Supporting Information for the manuscript "*DFT studies on catalytic properties of isolated and carbon nanotube supported Pd_9 cluster – II: hydro-isomerization of butene isomers*" by the authors Vincenza D'Anna, Dario Duca, Francesco Ferrante and Gianfranco La Manna.

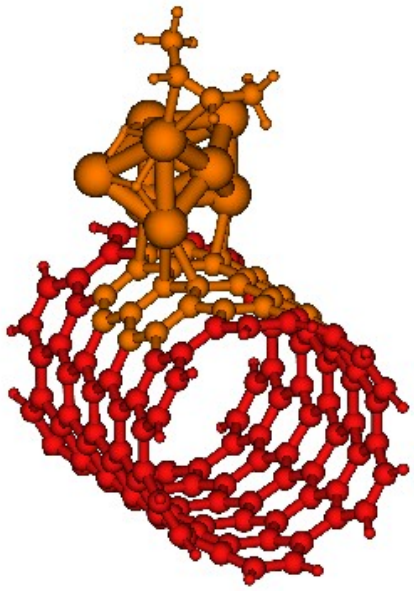

Figure S1. The definition of the ONIOM layers employed in the study of the supported systems: the model system, consisting of the Pd_9 cluster, the molecules adsorbed/fragmented on it and a coronene-lyke portion of the carbon nanotube surface, is in orange (the *cis*-but-2-ene/$Pd_9(H_2)$/nanotube system is reported as an example).

Optimized geometries of the most stable minima and transition states in xyz format; the normal modes of vibration with the imaginary frequency are reported for TSs by using the Gaussian03 format.

cis-but-2-ene/$Pd_9(H_2)$

23

H	-4.668555	1.957043	-0.831062
C	-3.753443	2.433600	-0.470479
C	-3.541830	2.440060	0.906413
H	-4.306621	1.967136	1.528905
Pd	-2.655273	0.456823	0.084757
Pd	-1.746312	-1.857327	-1.348789
Pd	-1.397799	-1.793021	1.535444
Pd	-0.006721	0.553054	1.231832
Pd	0.787530	-1.629935	-0.089940
Pd	-0.077756	0.567320	-1.490570
Pd	1.925112	1.990415	-0.024103
Pd	2.759140	-0.143914	1.335370
Pd	2.710742	-0.152781	-1.306388
H	-2.453478	-1.383269	0.225773
H	-1.665908	-0.088129	-1.501618
C	-3.027261	3.290856	-1.490701
C	-2.545154	3.305189	1.656284
H	-3.032229	4.229835	2.005675
H	-2.165259	2.784039	2.543672
H	-1.688638	3.590763	1.036847
H	-3.593493	4.217379	-1.678112
H	-2.021951	3.573131	-1.161261
H	-2.936231	2.764627	-2.448126

trans-but-2-ene/$Pd_9(H_2)$

23

Pd	0.340687	0.136206	-0.066485
Pd	0.264418	0.156881	2.649853
Pd	2.648569	-0.069867	1.429522
Pd	1.822925	-2.246947	2.691098
Pd	-0.548253	-1.976358	1.320469
Pd	1.744219	-2.341320	-0.044589
Pd	2.114796	-4.823397	1.549338
Pd	-0.218172	-4.079499	3.097163
Pd	-0.398671	-4.494186	0.199266
H	1.613223	-4.039765	0.063753
H	0.378936	-5.099894	1.852667
C	-1.235369	-4.308950	-1.923829
C	-2.297785	-4.595810	-1.063284
C	-3.310408	-3.572228	-0.576718
C	-0.539307	-5.343100	-2.793587
H	-1.069908	-3.265811	-2.201044
H	-2.597469	-5.642329	-0.955300
H	-0.939993	-5.301841	-3.819241
H	-0.693362	-6.360668	-2.413555
H	0.539862	-5.159779	-2.856894
H	-2.926788	-2.548845	-0.673245
H	-4.233833	-3.646083	-1.173558
H	-3.587018	-3.739824	0.471413

