Electronic Supplementary Information

for

Π-Bond Maximization of Graphene in Hydrogen Addition Reactions

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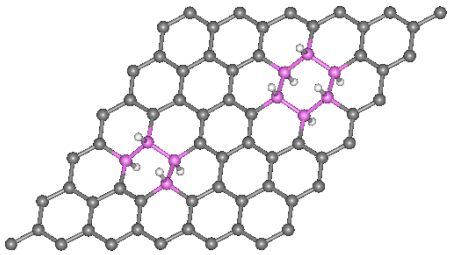
Fig. S1 Structures of graphene hydrides

Table S1 Carbon constitution, N_π and energies of graphene hydrides at PBE/DZP level of theory

Optimized Cartesian coordinates for graphene hydrides



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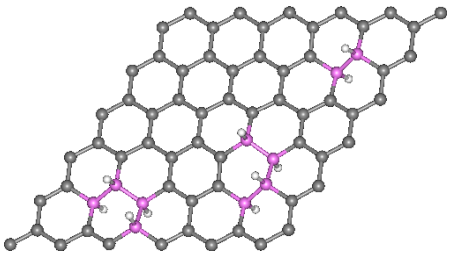

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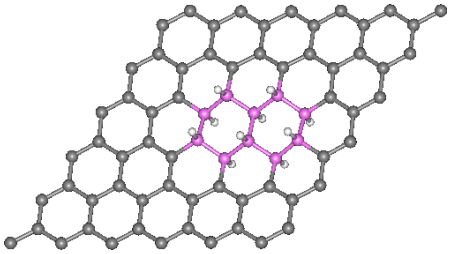

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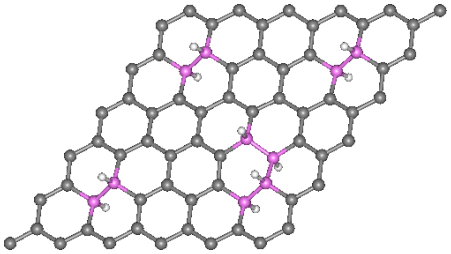

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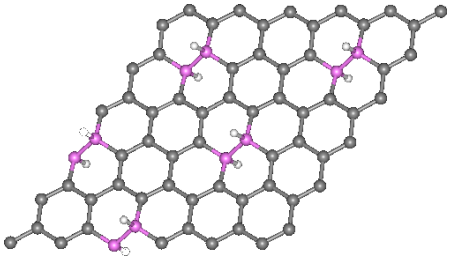

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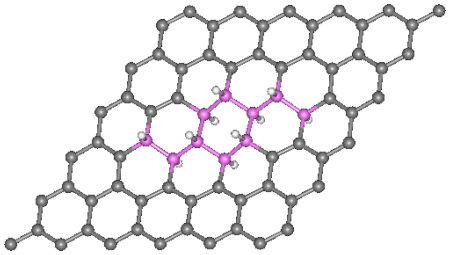

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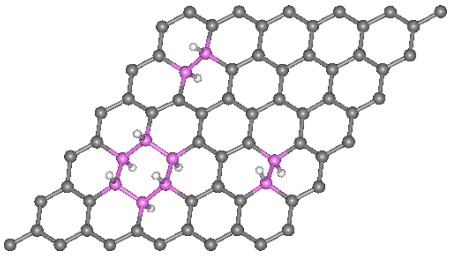

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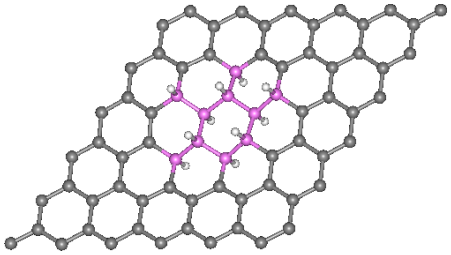

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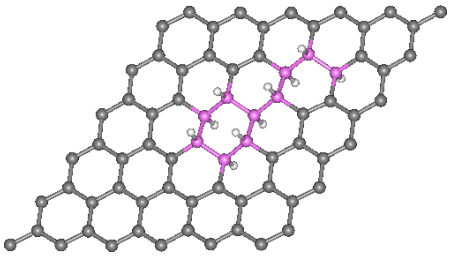

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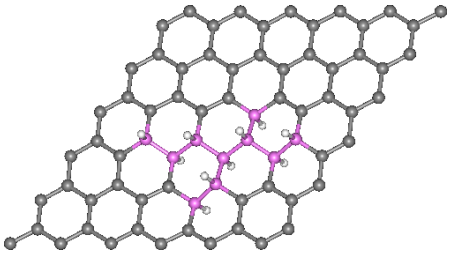

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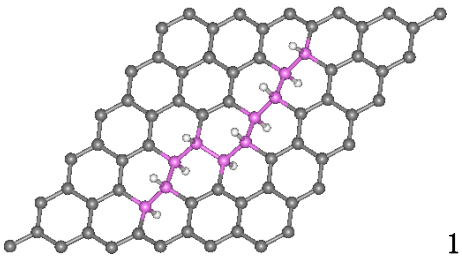

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Fig. S1 Structures of graphene hydrides.

