.0000	C	7.3993	2.8002	-0.0642	C	7.3709	2.7915	0.0702
C	8.6057	3.5104	-0.0002	C	8.6281	3.5143	-0.0698	C	8.6017	3.5032	0.0513
C	1.2434	4.9609	-0.0005	C	1.2510	4.9606	-0.0364	C	1.1816	4.8291	-0.1813
C	2.4664	5.6481	0.0008	C	2.4879	5.6223	-0.0549	C	2.3924	5.6641	-0.3881
C	3.6916	4.9565	0.0000	C	3.7113	4.9324	-0.0443	C	3.6958	4.9588	-0.0494
C	4.9191	5.6397	0.0003	C	4.9368	5.6186	-0.0359	C	4.8951	5.6220	0.0670
C	6.1467	4.9565	0.0000	C	6.1626	4.9335	-0.0434	C	6.1471	4.9364	0.1241
C	7.3719	5.6481	0.0008	C	7.3877	5.6223	-0.0305	C	7.3770	5.6223	0.1578
C	8.5949	4.9610	-0.0005	C	8.6223	4.9554	-0.0632	C	8.6069	4.9525	0.1074
C	-0.0009	5.5720	-0.0018	C	0.0153	5.6711	-0.0425	C	0.0554	5.5997	0.0477
H	-0.0009	-6.8280	0.0003	H	0.0183	-6.8270	0.2235	H	-0.0112	-6.8494	-0.0037
H	2.4590	-6.8284	0.0003	H	2.4783	-6.8269	0.2240	H	2.4492	-6.8504	-0.0034
H	4.9192	-6.8276	0.0003	H	4.9384	-6.8264	0.2235	H	4.9085	-6.8508	-0.0047
H	7.3794	-6.8284	0.0003	H	7.3979	-6.8269	0.2226	H	7.3692	-6.8505	-0.0060
H	2.4609	6.7392	0.0043	H	2.5112	6.7099	-0.0998	H	2.4565	5.7698	-1.4995
H	4.9191	6.7322	0.0010	H	4.9363	6.7112	-0.0239	H	4.9102	6.7148	0.0665
H	7.3775	6.7391	0.0043	H	7.3595	6.7100	0.0321	H	7.3626	6.7146	0.1751
				H	-0.7210	7.5816	-0.8085	H	-0.1012	7.8449	0.3738
				C	-0.0353	7.1517	-0.0627	C	0.5311	6.9798	0.1771
				C	0.6132	7.9944	0.7175	C	1.8861	7.0334	0.0195
				H	1.2893	7.9765	1.5688	H	2.4901	7.9385	0.0282
		Z3				Z4				X1	
C	-0.0062	-5.7649	-0.0477	C	-0.0128	-5.7585	-0.0149	C	0.0269	-5.7764	0.0797
C	1.2248	-5.0830	-0.0485	C	1.2177	-5.0752	-0.0187	C	1.2566	-5.0934	0.0642
C	2.4546	-5.7660	-0.0529	C	2.4479	-5.7588	-0.0205	C	2.4864	-5.7761	0.0801
C	3.6849	-5.0826	-0.0516	C	3.6774	-5.0750	-0.0137	C	3.7166	-5.0930	0.0641
C	4.9145	-5.7663	-0.0513	C	4.9073	-5.7587	-0.0082	C	4.9467	-5.7757	0.0797
C	6.1445	-5.0834	-0.0479	C	6.1377	-5.0760	0.0032	C	6.1767	-5.0930	0.0630
C	7.3744	-5.7665	-0.0473	C	7.3676	-5.7594	-0.0031	C	7.4063	-5.7761	0.0792
C	8.6032	-5.0827	-0.0454	C	8.5971	-5.0752	-0.0020	C	8.6367	-5.0937	0.0631

C	1.2237	-3.6429	-0.0363	C	1.2176	-3.6358	-0.0158	C	1.2567	-3.6539	0.0304
C	2.4533	-2.9363	-0.0257	C	2.4481	-2.9286	-0.0169	C	2.4863	-2.9471	0.0121
C	3.6840	-3.6423	-0.0392	C	3.6778	-3.6349	-0.0099	C	3.7167	-3.6533	0.0299
C	4.9146	-2.9362	-0.0262	C	4.9086	-2.9282	0.0062	C	4.9472	-2.9469	0.0107
C	6.1438	-3.6435	-0.0372	C	6.1375	-3.6360	0.0145	C	6.1770	-3.6536	0.0284
C	7.3728	-2.9362	-0.0257	C	7.3660	-2.9281	0.0199	C	7.4072	-2.9475	0.0097
C	8.6022	-3.6428	-0.0351	C	8.5966	-3.6351	0.0086	C	8.6371	-3.6540	0.0286
C	-0.0073	-2.9365	-0.0237	C	-0.0135	-2.9289	-0.0032	C	0.0272	-2.9471	0.0114
C	-0.0084	-1.5061	0.0059	C	-0.0146	-1.4984	-0.0045	C	0.0277	-1.5159	-0.0233
C	1.2228	-0.7976	0.0257	C	1.2173	-0.7894	-0.0178	C	1.2569	-0.8059	-0.0368
C	2.4535	-1.5057	0.0100	C	2.4490	-1.4983	-0.0165	C	2.4862	-1.5161	-0.0235
C	3.6861	-0.7992	0.0276	C	3.6798	-0.7903	-0.0083	C	3.7164	-0.8077	-0.0374
C	4.9160	-1.5046	0.0071	C	4.9098	-1.4966	0.0076	C	4.9476	-1.5157	-0.0246
C	6.1446	-0.7913	0.0216	C	6.1372	-0.7822	0.0164	C	6.1789	-0.8077	-0.0384
C	7.3721	-1.5045	0.0023	C	7.3645	-1.4966	0.0197	C	7.4082	-1.5164	-0.0249
C	8.6004	-0.7970	0.0195	C	8.5942	-0.7905	0.0069	C	8.6380	-0.8066	-0.0368
C	1.2231	0.6306	0.0526	C	1.2171	0.6359	-0.0255	C	1.2566	0.6249	-0.0512
C	2.4599	1.3307	0.0629	C	2.4542	1.3410	-0.0302	C	2.4860	1.3341	-0.0555
C	3.6893	0.6280	0.0547	C	3.6818	0.6382	-0.0149	C	3.7163	0.6221	-0.0533
C	4.9140	1.3488	0.0592	C	4.9061	1.3620	-0.0011	C	4.9491	1.3261	-0.0559
C	6.1457	0.6419	0.0491	C	6.1369	0.6521	0.0126	C	6.1808	0.6220	-0.0533
C	7.3758	1.3537	0.0526	C	7.3675	1.3618	0.0139	C	7.4107	1.3346	-0.0530
C	8.5986	0.6325	0.0464	C	8.5917	0.6379	0.0019	C	8.6389	0.6243	-0.0493
C	-0.0127	1.3386	0.0551	C	-0.0206	1.3407	-0.0157	C	0.0276	1.3362	-0.0490
C	-0.0159	2.7640	0.0497	C	-0.0273	2.7633	-0.0122	C	0.0258	2.7696	-0.0348
C	1.2293	3.4345	0.0493	C	1.2166	3.4442	-0.0299	C	1.2533	3.4763	-0.0361
C	2.4638	2.7546	0.0609	C	2.4605	2.7637	-0.0364	C	2.4858	2.7667	-0.0525
C	3.6796	3.4946	0.0463	C	3.6688	3.5093	-0.0224	C	3.7241	3.4589	-0.0494
C	4.9106	2.7838	0.0544	C	4.9038	2.7986	-0.0010	C	4.9519	2.7543	-0.0532
C	6.1413	3.4932	0.0354	C	6.1369	3.5021	0.0240	C	6.1791	3.4640	-0.0447
C	7.3771	2.7907	0.0440	C	7.3695	2.7979	0.0230	C	7.4128	2.7678	-0.0434
C	8.6055	3.5070	0.0276	C	8.6042	3.5082	0.0175	C	8.6405	3.4858	-0.0181
C	1.2490	4.8347	0.0008	C	1.2164	4.8296	-0.0173	C	1.2510	4.9250	0.0117
C	2.4016	5.5921	-0.0316	C	2.3883	5.6280	-0.0121	C	2.4965	5.5168	-0.0017
C	3.6759	4.9450	0.0025	C	3.6609	4.9685	-0.0082	C	3.7385	4.9035	-0.0339
C	4.9062	5.6156	-0.0177	C	4.9003	5.6292	0.0253	C	4.9575	5.5930	-0.0372
C	6.1340	4.9292	-0.0040	C	6.1367	4.9423	0.0376	C	6.1779	4.8985	-0.0383
C	7.3784	5.6164	-0.0375	C	7.3729	5.6288	0.0497	C	7.3999	5.5876	-0.0152
C	8.5920	4.9569	-0.0228	C	8.6115	4.9666	0.0319	C	8.6359	4.9293	0.0284
C	0.0475	5.6492	-0.0541	C	0.0433	5.6259	0.0156	C	0.0301	5.6582	0.0923
H	-0.0076	-6.8572	-0.0465	H	-0.0127	-6.8509	-0.0197	H	0.0269	-6.8685	0.1061
H	2.4530	-6.8586	-0.0462	H	2.4483	-6.8512	-0.0197	H	2.4866	-6.8682	0.1056
H	4.9124	-6.8591	-0.0485	H	4.9071	-6.8511	-0.0144	H	4.9466	-6.8678	0.1059
H	7.3739	-6.8590	-0.0498	H	7.3681	-6.8516	-0.0152	H	7.4059	-6.8682	0.1063
H	2.3491	7.5299	-1.0301	H	4.9158	6.7213	0.0416	H	2.0271	7.6629	-0.2229
H	4.9194	6.7077	-0.0466	H	7.3586	6.7211	0.0559	H	4.9544	6.6839	-0.0167
H	7.3629	6.7083	-0.0726	H	-0.1034	7.8878	0.0457	H	7.3560	6.6750	-0.0441
H	-0.1817	7.8387	-0.1962	C	0.5168	6.9935	0.0313	H	-0.9295	7.5256	0.6038
C	0.4495	6.9541	-0.1322	C	1.9110	6.9951	0.0171	C	0.0210	7.1005	0.2756

C	1.9635	7.0336	-0.1217	H	2.5285	7.8914	0.0277	C	1.0362	7.9753	0.1168
H	2.3300	7.6414	0.7255					H	0.8892	9.0363	0.3231
		Y1				Y2				Y3	
C	0.0074	-5.7489	0.1507	C	-0.0005	-5.7190	0.0284	C	-0.0026	-5.7468	0.1580
C	1.2378	-5.0669	0.1222	C	1.2299	-5.0361	0.0347	C	1.2278	-5.0641	0.1433
C	2.4677	-5.7493	0.1498	C	2.4596	-5.7196	0.0297	C	2.4575	-5.7474	0.1559
C	3.6975	-5.0660	0.1248	C	3.6895	-5.0354	0.0331	C	3.6873	-5.0642	0.1395
C	4.9276	-5.7486	0.1510	C	4.9195	-5.7192	0.0295	C	4.9175	-5.7469	0.1538
C	6.1576	-5.0657	0.1257	C	6.1496	-5.0355	0.0329	C	6.1478	-5.0641	0.1398
C	7.3870	-5.7492	0.1516	C	7.3795	-5.7196	0.0296	C	7.3776	-5.7474	0.1564
C	8.6169	-5.0667	0.1231	C	8.6092	-5.0361	0.0346	C	8.6072	-5.0640	0.1437
C	1.2383	-3.6283	0.0645	C	1.2298	-3.5962	0.0381	C	1.2278	-3.6247	0.1075
C	2.4674	-2.9217	0.0389	C	2.4588	-2.8887	0.0335	C	2.4575	-2.9185	0.0838
C	3.6978	-3.6270	0.0682	C	3.6894	-3.5952	0.0353	C	3.6874	-3.6248	0.1018
C	4.9285	-2.9211	0.0406	C	4.9198	-2.8883	0.0316	C	4.9177	-2.9188	0.0794
C	6.1586	-3.6269	0.0676	C	6.1500	-3.5952	0.0350	C	6.1480	-3.6247	0.1021
C	7.3887	-2.9212	0.0379	C	7.3808	-2.8888	0.0331	C	7.3780	-2.9185	0.0842
C	8.6178	-3.6280	0.0641	C	8.6096	-3.5962	0.0379	C	8.6075	-3.6246	0.1079
C	0.0082	-2.9223	0.0378	C	-0.0002	-2.8886	0.0328	C	-0.0023	-2.9183	0.0886
C	0.0082	-1.4916	-0.0092	C	0.0001	-1.4574	0.0082	C	-0.0021	-1.4876	0.0485
C	1.2370	-0.7819	-0.0287	C	1.2293	-0.7466	-0.0050	C	1.2279	-0.7790	0.0269
C	2.4663	-1.4916	-0.0122	C	2.4579	-1.4575	0.0153	C	2.4574	-1.4881	0.0421
C	3.6963	-0.7847	-0.0333	C	3.6887	-0.7502	0.0089	C	3.6873	-0.7805	0.0157
C	4.9285	-1.4911	-0.0133	C	4.9202	-1.4574	0.0196	C	4.9179	-1.4883	0.0355
C	6.1600	-0.7839	-0.0329	C	6.1519	-0.7501	0.0085	C	6.1487	-0.7805	0.0159
C	7.3898	-1.4910	-0.0120	C	7.3823	-1.4575	0.0149	C	7.3785	-1.4880	0.0424
C	8.6193	-0.7817	-0.0283	C	8.6112	-0.7466	-0.0054	C	8.6081	-0.7789	0.0271
C	1.2353	0.6487	-0.0488	C	1.2292	0.6842	-0.0334	C	1.2278	0.6505	-0.0100
C	2.4642	1.3557	-0.0545	C	2.4594	1.3897	-0.0283	C	2.4575	1.3582	-0.0321
C	3.6944	0.6436	-0.0557	C	3.6886	0.6778	-0.0089	C	3.6871	0.6482	-0.0239
C	4.9272	1.3465	-0.0616	C	4.9209	1.3812	-0.0104	C	4.9183	1.3545	-0.0415
C	6.1608	0.6447	-0.0557	C	6.1530	0.6779	-0.0097	C	6.1494	0.6483	-0.0235
C	7.3908	1.3573	-0.0551	C	7.3823	1.3901	-0.0295	C	7.3792	1.3584	-0.0315
C	8.6197	0.6491	-0.0489	C	8.6121	0.6843	-0.0340	C	8.6086	0.6506	-0.0097
C	0.0073	1.3628	-0.0499	C	0.0008	1.4002	-0.0509	C	-0.0018	1.3609	-0.0224
C	0.0069	2.7971	-0.0369	C	0.0011	2.8320	-0.0748	C	-0.0015	2.7925	-0.0443
C	1.2354	3.5059	-0.0282	C	1.2364	3.5390	-0.0677	C	1.2287	3.5004	-0.0535
C	2.4630	2.7874	-0.0480	C	2.4608	2.8199	-0.0341	C	2.4579	2.7891	-0.0523
C	3.6987	3.4807	-0.0492	C	3.6956	3.5167	-0.0084	C	3.6896	3.4908	-0.0647
C	4.9270	2.7728	-0.0590	C	4.9214	2.8072	-0.0080	C	4.9186	2.7835	-0.0611
C	6.1552	3.4800	-0.0492	C	6.1472	3.5172	-0.0108	C	6.1477	3.4912	-0.0640
C	7.3923	2.7897	-0.0481	C	7.3818	2.8204	-0.0363	C	7.3793	2.7895	-0.0514
C	8.6196	3.5109	-0.0272	C	8.6063	3.5397	-0.0696	C	8.6087	3.5010	-0.0527
C	1.2464	4.9474	0.0124	C	1.2683	4.9725	-0.0905	C	1.2393	4.9381	-0.0638
C	2.4796	5.6015	0.0038	C	2.4712	5.6358	-0.0228	C	2.4653	5.6152	-0.0719
C	3.7044	4.9146	-0.0287	C	3.7040	4.9489	0.0136	C	3.6920	4.9278	-0.0759
C	4.9275	5.6006	-0.0215	C	4.9216	5.6344	0.0380	C	4.9188	5.6132	-0.0879
C	6.1506	4.9125	-0.0274	C	6.1394	4.9496	0.0094	C	6.1457	4.9284	-0.0748
C	7.3722	5.6039	0.0072	C	7.3723	5.6371	-0.0299	C	7.3726	5.6161	-0.0700

