

Supplementary Information

Dissociative Chemisorption of Hydrogen Molecule on Defective Graphene Supported Aluminium Clusters: A Computational Study

Deepak Kumar,^{a,§} Thillai Govindaraja,^{b,§} Sailaja Krishnamurty,^{a,*} Selvaraj Kaliaperumal,^b and Sourav Pal^{c,*}

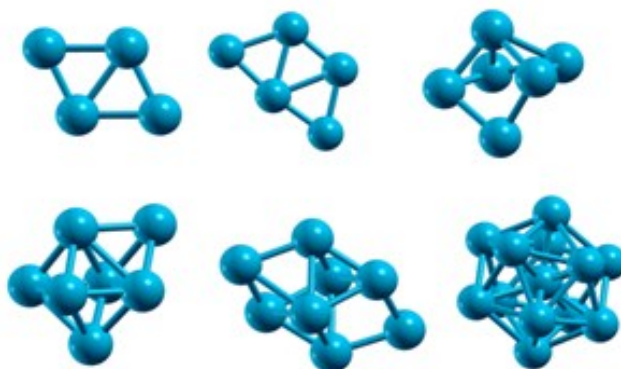
^a Physical Chemistry Division, CSIR-National Chemical Laboratory, Pune 411 008, India

^b Nano and Computational Material Lab., Catalysis Division, CSIR-National Chemical Laboratory, Pune 411 008, India

^c IISER Kolkata, Mohanpur 741 246, West Bengal, India

*Email: k.sailaja@ncl.res.in, s.pal@iiserkol.ac.in,

[§]equally contributing authors



Suppl-Figure 1. The optimized lowest energy conformations of Al_{4,8} and Al₁₃ clusters.

Suppl-Table 1. Interatomic distances in (i) free Al_n clusters (n = 4, 5), (ii) Al_n clusters (n = 4, 5) anchored on defective graphene and (iii) H₂ adsorbed on Al_n (n = 4, 5)--df_graphene complexes.

(i)	d_{Al-Al} (Å)	Unsaturated Carbons	d_{C-C} (Å)	(ii)	d_{Al-Al} (Å)	Unsaturated Carbons	d_{C-C} (Å)	(iii)	d_{Al-Al} (Å)	Unsaturated carbons	d_{C-C} (Å)
Al₄	2.47	C1-C2	2.38	Al₄--df_gp	2.61	C1-C2	2.84	H₂-Al₄--df_gp	2.75	C1-C2	2.86
	2.67	C2-C3	2.62		2.77	C2-C3	2.86		2.71	C2-C3	2.87
	2.77	C1-C3	2.60		2.67	C1-C3	2.84		2.55	C1-C3	2.82
	2.67				2.88				2.96		
	2.47				2.72				2.86		
Al₅	2.49	C1-C2	2.38	Al₅--df_gp	2.50	C1-C2	2.84	H₂-Al₅--df_gp	2.50	C1-C2	2.83
	2.52	C2-C3	2.62		2.58	C2-C3	2.87		2.54	C2-C3	2.85
	2.52	C1-C3	2.60		2.63	C1-C3	2.87		2.65	C1-C3	2.86
	2.62				2.70				2.78		
	2.62				2.52				2.55		
	2.78				2.80				2.84		
	2.76				2.68				2.58		

Suppl-Table 2. Charge distribution on various Al atoms of (a) free Al_n clusters and (b) Al_n – defective_graphene complexes as obtained by Bader analysis. Defective graphene is abbreviated as df_gp in the table.

Al_4 (e)	Al_4 --df_gp (e)	Al_5 (e)	Al_5 --df_gp (e)	Al_6 (e)	Al_6 --df_gp (e)	Al_7 (e)	Al_7 --df_gp (e)	Al_8 (e)	Al_8 --df_gp (e)	Al_{13} (e)	Al_{13} --df_gp (e)
-0.13	1.65	-0.23	1.95	0.06	1.65	-0.01	1.61	0.04	1.83	-1.14	1.88
0.14	0.63	0.15	0.41	-0.12	0.55	0.04	-0.04	-0.08	-0.35	0.12	0.56
-0.14	0.35	-0.06	0.04	0.09	0.10	-0.03	0.40	0.05	0.12	0.09	0.17
0.13	0.53	-0.02	-0.18	0.07	0.09	-0.02	0.15	-0.05	0.22	0.10	-0.25
		0.16	0.14	-0.08	0.56	0.00	0.06	-0.19	0.12	0.08	0.11
				0.00	0.02	-0.01	0.07	-0.15	0.08	0.11	-0.18
						0.03	0.00	0.20	0.50	0.10	0.11
								0.17	0.49	0.09	-0.49
										0.09	0.18
										0.10	0.01
										0.08	0.13
										0.11	0.39
										0.08	0.18

Suppl-Table 3. Charge distribution on unsaturated carbon centres in Al_n- defective_graphene complexes as obtained by Bader analysis. Defective graphene is abbreviated as df_gp in the table.