pre-*cis*/$Pd_9(H)$

23

Pd	-0.922768	1.513615	2.747802
Pd	-1.265652	-1.051999	2.411596
Pd	1.190294	-0.076308	2.858378
Pd	-1.921470	0.629914	0.247610
Pd	0.692146	1.555455	0.583582
Pd	0.399399	-1.043042	0.281097
Pd	1.712966	0.471050	-1.718441
Pd	-0.638962	2.303404	-1.754449
H	0.361462	1.172404	-2.528889
Pd	-0.915202	-0.400051	-2.099669
C	-1.183365	-0.756382	-4.105949
C	-1.118328	-2.286113	-4.165791
C	-2.501266	-0.108419	-4.554487
C	-3.768787	-0.586091	-3.808315
H	-0.325195	-0.290682	-4.604354
H	-1.812426	-2.766894	-3.461139
H	-0.106535	-2.655276	-3.961759
H	-1.404478	-2.634962	-5.174617
H	-2.409628	0.982206	-4.460503
H	-2.624886	-0.315660	-5.634690
H	-4.656201	-0.063229	-4.187166
H	-3.692758	-0.379605	-2.731344
H	-3.935588	-1.663106	-3.937505

pre-*trans*/$Pd_9(H)$

23

Pd	-1.072160	1.577825	2.878311
Pd	-1.347338	-1.045547	2.407818
Pd	1.025509	-0.033243	2.798371
Pd	-1.738131	0.581991	0.283381
Pd	0.684653	1.546070	0.636043
Pd	0.485607	-1.223804	0.280957
Pd	1.827939	0.446516	-1.658539
Pd	-0.566826	2.244095	-1.698964
H	0.457230	1.057894	-2.454009
Pd	-0.738727	-0.507453	-2.080107
C	-1.076767	-0.785117	-4.091728
C	-1.054005	-2.314398	-4.187247
C	-2.412446	-0.131069	-4.463307
H	-3.176946	-0.391518	-3.712820
H	-0.230078	-0.323916	-4.615121
H	-1.866811	-2.775797	-3.607253
H	-0.098081	-2.733917	-3.849089
H	-1.191844	-2.628438	-5.237375
C	-2.355728	1.398235	-4.649932
H	-2.760798	-0.591344	-5.407590
H	-3.338416	1.797444	-4.932738
H	-2.039924	1.893809	-3.718330
H	-1.635782	1.672113	-5.433049

but-1-ene/$Pd_9(H_2)$

23

C	-0.776863	1.679110	0.112413
Pd	1.037188	0.391227	-0.359509
Pd	3.708662	-0.836168	-0.099109
Pd	1.542569	-2.210779	-1.478104
Pd	2.564291	-3.044710	1.029956
Pd	0.003596	-2.059301	1.050474
Pd	0.385734	-1.789589	3.875699
Pd	0.886798	-4.146443	2.848213
Pd	2.879100	-2.734122	3.849925
Pd	2.071271	-0.636518	2.095983
C	0.316360	2.539687	0.046199
H	0.537966	3.021143	-0.910799
C	1.012287	3.143161	1.255750
H	-1.407355	1.502073	-0.757156
H	2.369746	-0.662405	-1.175178
H	-1.168729	1.343752	1.071119
H	0.264320	-1.459754	-0.527710
H	2.102318	3.106686	1.118243
C	0.586935	4.618446	1.478670
H	0.779221	2.551546	2.151632
H	1.110729	5.045439	2.343850
H	0.825698	5.234652	0.601250
H	-0.493057	4.690799	1.659220