C	8.6138	4.9561	0.0145	C	8.5754	4.9738	-0.0945	C	8.5987	4.9390	-0.0628
C	0.0152	5.6816	0.0624	C	0.0023	5.7192	-0.2129	C	-0.0009	5.6490	-0.0688
H	0.0083	-6.8404	0.1951	H	-0.0006	-6.8112	0.0154	H	-0.0028	-6.8391	0.1758
H	2.4682	-6.8410	0.1927	H	2.4588	-6.8121	0.0198	H	2.4574	-6.8397	0.1757
H	4.9282	-6.8407	0.1886	H	4.9194	-6.8121	0.0223	H	4.9175	-6.8392	0.1745
H	7.3880	-6.8408	0.1923	H	7.3800	-6.8121	0.0197	H	7.3775	-6.8397	0.1761
H	2.4916	6.6994	0.0294	H	2.4847	6.7272	-0.0208	H	2.4674	6.7062	-0.0723
H	4.9263	6.6928	0.0025	H	4.9215	6.7269	0.0538	H	4.9185	6.7053	-0.1078
H	7.3099	6.6908	0.0315	H	7.3586	6.7286	-0.0302	H	7.3707	6.7072	-0.0698
H	-1.0040	7.5871	0.2032	H	0.0415	8.6739	-1.7574	C	0.0051	7.0608	-0.0984
C	-0.0045	7.1300	0.1722	C	0.0100	7.0231	-0.4625	C	0.0245	8.2774	-0.1396
C	0.9912	8.0096	0.2554	C	0.0318	8.2989	-0.7279	H	0.0404	9.3458	-0.1925
H	1.0533	9.0901	0.3559	H	0.0391	9.0503	0.0693				

Table S5: Cartesian atomic coordinates (Angstrom) of the unit cell of acetylene and solid structures (i.e., transition states) with armchair and zigzag edges.

A0+C2H2=A1				A1=A2				A2=A3			
C	0.0111	21.2589	8.0066	C	0.0365	21.2713	8.0053	C	0.0162	21.2847	8.006
C	0.731	22.4666	8.0085	C	0.7568	22.4785	8.0051	C	0.7371	22.4916	8.0049
C	2.1034	22.4665	8.0085	C	2.1294	22.4789	8.0056	C	2.1093	22.4931	8.005
C	2.8234	21.2589	8.0066	C	2.8492	21.2714	8.0061	C	2.8301	21.2846	8.006
C	4.2706	21.2588	8.0067	C	4.2962	21.2714	8.0057	C	4.2757	21.2836	8.0061
C	4.991	22.4663	8.009	C	5.0157	22.4788	8.0061	C	4.9967	22.4904	8.0053
C	6.3637	22.4662	8.0091	C	6.3884	22.4792	8.0057	C	6.3691	22.492	8.0052
C	7.0839	21.2586	8.0066	C	7.1094	21.2719	8.005	C	7.0909	21.2843	8.0061
C	-0.0019	18.7871	8.0032	C	0.0244	18.8003	8.0021	C	0.005	18.8154	8.0056
C	0.7034	20.03	8.0046	C	0.7295	20.0426	8.0047	C	0.709	20.0548	8.006
C	2.1311	20.0301	8.0046	C	2.1572	20.0428	8.0051	C	2.1373	20.0557	8.006
C	2.8364	18.7874	8.003	C	2.8631	18.8008	8.0024	C	2.843	18.8141	8.0052
C	4.2574	18.7872	8.0027	C	4.2839	18.8011	8.0016	C	4.2646	18.8141	8.0055
C	4.9634	20.0298	8.0044	C	4.9891	20.0431	8.004	C	4.9693	20.0542	8.0062
C	6.3913	20.0298	8.0043	C	6.4168	20.0432	8.0035	C	6.3974	20.0549	8.0064
C	7.0972	18.7871	8.003	C	7.1233	18.8012	8.0013	C	7.1038	18.8131	8.006
C	0.0002	16.328	8.0126	C	0.0278	16.341	8.0019	C	0.0093	16.3549	8.0046
C	0.6985	17.556	8.0045	C	0.7258	17.5695	7.9998	C	0.7074	17.5831	8.0046
C	2.136	17.5565	8.0035	C	2.1631	17.57	7.9992	C	2.1423	17.5845	8.0042
C	2.8344	16.3285	8.007	C	2.8619	16.3424	7.9944	C	2.8424	16.355	8.004
C	4.2597	16.3285	8.0073	C	4.2871	16.343	7.9937	C	4.2684	16.3535	8.0043
C	4.9585	17.5563	8.003	C	4.9853	17.571	7.998	C	4.9677	17.583	8.0049
C	6.3962	17.5562	8.0042	C	6.4227	17.5709	7.9991	C	6.4024	17.583	8.0052
C	7.095	16.3281	8.0126	C	7.1224	16.3434	8.0024	C	7.1025	16.3514	8.0045
C	0.0058	13.8589	8.0704	C	0.0351	13.8693	8.0422	C	0.0164	13.8862	8.0086
C	0.705	15.0865	8.0305	C	0.7335	15.0988	8.0094	C	0.7149	15.1149	8.0069
C	2.1295	15.0874	8.0229	C	2.1578	15.1007	7.9966	C	2.1401	15.1179	8.007
C	2.8288	13.8599	8.0539	C	2.8571	13.8731	8.0018	C	2.8435	13.8887	8.0154
C	4.2663	13.8596	8.06	C	4.2943	13.8745	8.0106	C	4.2742	13.886	8.0108
C	4.9653	15.0874	8.0263	C	4.9929	15.1027	7.9999	C	4.9737	15.1139	8.0051
C	6.3896	15.087	8.0324	C	6.4179	15.103	8.0124	C	6.4006	15.1152	8.0045
C	7.0888	13.8589	8.0743	C	7.1184	13.876	8.0462	C	7.1021	13.8814	8.0046

C	0.0001	11.3871	8.1402	C	0.0331	11.389	8.0971	C	0.0182	11.4176	7.9918
C	0.7068	12.629	8.1064	C	0.736	12.6374	8.0673	C	0.7211	12.6545	8.0171
C	2.1285	12.6318	8.1052	C	2.1564	12.6435	8.0379	C	2.142	12.6575	8.0302
C	2.8342	11.3945	8.2057	C	2.8605	11.4068	8.1383	C	2.8506	11.4203	8.0597
C	4.2608	11.3935	8.2218	C	4.2884	11.4125	8.1706	C	4.2781	11.422	8.0321
C	4.9672	12.6314	8.1244	C	4.9951	12.6477	8.0716	C	4.9745	12.6477	8.0097
C	6.3886	12.6305	8.1278	C	6.4189	12.6485	8.0902	C	6.4054	12.6505	7.999
C	7.093	11.3866	8.1709	C	7.1244	11.4099	8.1258	C	7.1095	11.4156	7.9704
C	-0.0492	8.9839	8.1127	C	-0.0052	8.9467	7.858	C	0.0172	8.9459	7.8728
C	0.704	10.1534	8.1836	C	0.7289	10.1538	8.0862	C	0.7234	10.191	7.9939
C	2.1434	10.1697	8.3107	C	2.1662	10.1829	8.2708	C	2.1435	10.203	8.0768
C	2.849	8.9854	8.5807	C	2.8858	9.0398	8.6821	C	2.8645	8.9485	8.1439
C	4.2269	8.9854	8.5999	C	4.2671	9.0416	8.6992	C	4.2813	8.978	8.0894
C	4.9507	10.1674	8.3514	C	4.9846	10.1963	8.3396	C	4.9728	10.1682	8.0108
C	6.3951	10.1616	8.2452	C	6.4254	10.1864	8.1873	C	6.427	10.1737	7.9165
C	7.1106	8.9443	8.1452	C	7.1278	8.9935	7.9802	C	7.1439	8.984	7.8077
H	2.2888	8.0741	8.7766	H	2.3444	8.1656	9.0318	H	2.4992	8.2562	9.2087
H	4.754	8.0598	8.8284	H	4.8043	8.1475	9.0164	H	4.8036	8.0232	8.106
H	6.5623	8.0054	8.0589	H	6.5676	8.0702	7.8214	H	6.6261	8.0328	7.6942
H	0.2127	23.422	8.0099	H	0.2381	23.4338	8.0033	H	0.2182	23.447	8.0029
H	2.6217	23.4219	8.01	H	2.6471	23.4346	8.0043	H	2.6278	23.4485	8.0031
H	4.4727	23.4217	8.0114	H	4.497	23.434	8.0063	H	4.4779	23.4458	8.0039
H	6.8822	23.4215	8.0114	H	6.9061	23.4349	8.0057	H	6.8872	23.4476	8.0036
H	-0.543	6.6824	7.2212	H	-0.2802	6.9206	7.2054	H	0.1771	6.7794	7.7396
C	0.5034	6.8879	7.1024	C	0.5258	7.6719	7.3143	C	0.7281	7.7141	7.8422
C	1.6538	6.6785	6.7437	C	1.7118	7.3572	6.8568	C	2.1033	7.6902	8.0188
H	2.6982	6.6653	6.5071	H	2.6875	7.1022	6.4962	H	2.6838	6.7685	7.9624
	A3=A4+H				A2=A4+H				A0+C2H2=B1		
C	0.0214	21.2737	8.0034	C	0.0181	21.2846	8.005	C	0.0274	21.2519	8.0066
C	0.7438	22.4833	8.0014	C	0.7406	22.4942	8.0033	C	0.7476	22.4594	8.0054
C	2.1142	22.4833	8.0015	C	2.1109	22.4941	8.0032	C	2.1202	22.4594	8.0054
C	2.836	21.2736	8.0035	C	2.833	21.2844	8.0049	C	2.8397	21.2519	8.0064
C	4.2808	21.2737	8.0038	C	4.2775	21.2845	8.0051	C	4.2869	21.2518	8.0063
C	5.0028	22.4826	8.0028	C	4.9999	22.4933	8.0041	C	5.0068	22.4592	8.0057
C	6.374	22.4827	8.0027	C	6.3709	22.4934	8.0041	C	6.3796	22.4589	8.0058
C	7.0965	21.2738	8.0037	C	7.0936	21.2845	8.0051	C	7.1	21.2516	8.0065
C	0.0081	18.8038	8.0044	C	0.005	18.8153	8.0062	C	0.0142	18.7801	8.0057
C	0.7144	20.0456	8.0041	C	0.7113	20.0565	8.0057	C	0.7198	20.023	8.0067
C	2.1431	20.0456	8.0041	C	2.14	20.0566	8.0057	C	2.1475	20.0231	8.0065
C	2.8491	18.8038	8.0045	C	2.8462	18.8152	8.0061	C	2.8526	18.7803	8.0052
C	4.2676	18.8039	8.0046	C	4.2646	18.8153	8.0061	C	4.2736	18.7801	8.005
C	4.9742	20.0453	8.0044	C	4.9712	20.0561	8.0056	C	4.9793	20.0229	8.0062
C	6.4028	20.0454	8.0044	C	6.3999	20.0562	8.0057	C	6.4072	20.0227	8.0064
C	7.1095	18.8039	8.0045	C	7.1066	18.8151	8.0062	C	7.113	18.7799	8.0054
C	0.0119	16.3443	8.0052	C	0.0093	16.3562	8.0073	C	0.0159	16.3219	8.0024
C	0.7106	17.5708	8.0046	C	0.7079	17.5822	8.0067	C	0.7147	17.5496	8.0039
C	2.1468	17.5707	8.0044	C	2.1436	17.5826	8.0065	C	2.1523	17.5498	8.0033
C	2.8451	16.3443	8.0044	C	2.8425	16.3561	8.0066	C	2.8506	16.3222	8
C	4.272	16.3432	8.0047	C	4.2693	16.355	8.0068	C	4.2755	16.3218	7.9998