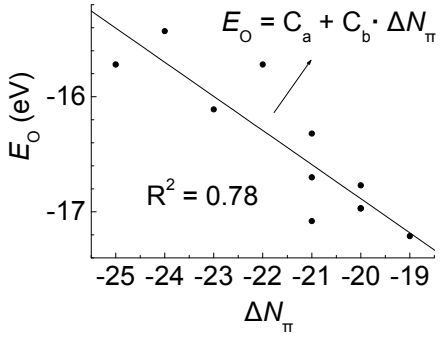

Fig. S2. Two-side epoxidation energies E_O with respect to the addition-induced π-bond reduction (ΔN_π), for graphene adducts with the same addition coverage. C_a and C_b are fitted to be - 22.81 (± 1.13) and - 0.30 (± 0.05), respectively.

Table S1 Carbon constitution, N_π and energies of graphene hydrides at PBE/DZP level of theory.

	n_0	n_I	n_{II}	n_{III}	N_π	energy (eV)
1	0	8	2	0	87	-14075.771004
2	0	4	6	0	85	-14074.568965
3	2	8	0	0	89	-14076.956441
4	0	2	8	0	84	-14073.489664
5	0	0	10	0	83	-14073.249018
6	2	6	2	0	88	-14076.418552
7	0	6	4	0	86	-14074.517142
8	4	2	4	0	88	-14076.283940
9	1	8	1	0	88	-14076.770820
10	2	4	4	0	87	-14076.309032
11	0	8	2	0	87	-14075.443719

Optimized Cartesian coordinates for graphene hydrides

1

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 Unit cell vectors (Ang):
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        7.550857    12.999179     0.000000
        0.000000     0.000000    16.000000

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C        2.544289     2.913161     8.051649
C        3.775370     5.112409     8.036753
C        5.031175     7.262449     8.009926
C        6.318856     9.420771     7.957767
C        7.570139    11.603060     7.951120
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C	2.534392	1.474844	8.040267
C	3.778427	3.630849	8.041755
C	4.992299	5.842907	7.959193
C	6.318623	7.985811	7.952240
C	7.567141	10.140365	7.950884
C	8.814630	12.326397	7.960542
C	3.770568	0.766245	8.052135
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C	6.288090	5.117292	7.655147
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C	8.806111	9.421910	7.956160
C	10.064530	11.602934	8.039550
C	6.262919	0.778120	7.954823
C	7.487716	2.923474	8.043376
C	8.772401	5.085951	7.734809
C	10.055385	7.271593	7.950174
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C	11.293748	5.132954	7.950878
C	12.508578	7.276047	7.966447
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C	15.056020	11.661445	7.963899
C	11.295650	0.798535	7.955366
C	12.541828	2.942459	7.955028
C	13.802717	5.112874	8.042408
C	15.061726	7.286050	7.746611
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C	15.043310	2.965391	8.038363
C	16.284041	5.114579	8.058558
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C	7.527915	5.807225	8.245991
C	8.789383	7.991215	7.946632
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C	11.288955	7.997796	7.960859
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C	20.079751	10.215743	8.041808
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H	6.394050	5.195982	6.536788
H	8.666099	4.992110	6.621452
H	13.878367	9.404827	6.625212
H	15.063018	7.369487	6.626619
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H	7.484140	5.695762	9.360045
H	8.835933	3.782721	9.429538
H	13.873439	8.042065	9.375067
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Unit cell vectors (Ang):

