

Supporting Information

Exploring the Possibility of Chemisorption of Ethylene on Graphene with and without Defects

P. Alamdari¹, F. Sharif^{1*}, S. Mazinani²

¹ Department of Polymer Engineering and Color Technology, Amirkabir University of Technology, Tehran, Iran.

² New Technologies Research Center (NTRC), Amirkabir University of Technology, Tehran, Iran.

The final optimized geometries are as follows:

Pristine graphene (PG)

C	0.000000000	-0.000000000	10.000000000
C	-1.230593763	2.131463248	10.000000000
C	-2.461199458	4.262923757	10.000000000
C	-3.691796127	6.394389479	10.000000000
C	2.461198202	-0.000006491	10.000000000
C	1.230593196	2.131463248	10.000000000
C	-0.000000568	4.262923796	10.000000000
C	-1.230600264	6.394384338	10.000000000
C	4.922399998	-0.000001279	10.000000000
C	3.691804011	2.131464040	10.000000000
C	2.461198323	4.262923757	10.000000000
C	1.230598561	6.394384338	10.000000000
C	7.383601794	-0.000006491	10.000000000
C	6.152995416	2.131464040	10.000000000
C	4.922399430	4.262918157	10.000000000
C	3.691794424	6.394389479	10.000000000
C	-0.000001436	1.420979783	10.000000000
C	-1.230602241	3.552433915	10.000000000
C	-2.461204597	5.683899063	10.000000000
C	-3.691798187	7.815357361	10.000000000
C	2.461199201	1.420975376	10.000000000
C	1.230598875	3.552433915	10.000000000
C	-0.000001930	5.683898168	10.000000000
C	-1.230604286	7.815361526	10.000000000
C	4.922398635	1.420977874	10.000000000
C	3.691800798	3.552435197	10.000000000
C	2.461200662	5.683899063	10.000000000
C	1.230599857	7.815361526	10.000000000
C	7.383598069	1.420975376	10.000000000
C	6.152995905	3.552435197	10.000000000
C	4.922398067	5.683897515	10.000000000
C	3.691793685	7.815357361	10.000000000

Graphene with single vacancy (SVG)

C	4.927605621	8.447508951	10.215073295
C	8.596880932	2.047211355	10.275761276
C	7.382795249	4.195513577	10.207787684
C	-3.650145307	6.344547641	10.185610868
C	2.479916229	-0.040487576	10.112878178
C	1.229882277	2.076606954	10.370555355
C	0.015662728	4.178785134	10.366810175
C	-1.192577865	6.320138007	10.109750741
C	4.932494950	-0.068088920	9.993505692
C	3.628689612	2.180746123	9.999456355
C	1.305609020	6.204149469	9.999814104
C	2.464753848	8.431011009	10.078862223
C	6.137216413	2.070714753	10.075068304
C	4.903412257	4.230641265	10.142633593
C	3.718154957	6.282408326	10.147262857
C	-0.011791055	1.345647417	10.292125464
C	-1.237602021	3.468501959	10.286781371
C	-2.428081462	5.617261805	10.182632027
C	-3.668774635	7.766540528	10.187576532
C	2.457845633	1.384279903	10.153503674
C	1.185407625	3.453201804	10.638595629
C	0.030111981	5.588455516	10.150475094
C	-1.214442229	7.751025573	10.030792588
C	4.890068384	1.397886069	9.996653368
C	3.614385793	3.657884936	9.988293509
C	2.577446170	5.452333599	9.991622043
C	1.258453590	7.687833542	9.997942431
C	7.367463642	1.337297952	10.135986623
C	6.137383350	3.489979263	10.152722756
C	4.979979683	5.643033938	10.182421092
C	3.693828628	7.721439828	10.159159609

Graphene with double vacancy (DVG)