n-butane/Pd_9

23

C	-0.370653	-0.301797	0.522355
C	0.137041	0.184944	1.895902
C	1.676069	0.189372	2.043930
C	2.382168	1.221971	1.141746
Pd	0.029660	3.443687	1.754328
Pd	-1.759413	4.794566	3.393699
Pd	-0.961314	5.983629	1.229948
Pd	1.662348	5.763812	1.953486
Pd	-0.119537	7.043490	3.584996
Pd	0.854512	4.474810	4.078458
Pd	3.515875	5.473663	3.964218
Pd	2.550894	7.962807	3.490861
Pd	1.795915	6.610303	5.586996
H	-0.303337	-0.439120	2.687642
H	-0.011316	0.337590	-0.294027
H	-1.467713	-0.301293	0.485733
H	-0.027145	-1.326619	0.323822
H	1.931897	0.397952	3.093121
H	2.060906	-0.817818	1.819869
H	3.463289	1.247487	1.330637
H	1.993274	2.241609	1.343848
H	2.229573	1.009774	0.076213
H	-0.242672	1.215510	2.084521

TS *cis*-but-2-ene/$Pd_9(H_2)$ → pre-*cis*/$Pd_9(H)$

23

Pd	-2.540611	0.226620	1.471743
Pd	-1.943911	1.936603	-0.421580
Pd	-2.982825	-0.440073	-1.041370
Pd	0.220877	0.978477	1.139930
Pd	-0.751545	-1.518007	0.431782
Pd	-0.235891	0.149947	-1.524298
Pd	1.412327	-2.095502	-1.142067
Pd	1.743540	-1.413960	1.647798
H	2.481914	-1.530979	0.111558
Pd	2.372188	0.441923	-0.433952
C	2.769360	2.596219	-0.522108
C	2.537983	3.195667	0.849692
C	4.009634	2.069921	-0.996628
C	5.302194	2.074778	-0.189795
H	2.049216	2.901332	-1.283924
H	3.288683	2.889529	1.584000
H	1.539253	2.900514	1.232500
H	2.534244	4.295834	0.792041
H	3.805580	0.349866	-1.120791
H	4.139428	2.079343	-2.079640
H	6.026200	1.364975	-0.603166
H	5.137033	1.814895	0.859961
H	5.752596	3.077883	-0.226856

1
A

Frequencies -- -684.3212
Red. masses -- 1.1953
Frc consts -- 0.3298
IR Inten -- 98.4038

Atom	AN	X	Y	Z
1	46	0.00	0.00	0.00
2	46	0.00	0.00	0.00
3	46	0.00	0.00	0.00
4	46	0.00	0.00	0.00
5	46	0.00	0.00	0.00
6	46	0.00	0.00	0.00
7	46	0.00	0.00	0.00
8	46	0.00	0.00	0.00
9	1	0.02	-0.02	0.00
10	46	-0.01	0.01	0.00
11	6	-0.03	-0.05	0.01
12	6	0.00	-0.01	0.00
13	6	0.02	-0.10	-0.03
14	6	0.02	0.02	0.00
15	1	0.03	0.04	0.00
16	1	0.00	0.00	0.00
17	1	0.00	0.00	0.00
18	1	0.00	-0.01	-0.02
19	1	0.25	0.93	0.03
20	1	0.07	0.21	-0.02
21	1	0.05	0.04	0.02
22	1	0.00	0.00	0.00
23	1	-0.03	0.03	0.01

TS pre-*trans*/$Pd_9(H)$ → *trans*-but-2-ene/$Pd_9(H_2)$

23

Pd	0.455967	0.109732	-0.438427
Pd	0.643191	0.338996	2.186271
Pd	2.837242	0.047999	0.712835
Pd	-0.563146	-1.960560	1.241174
Pd	1.681148	-2.355044	-0.180976
Pd	1.990512	-2.026545	2.428271
Pd	2.636634	-4.448927	1.294133
Pd	-0.174203	-4.322435	-0.061711
H	1.052107	-4.996988	0.978502
Pd	0.207136	-4.252333	2.689536
C	0.465790	-4.945736	4.775738
C	1.391813	-4.051625	5.583659
C	-0.942497	-4.687627	4.665668
H	-1.301234	-3.792309	5.179363
H	0.788299	-5.982647	4.656941
H	1.076352	-3.001232	5.545490
H	2.423425	-4.113869	5.221060
H	1.393628	-4.362536	6.642290
H	-1.290614	-3.954143	3.227323
C	-1.951002	-5.832751	4.581720