System		Al₄ (e)	Al₅ (e)	Al₆ (e)	Al₇ (e)	Al₈ (e)	Al₁₃ (e)
Net charge on defective_graphene		-3.16	-2.36	-2.97	-2.25	-3.01	-2.79
Net charge on Al cluster		3.16	2.36	2.97	2.25	3.01	2.79
Charge redistribution at defective sites	df_gp (e)	Al4--df_gp (e)	Al5--df_gp (e)	Al6--df_gp (e)	Al7--df_gp (e)	Al8--df_gp (e)	Al13--df_gp (e)
C1	-0.13	-0.76	-0.5	-0.6	-0.06	-0.97	-0.43
C2	0.08	-0.31	-0.48	-1.06	-0.43	-0.47	-0.56
C3	0.05	-0.93	-1.02	-1.06	-0.9	-0.96	-0.99
Sum of charges on defective sites		-2.0	-2.0	-2.72	-1.39	-2.4	-1.98

Suppl-Table 4. Charge distribution on unsaturated carbon centers in Al_n supported defective graphene before and after H₂ adsorption. Defective graphene is abbreviated as df_gp in the table.

Carbon site	Al ₄ --df_gp		Al ₅ --df_gp		Al ₆ --df_gp		Al ₇ --df_gp		Al ₈ --df_gp		Al ₁₃ --df_gp	
	(e)		(e)		(e)		(e)		(e)		(e)	
	(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)	(i)	(ii)
C1	-0.76	-0.89	-0.5	-0.48	-0.6	-0.56	-0.06	-0.51	-0.97	-1.04	-0.43	-1.02
C2	-0.31	-0.58	-0.48	-0.63	-1.06	-1.04	-0.43	-0.48	-0.47	-0.61	-0.56	-0.42
C3	-0.93	-0.9	-1.02	-1.03	-1.06	-1.02	-0.9	-0.92	-0.96	-0.93	-0.99	-1.09
Sum of charges on defective sites	-2	-2.37	-2	-2.14	-2.72	-2.62	-1.39	-1.91	-2.4	-2.58	-1.98	-2.53

(i) – before H₂ adsorption, (ii) – after H₂ adsorption

Cartesian coordinates of the optimized structures

Def_graphene			
C	9.926615	17.354302	3.505298
C	9.213081	16.121569	3.626027
C	9.933274	14.885349	3.685142
C	9.220017	13.651414	3.771192
C	9.916752	12.404806	3.802755
C	9.196335	11.165372	3.863027
C	9.902038	9.926615	3.858083
C	9.169431	8.704186	3.908235
C	9.902830	7.457847	3.954193
C	9.202994	6.219690	4.047226
C	7.770722	6.232729	4.134426
C	7.061748	4.991590	4.240328
C	5.633086	4.983870	4.294984
C	4.916174	3.743442	4.350227
C	3.487126	3.739731	4.376181
C	2.773765	2.500769	4.406902
C	1.341769	2.509282	4.428540
C	0.628219	1.274200	4.496344
C	0.620385	3.746510	4.404949
C	1.338537	4.982850	4.374949
C	0.628781	6.223608	4.348315
C	1.346210	7.464591	4.299513
C	0.641134	8.706579	4.238412
C	1.364969	9.939864	4.132606
C	0.638959	11.174417	4.038009
C	1.362085	12.398777	3.943815
C	2.807358	12.385198	3.900158
C	3.500467	13.630289	3.845160
C	4.925841	13.636862	3.852116
C	5.640719	14.878885	3.794206
C	7.068246	14.896602	3.765345
C	7.782496	16.129392	3.679560
C	2.775168	7.452083	4.323377
C	3.485145	6.216576	4.352460
C	2.768749	4.976691	4.367059
C	4.910368	6.215392	4.318578
C	7.051831	7.461732	4.125028
C	7.702052	8.723717	3.940437
C	7.031912	9.980457	3.868547
C	7.750001	11.182656	3.902951
C	7.790332	13.661997	3.805306
C	7.085262	12.441883	3.874176
C	5.663105	12.393472	3.891606
C	4.978488	11.173919	3.847358
C	3.556883	11.122505	3.935771
C	2.789265	9.929657	4.128239
C	3.504806	8.705300	4.306144
C	4.886453	8.632452	4.472915
C	5.633439	7.470903	4.298613