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C	10.008505	2.915641	7.950868
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H	11.266905	7.896617	9.378366
H	12.547731	5.714828	9.263310
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C	6.241876	9.409518	7.944706
C	7.492042	11.543900	8.044328
C	2.460053	1.476858	7.938554
C	3.706776	3.650644	7.853500
C	4.989385	5.818102	7.941682
C	6.237720	7.968361	7.940945
C	7.481312	10.137286	7.943735
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C	3.725205	0.758924	7.957321
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C	7.498256	7.247983	7.946997
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C	12.509815	11.582365	8.059701
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C	11.207968	5.054528	8.061787
C	12.503175	7.294625	7.972451
C	13.746045	9.420580	7.950600
C	15.001413	11.559622	8.033857
C	11.229801	0.775542	7.948369
C	12.515688	2.926782	7.647671
C	13.718563	5.116682	7.758006
C	15.028201	7.254589	8.044128
C	16.284163	9.420773	7.648580
C	17.498036	11.638110	7.966988
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C	15.008752	2.925163	7.976334
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C	17.505665	7.265038	8.047254
C	18.781215	9.419673	7.970293
C	20.022609	11.601941	7.969861
C	4.983410	1.442219	7.931297
C	6.186244	3.628982	8.244447
C	7.473838	5.821772	7.954244
C	8.764860	7.929701	7.944078
C	9.964286	10.119385	8.347551
C	11.250403	12.315464	8.046616
C	7.480891	1.496591	7.954491
C	8.727084	3.632128	7.953576
C	9.971160	5.780583	8.050767
C	11.260612	7.989381	7.969456
C	12.500187	10.126162	8.040550
C	13.751869	12.287596	8.063632
C	9.968709	1.492824	7.939012

C	11.211963	3.660259	7.937894
C	12.494351	5.832338	8.337471
C	13.736872	7.985734	7.951275
C	14.987259	10.155074	7.941293
C	16.269771	12.324250	7.954600
C	12.496606	1.452906	7.949950
C	13.715310	3.656965	8.249576
C	15.026957	5.842789	8.038420
C	16.270625	7.952828	8.022390
C	17.481694	10.146036	8.259022
C	18.760860	12.334813	7.953505
C	14.995417	1.518077	7.957138
C	16.246281	3.657208	7.963306
C	17.502422	5.826666	8.055467
C	18.771981	8.012543	7.953360
C	20.018245	10.149807	7.953878
C	21.264901	12.304500	8.049976
H	5.174842	2.966780	6.454907
H	8.958484	9.515721	6.545169
H	12.645323	2.981623	6.529421
H	13.610566	5.095317	6.641333
H	16.412122	9.448376	6.528554
H	6.010967	3.537240	9.354903
H	9.792163	10.011735	9.456732
H	12.617938	5.819817	9.456417
H	13.587889	3.674862	9.364789
H	17.347119	10.071383	9.377086

5

Unit cell vectors (Ang):

15.009870	-0.017970	0.000000
7.489451	12.970747	0.000000
0.000000	0.000000	16.000000

C	1.135648	0.636796	7.961041
C	2.403307	2.787368	7.962379
C	3.663715	4.947542	7.636669
C	4.904261	7.143613	7.957149
C	6.137429	9.275749	7.861909
C	7.374937	11.414985	7.941422
C	2.378542	1.357845	8.035363
C	3.643164	3.478281	7.951621
C	4.877081	5.649393	8.253692
C	6.129355	7.831175	7.923678
C	7.362325	9.992711	7.852454
C	8.622216	12.171581	7.959867
C	3.627098	0.646805	8.045788
C	4.882468	2.778435	8.038224
C	6.179705	4.914692	7.966655
C	7.413559	7.084296	7.952605
C	8.678795	9.263914	7.644707

C	9.872010	11.481689	8.054688
C	6.163825	0.631913	7.750612
C	7.425702	2.803875	8.040021
C	8.664406	4.928108	7.934661
C	9.891955	7.063942	7.958674
C	11.151856	9.255312	8.056763
C	12.384676	11.419019	8.062145
C	8.697293	0.620166	8.054768
C	9.942694	2.771510	8.033989
C	11.208707	4.924077	7.655358
C	12.405620	7.133515	8.038982
C	13.632831	9.266415	7.953220
C	14.867699	11.405130	8.032514
C	11.180667	0.610049	7.953716
C	12.423735	2.756450	8.031637
C	13.686480	4.907581	8.138562
C	14.917795	7.082787	8.035311
C	16.159752	9.254712	7.642608
C	17.384921	11.473025	7.960050
C	13.666548	0.602241	7.951080
C	14.918866	2.770862	7.957219
C	16.160322	4.919134	7.958351
C	17.397493	7.065227	7.962790
C	18.661519	9.247237	7.963767
C	19.898084	11.403328	7.953490
C	4.857331	1.361905	8.038161
C	6.177408	3.500092	7.963552
C	7.408867	5.635113	7.958298
C	8.642452	7.765736	7.937727
C	9.842697	9.981780	8.341151
C	11.102608	12.164445	8.048424
C	7.395406	1.334392	8.360114
C	8.657520	3.488792	7.964576
C	9.894992	5.647955	7.919176
C	11.156501	7.838538	7.964408
C	12.381151	9.974942	8.050651
C	13.618455	12.107136	8.038819
C	9.934707	1.325784	8.043463
C	11.173286	3.448843	7.959615
C	12.372565	5.639742	8.355222
C	13.631756	7.824085	7.970126
C	14.862949	9.986845	7.943061
C	16.145276	12.177204	7.963134
C	12.424544	1.326260	7.964378
C	13.675369	3.489604	8.043310
C	14.907395	5.626370	8.061483
C	16.141808	7.760393	7.950962
C	17.363091	9.976994	8.254783
C	18.640249	12.141119	7.947424
C	14.899019	1.328451	7.946538
C	16.153393	3.484435	7.942359
C	17.387126	5.651574	7.936128
C	18.661166	7.830977	7.939106
C	19.891906	9.967125	7.942608