C	0.013407974	-0.007741097	10.000000000
C	-1.142435424	2.143048206	10.000000000
C	-2.476830259	4.249423544	10.000000000
C	-3.808859324	6.306011732	10.000000000
C	2.479203978	0.145562084	10.000000000
C	1.367770491	2.391716853	10.000000000
C	-0.021310396	4.347436113	10.000000000
C	-1.334429510	6.454330181	10.000000000
C	4.926276126	0.020285498	10.000000000
C	3.937426607	2.375040364	10.000000000
C	1.146753833	6.370583032	10.000000000
C	7.417648095	-0.082146331	10.000000000
C	6.288977265	2.052954883	10.000000000
C	4.834267444	3.928414586	10.000000000
C	3.534996839	6.145463654	10.000000000
C	0.117057254	1.509348072	10.000000000
C	-1.214971763	3.565936297	10.000000000
C	-2.549366614	5.672311593	10.000000000
C	-3.705209819	7.823100570	10.000000000
C	2.618000784	1.669896169	10.000000000
C	1.318730164	3.886945196	10.000000000
C	-0.135979652	5.762404942	10.000000000
C	-1.264650251	7.897505807	10.000000000
C	5.006243790	1.444776815	10.000000000
C	2.215571039	5.440319488	10.000000000
C	1.226721690	7.795073944	10.000000000
C	7.487427136	1.361029636	10.000000000
C	6.174307995	3.467923692	10.000000000
C	4.785227129	5.423642965	10.000000000
C	3.673793847	7.669797417	10.000000000

Graphene with three vacancy (TVG 4×4×1)

C	0.020186782	0.029962417	10.000000000
C	-1.266463006	2.081261424	10.000000000
C	-2.461200566	4.233160409	10.000000000
C	-3.711122143	6.345295506	10.000000000
C	2.461199999	0.151939572	10.000000000
C	1.092877469	2.443522527	10.000000000
C	0.085419830	4.032151253	10.000000000
C	-1.211279558	6.345295506	10.000000000
C	4.902213216	0.029962417	10.000000000
C	3.829521961	2.443522527	10.000000000
C	1.233484834	6.334145948	10.000000000
C	7.383599997	-0.066819661	10.000000000
C	6.188862436	2.081261424	10.000000000
C	4.836979032	4.032151253	10.000000000
C	3.688913461	6.334145948	10.000000000
C	0.018056807	1.481422590	10.000000000
C	-1.229420943	3.496187885	10.000000000
C	-2.461202003	5.655831066	10.000000000
C	-3.673936340	7.849430352	10.000000000
C	2.461198636	1.819081449	10.000000000
C	0.039952144	5.529098730	10.000000000
C	-1.248468160	7.849430352	10.000000000
C	4.904340392	1.481422590	10.000000000
C	2.461198068	5.702251204	10.000000000
C	1.209230938	7.789757498	10.000000000
C	7.383598634	1.358042998	10.000000000
C	6.151817575	3.496187885	10.000000000
C	4.882443993	5.529098730	10.000000000
C	3.713164631	7.789757498	10.000000000

Graphene with three vacancy-bridge (TVGB 4×4×1)

C	0.074270658	-0.112041859	10.000643431
C	-0.914815431	2.074433105	9.999763801
C	-2.166135989	4.244280398	9.998792067
C	-3.573183931	6.269482779	10.000340118
C	2.434604895	-0.048926937	10.000423227
C	0.627699692	3.919810108	9.998766694
C	-0.886816758	6.502222553	10.000320881
C	4.893579701	0.193467118	10.000344746
C	3.405779408	2.174921009	9.999271765
C	2.038327839	4.314623213	9.999209432
C	0.911446916	6.567923751	10.000513573
C	7.415673697	0.048383865	10.000468034
C	6.212974486	2.207012187	9.999328472
C	4.836706644	4.237764677	9.998954755
C	3.570371938	6.369156149	10.000536317
C	0.344133559	1.271308054	10.000031533
C	-0.782848508	3.524630576	9.998972562
C	-2.150362165	5.664175424	9.999836129
C	-3.638000180	7.645722982	10.000725628
C	2.142295281	1.336924312	9.999808474
C	-1.178983536	7.888128537	10.000470355
C	4.828654108	1.569724838	9.999659652
C	3.421534718	3.594821172	9.998729875
C	2.170398151	5.764842964	10.000369069
C	1.181292080	7.951261410	10.000576472
C	7.530019085	1.469957259	9.999874755
C	6.263494795	3.601299329	9.998776396
C	4.887376616	5.632128398	9.999992504
C	3.684702231	7.790682629	10.000709284

Graphene with three vacancy (TVG 6×6×1)