v_gp_al4

C	9.921506	17.340285	3.446761
C	9.208257	16.105962	3.541549
C	9.921105	14.871302	3.566720
C	9.207813	13.638197	3.674008
C	9.927563	12.400518	3.648600
C	9.229246	11.169210	3.807040
C	9.926825	9.919316	3.767375
C	9.225983	8.676805	3.937678
C	9.925082	7.438812	3.884730
C	9.207578	6.207284	4.034736
C	7.782133	6.215187	4.191649
C	7.067148	4.976388	4.152104
C	5.633846	4.968705	4.118137
C	4.915232	3.739052	4.115690
C	3.482092	3.740773	4.107301
C	2.766159	2.506993	4.186894
C	1.337796	2.506127	4.217821
C	0.623763	1.271269	4.340788
C	0.626158	3.743927	4.191971
C	1.338394	4.981183	4.109556
C	0.629069	6.219257	4.115919
C	1.337790	7.459663	4.111128
C	0.632001	8.696828	4.124090
C	1.358151	9.938360	4.137119
C	0.631953	11.172877	3.995829
C	1.334898	12.407845	3.853668
C	2.757526	12.422569	3.903263
C	3.479028	13.650780	3.745195
C	4.912466	13.665662	3.801585
C	5.631302	14.882641	3.637821
C	7.063457	14.875852	3.666818
C	7.781823	16.108402	3.566808
C	2.762175	7.452726	4.184134
C	3.482880	6.210845	4.140992
C	2.768526	4.975980	4.087749
C	4.916751	6.194783	4.184568
C	7.082210	7.451964	4.421952
C	7.850874	8.695384	4.335762
C	7.278492	9.960391	4.662981
C	7.847666	11.188316	4.192715
C	7.778580	13.645196	3.817775
C	7.076509	12.437552	4.160514
C	5.601535	12.477499	4.189750
C	4.824232	11.385095	4.608477
C	3.463287	11.238874	4.282935
C	2.770706	9.948654	4.342785
C	3.459202	8.672482	4.453754
C	4.823891	8.537439	4.869658
C	5.614756	7.411368	4.487937
Al	5.640110	10.092807	5.747488
Al	5.212315	7.700963	6.973086
Al	7.791359	8.988756	6.885148
Al	7.815235	11.582989	6.583085

v_gp_al4_H2

C	5.656056	7.361555	4.517829
C	4.946970	6.144120	4.241254
C	5.662256	4.916089	4.139679
C	7.090814	4.916081	4.137556
C	7.804603	6.159286	4.141980
C	7.109898	7.385461	4.360084
C	7.878933	8.624484	4.294012
C	9.253554	8.617173	3.901544
C	9.951115	7.378123	3.847396
C	9.236181	6.147919	3.992468
C	7.305234	9.869278	4.655737
C	7.882620	11.121436	4.247927
C	9.262594	11.114609	3.855660
C	9.956759	9.862907	3.772865
C	7.098506	12.378264	4.206604
C	7.805604	13.591735	3.871166
C	9.232260	13.585421	3.725938
C	9.956637	12.347280	3.694929
C	7.088831	14.820202	3.697832
C	7.806862	16.049698	3.572736
C	9.233285	16.048027	3.546453
C	9.944873	14.817475	3.599119
C	3.511861	6.156622	4.207872
C	2.795047	4.924486	4.126326
C	3.508931	3.686989	4.129507
C	4.938668	3.686920	4.138030
C	1.367155	4.927569	4.140148
C	0.655433	3.689822	4.198112
C	1.365067	2.449043	4.211179
C	2.793428	2.450895	4.188658
C	2.789356	7.398584	4.255161
C	1.364604	7.406658	4.163892
C	0.655337	6.167000	4.157185
C	3.487629	8.618530	4.521728
C	2.796102	9.892212	4.372417
C	1.382796	9.881328	4.165729
C	0.656547	8.642246	4.166136
C	3.483332	11.178560	4.270663
C	2.780220	12.365129	3.896769
C	1.360661	12.351239	3.847507
C	0.658158	11.114092	3.998345
C	4.845210	11.331376	4.568007
C	5.625838	12.421168	4.171048
C	4.937710	13.613846	3.799901
C	3.505734	13.593646	3.740000
C	5.655846	14.831500	3.655149
C	4.861952	8.489192	4.933862
C	9.947188	17.281846	3.434061
C	0.651240	1.213602	4.322783
Al	5.675596	10.092804	5.710782
Al	7.691678	11.715974	6.513012
Al	7.661832	8.987739	6.876322
Al	5.034056	7.641392	7.034145
H	8.495740	13.030221	6.948246
H	8.726839	10.360034	7.035763