C	21.134834	12.117778	7.951107
H	3.793225	5.015340	6.518161
H	4.739599	5.576842	9.370059
H	8.897208	9.336436	6.541664
H	6.297000	0.704122	6.635570
H	11.395922	5.007242	6.548212
H	16.290117	9.320047	6.525025
H	9.665725	9.889232	9.449331
H	7.268296	1.270662	9.476831
H	12.156072	5.577753	9.459427
H	17.234391	9.910439	9.372840

6

Unit cell vectors (Ang):

14.968784	0.057613	0.000000
7.534023	13.033075	0.000000
0.000000	0.000000	16.000000

C	1.310441	0.758235	7.948783
C	2.567316	2.912732	7.950525
C	3.810526	5.073766	7.954267
C	5.078226	7.271490	8.058056
C	6.326899	9.433283	7.959667
C	7.585556	11.612575	7.947606
C	2.555577	1.475677	7.950795
C	3.808818	3.631762	7.948863
C	5.065903	5.793786	8.037711
C	6.318705	7.995180	8.057624
C	7.572851	10.160017	7.951859
C	8.832029	12.340223	7.947503
C	3.801808	0.774950	7.949149
C	5.059216	2.926596	7.949338
C	6.269887	5.079064	8.054534
C	7.566570	7.299762	8.139529
C	8.802332	9.445429	7.962613
C	10.071524	11.646385	7.942619
C	6.305615	0.778370	7.962617
C	7.567122	2.932934	8.024487
C	8.773366	5.134603	7.662753
C	10.084253	7.299148	7.753760
C	11.310366	9.517135	8.050896
C	12.580725	11.662588	7.943668
C	8.798759	0.788804	8.037977
C	10.048690	2.951122	8.028401
C	11.321088	5.120190	7.649978
C	12.572721	7.314515	7.854282
C	13.826054	9.509718	8.055248
C	15.076419	11.652190	7.949166
C	11.289058	0.799131	8.040572
C	12.540352	2.958595	8.033344
C	13.854584	5.098178	7.955269
C	15.050182	7.325502	7.650769

C	16.331053	9.474582	8.029489
C	17.565601	11.669118	7.965603
C	13.787549	0.802407	7.964319
C	15.053653	2.954907	7.946953
C	16.312064	5.112737	7.866388
C	17.563454	7.317170	7.963460
C	18.817669	9.482501	8.036731
C	20.069973	11.664052	7.950266
C	5.057890	1.481996	7.949595
C	6.296689	3.642097	7.969229
C	7.576182	5.786681	8.354025
C	8.773822	8.010826	8.028882
C	10.071772	10.182053	7.954205
C	11.328237	12.367476	7.947227
C	7.558976	1.496129	8.038608
C	8.807708	3.640298	7.944105
C	10.060225	5.815695	8.147786
C	11.305644	8.021414	8.346512
C	12.583164	10.203121	7.989249
C	13.835198	12.368388	7.948833
C	10.045005	1.504232	8.060708
C	11.309977	3.643884	7.951822
C	12.550503	5.824069	8.246751
C	13.851872	8.016644	8.334247
C	15.070682	10.202892	7.971850
C	16.325848	12.380453	7.961919
C	12.547744	1.507855	8.043382
C	13.822139	3.666502	7.960282
C	15.062172	5.807170	7.849758
C	16.360224	8.032955	7.946764
C	17.564531	10.200152	8.035446
C	18.821144	12.386525	7.964697
C	15.040824	1.516410	7.950667
C	16.299525	3.675183	7.939632
C	17.551748	5.839773	7.924740
C	18.820399	8.039427	8.044075
C	20.059242	10.204460	7.958859
C	21.317147	12.379445	7.949796
H	8.664183	5.278202	6.558378
H	10.206285	7.351581	6.637713
H	11.367289	5.219868	6.532489
H	12.572341	7.380322	6.736594
H	14.896057	7.477815	6.547143
H	7.730373	5.634147	9.457170
H	10.059075	5.744806	9.264632
H	11.260433	7.927092	9.464041
H	12.432127	5.766390	9.362386
H	13.960636	7.878404	9.439466