C	-0.014566166	0.008409780	10.000000000
C	-1.257631848	2.127857028	10.000000000
C	-2.486174393	4.268874591	10.000000000
C	-3.671075611	6.393056302	10.000000000
C	-4.929366179	8.512940449	10.000000000
C	-6.154499258	10.643207253	10.000000000
C	2.454661575	0.008349441	10.000000000
C	1.210304937	2.153893005	10.000000000
C	-0.055469300	4.222852090	10.000000000
C	-1.135373301	6.354237710	10.000000000
C	-2.368539806	8.484453872	10.000000000
C	-3.661862901	10.629631943	10.000000000
C	4.912093897	0.012486000	10.000000000
C	3.614327352	2.229107190	10.000000000
C	2.276506268	4.510532065	10.000000000
C	1.513678024	6.021102889	10.000000000
C	0.262727746	8.363768357	10.000000000
C	-1.157422037	10.582169851	10.000000000
C	7.377111950	-0.017283408	10.000000000
C	6.105425243	2.150897337	10.000000000
C	4.835035463	4.325110953	10.000000000
C	2.917009939	8.451746486	10.000000000
C	1.303981773	10.579324526	10.000000000
C	9.809158733	0.018652831	10.000000000
C	8.562019054	2.152337316	10.000000000
C	7.311514361	4.294149619	10.000000000
C	6.046462087	6.423361882	10.000000000
C	4.606617619	8.546403202	10.000000000
C	3.689768717	10.709792978	10.000000000
C	12.277604223	0.025212587	10.000000000
C	11.026740272	2.149162031	10.000000000
C	9.791628832	4.282086759	10.000000000
C	8.564579938	6.410278688	10.000000000
C	7.251298677	8.528528621	10.000000000
C	6.114425579	10.648079903	10.000000000
C	-0.020910435	1.430712473	10.000000000
C	-1.268816504	3.543459930	10.000000000
C	-2.421622400	5.682759795	10.000000000
C	-3.654621396	7.808489399	10.000000000
C	-4.911457897	9.934515078	10.000000000
C	-6.151898734	12.067254416	10.000000000
C	2.435267832	1.444756947	10.000000000
C	1.191115106	3.576592206	10.000000000
C	0.100887020	5.624232920	10.000000000
C	-1.073854959	7.763750995	10.000000000
C	-2.406157018	9.904649308	10.000000000

C	-3.684671258	12.059370336	10.000000000
C	4.864788691	1.464589677	10.000000000
C	3.539031436	3.715175767	10.000000000
C	1.684134985	7.543118074	10.000000000
C	0.114066060	9.821291151	10.000000000
C	-1.215061038	12.033930952	10.000000000
C	7.342279692	1.420415395	10.000000000
C	6.081815722	3.578999666	10.000000000
C	4.876419998	5.700051343	10.000000000
C	2.554313952	9.873693732	10.000000000
C	1.242374195	12.028987241	10.000000000
C	9.796078036	1.441165598	10.000000000
C	8.553260523	3.577226944	10.000000000
C	7.316002900	5.716674098	10.000000000
C	5.926678795	7.850701954	10.000000000
C	4.872737275	9.953349105	10.000000000
C	3.671465520	12.100278318	10.000000000
C	12.263852786	1.434915421	10.000000000
C	11.024552122	3.568946314	10.000000000
C	9.815623391	5.704372235	10.000000000
C	8.538622317	7.827855358	10.000000000
C	7.341036820	9.941798689	10.000000000
C	6.125111184	12.075933562	10.000000000

Graphene with three vacancy-bridge (TVGB $6\times 6\times 1$)

C	0.007708780	0.077511227	7.496255601
C	-1.309167126	2.154474725	7.487665252
C	-2.631858543	4.176072212	7.489460343
C	-3.679496432	6.345494460	7.499447263
C	-4.809573656	8.530928051	7.503058639
C	-6.060929052	10.725699115	7.501396067
C	2.463354238	0.142660631	7.498372508
C	1.109330752	2.354890844	7.492937651
C	-0.332216243	4.539732663	7.492254330
C	-1.128239509	5.985312935	7.501662813
C	-2.302098005	8.351165162	7.503953005
C	-3.598695189	10.648401226	7.499998993
C	4.912755843	0.064246725	7.498133801
C	3.583583016	2.377497958	7.506722472
C	2.194756219	4.657887105	7.512252344
C	0.189713621	8.210681265	7.520097610
C	-1.138674887	10.531109911	7.504473813
C	7.359162379	-0.041053529	7.495632429
C	6.044527482	2.252198794	7.494644902
C	4.738646149	4.599624467	7.498350957
C	2.714488659	8.225120551	7.482637741
C	1.309399640	10.462236719	7.496782223
C	9.801295679	-0.081101232	7.494716941
C	8.518601929	2.113153794	7.495219415
C	7.282127652	4.321785873	7.491141894
C	6.179461417	6.505502838	7.485178247
C	5.060018237	8.510196883	7.475451606
C	3.735653686	10.563992904	7.485320174
C	12.270752347	-0.019679966	7.494276510
C	10.965064310	2.066587139	7.496027724
C	9.726659202	4.239905963	7.497659255
C	8.620376315	6.417910388	7.496680081
C	7.510032485	8.594422954	7.496894516
C	6.211606626	10.677414610	7.494476002
C	-0.048154808	1.517352280	7.491452825
C	-1.373981561	3.569849988	7.484689883
C	-2.493078932	5.575335902	7.495731103
C	-3.595709962	7.759434295	7.501914139
C	-4.830838742	9.968562139	7.501819682
C	-6.112769443	12.162540019	7.498247018
C	2.377120254	1.620070675	7.500081676
C	0.971039657	3.856480224	7.491547707
C	-1.052813371	7.481685901	7.510279077
C	-2.357927426	9.829998975	7.502820155
C	-3.671234428	12.123512556	7.498933285
C	4.825210790	1.551707889	7.499674748