v_gp_al5

C	4.978659	8.636046	4.936776
C	5.785204	7.510210	4.521041
C	5.077567	6.303470	4.223437
C	3.640071	6.317622	4.176825
C	2.910635	7.556625	4.217500
C	3.602258	8.772652	4.515331
C	5.791134	5.076142	4.139930
C	7.219498	5.082391	4.161958
C	7.932647	6.329300	4.191843
C	7.237003	7.560759	4.408482
C	8.007354	8.807098	4.344285
C	9.384416	8.784679	3.964959
C	10.081779	7.546108	3.915132
C	9.363183	6.317917	4.050010
C	7.449867	10.067887	4.634222
C	8.003819	11.287294	4.181835
C	9.384461	11.274056	3.821288
C	10.086139	10.024504	3.795584
C	7.231796	12.530622	4.099672
C	7.929359	13.736349	3.792968
C	9.363244	13.737660	3.664026
C	10.081724	12.502941	3.648241
C	7.215738	14.979974	3.663327
C	7.931073	16.214227	3.575385
C	9.361362	16.212594	3.552358
C	10.075918	14.973371	3.576270
C	2.927001	5.083984	4.119956
C	3.641928	3.845729	4.141369
C	5.070692	3.845747	4.138753
C	1.497178	5.086175	4.136431
C	0.784266	3.849712	4.223637
C	1.496667	2.610873	4.259291
C	2.925683	2.611217	4.227557
C	1.491435	7.563003	4.129798
C	0.784731	6.324774	4.129365
C	2.922132	10.056379	4.398150
C	1.508344	10.044945	4.178895
C	0.784237	8.804473	4.149073
C	3.617908	11.345388	4.334168
C	2.912766	12.528153	3.953826
C	1.491594	12.515098	3.901595
C	0.785680	11.279481	4.035608
C	4.987949	11.490953	4.627267
C	5.769313	12.579660	4.177685
C	5.069888	13.769873	3.816415
C	3.636982	13.755189	3.787060
C	5.787538	14.987172	3.645529
C	10.075881	17.448675	3.469840
C	0.783225	1.376718	4.382743
Al	5.886024	10.209075	5.700249
Al	4.718456	8.221977	6.962231
Al	4.782668	8.381627	9.753373
Al	5.857518	10.181013	8.394996
Al	3.676158	6.473284	8.539622

v_gp_al5_H2

C	10.067580	17.443058	3.450770
C	9.353161	16.207215	3.538899
C	7.924097	16.208580	3.563559
C	7.207558	14.974532	3.653037
C	5.779059	14.980375	3.627746
C	5.063204	13.761443	3.790627
C	3.629472	13.746916	3.754443
C	2.904762	12.520842	3.915725
C	1.482629	12.509268	3.870427
C	0.776937	11.273759	4.007301
C	3.612543	11.337601	4.286408
C	2.912925	10.051080	4.354087
C	1.498837	10.039116	4.140612
C	4.982844	11.473990	4.582131
C	5.762604	12.571089	4.151277
C	7.225179	12.524187	4.090130
C	7.922784	13.731236	3.785199
C	9.355200	13.732000	3.651923
C	10.067291	14.967785	3.558066
C	10.070832	12.496126	3.624060
C	9.374110	11.267561	3.806152
C	7.997493	11.281528	4.182484
C	0.774717	8.798247	4.115992
C	3.591940	8.766082	4.464351
C	4.970614	8.635945	4.889843
C	2.897582	7.545495	4.174823
C	1.478940	7.553994	4.087924
C	0.772743	6.315933	4.092387
C	3.629576	6.307161	4.149766
C	2.915884	5.073232	4.090754
C	1.486388	5.077883	4.104120
C	0.774424	3.841667	4.199213
C	2.916582	2.601973	4.199278
C	3.631994	3.836809	4.113937
C	1.487038	2.603571	4.231151
C	0.772214	1.370170	4.357136
C	5.070441	6.295163	4.202595
C	5.782400	5.067247	4.123282
C	5.060257	3.837812	4.117404
C	5.780493	7.505546	4.485672
C	7.227782	7.555508	4.387878
C	7.923990	6.322402	4.175876
C	7.210954	5.075429	4.147452
C	7.439280	10.063186	4.638659
C	7.997335	8.805531	4.335073
C	9.373313	8.779878	3.947153
C	10.076997	10.017979	3.777216
C	10.070916	7.540502	3.896738
C	9.353998	6.311203	4.034052
Al	5.862871	10.201673	5.687255
Al	4.382844	8.114772	6.777471
Al	5.139057	10.106507	8.232622
Al	5.529808	8.541812	10.191647
Al	3.295330	8.103204	9.034043
H	6.255578	10.132288	9.541673
H	6.288674	8.492726	11.594321