H	-2.171225	-6.197430	5.595872
H	-2.893479	-5.515483	4.122344
H	-1.551566	-6.669380	3.997681

	1
	A
Frequencies --	-843.1552
Red. masses --	1.1527
Frc consts --	0.4828
IR Inten --	133.8897

Atom	AN	X	Y	Z
1	46	0.00	0.00	0.00
2	46	0.00	0.00	0.00
3	46	0.00	0.00	0.00
4	46	0.00	0.00	0.00
5	46	0.00	0.00	0.00
6	46	0.00	0.00	0.00
7	46	0.00	0.00	0.00
8	46	0.00	0.00	0.00
9	1	0.00	-0.02	0.03
10	46	0.00	0.00	-0.01
11	6	-0.03	0.03	-0.01
12	6	0.01	0.00	0.00
13	6	-0.06	0.03	0.07
14	1	0.15	-0.15	-0.03
15	1	0.02	-0.02	0.02
16	1	0.00	0.00	-0.01
17	1	0.02	-0.01	0.00
18	1	0.01	0.00	0.01
19	1	0.71	-0.59	-0.30
20	6	0.02	-0.01	0.00
21	1	0.02	0.00	-0.03
22	1	0.05	-0.01	0.01
23	1	-0.01	0.00	0.00

TS pre-*cis*/Pd$_9$(H) → but-1-ene/Pd$_9$(H$_2$)

23

C	2.569284	3.167897	0.832939
C	2.722586	2.598170	-0.564515
C	3.929446	2.039026	-1.068652
H	4.816379	2.015237	-0.437331
Pd	2.365956	0.427896	-0.465863
Pd	1.748317	-1.351898	1.677200
Pd	1.428853	-2.132421	-1.092468
Pd	-0.234129	0.095812	-1.559827
Pd	-0.736272	-1.500349	0.453777
Pd	0.214353	1.026384	1.082370
Pd	-1.951129	1.909441	-0.520654
Pd	-2.978598	-0.495815	-1.050562
Pd	-2.539025	0.266884	1.434197
H	2.488433	-1.538317	0.150870
H	1.980479	2.935918	-1.290622
H	3.372199	2.800698	1.485141
H	1.609662	2.806057	1.269519
C	2.543200	4.717999	0.835611
H	3.833165	0.301699	-1.072591
H	4.111953	2.039129	-2.141010
H	2.398530	5.096581	1.855182
H	3.484870	5.127582	0.447891
H	1.723165	5.099128	0.213201

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	A
Frequencies --	-724.3574
Red. masses --	1.1355
Frc consts --	0.3510
IR Inten --	162.0824

Atom	AN	X	Y	Z
1	6	0.00	0.00	0.00
2	6	-0.02	-0.05	0.01
3	6	0.04	-0.08	-0.01
4	1	0.06	0.16	-0.04
5	46	-0.01	0.00	0.00
6	46	0.00	0.00	0.00
7	46	0.00	0.00	0.00
8	46	0.00	0.00	0.00
9	46	0.00	0.00	0.00
10	46	0.00	0.00	0.00
11	46	0.00	0.00	0.00
12	46	0.00	0.00	0.00
13	46	0.00	0.00	0.00
14	1	0.02	-0.01	-0.01
15	1	0.02	0.01	-0.01
16	1	0.00	0.00	0.00
17	1	0.00	0.00	0.00
18	6	0.00	0.00	0.00
19	1	0.24	0.92	-0.11
20	1	0.07	0.18	-0.03
21	1	0.00	-0.01	0.00
22	1	0.00	0.00	0.00
23	1	0.00	0.00	0.00