C	3.495508855	3.871779471	7.514588491
C	1.841458543	6.040963717	7.526943476
C	1.490322173	7.424119928	7.511163893
C	0.102359653	9.705253002	7.509473890
C	-1.224969304	12.018565613	7.498508257
C	7.286110364	1.434024170	7.493772047
C	5.988145432	3.730654001	7.492289839
C	4.017619293	7.540800777	7.479076945
C	2.577110478	9.727439571	7.485417542
C	1.224545165	11.939560935	7.494856011
C	9.748850839	1.355706778	7.496899608
C	8.496423794	3.550562397	7.495088948
C	7.365989597	5.735515463	7.490898146
C	6.318233253	7.904377258	7.483277907
C	4.996281104	9.925791145	7.483017343
C	3.680917541	12.003803490	7.492763260
C	12.225103964	1.403132733	7.492833331
C	10.926014181	3.486597226	7.495585141
C	9.815321164	5.662942368	7.498115393
C	8.709326642	7.841035781	7.500972376
C	7.471661366	10.014344740	7.500015400
C	6.166967100	12.100482308	7.496053348
C	4.814478751	6.095230921	7.488024987

Ethylene physisorption on PG

C	0.002960220	-0.007010253	9.809321125
C	-1.227859682	2.124409194	9.801765261
C	-2.458054177	4.255990431	9.808446781
C	-3.688604731	6.387474727	9.811871362
C	2.464343031	-0.006934402	9.815088566
C	1.233516392	2.124830656	9.783694630
C	0.003621461	4.255411797	9.779556812
C	-1.227211253	6.387140725	9.810072731
C	4.925520386	-0.007216811	9.819366403
C	3.694543641	2.124882655	9.799974329
C	2.463819813	4.255316801	9.758916844
C	1.234079838	6.386561591	9.793106902
C	7.386593875	-0.007267309	9.810567115
C	6.155827581	2.124586081	9.813708233
C	4.925007094	4.256035658	9.797892029
C	3.694576757	6.386872389	9.794431089
C	0.002989026	1.414089616	9.798988006
C	-1.227323843	3.545496752	9.796508312
C	-2.457998862	5.676987686	9.811114118
C	-3.688704927	7.808447299	9.813110815
C	2.464040005	1.414208308	9.800357295
C	1.234240776	3.545433769	9.762204368
C	0.003451706	5.676359528	9.794091422
C	-1.227356914	7.808272500	9.818373960
C	4.925182032	1.413954645	9.815885281
C	3.694009737	3.545649877	9.781125255
C	2.464130527	5.675765403	9.775929995
C	1.233677826	7.807842269	9.810221857
C	7.386384145	1.413869985	9.813219433
C	6.155693068	3.545550432	9.809359866
C	4.925368051	5.676982572	9.800451212
C	3.694594979	7.807973830	9.806767559
C	1.369344938	3.809784659	13.117609098
C	2.561132374	4.432189670	13.132285313
H	1.287281022	2.712726053	13.093765254
H	0.428620213	4.380002230	13.122188026
H	3.508834602	3.873927745	13.120229866
H	2.632829272	5.529511240	13.150353477