v_gp_al6

C	10.031512	17.317288	3.581009
C	9.317302	16.083886	3.668680
C	10.031500	14.847596	3.697227
C	9.318722	13.611631	3.791823
C	10.038608	12.375534	3.772349
C	9.338382	11.145929	3.927600
C	10.039807	9.895437	3.890296
C	9.338481	8.654271	4.050041
C	10.038716	7.415538	4.014721
C	9.318815	6.186909	4.150970
C	7.888767	6.197750	4.294090
C	7.177194	4.951785	4.268950
C	5.750351	4.944304	4.252029
C	5.028466	3.714824	4.258454
C	3.602353	3.715983	4.269539
C	2.885742	2.481237	4.368247
C	0.742520	1.244391	4.495447
C	1.455529	2.481001	4.380298
C	0.742324	3.719542	4.334698
C	1.455407	4.956537	4.259247
C	0.742433	6.198672	4.253877
C	1.449760	7.436929	4.257964
C	0.741763	8.679511	4.276303
C	1.463593	9.917866	4.317467
C	0.741652	11.146861	4.160286
C	1.449754	12.382056	4.024996
C	2.870569	12.395225	4.115182
C	3.597423	13.628393	3.955817
C	5.034890	13.647928	3.990229
C	5.750405	14.860077	3.777131
C	7.177215	14.852912	3.793633
C	7.894221	16.085010	3.689590
C	7.955357	8.677948	4.416291
C	7.397406	9.934535	4.698787
C	7.955513	11.157526	4.295187
C	7.188149	12.410782	4.270573
C	5.744611	12.476601	4.398111
C	4.922892	11.430758	4.979918
C	3.563495	11.216431	4.542385
C	2.882173	9.929454	4.562139
C	3.563655	8.646098	4.663156
C	2.870692	7.432112	4.349666
C	2.885528	4.954484	4.247569
C	3.597162	6.188830	4.309264
C	5.034560	6.171373	4.346907
C	5.743993	7.376308	4.641446
C	7.188085	7.428203	4.511415
C	4.923040	8.474662	5.118114
C	7.888709	13.614757	3.936573
Al	5.909197	9.990843	5.869804
Al	4.685874	12.057196	6.974252
Al	7.138989	11.379052	8.215291
Al	7.143025	8.826191	8.332785
Al	4.692895	8.030164	7.162253
Al	4.722899	10.115666	8.600055

v_gp_al6_H2

C	7.891232	13.601729	3.918346
C	9.320540	13.599024	3.787560
C	10.034298	14.834642	3.696405
C	9.320073	16.072909	3.669490
C	7.896457	16.073924	3.681308
C	7.180821	14.839555	3.771905
C	7.187781	12.394997	4.253454
C	7.959127	11.142348	4.312210
C	9.341126	11.131673	3.939399
C	10.040824	12.360433	3.772370
C	7.405854	9.926148	4.744605
C	7.962422	8.665504	4.451135
C	9.342530	8.642000	4.073263
C	10.043897	9.882237	3.906197
C	7.193679	7.417446	4.530600
C	7.891151	6.188282	4.305296
C	9.323029	6.176261	4.164686
C	10.041930	7.403115	4.028647
C	5.738713	7.366167	4.637801
C	5.035273	6.161422	4.317322
C	5.752226	4.934003	4.231382
C	7.178503	4.941311	4.263527
C	3.600004	6.174728	4.272616
C	2.886864	4.939815	4.219335
C	3.604431	3.701878	4.245501
C	5.030637	3.702814	4.232031
C	1.458248	4.941728	4.247437
C	0.744897	3.706533	4.337018
C	1.457791	2.466571	4.380397
C	2.888798	2.466923	4.357420
C	2.872920	7.416004	4.330146
C	1.450675	7.422062	4.250250
C	0.742888	6.184512	4.247386
C	3.568027	8.627520	4.651851
C	2.885005	9.918463	4.558988
C	1.466282	9.905239	4.318100
C	0.744331	8.665891	4.275536
C	3.564270	11.200188	4.547655
C	2.873819	12.381237	4.119491
C	1.453756	12.368494	4.029575
C	0.744461	11.134636	4.166287
C	4.926257	11.432299	4.989001
C	5.748719	12.464127	4.368691
C	5.038069	13.635487	3.960697
C	3.599909	13.614910	3.947299
C	5.751982	14.847368	3.747571
C	4.928134	8.475556	5.080745
C	10.034353	17.305445	3.589279
C	0.746254	1.232369	4.500502
Al	5.887147	9.963030	5.889323
Al	4.685083	9.990079	8.429918
Al	4.612989	7.849201	7.133192
Al	6.937836	8.886439	8.472381
Al	7.026185	11.580107	8.309684
Al	4.977762	12.254228	6.890154
H	8.519083	8.596047	8.521855
H	4.150447	6.326622	7.218894