C	4.9711	17.571	8.0049	C	4.9685	17.5824	8.0067	C	4.9742	17.5495	8.0029
C	6.4058	17.571	8.0049	C	6.4026	17.5825	8.007	C	6.412	17.5493	8.0033
C	7.1049	16.3433	8.0052	C	7.102	16.3545	8.0077	C	7.1109	16.3215	8.0021
C	0.0157	13.8736	8.0055	C	0.0135	13.8859	8.0054	C	0.0215	13.8533	8.0062
C	0.7172	15.103	8.0056	C	0.7148	15.1151	8.0072	C	0.7211	15.0807	8.0012
C	2.1398	15.103	8.0047	C	2.1375	15.1156	8.0065	C	2.1456	15.0813	7.9981
C	2.8407	13.8737	8.0044	C	2.8395	13.886	8.0054	C	2.8445	13.8541	7.9997
C	4.2765	13.869	8.0022	C	4.2738	13.8813	8.0058	C	4.2821	13.8531	8.0015
C	4.9784	15.1035	8.0042	C	4.9758	15.1151	8.0068	C	4.9808	15.0807	7.9989
C	6.398	15.1034	8.005	C	6.3956	15.1155	8.0075	C	6.4052	15.0803	8.0016
C	7.1	13.8693	8.004	C	7.098	13.8802	8.0043	C	7.1043	13.8522	8.0076
C	0.0085	11.4064	7.9922	C	0.0081	11.4205	7.9807	C	0.0153	11.382	8.0254
C	0.7162	12.6455	8.005	C	0.715	12.658	8.0021	C	0.7228	12.6236	8.0138
C	2.1401	12.6456	8.0065	C	2.1388	12.6582	8.0049	C	2.1441	12.6252	8.0139
C	2.8474	11.4068	8.0059	C	2.8463	11.4194	8.014	C	2.8505	11.3851	8.0682
C	4.2683	11.3987	7.9943	C	4.2681	11.4119	8.0061	C	4.2769	11.3823	8.0736
C	4.9752	12.6426	7.9964	C	4.973	12.6524	8.0017	C	4.9827	12.6232	8.0205
C	6.4006	12.6422	7.9968	C	6.3995	12.6541	7.9954	C	6.4036	12.6222	8.0213
C	7.1069	11.399	7.9819	C	7.1068	11.411	7.9708	C	7.1076	11.3776	8.0351
C	0.0154	8.9431	7.9323	C	0.0184	8.9589	7.8973	C	-0.0343	8.9813	8.0005
C	0.7146	10.1807	7.9852	C	0.7167	10.195	7.9692	C	0.7193	10.1505	8.0552
C	2.141	10.1803	8.0057	C	2.1373	10.198	8.0181	C	2.1612	10.1586	8.1401
C	2.8403	8.9454	8.0086	C	2.8378	8.952	8.1106	C	2.8681	8.9597	8.3307
C	4.2385	8.9657	7.998	C	4.2503	8.9782	8.0159	C	4.2436	8.9568	8.3316
C	4.9558	10.1578	7.9778	C	4.9592	10.166	7.9781	C	4.9652	10.1519	8.1493
C	6.4179	10.1574	7.9488	C	6.4206	10.1704	7.9327	C	6.4107	10.1502	8.0716
C	7.1335	8.967	7.9004	C	7.141	8.9801	7.8732	C	7.1276	8.9323	8.008
H	2.332	7.2106	10.0549	H	2.8219	8.8385	9.9445	H	2.3141	8.0358	8.4869
H	4.7538	8.0067	8.0054	H	4.7638	8.0186	8.0145	H	4.7686	8.0161	8.4864
H	6.6179	8.0096	7.8473	H	6.6264	8.0225	7.8127	H	6.6086	7.9783	7.9425
H	0.2251	23.4386	7.9982	H	0.222	23.4495	8.0008	H	0.2292	23.4147	8.0032
H	2.6328	23.4385	7.9984	H	2.6296	23.4493	8.0007	H	2.6387	23.4146	8.0034
H	4.4845	23.4381	8.0007	H	4.4817	23.4489	8.0022	H	4.4884	23.4145	8.0043
H	6.8922	23.4382	8.0005	H	6.8892	23.4489	8.0022	H	6.8983	23.4141	8.0043
H	0.1794	6.7784	7.8873	H	0.1912	6.7951	7.7367	H	1.057	7.115	6.5708
C	0.7387	7.715	7.9274	C	0.7497	7.7264	7.8493	C	0.5876	6.7468	7.4627
C	2.1092	7.7085	8.0106	C	2.1046	7.717	7.9521	C	0.1606	5.9708	8.3055
H	2.6677	6.7852	7.805	H	2.668	6.7825	7.9331	H	-0.2789	5.4699	9.1448
		B1=B2				B2=A1				B2=D1+H	
C	0.0449	21.2799	8.0078	C	0.0324	21.2691	8.0062	C	0.0533	21.2749	8.0101
C	0.7673	22.4885	8.0077	C	0.7551	22.4784	8.0078	C	0.7741	22.4824	8.0106
C	2.1387	22.4883	8.0075	C	2.1259	22.4782	8.0081	C	2.1465	22.4828	8.0107
C	2.8596	21.28	8.0076	C	2.8477	21.2692	8.0065	C	2.8666	21.2752	8.0103
C	4.3048	21.2803	8.0076	C	4.2919	21.2689	8.0066	C	4.3134	21.2756	8.0103
C	5.0262	22.4889	8.008	C	5.014	22.4781	8.0086	C	5.0333	22.4833	8.0114
C	6.3978	22.4886	8.0081	C	6.385	22.478	8.0086	C	6.4057	22.4834	8.0113
C	7.1195	21.2804	8.0078	C	7.1079	21.2694	8.0064	C	7.1263	21.2758	8.0102
C	0.031	18.8093	8.0057	C	0.0196	18.7988	8.0027	C	0.0401	18.804	8.0081
C	0.7378	20.0514	8.007	C	0.7257	20.0408	8.0042	C	0.7462	20.0464	8.0094

C	2.1662	20.0512	8.0069	C	2.1545	20.0403	8.0043	C	2.174	20.0466	8.0094
C	2.8712	18.8101	8.0053	C	2.86	18.7993	8.0022	C	2.8798	18.8046	8.0079
C	4.2908	18.8102	8.0053	C	4.2791	18.7987	8.002	C	4.3003	18.8054	8.0077
C	4.9973	20.0519	8.0069	C	4.9853	20.0405	8.0043	C	5.0058	20.0473	8.0092
C	6.4256	20.0518	8.0071	C	6.4139	20.0404	8.0042	C	6.4336	20.0473	8.0092
C	7.131	18.8105	8.0058	C	7.1201	18.7993	8.0027	C	7.1395	18.8053	8.008
C	0.032	16.349	8.004	C	0.0224	16.3385	8.0125	C	0.0425	16.3446	8.0055
C	0.7324	17.5774	8.0037	C	0.7224	17.5667	8.0033	C	0.7413	17.5728	8.0062
C	2.1683	17.5774	8.0029	C	2.1572	17.5657	8.0016	C	2.1787	17.5735	8.0056
C	2.8658	16.3504	7.9993	C	2.8556	16.3389	8.0022	C	2.8771	16.3462	8.0019
C	4.2922	16.3502	7.9996	C	4.2827	16.3372	8.002	C	4.3025	16.3473	8.0019
C	4.9923	17.579	8.0032	C	4.982	17.5665	8.0012	C	5.0012	17.5749	8.0054
C	6.4274	17.5789	8.0041	C	6.4163	17.5664	8.0034	C	6.4384	17.5749	8.0061
C	7.1259	16.3513	8.0042	C	7.1159	16.3391	8.0127	C	7.1372	16.3475	8.0056
C	0.0328	13.8763	8.0184	C	0.0242	13.869	8.0723	C	0.0483	13.8713	8.0145
C	0.7356	15.1072	8.0057	C	0.7273	15.0992	8.0295	C	0.7476	15.1016	8.0058
C	2.1594	15.1084	7.999	C	2.1502	15.0978	8.0157	C	2.1717	15.104	8.0007
C	2.8577	13.8796	8.003	C	2.8507	13.8687	8.037	C	2.8703	13.8763	8.0026
C	4.2936	13.8792	8.0055	C	4.2856	13.8653	8.0445	C	4.3082	13.8783	8.0037
C	4.9958	15.1115	8.0003	C	4.9874	15.099	8.0183	C	5.0078	15.1069	8.0012
C	6.4191	15.111	8.0061	C	6.4099	15.0985	8.0309	C	6.4319	15.1071	8.006
C	7.1191	13.882	8.0192	C	7.1117	13.8697	8.0742	C	7.1318	13.879	8.0147
C	0.0278	11.3963	8.0415	C	0.0178	11.3986	8.1222	C	0.0458	11.3885	8.0308
C	0.7326	12.6443	8.0334	C	0.7256	12.641	8.1046	C	0.7485	12.6384	8.0261
C	2.1537	12.6501	8.0298	C	2.1486	12.6408	8.088	C	2.1688	12.6464	8.0236
C	2.8542	11.413	8.1146	C	2.8513	11.4053	8.1873	C	2.8716	11.4079	8.0977
C	4.2801	11.415	8.1213	C	4.2768	11.4015	8.216	C	4.2982	11.4141	8.1007
C	4.991	12.6534	8.0375	C	4.9836	12.6409	8.114	C	5.0078	12.6517	8.0272
C	6.4175	12.6516	8.0411	C	6.4103	12.638	8.1227	C	6.4319	12.6515	8.0285
C	7.1205	11.4165	8.0561	C	7.1128	11.4039	8.1539	C	7.1389	11.4123	8.0353
C	-0.0131	8.943	7.8952	C	-0.0117	8.9595	7.8589	C	0.0001	8.9351	7.9166
C	0.7258	10.1632	8.0573	C	0.7219	10.1729	8.1065	C	0.7409	10.1504	8.0516
C	2.1568	10.1823	8.2177	C	2.147	10.178	8.289	C	2.1828	10.176	8.1951
C	2.8821	9.013	8.5215	C	2.862	9.0134	8.6416	C	2.9139	9.008	8.4781
C	4.26	9.0178	8.5306	C	4.242	9.0135	8.6735	C	4.2889	9.0129	8.4687
C	4.9734	10.193	8.2377	C	4.9694	10.1775	8.3621	C	4.9944	10.1949	8.1967
C	6.4146	10.1861	8.0919	C	6.4132	10.1609	8.2127	C	6.4345	10.1915	8.0613
C	7.1016	8.9923	7.926	C	7.106	8.9745	7.9971	C	7.1262	8.9908	7.9283
H	2.3521	8.1018	8.7887	H	2.3174	8.1172	8.9331	H	2.3935	8.0846	8.7057
H	4.7961	8.1059	8.7911	H	4.7713	8.1054	8.9625	H	4.8225	8.0902	8.6894
H	6.5561	8.0598	7.7934	H	6.5586	8.0432	7.847	H	6.585	8.0532	7.8263
H	0.2489	23.444	8.0073	H	0.2361	23.4336	8.0087	H	0.2557	23.4379	8.0115
H	2.6575	23.4436	8.007	H	2.6447	23.4334	8.0092	H	2.6646	23.4383	8.0117
H	4.5081	23.4445	8.0082	H	4.4951	23.4332	8.0103	H	4.5152	23.4388	8.013
H	6.9164	23.444	8.0081	H	6.9037	23.4334	8.0104	H	6.9236	23.4391	8.0129
H	1.2131	7.2129	6.6597	H	0.2216	7.1579	6.3093	H	1.0626	5.9488	5.2523
C	0.4997	7.6583	7.5861	C	0.6343	7.8598	7.259	C	0.5154	7.6163	7.773
C	0.5365	6.367	7.4738	C	1.5115	7.0612	6.7352	C	0.7617	6.4302	7.6406
H	0.497	5.4391	8.0557	H	2.3217	6.3816	7.0233	H	1.0333	5.396	7.6311

C2=D1+H				B2=B3				B3=B4			
C	0.0502	21.2493	8.0107	C	0.0559	21.2748	8.006	C	0.0273	21.2549	8.0127
C	0.7707	22.4573	8.0119	C	0.7769	22.4822	8.005	C	0.7478	22.4626	8.0136
C	2.143	22.4578	8.0117	C	2.1495	22.4824	8.005	C	2.1203	22.4627	8.0139
C	2.8635	21.2498	8.0104	C	2.8693	21.275	8.006	C	2.84	21.2548	8.0132
C	4.3103	21.2501	8.0102	C	4.3162	21.2747	8.0061	C	4.2871	21.2538	8.0132
C	5.0299	22.4582	8.0112	C	5.0363	22.4822	8.0051	C	5.007	22.4614	8.014
C	6.4022	22.4582	8.0113	C	6.4086	22.4824	8.005	C	6.3796	22.4615	8.0138
C	7.1233	21.2502	8.0106	C	7.1289	21.2748	8.0061	C	7.1001	21.2539	8.0127
C	0.0383	18.777	8.0081	C	0.0417	18.8043	8.0062	C	0.014	18.7837	8.013
C	0.7435	20.0202	8.0095	C	0.7484	20.0464	8.0062	C	0.7198	20.0263	8.0126
C	2.1716	20.0206	8.0094	C	2.1762	20.0467	8.0062	C	2.1477	20.0263	8.0128
C	2.8777	18.7777	8.0077	C	2.8817	18.8049	8.0062	C	2.8531	18.7836	8.0129
C	4.2983	18.7784	8.0074	C	4.3022	18.8043	8.0062	C	4.2738	18.7817	8.0128
C	5.003	20.0213	8.009	C	5.0082	20.0462	8.0064	C	4.9794	20.0247	8.0127
C	6.4311	20.0212	8.0092	C	6.4358	20.0463	8.0064	C	6.4073	20.0248	8.0125
C	7.1374	18.7783	8.0079	C	7.1409	18.8041	8.0062	C	7.1131	18.7818	8.0128
C	0.0421	16.3164	8.0063	C	0.0425	16.3461	8.0064	C	0.0157	16.3261	8.0159
C	0.74	17.545	8.0064	C	0.7423	17.5738	8.0062	C	0.7148	17.5534	8.014
C	2.1774	17.5458	8.0058	C	2.1799	17.5747	8.0063	C	2.1525	17.5534	8.0137
C	2.8765	16.3183	8.0036	C	2.8781	16.3478	8.0069	C	2.8512	16.3262	8.0141
C	4.302	16.3194	8.0038	C	4.3033	16.3457	8.0066	C	4.2763	16.3215	8.0139
C	4.9999	17.5473	8.0055	C	5.0022	17.5734	8.006	C	4.9745	17.5499	8.0132
C	6.4369	17.5472	8.006	C	6.4394	17.5735	8.0058	C	6.412	17.5501	8.0137
C	7.1366	16.3193	8.006	C	7.1373	16.3457	8.0061	C	7.1104	16.322	8.0157
C	0.0498	13.8428	8.0168	C	0.047	13.8762	8.0084	C	0.021	13.86	8.0198
C	0.748	15.0735	8.0082	C	0.7474	15.105	8.0074	C	0.7212	15.0868	8.0175
C	2.1721	15.0762	8.0051	C	2.172	15.1075	8.0081	C	2.1458	15.087	8.0153
C	2.8718	13.8484	8.0131	C	2.871	13.8813	8.0092	C	2.8461	13.8608	8.0141
C	4.3091	13.8508	8.0158	C	4.3087	13.8752	8.0094	C	4.2834	13.8479	8.0153
C	5.0082	15.0794	8.0066	C	5.0077	15.104	8.0078	C	4.9814	15.0781	8.0155
C	6.4322	15.0794	8.0094	C	6.4318	15.1042	8.0076	C	6.4051	15.0786	8.0174
C	7.1331	13.8507	8.0196	C	7.1304	13.8761	8.0095	C	7.1033	13.8491	8.0201
C	0.0497	11.359	8.0182	C	0.0394	11.4021	8.0105	C	0.0059	11.3983	7.9989
C	0.7511	12.6092	8.025	C	0.7472	12.6467	8.0083	C	0.7212	12.6348	8.015
C	2.1715	12.6175	8.0305	C	2.1689	12.6547	8.0076	C	2.1461	12.6354	8.0119
C	2.874	11.3772	8.0943	C	2.8771	11.4193	8.0031	C	2.8615	11.4009	8.011
C	4.3011	11.3857	8.1091	C	4.3041	11.4013	8.0048	C	4.2873	11.3624	8.0159
C	5.0094	12.623	8.0442	C	5.0085	12.6454	8.0096	C	4.9842	12.6139	8.017
C	6.4345	12.6235	8.0393	C	6.4298	12.6454	8.0106	C	6.4019	12.6154	8.0196
C	7.143	11.3838	8.0375	C	7.1339	11.4048	8.0095	C	7.101	11.3675	8.0082
C	0.0021	8.9071	7.8642	C	0.0317	8.937	8.0129	C	0.07	8.9439	7.8904
C	0.7458	10.1198	8.0036	C	0.7331	10.1755	8.0138	C	0.7129	10.1932	7.9611
C	2.1858	10.142	8.135	C	2.1774	10.1955	8.0035	C	2.1454	10.1912	7.9979
C	2.9178	8.9565	8.3641	C	2.908	9.0133	7.9875	C	2.8323	8.9902	8.0194
C	4.299	8.9712	8.3814	C	4.2685	8.9544	7.9824	C	4.2017	8.9039	8.0297
C	5.0001	10.1628	8.1841	C	4.9938	10.1682	7.998	C	4.9645	10.1111	8.0151
C	6.441	10.1632	8.0578	C	6.4461	10.1679	8.0003	C	6.4338	10.112	7.9938
C	7.1315	8.9639	7.9051	C	7.1616	8.9676	7.9916	C	7.1961	8.9186	7.9217