Ethylene chemisorption on SVG

C	-4.909059008	8.445076467	9.792694843
C	-1.221876868	2.045184073	9.763209938
C	-2.446564745	4.190429497	9.691555361
C	6.170390867	6.321645344	9.803244538
C	2.475616900	-0.055597215	9.935107063
C	1.224950839	2.070464386	10.153654758
C	-0.027977157	4.178281410	10.049997983
C	-1.217203156	6.319134107	9.833481940
C	0.014983273	8.444801268	9.819935237
C	3.719525181	2.076630439	10.151875688
C	1.261786226	6.262351763	9.821548562
C	2.474486375	8.423730016	9.706623288
C	6.169310332	2.045518818	9.762440982
C	4.976434612	4.183654650	10.007644522
C	3.691060913	6.266173424	9.782816289
C	0.018007076	1.352316092	9.854074577
C	-1.222901779	3.468982516	9.770240998
C	-2.446227135	5.607676635	9.785635417
C	-3.674333055	7.750517298	9.837529199
C	2.474281057	1.365490984	10.156445362
C	1.122438315	3.471344706	10.519735977
C	-0.004076225	5.595097454	9.920337574
C	-1.218744741	7.748570120	9.859681336
C	4.928940015	1.354032563	9.864240415
C	3.821659928	3.489766637	10.490201018
C	2.476950662	5.545730679	9.729283534
C	1.247291174	7.712630619	9.759311652
C	7.395853561	1.330435649	9.707064327
C	6.172828142	3.469615578	9.752450729
C	4.956320543	5.598266300	9.868956341
C	3.703495361	7.714630098	9.733795041
C	1.717885243	3.892327822	11.854761653
C	3.256226720	3.942654059	11.828283828
H	1.359515469	3.154460877	12.605552033
H	1.304011348	4.876767391	12.142708660
H	3.690024763	3.273755256	12.603999841
H	3.611398974	4.967352219	12.045609496

Ethylene chemisorption on DVG-H

C	-4.902230423	8.626416434	9.636061782
C	-1.161142540	2.238726982	9.850981137
C	7.406231087	4.364824865	9.855581250
C	6.103693884	6.447272187	9.688986804
C	2.485572135	0.178604109	9.682041711
C	1.333584079	2.356685522	9.704054926
C	0.019411082	4.427703982	10.065691643
C	-1.273961896	6.540294122	9.876455201
C	4.940925521	0.138003603	9.932037633
C	3.806021406	2.450445954	10.137702633
C	1.205086732	6.485634675	9.818153218
C	2.501168263	8.587004624	9.803212805
C	6.240933099	2.188587474	9.940181610
C	4.909357629	4.179176527	9.664421319
C	3.613743046	6.352128870	9.658754064
C	0.079498888	1.568089704	9.697155811
C	-1.182747201	3.674178041	9.951868893
C	-2.491468621	5.785469652	9.807414240
C	-3.678690088	7.919122498	9.631546888
C	2.541041785	1.659948364	9.693311448
C	1.389748191	3.843430560	10.157995881
C	-0.056907187	5.824290939	9.963064832
C	-1.235851882	7.965250536	9.837951099
C	4.993825290	1.555701233	10.035385008
C	2.332671143	5.666938539	9.672092415
C	1.244471081	7.921163210	9.848901821
C	7.468790520	1.492888226	9.868998280
C	6.182906541	3.612825525	9.808803828
C	4.860999279	5.631064642	9.656336102
C	3.699855066	7.836193787	9.691026844
C	3.411679396	2.964496437	11.564114977
C	2.057919812	3.752981901	11.573389062
H	4.231309134	3.580124833	11.978941277
H	3.310671513	2.065971371	12.209193583
H	2.198586497	4.766543092	11.991332784
H	1.337337738	3.218476981	12.226877191

Ethylene chemisorption on DVG-P

C	-4.996429641	8.571167123	9.620082373
C	-1.295799455	2.190041725	9.701055750
C	7.276541427	4.311916408	9.839234397
C	6.021080333	6.399995532	9.849967448
C	2.394571509	0.115975940	9.841302344
C	1.131456372	2.213321171	10.009389186
C	-0.134584739	4.298973504	10.304275484
C	-1.329910950	6.454917602	10.047728690
C	4.829829393	0.072806116	9.821335375
C	3.719313999	2.341169306	9.837348282
C	1.132710803	6.498912160	10.289081928
C	2.381599572	8.557765230	9.691569770
C	6.115076046	2.157235593	9.674754152
C	4.756339386	4.138603171	9.850721322
C	3.572102187	6.442389050	10.010541978
C	-0.065271310	1.486210208	9.679519723
C	-1.323383441	3.607262243	9.887490616
C	-2.573434164	5.728259883	9.922740137
C	-3.781238068	7.870595719	9.785915943
C	2.444148118	1.603657701	9.893639359
C	0.999229137	3.488144696	10.611296058
C	-0.118999973	5.756055545	10.326601573
C	-1.320825661	7.894582749	9.911616808
C	4.853053975	1.509228614	9.741350971
C	2.398126026	5.922832951	10.607439019
C	1.139388123	7.872713167	9.868729230
C	7.321720941	1.460321040	9.633666157
C	6.044744390	3.573418808	9.754839257
C	4.757241877	5.611732317	9.905289550
C	3.605446363	7.842367557	9.677496510
C	1.855006121	3.735722503	11.828647719
C	2.584971843	5.075773962	11.842979773
H	2.574506018	2.905624783	11.937947839
H	1.151755878	3.662544922	12.688827527
H	3.664625556	4.922105924	12.021181316
H	2.210592015	5.710735072	12.675886433