7

Unit cell vectors (Ang):

15.011425	0.035944	0.000000

	7.536784	13.002722	0.000000
	0.000000	0.000000	16.000000
C	1.305993	0.764525	7.940568
C	2.551964	2.916600	7.939880
C	3.793905	5.124801	8.045851
C	5.024520	7.302106	8.041905
C	6.279556	9.485475	7.959043
C	7.560746	11.613591	8.032662
C	2.549842	1.481489	7.943276
C	3.801266	3.635508	7.955452
C	4.996689	5.858201	8.031916
C	6.278543	8.051970	7.950681
C	7.522962	10.209779	7.932473
C	8.840616	12.326507	7.952641
C	3.791795	0.772373	7.942936
C	5.009130	2.917928	7.967261
C	6.291261	5.126499	7.748130
C	7.559609	7.344418	7.953632
C	8.826527	9.482179	7.567399
C	10.068328	11.631828	7.967366
C	6.288245	0.769452	8.042240
C	7.530381	2.945446	7.742020
C	8.790612	5.132108	7.752448
C	10.061866	7.278277	8.035567
C	11.352016	9.419659	8.043435
C	12.556360	11.618012	7.967937
C	8.772931	0.781989	8.045902
C	10.069737	2.923998	7.959338
C	11.314252	5.134277	8.035947
C	12.564436	7.269834	8.036654
C	13.824735	9.425451	7.959135
C	15.071449	11.621607	8.035325
C	11.289579	0.792964	7.942106
C	12.526464	2.929864	7.962674
C	13.806426	5.099531	7.642522
C	15.070595	7.291919	8.036516
C	16.312960	9.463526	7.968615
C	17.565989	11.636704	7.962210
C	13.797901	0.792923	7.968166
C	15.097153	2.933156	7.970577
C	16.293669	5.149256	8.029815
C	17.553032	7.307245	8.053026
C	18.801714	9.500959	8.039294
C	20.053948	11.661171	8.038084
C	5.028715	1.487194	7.957437
C	6.284591	3.671593	8.254604
C	7.544638	5.857405	8.265312
C	8.788745	7.988541	7.859060
C	10.033430	10.141030	8.255231
C	11.317824	12.333184	7.951220
C	7.543936	1.468649	8.038179
C	8.779464	3.670648	8.248634
C	10.087383	5.855830	8.044519

C	11.320657	7.989842	8.052221
C	12.558268	10.143306	7.964097
C	13.812015	12.339318	8.041105
C	10.052154	1.506246	7.954906
C	11.303125	3.640769	7.951744
C	12.538142	5.851402	7.959427
C	13.820664	8.002725	8.020132
C	15.072448	10.161127	7.959589
C	16.309070	12.340772	8.040315
C	12.536497	1.506214	7.946583
C	13.805491	3.688252	8.255569
C	15.081328	5.861925	7.955896
C	16.305605	8.017122	8.041215
C	17.557498	10.204192	7.968380
C	18.813793	12.357691	7.962019
C	15.077106	1.509199	7.948673
C	16.311758	3.659172	7.954358
C	17.545181	5.871000	8.061932
C	18.792776	8.044978	8.051965
C	20.038404	10.227433	8.044827
C	21.315718	12.381626	8.044151
H	6.371487	5.089566	6.628278
H	8.955823	9.603948	6.454382
H	7.521761	3.021709	6.621117
H	8.723391	5.102624	6.631814
H	13.808186	4.956041	6.526094
H	6.360014	3.705221	9.374741
H	7.532979	5.775020	9.384958
H	9.828929	10.059811	9.364445
H	8.712013	3.699873	9.369374
H	13.805385	3.844901	9.369457

8

Unit cell vectors (Ang):

15.031369	0.052065	0.000000
7.560781	12.991854	0.000000
0.000000	0.000000	16.000000

C	1.330590	0.772370	8.050766
C	2.588295	2.913782	8.038835
C	3.844515	5.082440	8.038468
C	5.100111	7.258046	7.973299
C	6.356711	9.419596	7.965269
C	7.628730	11.609805	7.955146
C	2.579627	1.485107	8.050893
C	3.839848	3.651763	8.050874
C	5.089712	5.820894	8.042184
C	6.341048	7.981565	8.029547
C	7.624769	10.182599	7.953183
C	8.877429	12.324892	8.023697
C	3.846407	0.767681	8.041005
C	5.094162	2.936920	8.054949
C	6.327730	5.112371	8.034000