H	2.5324	8.3494	10.3435	H	1.1133	5.5975	8.0728	H	1.4161	5.7334	8.2827
H	4.8288	8.0381	8.5625	H	4.7763	7.9917	7.9617	H	4.7057	7.9373	8.0604
H	6.5908	8.0278	7.793	H	6.6345	8.0167	7.9657	H	6.6944	7.9536	7.8562
H	0.2514	23.4123	8.0136	H	0.259	23.4379	8.0035	H	0.2293	23.4179	8.0153
H	2.6609	23.4133	8.0134	H	2.6675	23.438	8.0036	H	2.6388	23.418	8.0155
H	4.5112	23.4134	8.0124	H	4.5182	23.4378	8.0033	H	4.4885	23.4167	8.0159
H	6.92	23.4138	8.0126	H	6.9269	23.4379	8.0032	H	6.8981	23.4168	8.0157
H	2.4087	8.0001	8.3865	H	1.9876	7.9793	7.9397	H	1.3943	7.638	6.7317
C	0.509	7.5919	7.6483	C	0.7579	7.6839	8.007	C	0.9464	7.7517	7.7259
C	0.7495	6.4159	7.452	C	0.3881	6.4104	8.139	C	0.8703	6.6445	8.5277
H	1.0234	5.3929	7.3012	H	-0.6533	6.1214	8.325	H	0.3164	6.6656	9.4668
	B4=B5				B5=B6+H				B4=B6+H		
C	0.0258	21.2553	8.0074	C	0.0464	21.268	8.0048	C	0.0105	21.2443	8.0015
C	0.7471	22.4638	8.0063	C	0.7672	22.4758	8.0035	C	0.7308	22.4524	7.9985
C	2.1189	22.4639	8.0064	C	2.1398	22.4759	8.0033	C	2.1031	22.4524	7.9985
C	2.8399	21.2553	8.0074	C	2.8601	21.2679	8.0038	C	2.8235	21.2442	8.0015
C	4.2857	21.2529	8.0074	C	4.3068	21.2655	8.0034	C	4.2704	21.2418	8.0016
C	5.0065	22.4612	8.0064	C	5.0264	22.4734	8.0023	C	4.991	22.4499	7.9995
C	6.3782	22.4612	8.0064	C	6.3984	22.4736	8.0025	C	6.3632	22.4499	7.9995
C	7.0999	21.253	8.0075	C	7.1195	21.2659	8.0044	C	7.0836	21.2418	8.0016
C	0.0131	18.7847	8.0078	C	0.0336	18.7979	8.0027	C	-0.0032	18.773	8.0023
C	0.7189	20.027	8.008	C	0.7397	20.0399	8.0044	C	0.7027	20.0157	8.0026
C	2.1476	20.027	8.008	C	2.1679	20.0399	8.0037	C	2.131	20.0157	8.0026
C	2.8538	18.7847	8.0078	C	2.8747	18.7981	8.0015	C	2.8368	18.773	8.0023
C	4.2738	18.7801	8.0076	C	4.2951	18.7933	8.0017	C	4.2574	18.7685	8.002
C	4.9788	20.0234	8.008	C	4.9995	20.0365	8.0035	C	4.9629	20.0121	8.0024
C	6.407	20.0234	8.008	C	6.4272	20.0365	8.0043	C	6.391	20.0122	8.0024
C	7.1129	18.7802	8.0077	C	7.133	18.7935	8.0028	C	7.0963	18.7685	8.002
C	0.0159	16.3281	8.0034	C	0.0367	16.3423	7.9945	C	-0.0018	16.3168	7.9991
C	0.7155	17.5544	8.0065	C	0.7361	17.5688	7.9987	C	0.6979	17.5432	8.0011
C	2.1526	17.5543	8.0066	C	2.1739	17.5687	7.9982	C	2.1355	17.5432	8.0011
C	2.8527	16.3281	8.0038	C	2.8744	16.3424	7.9938	C	2.835	16.3168	7.9991
C	4.2786	16.3167	8.0037	C	4.2996	16.3309	7.995	C	4.2604	16.3059	7.9991
C	4.9757	17.5463	8.0062	C	4.9959	17.5602	7.9991	C	4.9582	17.5349	8.0006
C	6.4115	17.5463	8.0061	C	6.4329	17.5601	7.9995	C	6.3954	17.5349	8.0006
C	7.1098	16.3169	8.0033	C	7.1311	16.3312	7.9956	C	7.0928	16.3059	7.9991
C	0.0205	13.8662	7.9917	C	0.0431	13.8805	7.9951	C	0.0025	13.855	7.9968
C	0.7228	15.0921	7.998	C	0.7443	15.1064	7.9901	C	0.7043	15.0807	7.9968
C	2.1471	15.0918	7.9984	C	2.1688	15.1062	7.9897	C	2.1286	15.0808	7.9968
C	2.8502	13.8661	7.9923	C	2.8712	13.8807	7.9935	C	2.8302	13.855	7.9967
C	4.2868	13.8363	7.9972	C	4.3088	13.8513	8.0003	C	4.2679	13.8259	8.0009
C	4.9834	15.0704	8.0006	C	5.0044	15.0835	7.995	C	4.965	15.0586	7.9991
C	6.4056	15.0703	8.0002	C	6.4276	15.0834	7.9954	C	6.3881	15.0586	7.9992
C	7.1038	13.8365	7.9964	C	7.1254	13.8515	8.0018	C	7.0848	13.8259	8.001
C	-0.0077	11.4202	7.9902	C	0.0143	11.4352	8.059	C	-0.0281	11.408	8.0109
C	0.721	12.6487	7.9818	C	0.743	12.6625	8.009	C	0.7008	12.6364	7.996
C	2.1513	12.6481	7.9815	C	2.1735	12.6623	8.0076	C	2.1315	12.6365	7.996
C	2.881	11.4194	7.9872	C	2.9039	11.4354	8.0566	C	2.8602	11.4081	8.011
C	4.303	11.3361	8.0072	C	4.3254	11.3518	8.0747	C	4.2817	11.3255	8.0287

C	4.9883	12.595	8.0013	C	5.0113	12.6102	8.0269	C	4.9697	12.5845	8.0122
C	6.4029	12.5951	8.0011	C	6.4242	12.6101	8.0282	C	6.3829	12.5845	8.0122
C	7.0901	11.3367	8.0092	C	7.1127	11.3522	8.0769	C	7.0704	11.3254	8.0286
C	0.2021	8.9607	8.0832	C	0.2254	8.9809	8.2426	C	0.1751	8.9499	8.0917
C	0.7294	10.2552	8.0084	C	0.7492	10.2704	8.1287	C	0.7055	10.2389	8.0307
C	2.1443	10.2542	8.0052	C	2.1699	10.2708	8.1286	C	2.1264	10.239	8.0309
C	2.6707	8.9586	8.0749	C	2.6946	8.9823	8.2461	C	2.6569	8.9501	8.0918
C	4.096	8.8668	8.0846	C	4.115	8.8896	8.2488	C	4.0753	8.8584	8.1097
C	4.9359	10.0382	8.0431	C	4.9591	10.0584	8.1575	C	4.9163	10.0311	8.0717
C	6.4575	10.0387	8.047	C	6.4804	10.0585	8.1586	C	6.4356	10.0311	8.0717
C	7.2974	8.8682	8.0975	C	7.3245	8.8896	8.2501	C	7.2766	8.8583	8.1097
H	2.3731	6.1474	8.7658	H	2.4421	5.778	6.3058	H	2.3484	6.178	8.6615
H	4.5822	7.8892	8.1185	H	4.5979	7.9131	8.3274	H	4.5589	7.88	8.1477
H	6.8113	7.891	8.1424	H	6.8403	7.9139	8.3314	H	6.7931	7.8798	8.148
H	0.2279	23.4189	8.0048	H	0.2488	23.4313	8.0007	H	0.2124	23.4078	7.9934
H	2.6375	23.4192	8.0049	H	2.6576	23.4316	8.0009	H	2.6217	23.4077	7.9935
H	4.4871	23.4161	8.0051	H	4.5074	23.4285	7.9997	H	4.4723	23.4051	7.9955
H	6.8971	23.4164	8.005	H	6.9167	23.429	7.9995	H	6.882	23.405	7.9955
H	1.4262	7.1907	7.271	H	0.5398	6.1789	8.6453	H	1.4186	7.9595	6.2128
C	1.4349	8.0666	8.1439	C	1.4606	8.0785	8.3532	C	1.4163	8.0314	8.1498
C	1.4315	6.6599	8.5888	C	1.4663	6.7478	8.5628	C	1.4168	6.7259	8.5213
H	0.4875	6.157	8.7811	H	2.3989	6.1972	8.6892	H	0.4856	6.1773	8.6616
		B1=C1				C1=C2				B2=C1	
C	0.0557	21.2609	8.0063	C	0.0417	21.2517	8.0109	C	0.0583	21.271	8.0073
C	0.7767	22.4688	8.0056	C	0.7651	22.4612	8.0133	C	0.7807	22.4798	8.0092
C	2.1489	22.469	8.0057	C	2.1356	22.4614	8.0134	C	2.1522	22.4796	8.0091
C	2.8693	21.2611	8.0064	C	2.8577	21.2511	8.0111	C	2.8736	21.2712	8.0073
C	4.3159	21.2614	8.0064	C	4.3017	21.2514	8.0112	C	4.3185	21.2715	8.0075
C	5.0359	22.4694	8.0059	C	5.024	22.4608	8.0133	C	5.0402	22.4803	8.0097
C	6.4081	22.4694	8.0059	C	6.3947	22.4609	8.013	C	6.4116	22.4799	8.0097
C	7.129	21.2616	8.0063	C	7.1177	21.2511	8.0109	C	7.1332	21.2715	8.0075
C	0.0429	18.7895	8.0041	C	0.0292	18.7808	8.0077	C	0.0443	18.8003	8.0029
C	0.7488	20.0322	8.0059	C	0.7353	20.0218	8.009	C	0.7513	20.0425	8.0049
C	2.1768	20.0324	8.0059	C	2.1645	20.0226	8.0091	C	2.1798	20.0422	8.0049
C	2.8828	18.79	8.0037	C	2.8702	18.7801	8.0074	C	2.885	18.8011	8.0023
C	4.3031	18.7905	8.0035	C	4.2893	18.7803	8.0078	C	4.3047	18.8011	8.0023
C	5.0084	20.0329	8.0056	C	4.995	20.0216	8.0095	C	5.011	20.043	8.0051
C	6.4364	20.0329	8.0056	C	6.4238	20.0221	8.0094	C	6.4394	20.0428	8.0051
C	7.1424	18.7905	8.004	C	7.1296	18.7795	8.0083	C	7.1444	18.8014	8.0031
C	0.0459	16.3301	8.0021	C	0.0331	16.3193	8.009	C	0.0453	16.3399	8.0086
C	0.7445	17.558	8.0018	C	0.7326	17.5459	8.0064	C	0.746	17.5682	8.0022
C	2.1819	17.5583	8.0009	C	2.1672	17.5474	8.0056	C	2.1818	17.5681	8.0007
C	2.8806	16.3311	7.996	C	2.8671	16.3188	8.0032	C	2.8796	16.3411	8
C	4.3061	16.3318	7.9958	C	4.2934	16.3176	8.0037	C	4.3063	16.3405	8
C	5.0043	17.5594	8.0003	C	4.9927	17.5457	8.0066	C	5.0061	17.5696	8.0007
C	6.4413	17.5595	8.0016	C	6.4258	17.5468	8.0079	C	6.4408	17.5694	8.0024
C	7.1403	16.3321	8.0023	C	7.1254	16.3158	8.0098	C	7.1392	16.3418	8.0087
C	0.0523	13.8581	8.0228	C	0.0368	13.8501	8.0382	C	0.046	13.8684	8.0583
C	0.7516	15.0878	8.0045	C	0.7389	15.0789	8.0156	C	0.7492	15.0988	8.0221