Hydrogenated graphene as final product of the interaction of ethylene with DVG-H

C	-0.017057255	-0.027900074	9.617523260
C	-1.237746105	2.107301519	9.689232965
C	-2.470065729	4.228546405	9.828402257
C	-3.717414666	6.365604025	9.728969323
C	2.449513357	-0.013258989	9.654815410
C	1.216346437	2.127858734	9.834272855
C	0.000916582	4.231769694	9.877857460
C	-1.248235981	6.371116012	9.745766644
C	4.899868223	-0.014148558	9.731176377
C	3.679141642	2.093340644	10.044821366
C	1.187000391	6.394778842	10.030427504
C	7.372329943	-0.024353708	9.779184799
C	6.149981845	2.118461471	9.909461095
C	4.992217532	4.286009688	10.562950016
C	3.693698622	6.355637582	9.950836903
C	-0.005642359	1.404225719	9.654815427
C	-1.231589543	3.525850559	9.731176415
C	-2.476657109	5.661961086	9.779184855
C	-3.707435220	7.786637539	9.617523303
C	2.465205701	1.406830370	9.834272965
C	1.203912949	3.522415545	10.044821461
C	-0.009750988	5.674785031	9.909461146
C	-1.247950459	7.797090873	9.689233038
C	4.894961061	1.406192076	9.877857335
C	2.446282629	5.755905801	10.562950041
C	1.205259683	7.790493791	9.828402305
C	7.372263496	1.394067783	9.745766703
C	6.175138901	3.514875586	10.030427506
C	4.887892394	5.666168932	9.950837049
C	3.679679064	7.778786674	9.728969483
C	2.349472915	4.211361065	10.771505945
C	3.703007679	3.429897625	10.771505988
H	3.814151661	3.068535654	11.817997545
H	1.980952290	4.126933805	11.817997578
H	5.326191514	4.535959940	11.604797821
H	2.495759098	6.170110879	11.604797858

Hydrogenated Stone wale as final product of the interaction of ethylene with DVG-P

C	-4.931010333	8.520028194	9.146631814
C	-1.280043639	2.127062093	9.598538689
C	7.367045775	4.246575863	9.983597645
C	6.224401890	6.393364481	9.472145446
C	2.487825272	-0.077652232	9.475529659
C	1.178819382	2.019151387	9.634516397
C	0.094409974	4.166501446	10.124637452
C	-1.141095967	6.331598950	9.922462340
C	4.918586592	0.005995765	9.984616376
C	3.404742608	1.927693599	10.616864987
C	1.351709270	6.344392747	10.122035143
C	2.430548573	8.554431952	9.596488627
C	6.047423954	2.181263383	10.029914543
C	4.945661241	4.597343656	10.612613420
C	3.753356277	6.478318966	9.628546009
C	-0.058356580	1.403046008	9.325740572
C	-1.205159386	3.522431127	9.894584327
C	-2.403843651	5.669583910	9.815424120
C	-3.665234289	7.789204462	9.192362315
C	2.382353784	1.274859224	9.753572318
C	1.280066334	3.313377692	10.177184483
C	0.102801111	5.613575846	10.174041930
C	-1.199264290	7.756152415	9.817056251
C	4.837791368	1.438567500	10.159308222
C	2.683300814	5.743584704	10.172045924
C	1.259567070	7.791875858	9.892712038
C	7.297432980	1.459644646	9.683339267
C	6.085879710	3.600251523	10.157649346
C	4.999658692	5.807951945	9.747697184
C	3.668271602	7.858383677	9.322421916
C	2.623653261	3.291194181	10.967906045
C	3.374964397	4.592976530	10.964753849
H	3.331689535	1.356290751	11.580081656
H	3.365334581	4.983465072	12.008324510
H	5.404280458	4.948937754	11.574754697
H	2.283948152	3.107354825	12.013039282