v_gp_al7

C	10.021284	17.317016	4.872518
C	9.309599	16.083025	4.867513
C	10.024048	14.849763	4.842145
C	9.312427	13.617276	4.836996
C	7.882905	16.086662	4.854255
C	7.171673	14.854067	4.830348
C	7.882335	13.611591	4.913884
C	5.749911	14.863481	4.765787
C	7.180322	12.398438	5.147858
C	5.723445	12.441148	5.161128
C	5.033679	13.640613	4.835434
C	3.608075	13.624387	4.765017
C	4.945518	11.334303	5.540934
C	3.583674	11.203562	5.232963
C	2.887020	12.394556	4.866480
C	1.469998	12.384517	4.799570
C	0.767667	11.149123	4.878605
C	1.488195	9.915366	5.000665
C	2.889777	9.919959	5.275043
C	0.767456	8.684509	4.898340
C	1.474554	7.451208	4.857734
C	0.770428	6.220484	4.752612
C	2.882555	7.441404	5.030608
C	3.562178	8.636993	5.414406
C	3.608629	6.211014	4.947499
C	2.902585	4.989606	4.761884
C	1.479118	4.988526	4.720754
C	0.765938	3.753593	4.715671
C	1.475949	2.519855	4.688578
C	0.762892	1.285716	4.741146
C	2.900792	2.523881	4.674853
C	3.614409	3.757655	4.703597
C	5.037558	3.762271	4.744264
C	5.750936	4.985821	4.876549
C	5.037497	6.201683	5.043774
C	7.172924	4.988220	4.927197
C	7.880134	6.226410	5.054823
C	9.308030	6.219723	4.921328
C	10.023512	7.447644	4.850916
C	10.029126	9.916166	4.843084
C	9.328695	11.158822	4.900940
C	10.028529	12.389092	4.791406
C	7.943974	11.159547	5.228837
C	5.729582	7.385433	5.439700
C	4.919891	8.485822	5.896432
C	7.181019	7.440681	5.336492
C	7.945767	8.684655	5.325079
C	7.376963	9.933446	5.645495
C	9.323766	8.677617	4.956234
Al	5.783135	10.073671	6.690347
Al	4.765423	10.624088	9.240617
Al	4.379009	8.208161	7.941200
Al	3.684796	8.492092	10.364603
Al	6.254739	9.294947	11.338653
Al	5.997913	7.102289	9.877564
Al	7.190593	9.589364	9.011520

v_gp_al7_H2

C	9.474162	8.771688	4.975263
C	10.171436	7.541892	4.866968
C	9.455529	6.313064	4.926262
C	8.027225	6.317415	5.042244
C	7.331092	7.530518	5.320032
C	8.099116	8.772642	5.350845
C	5.880602	7.480046	5.380072
C	5.186591	6.295318	4.992967
C	5.898548	5.074727	4.857176
C	7.319160	5.078117	4.921682
C	3.757235	6.309100	4.896248
C	3.049355	5.084102	4.735628
C	3.761443	3.850004	4.713174
C	5.184081	3.849176	4.763923
C	1.624871	5.083984	4.717320
C	0.912794	6.315455	4.768312
C	1.616935	7.546487	4.857413
C	3.029479	7.538670	4.991869
C	3.710276	8.730650	5.387275
C	3.028045	10.016581	5.325260
C	1.629325	10.011966	5.045821
C	0.910205	8.779035	4.922813
C	3.723218	11.301959	5.332897
C	3.031542	12.492128	4.963103
C	1.616674	12.481738	4.863380
C	0.912098	11.246562	4.925786
C	3.753906	13.719098	4.856867
C	5.179112	13.729183	4.937819
C	5.864308	12.530087	5.288461
C	5.079852	11.426197	5.674878
C	5.894639	14.949383	4.835165
C	7.316175	14.942125	4.897872
C	8.023422	13.697584	5.000735
C	7.324373	12.485227	5.255351
C	9.454559	13.708075	4.900684
C	10.166584	14.941738	4.883798
C	9.454235	16.176433	4.899453
C	8.028992	16.175495	4.883155
C	8.094342	11.244087	5.311266
C	9.473122	11.250912	4.956135
C	10.171419	12.480987	4.844166
C	5.072120	8.582845	5.823353
C	3.048272	2.616487	4.723686
C	1.624039	2.615428	4.720077
C	0.912637	3.849726	4.731097
C	7.538537	10.009882	5.713206
C	10.176122	10.011274	4.873055
C	10.167337	17.410725	4.893792
C	0.911188	1.382513	4.782116
Al	5.937976	10.097805	6.731015
Al	4.638790	8.061269	7.809044
Al	3.150770	7.331199	9.814662
Al	5.898880	7.715738	10.255144
Al	4.359139	9.421342	11.696429
Al	2.863088	9.883476	9.692787
Al	5.538414	10.108730	9.362848
H	4.610903	6.527009	10.462723
H	5.587847	8.190441	11.989607