C	7.570729	7.250720	8.043064
C	8.867906	9.494710	7.953152
C	10.116093	11.619888	7.943173
C	6.342591	0.782689	8.053281
C	7.605317	2.929526	8.040397
C	8.856288	5.109144	7.640997
C	10.106984	7.279880	7.727737
C	11.397256	9.437544	7.589345
C	12.657745	11.631408	7.953940
C	8.845396	0.793655	8.052691
C	10.092274	2.937933	8.024000
C	11.374560	5.125499	7.655358
C	12.664107	7.281030	7.755095
C	13.887574	9.503888	8.056262
C	15.151411	11.634365	8.048607
C	11.348392	0.793907	8.053031
C	12.586834	2.959315	8.032201
C	13.909316	5.081537	7.971555
C	15.170445	7.272107	8.046024
C	16.385783	9.462458	8.047685
C	17.636285	11.631230	8.048956
C	13.844291	0.804693	8.040360
C	15.131192	2.948435	7.958028
C	16.394672	5.121205	7.941812
C	17.636060	7.290163	7.949119
C	18.894761	9.447954	7.961342
C	20.155742	11.637596	7.961461
C	5.100155	1.486601	8.051205
C	6.328102	3.655415	8.044367
C	7.565842	5.851719	7.955534
C	8.868929	8.002981	8.265517
C	10.097866	10.199883	7.857023
C	11.402267	12.342286	7.955314
C	7.605035	1.501120	8.056471
C	8.847695	3.629135	7.955222
C	10.109653	5.816400	8.156468
C	11.385384	8.009728	8.154540
C	12.675635	10.195240	7.933004
C	13.902577	12.344416	8.042178
C	10.092363	1.502918	8.058443
C	11.362091	3.639318	7.950897
C	12.609794	5.825157	8.238663
C	13.878777	8.007322	8.345366
C	15.142399	10.205300	8.058223
C	16.403491	12.349677	8.051766
C	12.598350	1.512073	8.055912
C	13.884042	3.679529	7.952728
C	15.149625	5.844387	7.956614
C	16.390944	8.002546	7.989393
C	17.623335	10.174182	8.035348
C	18.909316	12.349193	8.037267
C	15.118409	1.525862	8.038524
C	16.377462	3.675498	7.958997
C	17.630915	5.854434	7.959434

C	18.892142	8.022614	7.949399
C	20.151416	10.173368	7.950005
C	21.396138	12.369115	7.964062
H	8.918543	5.149278	6.515992
H	10.054478	7.306855	6.608461
H	11.430996	9.337557	6.469131
H	11.412421	5.222661	6.536530
H	12.765759	7.278620	6.641584
H	8.973893	7.993104	9.387840
H	10.099445	5.756239	9.273126
H	11.373421	8.091095	9.271697
H	12.492127	5.834669	9.355897
H	13.769989	7.943930	9.464516

9

Unit cell vectors (Ang):

15.019879	0.032210	0.000000
7.537836	12.990217	0.000000
0.000000	0.000000	16.000000

C	1.295711	0.744625	7.946308
C	2.561063	2.893593	7.949314
C	3.822392	5.048548	8.038788
C	5.061573	7.218923	8.053259
C	6.331505	9.389416	8.054209
C	7.586602	11.570690	7.963037
C	2.550821	1.469152	7.947829
C	3.804137	3.610467	7.962544
C	5.055532	5.772590	8.038429
C	6.321074	7.960212	8.056352
C	7.570898	10.117207	8.042240
C	8.821232	12.299631	7.948660
C	3.795406	0.767858	7.950578
C	5.047916	2.904464	7.950284
C	6.306186	5.054602	7.957645
C	7.560120	7.252645	8.043182
C	8.805114	9.403250	8.042806
C	10.074014	11.590326	7.947309
C	6.313235	0.761156	7.943600
C	7.555884	2.909164	7.946118
C	8.772818	5.055921	7.962943
C	10.072931	7.253338	7.740351
C	11.316938	9.483821	7.972099
C	12.563867	11.612642	7.948523
C	8.810514	0.753006	7.959465
C	10.066006	2.910088	8.041221
C	11.331481	5.086229	7.756030
C	12.593022	7.253914	7.845236
C	13.843278	9.410915	7.750257
C	15.100879	11.622075	7.964915
C	11.309459	0.762455	8.052761
C	12.545054	2.916123	8.043281
C	13.870149	5.049552	8.058340