C	2.1754	15.0892	7.9953	C	2.1624	15.0808	8.0064	C	2.173	15.0995	8.0105
C	2.8748	13.861	7.9963	C	2.8659	13.8499	8.0142	C	2.8718	13.871	8.0278
C	4.3123	13.8626	8.002	C	4.2975	13.8452	8.011	C	4.3074	13.8696	8.032
C	5.0117	15.0916	7.9974	C	4.9985	15.0761	8.0054	C	5.0096	15.1022	8.0119
C	6.4351	15.0917	8.0061	C	6.4208	15.0788	8.012	C	6.4326	15.1015	8.0227
C	7.1354	13.8635	8.0253	C	7.1235	13.8422	8.0265	C	7.1326	13.873	8.0594
C	0.0484	11.3797	8.047	C	0.0366	11.3824	8.0835	C	0.0403	11.3905	8.1079
C	0.7528	12.6267	8.0357	C	0.7406	12.6209	8.0726	C	0.7462	12.6375	8.0901
C	2.1741	12.6315	8.0197	C	2.1635	12.6238	8.0591	C	2.1676	12.6423	8.0746
C	2.8783	11.3923	8.1037	C	2.8715	11.3859	8.1475	C	2.8688	11.4058	8.1604
C	4.3048	11.3976	8.1252	C	4.3	11.3753	8.097	C	4.2946	11.4062	8.1758
C	5.0125	12.6364	8.0418	C	4.9979	12.607	8.0288	C	5.0045	12.6447	8.0893
C	6.4357	12.6365	8.0531	C	6.4269	12.6139	8.0315	C	6.431	12.6424	8.1005
C	7.1426	11.3963	8.0742	C	7.1328	11.371	8.0451	C	7.133	11.4081	8.1252
C	0.0102	8.9357	7.8423	C	0.0595	8.9309	7.9263	C	0.0029	8.9404	7.9209
C	0.7431	10.1422	8.0306	C	0.751	10.1574	8.1406	C	0.7395	10.1602	8.1061
C	2.1842	10.1629	8.2108	C	2.166	10.1841	8.3202	C	2.1695	10.176	8.2604
C	2.9099	9.0079	8.5688	C	2.871	8.9512	8.6149	C	2.8917	9.0049	8.5669
C	4.2897	9.0105	8.574	C	4.292	8.9583	8.4626	C	4.2695	9.0078	8.5837
C	5.0017	10.1789	8.2564	C	4.9917	10.1173	8.1507	C	4.9865	10.1832	8.2998
C	6.4443	10.171	8.1153	C	6.4489	10.1269	8.0295	C	6.429	10.1744	8.1608
C	7.1432	8.9756	7.9286	C	7.1838	8.942	7.8826	C	7.1167	8.9821	7.9862
H	2.3782	8.1047	8.8575	H	2.4995	8.3683	9.4687	H	2.357	8.096	8.8343
H	4.8269	8.1017	8.8436	H	4.8408	8.0469	8.6998	H	4.8025	8.0945	8.8462
H	6.5998	8.0428	7.7788	H	6.6738	7.9919	7.7236	H	6.5717	8.0491	7.8527
H	0.2579	23.4239	8.0038	H	0.2466	23.4165	8.0167	H	0.2623	23.4352	8.0108
H	2.6672	23.4244	8.0041	H	2.6549	23.4162	8.0168	H	2.6711	23.4347	8.0106
H	4.5172	23.4245	8.0046	H	4.5059	23.4163	8.0163	H	4.5219	23.4357	8.0117
H	6.9265	23.4248	8.0046	H	6.9138	23.4159	8.0159	H	6.9305	23.4351	8.0117
H	1.5276	7.7418	6.8095	H	2.0745	8.0586	7.8177	H	1.2908	7.3982	6.587
C	0.6363	7.6453	7.4538	C	0.7918	7.6968	7.6702	C	0.5315	7.6912	7.5275
C	0.1978	6.4508	7.7644	C	0.568	6.4716	7.4248	C	0.6315	6.4218	7.2776
H	-0.1441	5.4788	8.059	H	0.9096	5.4734	7.2105	H	0.703	5.4535	7.7848
	A0+C2H2=C1				C1=D1+H				B4=>A3		
C	0.0713	21.2403	8.0041	C	0.0596	21.2505	8.006	C	-0.0101	21.2351	8.0057
C	0.7915	22.448	8.0058	C	0.7804	22.4584	8.0091	C	0.7111	22.4442	8.0077
C	2.1643	22.448	8.006	C	2.1529	22.4588	8.009	C	2.0825	22.4445	8.0075
C	2.8845	21.2403	8.0045	C	2.873	21.2508	8.006	C	2.8048	21.2348	8.0059
C	4.3318	21.2403	8.0044	C	4.3199	21.2512	8.0059	C	4.25	21.2327	8.0062
C	5.0516	22.4481	8.0059	C	5.04	22.4593	8.0084	C	4.9718	22.4414	8.0084
C	6.4241	22.4479	8.0058	C	6.4122	22.4593	8.0085	C	6.343	22.4421	8.0084
C	7.144	21.2402	8.0041	C	7.1326	21.2512	8.006	C	7.0649	21.233	8.0059
C	0.0582	18.7679	8.001	C	0.046	18.7782	8.0027	C	-0.0218	18.7643	8.006
C	0.7639	20.0111	8.0023	C	0.7521	20.0214	8.0035	C	0.683	20.0059	8.0044
C	2.192	20.0112	8.0024	C	2.1803	20.0217	8.0037	C	2.1121	20.0062	8.0048
C	2.898	18.768	8.0007	C	2.8859	18.7787	8.0023	C	2.8191	18.7634	8.0067
C	4.319	18.7677	8.0007	C	4.3064	18.7794	8.0023	C	4.2392	18.7599	8.0066
C	5.0241	20.0111	8.0023	C	5.0119	20.0223	8.0037	C	4.9439	20.0026	8.005
C	6.452	20.011	8.0022	C	6.4399	20.0223	8.0037	C	6.3725	20.003	8.0048

C	7.1572	18.7676	8.001	C	7.1453	18.7793	8.0028	C	7.0784	18.7596	8.0063
C	0.0607	16.3091	8.0119	C	0.0478	16.3179	8.0148	C	-0.0169	16.3064	8.0262
C	0.7594	17.537	8.0025	C	0.7469	17.5463	8.0045	C	0.6816	17.5323	8.0136
C	2.1971	17.5371	8.0015	C	2.1844	17.5469	8.0027	C	2.1174	17.5327	8.0143
C	2.8963	16.3092	8.0066	C	2.8824	16.3191	8.0047	C	2.8195	16.3056	8.0286
C	4.3214	16.3086	8.0069	C	4.308	16.3201	8.0047	C	4.2454	16.2962	8.0242
C	5.0195	17.5366	8.0015	C	5.0069	17.5479	8.0025	C	4.9429	17.5253	8.0122
C	6.457	17.5364	8.0025	C	6.4441	17.548	8.0045	C	6.3772	17.5256	8.0117
C	7.1556	16.3083	8.0119	C	7.1424	16.3204	8.015	C	7.0763	16.2949	8.0212
C	0.0669	13.8408	8.0767	C	0.0529	13.8453	8.0727	C	-0.0103	13.8442	8.0653
C	0.7664	15.0681	8.0329	C	0.7526	15.0752	8.0319	C	0.6906	15.0705	8.0531
C	2.191	15.0681	8.0261	C	2.1765	15.0771	8.0188	C	2.1149	15.0705	8.0562
C	2.8908	13.8404	8.0617	C	2.8747	13.8489	8.0388	C	2.8208	13.8429	8.0778
C	4.3286	13.8392	8.0649	C	4.3126	13.8512	8.0459	C	4.2544	13.8171	8.049
C	5.0267	15.0673	8.028	C	5.0129	15.0797	8.022	C	4.9517	15.0499	8.0323
C	6.4508	15.0668	8.0342	C	6.4367	15.0803	8.0348	C	6.3741	15.0518	8.0276
C	7.1495	13.8388	8.0794	C	7.1362	13.8526	8.0776	C	7.0743	13.8142	8.0331
C	0.0607	11.371	8.1578	C	0.0479	11.3634	8.1164	C	-0.033	11.3991	8.0184
C	0.7684	12.6118	8.1193	C	0.7524	12.6126	8.0986	C	0.6916	12.6241	8.0886
C	2.1906	12.612	8.1174	C	2.1731	12.6192	8.082	C	2.1224	12.6221	8.1005
C	2.8979	11.3733	8.2132	C	2.8749	11.3798	8.1683	C	2.8523	11.3916	8.06
C	4.3245	11.3703	8.2217	C	4.3014	11.3875	8.1967	C	4.2752	11.3233	7.9809
C	5.0291	12.6101	8.1275	C	5.0114	12.6252	8.1085	C	4.9583	12.5722	8.0132
C	6.45	12.6087	8.1314	C	6.4355	12.6261	8.1205	C	6.3759	12.5775	7.9994
C	7.1534	11.3636	8.1749	C	7.1414	11.3862	8.1431	C	7.0673	11.3199	7.9475
C	0.0144	8.9727	8.1206	C	-0.0001	8.919	7.9338	C	0.1667	8.9534	7.7468
C	0.7656	10.1406	8.2022	C	0.7425	10.1254	8.1053	C	0.7063	10.2273	7.9496
C	2.2068	10.1484	8.3144	C	2.1839	10.1481	8.2612	C	2.1169	10.2237	8.0021
C	2.9134	8.9561	8.552	C	2.9074	8.9834	8.582	C	2.6617	8.93	7.8064
C	4.291	8.954	8.5605	C	4.2849	8.9933	8.6159	C	4.1033	8.8686	7.6882
C	5.013	10.1413	8.3335	C	4.9959	10.1696	8.3292	C	4.9193	10.0263	7.8213
C	6.4582	10.1342	8.2309	C	6.4373	10.1649	8.1863	C	6.4344	10.0349	7.8119
C	7.1755	8.9169	8.1285	C	7.1268	8.9678	8.006	C	7.2773	8.867	7.6872
H	2.3562	8.0369	8.729	H	2.3768	8.0645	8.8158	H	2.6103	6.7281	9.0876
H	4.8197	8.0218	8.7524	H	4.8187	8.0805	8.8768	H	4.5861	7.9026	7.5309
H	6.6553	7.9663	8.0168	H	6.5798	8.0362	7.8773	H	6.7963	7.8966	7.5481
H	0.273	23.4034	8.0062	H	0.2618	23.4137	8.0121	H	0.192	23.3992	8.0098
H	2.6826	23.4034	8.0067	H	2.6716	23.414	8.012	H	2.6009	23.3999	8.0092
H	4.5329	23.4033	8.0067	H	4.5216	23.4147	8.0112	H	4.4522	23.3963	8.0103
H	6.9428	23.4031	8.0064	H	6.9309	23.4145	8.0114	H	6.8613	23.3975	8.0108
H	1.392	7.7103	6.3903	H	1.8997	8.1609	6.2481	H	1.4048	7.2393	6.8999
C	0.8172	7.0323	6.9931	C	0.5094	7.6109	7.645	C	1.4033	7.9943	7.6942
C	0.3366	5.9942	7.4209	C	0.5509	6.392	7.5282	C	1.8918	7.5432	9.0225
H	-0.1583	5.1775	7.9068	H	0.7086	5.357	7.3066	H	1.5389	8.0167	9.9345

A1=B1			
C	0.04236	21.25718	8.004709
C	0.762518	22.46512	8.003587
C	2.135158	22.46548	8.003974
C	2.855025	21.2576	8.005076

C	4.30219	21.25779	8.005016
C	5.021472	22.46582	8.00505
C	6.394207	22.46578	8.004879
C	7.115061	21.25797	8.004796
C	0.030654	18.78442	8.003035
C	0.735514	20.02797	8.004496
C	2.16341	20.02834	8.004505
C	2.86954	18.78537	8.002465
C	4.290282	18.78591	8.00233
C	4.994994	20.02902	8.004158
C	6.422957	20.02886	8.00408
C	7.129596	18.78586	8.002869
C	0.035137	16.32308	8.001411
C	0.73243	17.55237	8.000871
C	2.170015	17.55321	7.999791
C	2.869291	16.32528	7.994599
C	4.294738	16.32655	7.994623
C	4.99195	17.55484	7.999735
C	6.429609	17.55451	8.001248
C	7.129703	16.32646	8.002372
C	0.04431	13.84797	8.016939
C	0.741554	15.07958	8.002121
C	2.165586	15.0825	7.992406
C	2.865575	13.85412	7.989786
C	4.303515	13.85738	7.993224
C	5.00146	15.08611	7.99422
C	6.425949	15.08546	8.004199
C	7.127379	13.85705	8.017001
C	0.045234	11.36126	8.029599
C	0.745549	12.6138	8.028455
C	2.16626	12.62314	8.013063
C	2.871327	11.38408	8.10044
C	4.299333	11.39266	8.105677
C	5.005494	12.63042	8.020893
C	6.42964	12.62893	8.027397
C	7.137554	11.38766	8.025548
C	0.005617	8.91216	7.796006
C	0.739495	10.1182	8.040216
C	2.18048	10.15616	8.239299
C	2.920907	9.026288	8.645571
C	4.298994	9.019654	8.600533
C	5.001728	10.17573	8.224038
C	6.437398	10.16582	8.041911
C	7.13483	8.969409	7.836578
H	2.408546	8.156324	9.041277
H	4.84436	8.122951	8.894086
H	6.579759	8.042235	7.698341
H	0.24344	23.42021	8.000989
H	2.653357	23.42095	8.001713