Ethylene chemisorption on TVG-1

C	0.047764715	0.154645863	9.835110167
C	8.586434010	2.220461050	9.871888125
C	7.421647377	4.367429280	9.995107347
C	6.201859032	6.520596966	9.908946283
C	2.491998600	0.228504871	9.836670657
C	1.118480136	2.469358375	9.802114929
C	0.108591895	4.176798418	9.902283130
C	-1.144758084	6.455735382	9.925952843
C	4.951877316	0.119075390	9.884256966
C	3.760136603	2.375559448	9.752316445
C	1.323347181	6.453848363	10.192479274
C	2.485553878	8.617634731	9.956441463
C	6.176600431	2.253747508	10.007794304
C	4.937707947	4.351794286	10.421717157
C	3.762770867	6.548598229	10.219037718
C	0.020898223	1.594576606	9.810566926
C	-1.197994778	3.629900047	9.888985716
C	-2.392686325	5.791053640	9.936100636
C	-3.640199125	7.983055765	9.840056569
C	2.453180269	1.779651834	9.807014571
C	0.124441218	5.645581095	10.022728592
C	-1.193504809	7.951507727	9.876514240
C	4.917172633	1.576653698	9.868134603
C	2.565032882	5.865990374	10.560817801
C	1.270662347	7.892418171	9.990464938
C	7.387962605	1.520312567	9.932776471
C	6.188863958	3.652779566	10.158121251
C	4.984047458	5.807275204	10.105101857
C	3.741328454	7.953561156	9.956880050
C	4.140789977	4.208949610	11.725339907
C	2.686486953	4.649860532	11.463430471
H	4.619610367	4.875346506	12.480178821
H	4.165700233	3.173902219	12.114674964
H	2.197986588	4.932540831	12.422538205
H	2.123768968	3.790584692	11.081036602

Ethylene chemisorption on TVG-2

C	0.001226303	-0.094139212	9.940984490
C	8.616294155	2.025393314	10.122890392
C	7.375040640	4.154607915	9.838773711
C	6.142213003	6.280205566	9.697006774
C	2.454831968	-0.115766249	9.820467652
C	1.266626152	1.950669814	10.581459568
C	-0.013677740	4.148013574	9.644446200
C	-1.236887813	6.280561418	9.683078774
C	4.907951529	-0.095304808	9.933886955
C	3.648733206	1.948890869	10.587110643
C	1.233895732	6.276988670	9.647883436
C	2.454098240	8.412806398	9.964220607
C	6.138843623	2.023080814	10.127675001
C	4.916090308	4.146320608	9.686396969
C	3.672842431	6.276292527	9.667268301
C	0.014243580	1.319089140	10.241660507
C	-1.206744555	3.442509713	9.906516614
C	-2.470260540	5.566994039	9.697428103
C	-3.701708282	7.706912966	9.783011192
C	2.456081381	1.256544741	10.212657062
C	-0.002137482	5.555118737	9.636212672
C	-1.234833547	7.705934860	9.775842877
C	4.898122807	1.315299380	10.243725652
C	2.453778848	5.579617206	9.574526193
C	1.226200568	7.713081764	9.832842023
C	7.377735542	1.317999344	10.091245518
C	6.113885461	3.441472540	9.922499524
C	4.907285263	5.553203236	9.667658478
C	3.682278297	7.713358050	9.842933256
H	3.590417109	2.467357231	12.663513222
H	1.234475460	2.638263627	12.625309409
C	3.242573156	2.920637397	11.708240894
C	1.674308711	2.971732373	11.660343403
H	3.672807017	3.931391020	11.641172068
H	1.335109466	4.000911416	11.471831859

Ethylene chemisorption on TVG-3

C	0.168174136	-0.080623967	9.846140222
C	8.703694964	1.988615072	9.875148254
C	7.589749506	4.161135058	9.916600753
C	6.371712268	6.308177116	9.880509192
C	2.606431322	-0.039108298	9.736243647
C	1.253837431	2.190224103	9.762376396
C	0.257504270	3.946083086	9.774872759
C	-0.982815885	6.245070534	9.770158776
C	5.081974102	-0.088078996	10.021475486
C	3.735642698	2.004111771	10.448063187
C	1.461336016	6.241460181	9.929632917
C	2.613045118	8.401334582	10.047512425
C	6.284944800	2.045932646	10.308182669
C	5.344702880	4.319369178	10.822862304
C	3.911689129	6.305041862	10.175091694
C	0.120173359	1.346052966	9.773938391
C	-1.040415937	3.405018462	9.816060372
C	-2.235968423	5.579676314	9.826949805
C	-3.519224480	7.739752791	9.740120406
C	2.515777220	1.437280998	9.875414071
C	0.274147987	5.432534211	9.796888023
C	-1.047931542	7.722116299	9.828692913
C	5.046489550	1.341929309	10.273956835
C	2.712112728	5.598447569	10.031415624
C	1.391423163	7.683078819	10.022645370
C	7.500951141	1.306461792	10.063768341
C	6.389124086	3.492221745	10.330054557
C	5.191635452	5.630089470	10.287256884
C	3.872755440	7.728511820	10.022446211
H	2.738861838	4.508864910	9.920602413
H	4.158961675	4.627017461	12.618800057
C	3.482971689	3.029992352	11.334576556
C	4.558202467	3.801348546	12.003267199
H	2.431323420	3.321058589	11.482957840
H	5.220316417	3.157721651	12.621637451