C	15.136032	7.221343	8.066191
C	16.336365	9.412951	7.658209
C	17.622778	11.553030	8.029396
C	13.822439	0.762966	7.963434
C	15.081371	2.921817	7.945749
C	16.348536	5.058854	7.969895
C	17.602467	7.213425	8.028959
C	18.861293	9.412850	8.041718
C	20.111843	11.570492	8.039872
C	5.044228	1.475734	7.947080
C	6.303545	3.622311	7.947764
C	7.550192	5.773591	7.957293
C	8.784929	7.979119	8.033119
C	10.065039	10.160956	7.962054
C	11.322064	12.317399	7.951059
C	7.564069	1.465466	7.948622
C	8.790392	3.631012	7.956526
C	10.070871	5.803071	8.250631
C	11.311573	7.988002	8.264287
C	12.537817	10.184507	7.943045
C	13.856681	12.320969	7.945392
C	10.065950	1.482294	8.042298
C	11.309383	3.610490	8.036149
C	12.571218	5.790019	8.335732
C	13.835948	7.988429	8.337995
C	15.100217	10.132443	8.247047
C	16.346948	12.306245	7.957414
C	12.550747	1.484773	8.042899
C	13.834855	3.638889	7.970955
C	15.108260	5.770907	8.045824
C	16.346491	7.908321	7.951840
C	17.640327	10.131525	7.959918
C	18.861268	12.281713	8.052394
C	15.070129	1.477364	7.947564
C	16.327503	3.631956	7.947954
C	17.594694	5.783201	8.040487
C	18.849061	7.951205	8.045056
C	20.103787	10.135565	8.054082
C	21.361687	12.316052	7.965309
H	10.145008	7.212021	6.619983
H	11.366833	5.185407	6.638603
H	12.635903	7.233698	6.726589
H	13.953444	9.307937	6.639147
H	16.229620	9.488647	6.540702
H	10.129613	5.842290	9.371841
H	11.254967	7.921557	9.385829
H	12.457073	5.797826	9.452065
H	13.756366	8.078876	9.453007
H	15.150056	10.035641	9.361998

10

Unit cell vectors (Ang):

15.029311	0.039357	0.000000

	7.548759	12.990853	0.000000
	0.000000	0.000000	16.000000
C	1.288136	0.682987	8.039401
C	2.545038	2.868017	7.943355
C	3.792174	5.024477	7.941676
C	5.050992	7.174986	7.953460
C	6.322190	9.375738	7.942947
C	7.571793	11.526714	8.039070
C	2.535824	1.427388	7.960146
C	3.786852	3.593704	7.945626
C	5.040504	5.750232	7.958607
C	6.319414	7.930981	7.957013
C	7.560583	10.094793	7.963748
C	8.826111	12.252698	8.048258
C	3.781713	0.719296	7.963766
C	5.030735	2.877942	7.957260
C	6.265647	5.021272	8.051099
C	7.544775	7.253773	8.061553
C	8.810275	9.394803	7.975501
C	10.083138	11.550077	8.049402
C	6.313869	0.714822	8.039932
C	7.569466	2.892223	8.050613
C	8.770127	5.093864	7.731678
C	10.059488	7.269652	8.049920
C	11.299864	9.402833	8.033768
C	12.584779	11.536320	8.050491
C	8.801208	0.696628	8.041820
C	10.061408	2.877451	7.648267
C	11.311766	5.042501	7.744881
C	12.568923	7.225893	7.652762
C	13.840533	9.403396	8.028706
C	15.088566	11.548888	8.055642
C	11.283927	0.707975	8.048195
C	12.602223	2.835305	8.056476
C	13.846996	5.048906	7.747114
C	15.073773	7.277235	8.047180
C	16.332864	9.403929	7.959433
C	17.601170	11.546637	8.037595
C	13.821869	0.705811	8.051696
C	15.073800	2.862801	8.042102
C	16.350492	5.044663	8.040327
C	17.591745	7.218050	7.955635
C	18.844993	9.390802	7.948166
C	20.101993	11.546364	8.039303
C	5.032097	1.452824	7.962755
C	6.281086	3.619045	8.038645
C	7.547554	5.764781	8.354824
C	8.802584	7.968874	8.043526
C	10.062244	10.112884	8.043469
C	11.324101	12.262812	8.040145
C	7.551192	1.415976	8.049745
C	8.760266	3.597968	7.936381
C	10.057945	5.757824	8.255331