H	4.502586	23.42095	8.0043								
H	6.912587	23.42124	8.004083								
H	1.468204	7.211802	7.932488								
C	0.596492	7.595776	7.401383								
C	0.137197	6.845072	6.421161								
H	-0.6239	6.845917	5.646221								
	Z0+C2H2=Z1				Z1=Z2				Z2=Z3		
C	0.0077	-5.7321	0.1226	C	0.0207	-5.7614	0.0717	C	-0.0086	-5.7608	-0.0387
C	1.2378	-5.0491	0.1	C	1.2506	-5.0784	0.0683	C	1.2218	-5.0783	-0.0358
C	2.4676	-5.7324	0.1231	C	2.4804	-5.7612	0.0723	C	2.4518	-5.7612	-0.0403
C	3.6974	-5.049	0.1001	C	3.7104	-5.078	0.0692	C	3.6817	-5.0779	-0.0349
C	4.9277	-5.732	0.1229	C	4.9407	-5.7607	0.0731	C	4.9113	-5.7612	-0.0377
C	6.1579	-5.049	0.1	C	6.1707	-5.078	0.0692	C	6.1418	-5.0789	-0.0307
C	7.3877	-5.7324	0.1231	C	7.4003	-5.7613	0.072	C	7.3717	-5.7619	-0.0369
C	8.6175	-5.049	0.1	C	8.6305	-5.0784	0.0686	C	8.6009	-5.0781	-0.0319
C	1.2378	-3.6097	0.0541	C	1.2505	-3.6388	0.0604	C	1.2219	-3.6386	-0.0233
C	2.4673	-2.9031	0.0326	C	2.4799	-2.9322	0.054	C	2.452	-2.9319	-0.0156
C	3.6973	-3.6096	0.0541	C	3.7104	-3.6382	0.0602	C	3.6824	-3.638	-0.0207
C	4.9277	-2.9034	0.0323	C	4.9411	-2.932	0.0544	C	4.9126	-2.9318	-0.0045
C	6.1579	-3.6097	0.054	C	6.171	-3.6384	0.0611	C	6.1419	-3.6392	-0.0121
C	7.3877	-2.9031	0.0326	C	7.401	-2.932	0.0563	C	7.3707	-2.932	0.0002
C	8.6175	-3.6096	0.0542	C	8.6307	-3.6386	0.0617	C	8.6005	-3.6383	-0.0147
C	0.0077	-2.9031	0.0325	C	0.0209	-2.9319	0.0563	C	-0.0086	-2.9323	-0.0099
C	0.0076	-1.4722	-0.0084	C	0.021	-1.5007	0.0393	C	-0.0092	-1.502	0.007
C	1.2375	-0.7635	-0.0251	C	1.2502	-0.7915	0.0213	C	1.222	-0.7939	0.002
C	2.4672	-1.4724	-0.0084	C	2.4795	-1.5013	0.033	C	2.4528	-1.5018	-0.0013
C	3.6973	-0.7643	-0.0251	C	3.71	-0.7939	0.0137	C	3.6844	-0.7934	0.0121
C	4.9276	-1.4726	-0.0085	C	4.9414	-1.501	0.0322	C	4.9138	-1.4998	0.0169
C	6.1578	-0.7643	-0.0252	C	6.1724	-0.7929	0.0181	C	6.1421	-0.7865	0.0317
C	7.3878	-1.4724	-0.0084	C	7.4018	-1.5009	0.0376	C	7.3697	-1.5004	0.0236
C	8.6176	-0.7635	-0.025	C	8.6316	-0.7912	0.0257	C	8.5987	-0.7942	0.0245
C	1.2373	0.6663	-0.0471	C	1.2498	0.6383	-0.018	C	1.2218	0.634	-0.0044
C	2.4673	1.3737	-0.0531	C	2.4792	1.345	-0.0543	C	2.4576	1.339	-0.0153
C	3.6973	0.6652	-0.0472	C	3.7095	0.6342	-0.0342	C	3.6868	0.635	0.0101
C	4.9275	1.3733	-0.0534	C	4.9422	1.3384	-0.0587	C	4.911	1.3561	0.0261
C	6.1576	0.6651	-0.0473	C	6.1741	0.6357	-0.0267	C	6.1423	0.6468	0.0393
C	7.3873	1.3737	-0.0531	C	7.4043	1.3479	-0.0404	C	7.3732	1.3562	0.0397
C	8.6175	0.6665	-0.0472	C	8.6328	0.6391	-0.0099	C	8.5964	0.634	0.03
C	0.0075	1.3761	-0.0531	C	0.0215	1.3512	-0.0274	C	-0.0145	1.3376	0.0077
C	0.0074	2.8084	-0.058	C	0.0222	2.7843	-0.0547	C	-0.0188	2.7615	-0.0052
C	1.24	3.5112	-0.0572	C	1.2516	3.492	-0.0918	C	1.2198	3.4362	-0.0507
C	2.4685	2.8051	-0.0577	C	2.4792	2.7752	-0.1072	C	2.4612	2.7628	-0.0411
C	3.6982	3.5113	-0.057	C	3.7144	3.4702	-0.1518	C	3.6794	3.5047	-0.0173
C	4.9274	2.8042	-0.0576	C	4.9431	2.7644	-0.1182	C	4.9096	2.792	0.0213
C	6.1563	3.5116	-0.0563	C	6.1712	3.4726	-0.1327	C	6.1436	3.4986	0.0408
C	7.3858	2.8051	-0.0571	C	7.4065	2.7799	-0.084	C	7.376	2.7918	0.0399
C	8.6145	3.5108	-0.0572	C	8.6352	3.4982	-0.0735	C	8.6055	3.5066	0.026
C	1.2482	4.9608	-0.0537	C	1.2632	4.9324	-0.0951	C	1.2097	4.8337	-0.0488
C	2.4753	5.6424	-0.0526	C	2.4907	5.588	-0.2242	C	2.3954	5.6191	-0.0833

C	3.6994	4.9503	-0.0531	C	3.7185	4.9019	-0.2336	C	3.6955	4.9537	-0.0103
C	4.9269	5.6335	-0.0456	C	4.9432	5.5878	-0.2729	C	4.9088	5.6218	0.0352
C	6.1544	4.9507	-0.047	C	6.1681	4.9051	-0.1966	C	6.1464	4.9347	0.0468
C	7.3791	5.6418	-0.0354	C	7.393	5.5958	-0.1566	C	7.3809	5.6219	0.0537
C	8.6066	4.9606	-0.0485	C	8.63	4.9434	-0.0657	C	8.6006	4.957	0.0425
C	0.0074	5.5899	-0.0517	C	0.0346	5.6603	0.0369	C	0.0512	5.6296	0.0449
H	0.0077	-6.8242	0.1581	H	0.0206	-6.8538	0.0777	H	-0.0088	-6.8533	-0.0433
H	2.4676	-6.8244	0.1588	H	2.4805	-6.8536	0.0787	H	2.452	-6.8538	-0.0439
H	4.9277	-6.824	0.1584	H	4.9408	-6.8532	0.0794	H	4.9109	-6.8537	-0.0429
H	7.3878	-6.8244	0.1588	H	7.4002	-6.8537	0.0777	H	7.372	-6.8544	-0.0435
H	2.4711	6.7323	-0.0499	H	2.5046	6.6743	-0.3136	H	2.2697	6.3844	-1.1143
H	4.9262	6.7259	-0.0373	H	4.9409	6.6789	-0.331	H	4.9249	6.7147	0.0437
H	7.3764	6.7319	-0.0022	H	7.3436	6.6831	-0.2063	H	7.3662	6.7144	0.0554
H	-0.4419	7.9774	-1.0041	H	-0.9928	7.5298	0.3696	H	-0.1523	7.8652	0.1079
C	-0.0105	8.0414	-0.0246	C	0.0138	7.0853	0.3592	C	0.4785	6.98	0.0796
C	0.455	8.4712	1.0176	C	0.9872	7.9034	0.718	C	1.8926	7.0296	0.0162
H	0.8869	8.6768	1.9762	H	1.7876	8.5461	1.0277	H	2.5265	7.9078	0.1067
	Z3=Z4+H				Z1=Y1				Y1=Y2		
C1	-0.0083	-5.7544	-0.0846	C1	0.0096	-5.7423	0.1616	C1	0.008	-5.7378	0.1223
C	1.2223	-5.0711	-0.0727	C	1.2396	-5.0599	0.1301	C	1.2382	-5.0549	0.1014
C1	2.4523	-5.755	-0.0843	C1	2.4694	-5.7425	0.1612	C1	2.4677	-5.738	0.1225
C	3.6818	-5.0713	-0.0735	C	3.6992	-5.0594	0.1299	C	3.6977	-5.0546	0.1009
C1	4.912	-5.7551	-0.0863	C1	4.9296	-5.7416	0.1616	C1	4.9279	-5.7375	0.1219
C	6.1423	-5.0724	-0.0745	C	6.1597	-5.0593	0.1301	C	6.1582	-5.0547	0.1007
C1	7.3721	-5.7558	-0.0856	C1	7.3894	-5.7425	0.1617	C1	7.3881	-5.738	0.1225
C	8.6016	-5.0714	-0.0734	C	8.6193	-5.0599	0.1303	C	8.6178	-5.0548	0.1014
C	1.222	-3.6318	-0.0487	C	1.2392	-3.6214	0.0649	C	1.2385	-3.6154	0.0588
C	2.4524	-2.9249	-0.0358	C	2.4684	-2.9151	0.0359	C	2.4676	-2.909	0.0383
C	3.6822	-3.6312	-0.0493	C	3.6988	-3.6208	0.0645	C	3.698	-3.6153	0.0579
C	4.9131	-2.9246	-0.0364	C	4.9292	-2.915	0.0353	C	4.9288	-2.9096	0.0367
C	6.142	-3.6323	-0.0498	C	6.1597	-3.6209	0.0644	C	6.1589	-3.6155	0.0574
C	7.3703	-2.9245	-0.0364	C	7.3897	-2.9151	0.0356	C	7.3893	-2.909	0.0374
C	8.6008	-3.6313	-0.0492	C	8.6192	-3.6213	0.0649	C	8.6183	-3.6152	0.0584
C	-0.0091	-2.9251	-0.0356	C	0.0093	-2.915	0.0362	C	0.0087	-2.9082	0.0385
C	-0.0106	-1.4949	-0.0053	C	0.0089	-1.4843	-0.0139	C	0.0093	-1.4776	-0.0012
C	1.2213	-0.786	0.0104	C	1.238	-0.7751	-0.0317	C	1.2388	-0.7681	-0.0181
C	2.4531	-1.4949	-0.0057	C	2.4673	-1.4849	-0.0142	C	2.4676	-1.4784	-0.0013
C	3.6837	-0.7872	0.0095	C	3.6971	-0.7775	-0.033	C	3.6986	-0.772	-0.0203
C	4.9141	-1.4932	-0.0063	C	4.9289	-1.4847	-0.0154	C	4.9296	-1.4791	-0.0039
C	6.1413	-0.7791	0.0092	C	6.1601	-0.7774	-0.0342	C	6.1608	-0.7716	-0.0217
C	7.3685	-1.4933	-0.0062	C	7.39	-1.4849	-0.0155	C	7.3908	-1.4783	-0.0031
C	8.5981	-0.7873	0.01	C	8.6194	-0.7752	-0.0332	C	8.6201	-0.7679	-0.0197
C	1.2208	0.6388	0.0368	C	1.2367	0.6553	-0.0522	C	1.2389	0.6622	-0.0421
C	2.4576	1.3437	0.0459	C	2.4653	1.3632	-0.057	C	2.4691	1.367	-0.0483
C	3.6855	0.641	0.036	C	3.6955	0.6513	-0.0547	C	3.6989	0.6559	-0.0451
C	4.9097	1.3647	0.0455	C	4.9281	1.3544	-0.061	C	4.9313	1.3597	-0.0544
C	6.1406	0.6551	0.0357	C	6.1608	0.6514	-0.0568	C	6.1628	0.6565	-0.0473
C	7.3709	1.3646	0.0459	C	7.3906	1.3631	-0.0619	C	7.3924	1.3688	-0.0535
C	8.595	0.6409	0.0364	C	8.6198	0.6553	-0.0553	C	8.6216	0.6627	-0.0451

C	-0.0172	1.3435	0.046	C	0.0082	1.3681	-0.0572	C	0.0106	1.377	-0.0506
C	-0.0244	2.7659	0.0579	C	0.0076	2.802	-0.0555	C	0.0116	2.8099	-0.053
C	1.2197	3.4464	0.0605	C	1.2355	3.5127	-0.0413	C	1.2465	3.5134	-0.0365
C	2.4637	2.7663	0.0581	C	2.4635	2.7949	-0.0528	C	2.4715	2.797	-0.0444
C	3.6717	3.5114	0.0645	C	3.6988	3.4886	-0.0516	C	3.7064	3.494	-0.0443
C	4.907	2.8013	0.0606	C	4.9274	2.7814	-0.0613	C	4.9325	2.7861	-0.0571
C	6.14	3.5049	0.0685	C	6.1557	3.4883	-0.063	C	6.1585	3.4961	-0.0553
C	7.3723	2.8009	0.061	C	7.3913	2.7949	-0.0656	C	7.3929	2.7998	-0.0575
C	8.6069	3.511	0.0645	C	8.6192	3.5125	-0.0616	C	8.618	3.5181	-0.0533
C	1.2188	4.8316	0.0657	C	1.2434	4.9557	-0.0101	C	1.2759	4.9497	-0.0057
C2	2.3918	5.6298	0.0747	C2	2.4791	5.6124	-0.0328	C2	2.486	5.6117	0.0354
C	3.6643	4.9704	0.0762	C	3.7024	4.9226	-0.0461	C	3.7161	4.926	-0.0103
C2	4.9028	5.6317	0.091	C2	4.9268	5.6082	-0.044	C2	4.9323	5.6118	-0.0044
C	6.14	4.9454	0.0859	C	6.151	4.9218	-0.0466	C	6.1506	4.9292	-0.0303
C2	7.3754	5.6316	0.0929	C2	7.3735	5.6118	-0.015	C2	7.3816	5.614	-0.008
C	8.6141	4.9693	0.0756	C	8.6128	4.9559	-0.0379	C	8.594	4.9567	-0.0374
C2	0.0465	5.6275	0.0708	C2	0.0088	5.6772	0.0098	C2	0.0147	5.6744	-0.0461
H	-0.0081	-6.8467	-0.1041	H	0.0097	-6.8338	0.2119	H	0.0077	-6.83	0.1547
H	2.4525	-6.8472	-0.1037	H	2.4698	-6.8339	0.2113	H	2.4675	-6.8302	0.155
H	4.9116	-6.8474	-0.1063	H	4.9298	-6.833	0.2119	H	4.9276	-6.8296	0.1549
H	7.3727	-6.848	-0.1054	H	7.3894	-6.8338	0.2122	H	7.3878	-6.8302	0.1556
H	2.2605	7.4517	-2.5051	H	2.5017	6.7018	-0.0505	H	2.5188	6.6999	0.1147
H	4.9175	6.7239	0.1064	H	4.9265	6.7006	-0.0326	H	4.929	6.7043	0.0141
H	7.3613	6.7237	0.1113	H	7.3247	6.6975	0.0498	H	7.3426	6.7052	0.061
H	-0.1009	7.888	0.0812	H	-0.9321	7.5865	-0.4025	H	-0.8291	7.7763	-0.1086
C	0.5196	6.994	0.0785	C	-0.0377	7.1467	0.0708	C	0.107	7.0342	-0.0656
C	1.9167	6.9956	0.0796	C	0.8073	7.9884	0.6238	C	0.5636	8.2317	-0.407
H	2.5359	7.8899	0.1012	H	1.4824	8.6691	1.1031	H	0.6295	9.0335	0.3503
		Y2=Y3+H				Y1=Y3+H				Y1=X1	
C	-0.0003	-5.7313	0.0691	C	0.0214	-5.7575	0.1657	C	0.013	-5.7511	0.122
C	1.2299	-5.048	0.0651	C	1.2512	-5.0752	0.1349	C	1.2427	-5.0686	0.0981
C	2.4596	-5.7318	0.0688	C	2.481	-5.7574	0.1657	C	2.4728	-5.7513	0.1221
C	3.6894	-5.0479	0.065	C	3.7111	-5.0749	0.1344	C	3.7024	-5.0685	0.0979
C	4.9196	-5.7312	0.069	C	4.9414	-5.757	0.1654	C	4.933	-5.751	0.1216
C	6.1499	-5.0479	0.0649	C	6.1714	-5.0747	0.1343	C	6.1628	-5.0687	0.0976
C	7.3797	-5.7318	0.0687	C	7.4009	-5.7575	0.1654	C	7.3929	-5.7516	0.122
C	8.6094	-5.048	0.065	C	8.6311	-5.0753	0.1346	C	8.6223	-5.0687	0.0981
C	1.2299	-3.6079	0.0569	C	1.2511	-3.6369	0.0701	C	1.2406	-3.6299	0.0501
C	2.4595	-2.9011	0.0519	C	2.4805	-2.9308	0.0411	C	2.4694	-2.924	0.0272
C	3.6894	-3.6078	0.0567	C	3.7109	-3.6364	0.0697	C	3.7003	-3.6296	0.0497
C	4.9198	-2.9012	0.0516	C	4.9415	-2.9306	0.0405	C	4.9301	-2.9238	0.0267
C	6.1501	-3.6078	0.0567	C	6.1715	-3.6364	0.0694	C	6.1608	-3.6299	0.0494
C	7.3801	-2.9011	0.0519	C	7.4016	-2.9308	0.0409	C	7.3897	-2.924	0.027
C	8.6096	-3.6079	0.0568	C	8.6314	-3.6368	0.0701	C	8.6203	-3.6297	0.05
C	-0.0002	-2.901	0.0518	C	0.0215	-2.9306	0.0415	C	0.0099	-2.9238	0.0275
C	-0.0001	-1.4696	0.0361	C	0.0216	-1.5	-0.0089	C	0.0068	-1.4936	-0.0142
C	1.2297	-0.7606	0.0245	C	1.2507	-0.7907	-0.0283	C	1.2358	-0.785	-0.0308
C	2.4593	-1.47	0.0363	C	2.4799	-1.5006	-0.0098	C	2.4662	-1.494	-0.0151
C	3.6892	-0.7621	0.0246	C	3.71	-0.7931	-0.0295	C	3.6953	-0.7864	-0.0317