v_gp_al8

C	5.617800	12.582528	5.060335
C	4.935869	13.775529	4.667406
C	5.656361	14.996609	4.565429
C	7.079816	14.987263	4.651857
C	7.789785	13.748062	4.796769
C	7.085227	12.533810	5.074907
C	9.220814	13.755586	4.719207
C	9.932173	14.992433	4.678237
C	9.221022	16.222467	4.655635
C	7.796226	16.222940	4.623788
C	7.853462	11.313740	5.200762
C	9.232924	11.296644	4.841765
C	9.937255	12.525292	4.699131
C	9.934126	17.456642	4.633983
C	3.508235	13.761134	4.557785
C	2.781228	12.530711	4.660733
C	1.365418	12.517768	4.544991
C	0.660182	11.280119	4.625297
C	1.378161	10.046610	4.776590
C	2.779532	10.048501	5.063294
C	3.470350	11.343337	5.056402
C	0.657028	8.810725	4.685898
C	1.364997	7.575234	4.664364
C	2.779435	7.569703	4.816981
C	3.453342	8.772225	5.183098
C	0.660322	6.337202	4.592183
C	1.371240	5.104799	4.571355
C	2.800200	5.103962	4.596477
C	3.507686	6.331962	4.740379
C	3.514634	3.867559	4.581036
C	4.943516	3.868042	4.638766
C	5.656839	5.096452	4.721022
C	4.937632	6.315834	4.826798
C	7.085238	5.101189	4.802399
C	7.794584	6.338558	4.913894
C	7.085204	7.565198	5.172165
C	5.627980	7.514551	5.212068
C	9.220521	6.333539	4.811385
C	9.938992	7.568426	4.737975
C	9.241242	8.800125	4.846162
C	7.857678	8.800049	5.227263
C	2.798137	2.632056	4.584331
C	1.371302	2.629813	4.570257
C	0.657821	3.867080	4.584562
C	4.815374	11.491893	5.429781
C	9.941196	10.046288	4.765899
C	7.321393	10.059682	5.695910
C	4.804624	8.606535	5.678604
C	0.658068	1.392566	4.616081
Al	5.561341	10.193460	6.561921
Al	5.707439	9.926034	9.261202
Al	8.247236	8.953107	10.168295
Al	6.171075	9.098901	11.696348
Al	5.290768	7.230659	10.151248
Al	7.493422	6.860517	8.790970
Al	7.755607	9.363505	7.644029
Al	5.186301	7.874675	7.628719

v_gp_al8_H2

C	9.241350	6.376548	4.745438
C	7.817591	6.383027	4.840570
C	7.107070	7.611432	5.079048
C	7.879908	8.844102	5.130902
C	9.261564	8.841214	4.758066
C	9.960360	7.608940	4.662300
C	7.343076	10.113012	5.591041
C	7.876428	11.362139	5.069541
C	9.257350	11.337674	4.719165
C	9.965041	10.089211	4.667391
C	7.104733	12.575391	4.909532
C	7.812367	13.787731	4.613869
C	9.240995	13.793604	4.544362
C	9.960779	12.564476	4.549712
C	5.640477	12.628390	4.881196
C	4.960360	13.814161	4.464314
C	5.681825	15.033528	4.345864
C	7.104534	15.022680	4.441825
C	3.535628	13.797494	4.339325
C	2.804044	12.571699	4.450609
C	3.489790	11.389375	4.867936
C	4.829046	11.543049	5.250984
C	1.391664	12.558143	4.324925
C	0.685811	11.319277	4.414466
C	1.403482	10.089809	4.588661
C	2.800527	10.095682	4.889001
C	0.683127	8.853236	4.512055
C	1.392079	7.617671	4.513349
C	2.804950	7.611755	4.673583
C	3.477730	8.820894	5.028384
C	3.534726	6.377506	4.622453
C	4.962044	6.361946	4.725519
C	5.648720	7.565919	5.097100
C	4.828416	8.669735	5.515910
C	0.686356	6.381102	4.457262
C	1.400861	5.146935	4.461530
C	2.826460	5.145125	4.493858
C	3.542928	3.909793	4.508249
C	4.968538	3.909446	4.579325
C	5.683371	5.140321	4.647797
C	7.106988	5.144294	4.740423
C	9.955771	15.028067	4.486010
C	9.243502	16.259495	4.437228
C	7.821093	16.258458	4.396045
C	2.826237	2.674498	4.527533
C	1.400635	2.673593	4.502362
C	0.685651	3.910330	4.495157
C	9.958434	17.491532	4.400061
C	0.684731	1.437702	4.561898
Al	5.562466	10.259520	6.399415
Al	5.637267	10.133692	9.111879
Al	8.195770	9.292501	10.032421
Al	5.816507	8.246449	10.808734
Al	5.184717	6.162866	9.351250
Al	7.542711	7.087206	8.747949
Al	7.818864	9.512648	7.521476
Al	5.152008	7.995171	7.523961
H	5.925428	8.362161	12.401456
H	4.331650	4.814595	9.455764