C	11.271766	7.974830	7.956968
C	12.573318	10.119500	8.043391
C	13.853419	12.260442	8.050186
C	10.050443	1.397590	7.960978
C	11.290546	3.595593	8.252722
C	12.572570	5.779157	8.183119
C	13.853479	7.981747	7.957523
C	15.086285	10.115192	8.042269
C	16.346093	12.257567	8.054554
C	12.578558	1.417075	8.049296
C	13.831910	3.545070	8.031376
C	15.061347	5.774592	8.346494
C	16.321382	7.973968	7.970049
C	17.608080	10.108090	7.959344
C	18.843671	12.260801	8.056899
C	15.068922	1.428528	8.053677
C	16.333501	3.633333	7.970316
C	17.584278	5.777415	7.958694
C	18.836447	7.928454	7.944470
C	20.095730	10.120986	7.959979
C	21.362611	12.263025	8.048487
H	8.738650	5.268906	6.619558
H	10.207785	2.931156	6.529972
H	11.291963	5.022329	6.625167
H	12.571037	7.140261	6.529336
H	13.932096	5.141389	6.631432
H	7.679339	5.664721	9.471779
H	10.046308	5.615103	9.369777
H	11.127456	3.631879	9.362156
H	12.575507	5.824042	9.301651
H	14.949652	5.707728	9.465851

11

Unit cell vectors (Ang):

14.997824	0.013263	0.000000
7.510325	12.950403	0.000000
0.000000	0.000000	16.000000

C	1.236922	0.680586	7.950694
C	2.487046	2.855271	7.932607
C	3.729030	5.004831	7.949233
C	4.987607	7.141377	8.051466
C	6.239836	9.305127	8.053826
C	7.481930	11.479023	8.034541
C	2.484910	1.408935	7.927981
C	3.726023	3.575454	7.863278
C	4.976223	5.716048	7.955914
C	6.234960	7.864535	8.044493
C	7.476732	10.045584	8.036496
C	8.727735	12.197328	7.963534
C	3.742856	0.700897	7.861316
C	4.990354	2.860947	7.747289
C	6.235108	4.999326	7.836055

C	7.483309	7.143162	7.956826
C	8.732248	9.333338	7.959888
C	9.988554	11.487872	7.953127
C	6.238864	0.678533	7.822702
C	7.520406	2.827651	7.418753
C	8.754279	5.012211	7.545892
C	9.990187	7.222145	7.942365
C	11.226729	9.350767	7.869349
C	12.466414	11.481755	7.956141
C	8.713406	0.669545	7.950215
C	10.004957	2.810913	7.948569
C	11.246662	5.009924	7.734402
C	12.517087	7.146752	7.759194
C	13.777382	9.328961	7.847796
C	14.967392	11.519061	8.156091
C	11.218888	0.675507	8.049735
C	12.469357	2.824674	8.037258
C	13.737587	4.997290	8.152643
C	14.983027	7.152483	8.263106
C	16.240579	9.312918	8.346133
C	17.478773	11.479934	8.236805
C	13.724183	0.686539	8.042544
C	14.971088	2.862394	7.960710
C	16.222776	5.015999	8.043924
C	17.478133	7.158260	8.149071
C	18.722320	9.310216	8.150383
C	19.967923	11.480387	8.068960
C	4.975145	1.409274	7.758481
C	6.214332	3.575621	7.664788
C	7.464017	5.732160	7.834299
C	8.731769	7.906245	7.948801
C	9.980130	10.058609	7.943669
C	11.231105	12.202579	7.937667
C	7.483419	1.358638	7.764380
C	8.692779	3.571623	8.062868
C	9.955693	5.720149	8.163138
C	11.202492	7.907071	7.852848
C	12.458080	10.070868	7.933370
C	13.740792	12.203659	7.963309
C	9.986364	1.385082	7.962231
C	11.223304	3.508590	7.955058
C	12.435407	5.734022	8.351888
C	13.670532	7.911783	8.422794
C	14.927999	10.065737	8.546149
C	16.213442	12.201055	8.145898
C	12.466473	1.396299	8.051926
C	13.726850	3.588667	8.044098
C	14.970022	5.732911	8.149638
C	16.215846	7.875007	8.253046
C	17.461870	10.023343	8.254491
C	18.710720	12.185204	8.137328
C	14.963671	1.414925	7.963075
C	16.216268	3.589424	7.959301
C	17.468944	5.732034	8.050250

C	18.722967	7.871924	8.138796
C	19.960826	10.041005	8.069319
C	21.213056	12.204989	8.048939
H	7.695037	2.853521	6.306321
H	8.886735	4.987532	6.432185
H	11.346152	5.136802	6.622588
H	12.774149	7.039351	6.674105
H	14.049067	9.246477	6.763073
H	8.466035	3.631196	9.160222
H	9.854563	5.588405	9.273701
H	12.262026	5.825056	9.455881
H	13.433745	8.011471	9.512918
H	14.708001	10.047686	9.648982