C	4.9199	-1.47	0.036	C	4.9416	-1.5003	-0.0107	C	4.9273	-1.4934	-0.0154
C	6.1508	-0.762	0.0246	C	6.1727	-0.7929	-0.0299	C	6.1569	-0.785	-0.0317
C	7.3805	-1.47	0.0363	C	7.4024	-1.5005	-0.01	C	7.3869	-1.4938	-0.0151
C	8.6101	-0.7606	0.0245	C	8.6322	-0.7908	-0.0281	C	8.6155	-0.7855	-0.0303
C	1.2295	0.6691	-0.0045	C	1.2501	0.6397	-0.0506	C	1.232	0.6443	-0.0495
C	2.4591	1.3768	-0.0185	C	2.4788	1.348	-0.057	C	2.4613	1.3519	-0.0552
C	3.6888	0.6669	-0.0037	C	3.709	0.6359	-0.0534	C	3.6919	0.6423	-0.0522
C	4.9202	1.3727	-0.0179	C	4.9418	1.3394	-0.0592	C	4.9218	1.3494	-0.0566
C	6.1515	0.6669	-0.0038	C	6.174	0.636	-0.0535	C	6.1546	0.6445	-0.0515
C	7.3812	1.377	-0.0186	C	7.404	1.3481	-0.0566	C	7.3836	1.3551	-0.053
C	8.6106	0.6692	-0.0045	C	8.6332	0.6398	-0.0503	C	8.6122	0.6438	-0.0481
C	0.0001	1.3798	-0.0196	C	0.022	1.3524	-0.0531	C	0.0002	1.3533	-0.0495
C	0.0003	2.8115	-0.0453	C	0.0221	2.7863	-0.0453	C	-0.0047	2.784	-0.0373
C	1.2304	3.5195	-0.0547	C	1.2499	3.4977	-0.0394	C	1.225	3.4858	-0.0336
C	2.4593	2.8075	-0.0424	C	2.4785	2.78	-0.0547	C	2.4584	2.7824	-0.0522
C	3.6914	3.5082	-0.0502	C	3.7138	3.474	-0.0539	C	3.6895	3.4862	-0.0515
C	4.9204	2.8013	-0.0409	C	4.9421	2.7662	-0.0599	C	4.9195	2.7789	-0.0565
C	6.1495	3.5086	-0.0503	C	6.1697	3.4738	-0.0535	C	6.1475	3.486	-0.0478
C	7.3815	2.8079	-0.0425	C	7.4054	2.7802	-0.0536	C	7.3819	2.7874	-0.0465
C	8.6105	3.52	-0.0548	C	8.6346	3.4972	-0.0376	C	8.6095	3.5013	-0.0247
C	1.2415	4.957	-0.0784	C	1.262	4.9389	-0.0018	C	1.2279	4.9212	0.0091
C	2.4674	5.6325	-0.0782	C	2.4957	5.5981	-0.0078	C	2.4521	5.5757	0.0013
C	3.694	4.9447	-0.0642	C	3.7178	4.9077	-0.0376	C	3.6945	4.9304	-0.0341
C	4.9205	5.6297	-0.0677	C	4.9417	5.5957	-0.0335	C	4.919	5.6132	-0.0334
C	6.1472	4.9453	-0.0643	C	6.1649	4.9076	-0.0371	C	6.1433	4.9214	-0.0344
C	7.374	5.6333	-0.0785	C	7.3874	5.5948	-0.0065	C	7.3688	5.608	-0.003
C	8.5999	4.9579	-0.0786	C	8.6227	4.9402	0.0009	C	8.6026	4.9447	0.0189
C	0.0009	5.6693	-0.104	C	0.0174	5.6623	0.0471	C	0.0027	5.6554	0.0715
H	-0.0004	-6.8239	0.0764	H	0.0213	-6.8488	0.2156	H	0.0141	-6.8429	0.1595
H	2.4597	-6.8244	0.0761	H	2.4812	-6.8487	0.2156	H	2.4741	-6.843	0.1599
H	4.9196	-6.8238	0.0763	H	4.9415	-6.8483	0.2153	H	4.9342	-6.8427	0.1597
H	7.3795	-6.8244	0.0759	H	7.4006	-6.8488	0.2152	H	7.3942	-6.8433	0.1598
H	2.4708	6.7233	-0.0914	H	2.5175	6.6869	0.0168	H	2.2085	6.8954	0.0714
H	4.9201	6.7218	-0.0774	H	4.9428	6.6877	-0.0148	H	4.9187	6.7048	-0.0167
H	7.3706	6.7243	-0.0919	H	7.3748	6.6925	0.0212	H	7.3319	6.6969	-0.0006
H	0.0469	9.3242	-2.8865	H	-1.5994	8.0155	0.1721	H	-0.8706	7.6457	0.3295
C	0.0052	7.078	-0.1622	C	0.1081	7.0824	0.1551	C	0.0689	7.0987	0.1973
C	0.018	8.2949	-0.2292	C	0.6819	8.1702	0.2644	C	1.2268	7.7774	0.1866
H	0.0272	9.3642	-0.2441	H	0.9295	9.2085	0.3582	H	1.3907	8.85	0.2913
		X1=Z3				Z0+C2H2=Y1				Z0+C2H2=Z1	
C	0.027	-5.7767	0.0657	C	-0.0059	-5.7257	0.1754	C	0.0084	-5.7319	0.1188
C	1.2567	-5.0937	0.0545	C	1.2242	-5.0428	0.1443	C	1.2384	-5.0488	0.0966
C	2.4865	-5.7767	0.0651	C	2.4542	-5.7259	0.1748	C	2.4682	-5.7322	0.1191
C	3.7168	-5.0937	0.0537	C	3.6839	-5.0426	0.1444	C	3.6981	-5.0488	0.0966
C	4.947	-5.7765	0.0647	C	4.9142	-5.7252	0.1755	C	4.9284	-5.7317	0.1188
C	6.1767	-5.0934	0.0541	C	6.1445	-5.0425	0.1445	C	6.1585	-5.0488	0.0965
C	7.4065	-5.7766	0.0653	C	7.3743	-5.7259	0.1752	C	7.3883	-5.7322	0.1192
C	8.6366	-5.0938	0.0547	C	8.604	-5.0427	0.1446	C	8.6181	-5.0488	0.0967
C	1.2565	-3.6538	0.0278	C	1.224	-3.6039	0.0805	C	1.2384	-3.6094	0.052

C	2.4859	-2.9471	0.0111	C	2.4536	-2.8974	0.0525	C	2.4679	-2.9028	0.0309
C	3.7166	-3.6537	0.027	C	3.6837	-3.6038	0.0802	C	3.6979	-3.6093	0.0519
C	4.9467	-2.947	0.0108	C	4.914	-2.8976	0.0523	C	4.9282	-2.9031	0.0304
C	6.1767	-3.6537	0.0274	C	6.1444	-3.6037	0.0804	C	6.1585	-3.6094	0.0516
C	7.4065	-2.9468	0.0114	C	7.3744	-2.8973	0.0526	C	7.3882	-2.9028	0.0306
C	8.6365	-3.6536	0.0279	C	8.604	-3.6039	0.0806	C	8.618	-3.6093	0.0519
C	0.0268	-2.9467	0.0116	C	-0.0061	-2.8973	0.0528	C	0.0083	-2.9028	0.0308
C	0.0265	-1.5154	-0.0228	C	-0.0063	-1.4664	0.0044	C	0.0081	-1.4719	-0.0096
C	1.2557	-0.8055	-0.0375	C	1.2233	-0.7574	-0.0151	C	1.2379	-0.7632	-0.0258
C	2.4852	-1.5157	-0.0229	C	2.453	-1.4668	0.004	C	2.4676	-1.472	-0.0095
C	3.7155	-0.807	-0.037	C	3.683	-0.7591	-0.0157	C	3.6977	-0.764	-0.026
C	4.9463	-1.5154	-0.0232	C	4.9138	-1.4669	0.0037	C	4.9281	-1.4723	-0.0099
C	6.1761	-0.8057	-0.0379	C	6.1445	-0.7587	-0.0156	C	6.1582	-0.764	-0.0264
C	7.4063	-1.515	-0.0231	C	7.3746	-1.4666	0.0041	C	7.3882	-1.472	-0.0099
C	8.6361	-0.8056	-0.037	C	8.6041	-0.7572	-0.015	C	8.618	-0.7632	-0.0261
C	1.2547	0.6257	-0.0551	C	1.2226	0.673	-0.0413	C	1.2377	0.6667	-0.0472
C	2.4841	1.3346	-0.0548	C	2.4526	1.3796	-0.0488	C	2.4675	1.3741	-0.0528
C	3.7142	0.6231	-0.0531	C	3.6825	0.67	-0.042	C	3.6975	0.6655	-0.0474
C	4.9434	1.3323	-0.0572	C	4.9132	1.3765	-0.0488	C	4.9277	1.3736	-0.0534
C	6.1755	0.6249	-0.0564	C	6.1447	0.6708	-0.0418	C	6.1578	0.6654	-0.0477
C	7.4057	1.3352	-0.0604	C	7.3748	1.3805	-0.0486	C	7.3875	1.3739	-0.0532
C	8.6355	0.6254	-0.0556	C	8.6042	0.6731	-0.0411	C	8.6178	0.6668	-0.0475
C	0.0249	1.3374	-0.0598	C	-0.0068	1.3841	-0.0476	C	0.0078	1.3764	-0.0531
C	0.0229	2.7705	-0.0501	C	-0.007	2.8177	-0.0516	C	0.0076	2.8087	-0.0575
C	1.2537	3.4745	-0.024	C	1.2252	3.52	-0.0519	C	1.2401	3.5115	-0.0561
C	2.4825	2.7669	-0.0353	C	2.4532	2.811	-0.0539	C	2.4686	2.8054	-0.0566
C	3.7119	3.4752	-0.0213	C	3.6842	3.5132	-0.0542	C	3.6982	3.5117	-0.0553
C	4.941	2.7639	-0.0488	C	4.9127	2.8059	-0.0541	C	4.9274	2.8046	-0.0567
C	6.1703	3.4691	-0.0543	C	6.1413	3.5126	-0.0545	C	6.1563	3.5118	-0.0552
C	7.4046	2.7675	-0.0594	C	7.3739	2.8126	-0.054	C	7.3858	2.8052	-0.0566
C	8.6317	3.4825	-0.0418	C	8.6018	3.5226	-0.0518	C	8.6144	3.5108	-0.0566
C	1.2626	4.9169	0.062	C	1.2343	4.9708	-0.0468	C	1.2482	4.961	-0.0517
C	2.4694	5.564	0.2654	C	2.4644	5.6426	-0.0477	C	2.4751	5.643	-0.0484
C	3.7127	4.9252	0.0661	C	3.686	4.9504	-0.0515	C	3.6993	4.9508	-0.0495
C	4.9422	5.5973	0.034	C	4.912	5.6333	-0.0522	C	4.9268	5.6337	-0.0413
C	6.163	4.904	-0.0482	C	6.1376	4.949	-0.0565	C	6.1542	4.9508	-0.0444
C	7.3939	5.5885	-0.0621	C	7.3596	5.641	-0.0633	C	7.3789	5.6417	-0.0329
C	8.6165	4.9227	-0.0211	C	8.5955	4.9755	-0.0521	C	8.6062	4.9603	-0.0475
C	0.022	5.6451	0.0469	C	-0.0028	5.6113	-0.0434	C	0.0071	5.5888	-0.0511
H	0.027	-6.8691	0.0827	H	-0.0059	-6.8172	0.2262	H	0.0084	-6.824	0.1539
H	2.4865	-6.8691	0.082	H	2.4542	-6.8173	0.2255	H	2.4683	-6.8242	0.1541
H	4.9471	-6.8689	0.0816	H	4.9143	-6.8167	0.2264	H	4.9285	-6.8238	0.1539
H	7.4064	-6.869	0.0822	H	7.3744	-6.8173	0.226	H	7.3884	-6.8242	0.1546
H	1.981	7.4951	-0.7922	H	2.4652	6.7302	-0.0445	H	2.4709	6.7328	-0.0436
H	4.947	6.688	0.0758	H	4.9119	6.7258	-0.0466	H	4.9264	6.7261	-0.0311
H	7.3684	6.6784	-0.087	H	7.3177	6.7288	-0.0896	H	7.3753	6.7317	0.0023
H	-0.7595	7.564	0.6267	H	-1.1121	7.8686	0.2805	H	-0.489	7.9834	-0.9802
C	0.0979	7.0492	0.1832	C	-0.0532	8.0202	0.2502	C	-0.0288	8.0532	-0.0146
C	1.2352	7.7823	-0.0562	C	0.9958	8.645	0.2863	C	0.4647	8.4672	1.02