TS pre-*cis*/Pd$_9$(H) → *n*-butane/Pd$_9$

23

Pd	0.096798	0.258721	0.132023
Pd	0.497445	0.076931	2.826417
Pd	2.627042	-0.082945	1.065962
Pd	-1.085440	-1.831446	1.604726
Pd	1.288368	-2.122479	-0.021687
Pd	1.664810	-2.273983	2.575542
Pd	1.936964	-4.686942	1.099056
Pd	-0.504053	-4.087129	-0.108105
H	0.698182	-5.500508	2.254704
Pd	-0.304475	-4.191414	2.618238
C	-0.120386	-6.314501	3.336562
C	-0.316887	-5.905095	4.810837
C	-1.271507	-7.110147	2.686969
C	-2.663575	-6.445734	2.730257
H	0.793403	-6.921401	3.279259
H	-1.158690	-5.216652	4.967000
H	0.587934	-5.441827	5.220706
H	-0.530670	-6.809674	5.407290
H	-1.004120	-7.324911	1.643921
H	-1.326841	-8.085795	3.203160
H	-3.407614	-7.085460	2.237858
H	-2.651299	-5.478705	2.207017
H	-3.001458	-6.272768	3.760180

	1
	A
Frequencies --	-907.5420
Red. masses --	1.0820
Frc consts --	0.5250
IR Inten --	6.4386

Atom	AN	X	Y	Z
1	46	0.00	0.00	0.00
2	46	0.00	0.00	0.00
3	46	0.00	0.00	0.00
4	46	0.00	0.00	0.00
5	46	0.00	0.00	0.00
6	46	0.00	0.00	0.00
7	46	0.00	0.00	0.00
8	46	0.00	0.00	0.00
9	1	0.69	0.64	-0.12
10	46	-0.01	0.00	0.00
11	6	0.01	-0.07	-0.02
12	6	-0.01	-0.01	0.00
13	6	0.01	0.00	0.00
14	6	0.00	0.00	0.00
15	1	0.28	0.08	-0.08
16	1	-0.01	-0.03	0.01
17	1	0.00	0.01	0.00
18	1	-0.01	-0.02	0.02
19	1	0.02	0.00	0.01
20	1	0.00	0.01	0.01
21	1	0.00	0.00	0.00
22	1	0.00	0.00	0.00
23	1	0.00	0.00	0.00