v_gp_all3

C	4.863771	13.731371	1.829818
C	5.608157	12.542460	2.080120
C	7.026913	12.479037	1.747271
C	7.670642	13.679126	1.338292
C	6.955947	14.925656	1.335679
C	5.548760	14.944095	1.543392
C	9.061402	13.670763	0.976977
C	9.760963	12.440021	0.828589
C	9.089181	11.213997	1.097411
C	7.788657	11.231784	1.685095
C	7.656889	16.153383	1.146602
C	9.058945	16.141313	0.896019
C	9.756651	14.903719	0.793576
C	4.913785	11.466616	2.687348
C	9.766068	9.964612	0.928389
C	9.089977	8.731598	1.201855
C	7.798857	8.763738	1.815346
C	7.043463	7.518501	2.004309
C	7.680168	6.289317	1.645482
C	9.063301	6.269651	1.263324
C	9.761475	7.491271	1.022658
C	5.648387	7.474297	2.383254
C	4.885296	6.286571	2.179270
C	5.556542	5.056781	1.935282
C	6.965211	5.049148	1.721398
C	3.461807	6.312001	2.364824
C	2.733641	5.088290	2.373333
C	3.427839	3.845613	2.247776
C	4.834290	3.833715	2.020756
C	2.766083	7.553947	2.551728
C	1.345611	7.570003	2.677126
C	0.633729	6.340485	2.750561
C	1.324488	5.099381	2.611991
C	3.520357	8.739920	2.804453
C	2.835417	10.044885	2.875656
C	1.375060	10.044564	2.801998
C	0.650744	8.809298	2.833794
C	0.651022	11.282164	2.742250
C	1.340124	12.512116	2.489952
C	2.753506	12.514915	2.320297
C	3.522284	11.345999	2.624880
C	2.724007	2.616557	2.433242
C	1.322099	2.627795	2.694953
C	0.623379	3.867667	2.791437
C	4.945220	8.581134	3.011866
C	7.293717	10.014785	2.204465
C	3.444369	13.730966	2.024611
C	0.628110	1.397047	2.931128
C	9.758095	17.372082	0.708261
AI	5.975862	10.164108	3.578939
AI	4.935103	8.085985	5.046884
AI	2.914021	8.091512	6.709031
AI	4.179355	9.109980	8.740386
AI	6.619280	10.586019	8.520942
AI	7.267817	10.270691	5.931510
AI	6.202967	8.156327	7.368799
AI	4.686218	10.325709	6.433542
AI	5.951579	12.665290	6.711690
AI	4.178744	11.811397	8.716769
AI	2.078198	10.494088	7.793456
AI	2.454965	10.238679	5.113647

Al	3.237218	12.595142	6.249642
v_gp_all3_H2			
C	3.288584	13.917422	4.760728
C	4.721509	13.931427	4.836316
C	5.407748	12.724930	5.176831
C	4.611346	11.621876	5.519578
C	3.255564	11.485597	5.183277
C	2.557307	12.684847	4.842185
C	6.878128	12.677723	5.187594
C	7.580116	13.902799	4.922417
C	6.868998	15.147729	4.815102
C	5.439749	15.158263	4.759412
C	9.012042	13.912443	4.826748
C	9.731395	12.681662	4.791589
C	9.032109	11.448973	4.942777
C	7.652869	11.459533	5.309183
C	9.723479	15.153510	4.795487
C	9.012637	16.386614	4.808107
C	7.584047	16.388242	4.798834
C	7.137429	10.196091	5.837442
C	7.649429	8.937879	5.330222
C	9.028601	8.946597	4.944655
C	9.738179	10.196670	4.872013
C	6.874686	7.709920	5.252003
C	7.580596	6.486221	4.961306
C	9.009506	6.480521	4.845408
C	9.727988	7.716757	4.799384
C	6.871695	5.245643	4.843348
C	5.441646	5.241868	4.798400
C	4.726855	6.463281	4.943788
C	5.423785	7.654115	5.328841
C	3.288284	6.473398	4.872561
C	2.556348	7.710519	4.942140
C	3.234961	8.909416	5.312751
C	4.587810	8.723990	5.837754
C	2.578483	5.245610	4.725460
C	3.294158	4.008014	4.684001
C	4.724985	4.010680	4.711953
C	1.139135	7.720967	4.790596
C	0.434667	6.481382	4.725426
C	1.147098	5.246822	4.705629
C	0.433336	4.006793	4.725082
C	1.147048	2.768211	4.683296
C	2.577455	2.770015	4.670668
C	2.564589	10.188537	5.193623
C	1.153838	10.192290	4.924967
C	0.430793	8.957770	4.827661
C	1.137601	12.675363	4.762202
C	0.433287	11.431954	4.817218
C	9.725489	17.625254	4.800160
C	0.428356	1.530295	4.711935
Al	5.360849	10.326890	6.657112
Al	4.149524	12.391142	9.665055
Al	2.822004	10.221540	8.955873
Al	3.754046	10.419657	11.562163
Al	6.071931	11.771619	11.558110
Al	6.701065	12.464824	8.949773
Al	5.468982	10.117972	9.378250
Al	6.786572	7.860877	8.952563
Al	7.772886	10.132419	7.846931
Al	8.086953	10.474544	10.427533
Al	6.223628	8.794796	11.613636

Al	3.837494	8.034425	10.422392
Al	4.332015	8.135153	7.846109
H	6.636824	8.078596	12.974740
H	7.010589	7.425399	10.562283