H	1.3033	8.8067	0.3257	H	1.9768	9.0736	0.3075	H	0.9231	8.6655	1.9676

Selection of computational parameters

The modelling of graphene bulk is done by defining a primitive cell which will be repeated in each direction respecting the Periodic Boundary Conditions (PBCs), in this way a three-dimensional material will be represented. Graphene has been modelled as graphene nanoribbons (GNRs) since they are simple systems and representative for the aim of the work. GNRs are composed of hexagonal two-dimensional lattice, and they can have two different edges: armchair and zigzag. The monolayers of graphene have been studied in their form with hydrogen saturating all the carbon atoms at the edges (except the C2H2 addition site), that is because both structures tend to reconstruct when they are self-passivated. The ribbons' width is finite defined by the number of rings repeated in the layer, while the direction perpendicular to the width is infinite. The fundamentals parameter to be used in input to QE (i.e., energy cut-off, k-points and lattice parameters) were selected prior to perform DFT calculations by means of rigorous convergence tests:

1) ***Ecut(wfc)* and *Ecut(wfc)***: For both the armchair and zigzag, the optimal kinetic energy cut-off of wave functions $Ecut(wfc)$ and kinetic energy cut-off of charge density $Ecut(rho)$ have been evaluated for the bulk graphene structure by evaluating the total energy per atom for different $Ecut(rho)$. The values of 200 Ry for $Ecut(rho)$ and 40 Ry for $Ecut(wfc)$ are selected (for both the armchair and zigzag system) since for these values the total energy of the system per atom goes to convergence (Figure 1).

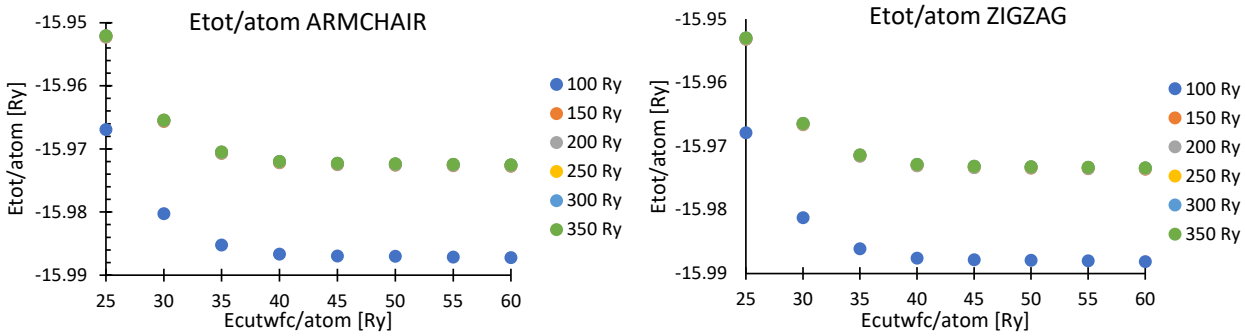

Figure S5: Total energy of the system per atom [Ry] with respect to $Ecut\ (rho)$ and $Ecut\ (wfc)$ for armchair (left) and zig-zag (right) graphene.

2) **k-points:** The optimal values of points in k-space have been chosen by computing the total energy of the system by varying k-points (from 2 to 7) and by choosing the one for which the total energy converges. Thus, an optimal value of k-points of 5 is chosen for both armchair and zigzag system (Figure 2).

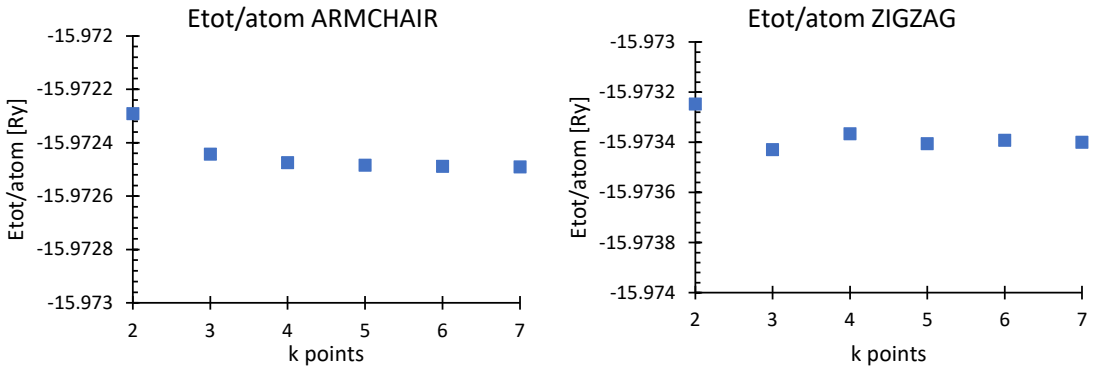

Figure S6: Total energy of the system [Ry] per atom with respect to k-points for armchair (left) and zig-zag (right) graphene.

3) **Unit cells dimension**: In order to assess an optimal dimension of the slabs studied in this work, the methodology consisted in performing a thorough binding energy convergence analysis for the addition of

acetylene on graphene. Thus, we calculated the variation of the C-H binding energy for an H-passivated edge (E_{C-H}) and the acetylene binding energy $E_{C2H2-binding}$ (R1 and R2) at different dimensions of the unit cell, by changing the width of graphene along the x direction, the width of graphene along the y direction and the void space between two repeated images along the z direction.

R1. $$E_{C-H} = \left(E_{graphene\_H} + \frac{1}{2}E_{H2}\right) - E_{graphene}$$

R2. $$E_{C2H2-binding} = \left(E_{graphene\_H} + \frac{1}{2}E_{C2H2}\right) - E_{graphene+C2H2}$$

Here, $E_{graphene\_H}$ is the energy of graphene with one non-saturated carbon atom, E_{H2} is the energy of a H_2 molecule, $E_{graphene}$ is the energy of a completely passivated graphene, $E_{graphene+C2H2}$ is the energy of a graphene with one non-saturated carbon atom together with a C_2H_2 molecule and E_{C2H2} is the energy of a C_2H_2 molecule alone.

These energies have been obtained by relaxing the cell and atoms positions in the cell: the results are ground state energies for the configurations of interest. So, a relaxation of all the structures involved in *H* scission and C_2H_2 binding has been done at various values of celldm(2) (width of graphene along the x direction), and after that E_{C-H} and $E_{C2H2-binding}$ are plotted to check to find the values where the energy values reach convergence. Thus values of celldm(2) of 2.8 and 2.3 are selected for the armchair and zigzag cells, respectively (Figure 3).

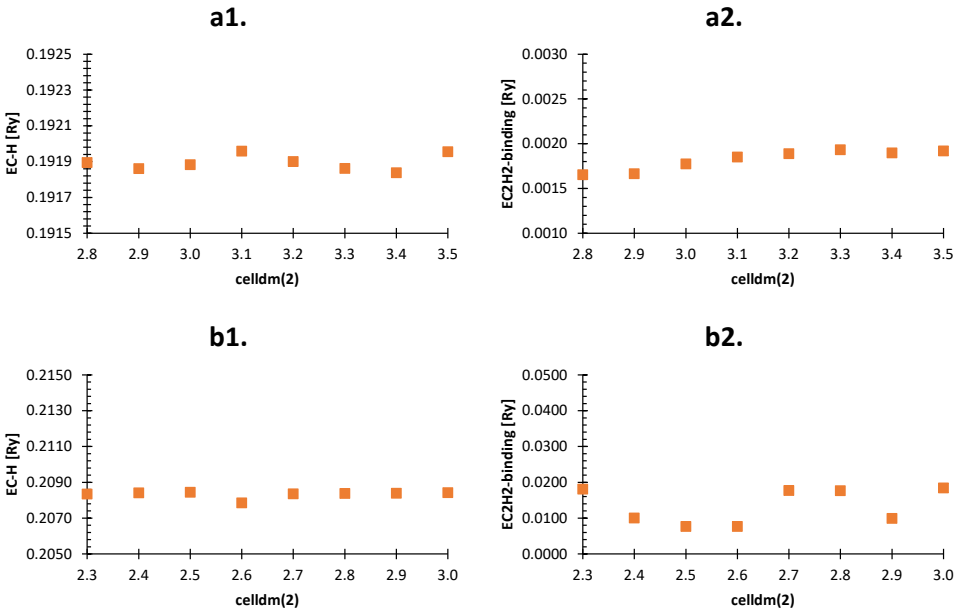

Figure S7: *H* scission energy [E_{C-H}, Ry] and C_2H_2 binding energy [$E_{C2H2-binding}$, Ry] varying the width of graphene along the x direction (i.e., celldm(2)) for armchair (a1. and a2., respectively) and zigzag (b1. and b2., respectively) graphene edges.

Hindered rotor effects

The hindered rotor (HR) treatment can significantly influence the estimation of kinetic rates and overall reactivity in reactions involving molecules in which atoms can rotate along a chemical bond. Thus, in the investigated system, it is important to account for this aspect in the entrance and exit channels involving intermediates with the ethenyl group (R-CH=ĊH) at the edge (A1, B1, C1, and Z1, X1 in the armchair and zigzag systems, respectively). However, after verifying that the influence on analogous gas phase processes was minimal (Figure S9), we decided to adopt a slightly different approach that still allows us to address this aspect, as discussed below.

For the armchair system, all configurations resulting from the addition of C2H2 at the carbon site were considered as distinct species. Thus, all three isomers A1, B1, and C1 are included in the potential energy surface (see Figure 3 in the main text). The barrier associated with surface-C2H2 torsion between A1 and B1 is accounted for in the potential energy surface and yields results very similar to the torsion observed in the gas phase system (5.3 and 4.6 kcal/mol for the solid and gas system, respectively). Considering that the partition functions of different configurations provide an overall statistical averaging in the final lumped rate constants, we considered that the net result should closely resemble that of a hindered rotor treatment.

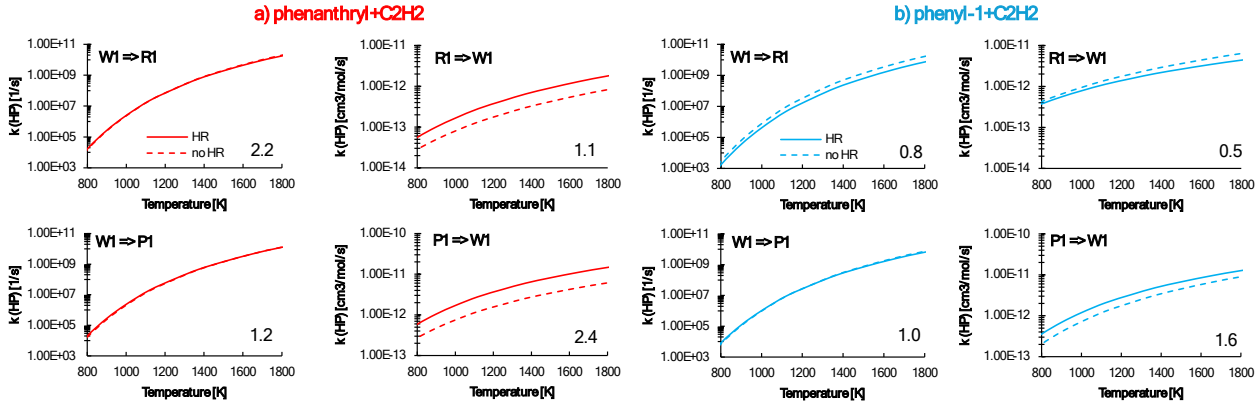

Figure S8: Comparison of rate constants with (solid lines) and without (dotted lines) the HR treatment for the phenanthryl+C2H2 (a) and phenyl+C2H2 (b) systems. R1 denotes the entrance channel (phenanthryl/phenyl+C2H2), W1 denotes the radicals formed by the addition of C2H2, and P1 denotes the ethynylphenanthrene/1-ethynylnaphthalene+H products. The number reported in the bottom right of each plot corresponds to the correction factors applied to the solid phase rates of analogous steps reported in Table S2.

In the zigzag system, only the two isomers Z1 and X1, with the H atoms of the C2H2 fragment in cis and trans positions, were considered. The torsion of C2H2 in these intermediates produces equivalent species that were not explicitly included. After confirming the consistency of the torsional barrier with the analogous gas-phase system (Figure S9), a correction was applied to the kinetic constant of the C2H2 addition and H elimination step to address the effects of the hindered rotor treatment. The corrective factors were derived as the maximum deviation within the temperature range of interest (800-1800 K) of the rates in the analogous gas phase steps, with and without the HR treatment (Figure S9b). In Table S3, the original pre-exponential factors of these reactions (marked with an *) are reported in brackets.

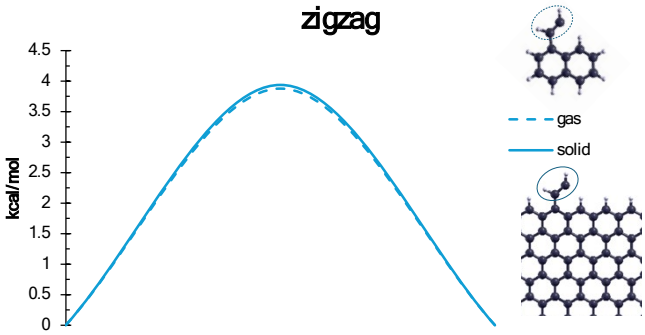

Figure S9: Torsional potential [kcal/mol] related to the torsion in the ethenyl group (R-CH=ĊH) at the zigzag edge (solid line) and in the analogous gas phase molecule (dotted line).

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