Ethylene chemisorption on TVGB-1

C	0.072618682	-0.115589020	9.984297447
C	-1.172423132	2.038127868	9.882427732
C	-2.196865183	4.211051180	9.770312018
C	-3.567857472	6.280921998	9.853379430
C	2.550210906	-0.098084527	10.201304075
C	0.752215427	3.314770784	9.845289397
C	-0.864852640	6.405343563	9.781281841
C	4.979885076	0.062079549	9.855907552
C	3.709401203	2.083219354	10.191231674
C	2.075541366	4.057130499	9.866254385
C	0.905302635	6.379752235	9.744178832
C	7.401953056	-0.076579500	9.782679561
C	6.227094814	2.129113732	9.781047435
C	4.904783502	4.181270078	9.817537457
C	3.581033786	6.268787509	9.783652059
C	0.038754821	1.361759248	10.330224449
C	-0.894500101	3.404471285	9.772353324
C	-2.180405795	5.632285622	9.793545669
C	-3.623125457	7.698840372	10.065938146
C	2.633256647	1.243599914	10.669161737
C	-1.121149693	7.790608744	9.882444579
C	4.972153443	1.450421492	9.908315467
C	3.548700625	3.470028222	9.962945878
C	2.136195574	5.561615012	9.766940257
C	1.216835013	7.789769252	9.758715500
C	7.427373304	1.360848405	9.780620036
C	6.274982155	3.545182426	9.801635808
C	4.923241236	5.596236345	9.791712601
C	3.708230945	7.708137973	9.813495740
H	2.158281401	2.758968502	12.115018572
H	-0.142244383	2.453994578	12.216130182
C	1.894620228	1.704517703	11.912884076
C	0.366649525	1.552325945	11.824024515
H	2.305330993	1.095691523	12.748668767
H	0.003997491	0.676092136	12.399833804

Ethylene chemisorption on TVGB-2

C	0.109781848	-0.219374584	9.663107337
C	-0.861477376	1.986952101	9.748571574
C	-2.202995195	4.117693952	10.140247185
C	-3.567300355	6.155256458	9.895266203
C	2.457914183	-0.157037979	9.711873894
C	0.398130811	3.966289002	10.617804589
C	-0.905054332	6.377991824	9.814799907
C	4.941193760	0.055094086	9.618740665
C	3.458984297	2.066432441	9.856470580
C	2.171545967	4.220376618	10.489940128
C	0.999635838	6.425873498	9.757650828
C	7.456446706	-0.066639503	9.609165157
C	6.250839553	2.076832986	9.829828925
C	4.891338384	4.104477974	10.107452619
C	3.613697635	6.251328704	9.849285490
C	0.406250264	1.182891420	9.695835109
C	-0.844274482	3.397270944	10.117949026
C	-2.166548146	5.529676606	9.975717923
C	-3.618609350	7.531633753	9.726085327
C	2.148990399	1.225722547	9.754941384
C	-1.154622524	7.754561225	9.696285585
C	4.879960833	1.435762557	9.733550191
C	3.519193373	3.442040169	10.109073433
C	2.219099257	5.642875768	9.932555022
C	1.232497364	7.828683476	9.606707279
C	7.575434066	1.361005262	9.687381905
C	6.269446193	3.465697254	10.069424853
C	4.920300821	5.513323216	9.994294285
C	3.728938692	7.670734155	9.671368253
H	2.677901404	5.183192891	12.475578299
H	0.285368549	5.751114698	11.961231388
C	2.037070007	4.386946156	12.050584656
C	0.515406726	4.664274762	11.972078256
H	2.255710364	3.419606073	12.540631134
H	-0.115215533	4.190669491	12.749661609