cis-but-2-ene/$Pd_9(H_2)$/nanotube

C	2.675356	-5.933252	4.451544
C	3.241131	-4.640271	4.459937
C	2.307020	-3.508443	4.238400
C	1.085451	-3.740301	3.594387
C	0.731305	-5.128501	3.201285
C	1.441292	-6.174035	3.827804
C	2.798297	-2.131299	4.388827
C	1.922530	-1.053220	4.189405
C	0.641730	-1.286873	3.461980
C	0.321747	-2.586350	3.053784
C	2.463614	0.317119	4.230467
C	1.549066	1.452153	4.011001
C	0.267604	1.203303	3.289438
C	-0.047474	-0.156680	2.882484
C	2.068990	2.753874	4.046398
C	1.201296	3.894095	3.723063
C	-0.025813	3.670984	3.085967
C	-0.418424	2.280467	2.732828
C	-1.285419	2.096102	1.585066
C	-1.605149	3.261809	0.765558
C	-1.556950	4.627248	1.363788
C	-0.763156	4.831767	2.522890
C	-1.389521	0.777857	1.002099
C	-1.560939	0.658172	-0.450452
C	-1.537004	1.853123	-1.256718
C	-1.732113	3.135783	-0.612546
C	-0.838294	1.844855	-2.520965
C	-0.488885	3.150399	-3.143587
C	-1.142284	4.337709	-2.724423
C	-1.795667	4.358657	-1.458726
C	-0.215873	0.684859	-2.971577
C	1.032003	0.802358	-3.776989
C	1.527333	2.098419	-4.063627
C	0.699731	3.239088	-3.911866
C	2.919328	2.286459	-4.197023
C	3.442240	3.598799	-4.178868
C	2.591042	4.702289	-4.427562
C	1.185033	4.518367	-4.290464
C	3.784674	1.188166	-4.001023
C	5.054878	1.414407	-3.425035
C	5.416948	2.727120	-3.055918
C	4.716027	3.822669	-3.597609
C	6.195030	2.921437	-1.895964
C	6.252786	4.205594	-1.320472
C	5.901232	5.339300	-2.094667
C	5.108154	5.142763	-3.263577
C	6.585827	1.797903	-1.137614
C	6.652590	1.906579	0.269754
C	6.343393	3.144071	0.874551
C	6.330164	4.320079	0.090675
C	5.738723	3.157298	2.149048
C	5.123336	4.354782	2.595371
C	5.449719	5.590877	1.977729
C	6.074697	5.572754	0.698250
C	5.497047	1.927178	2.811614
C	4.363485	1.849201	3.767720
C	3.525864	2.962089	3.910344
C	3.998991	4.289790	3.456414
C	1.760862	5.267666	3.773152
C	3.171082	5.433781	3.617060
C	-0.880816	-0.364784	1.737451
C	-0.497697	-0.577556	-2.335414
C	-1.192711	-0.598376	-1.083545
C	3.270618	-0.127894	-4.033378
C	1.876632	-0.327595	-3.911870
C	6.544632	0.517258	-1.725187
C	5.767886	0.322195	-2.889439
C	6.092851	0.727658	2.333728
C	6.685601	0.727911	1.049555
C	3.846588	0.515480	4.117570
C	-1.160357	-1.805143	-0.279186
C	-0.959948	-1.677673	1.156405
C	1.395064	-1.626269	-3.614397
C	0.154230	-1.770528	-2.804316
C	5.413485	-0.990880	-3.261555
C	4.144397	-1.221632	-3.838280
C	7.010290	-0.502795	0.434455
C	6.943035	-0.606487	-0.973251
C	4.735415	-0.644983	3.939882
C	5.860861	-0.518068	2.979263
C	-0.486727	-2.805256	1.886668
C	-0.108780	-2.993720	-2.189806
C	-0.777644	-3.032820	-0.916674
C	3.639936	-2.540062	-3.871716
C	2.251064	-2.749089	-3.738069
C	6.909781	-1.885493	-1.567528
C	6.133218	-2.080940	-2.728327
C	6.461403	-1.702250	2.481772
C	7.060544	-1.684694	1.204689
C	4.255171	-1.923445	4.249090
C	-0.632320	-4.219127	-0.114618
C	-0.490302	-4.113912	1.265222
C	1.788146	-4.051325	-3.420511
C	0.611582	-4.211543	-2.645770
C	5.792205	-3.394443	-3.106933
C	4.521154	-3.629382	-3.689838
C	7.403659	-2.907683	0.584831
C	7.324977	-3.009423	-0.827248
C	5.102555	-3.104893	3.966799
C	6.212200	-2.955630	3.097053
C	-0.063271	-5.316711	2.039494
C	0.322832	-5.470241	-2.058700
C	-0.323583	-5.510160	-0.789118
C	4.032872	-4.955633	-3.774417
C	2.631794	-5.172563	-3.635265
C	7.333211	-4.288720	-1.436840
C	6.543294	-4.487357	-2.607542
C	6.894776	-4.114871	2.642836
C	7.510363	-4.087908	1.358932
C	4.641148	-4.407810	4.297780
C	-0.351703	-6.666129	0.018728
C	-0.219184	-6.570485	1.412235
C	2.092328	-6.454738	-3.400585
C	0.951058	-6.602412	-2.611258
C	6.218414	-5.771917	-3.086476
C	4.971126	-6.004275	-3.670240
C	7.940319	-5.261880	0.704357
C	7.847692	-5.363148	-0.685229
C	5.555420	-5.468731	4.155109
C	6.680332	-5.320151	3.343610
C	-2.052656	5.687873	0.577495
C	-2.175388	5.554260	-0.813438
C	-0.398539	6.112116	2.989894
C	0.842924	6.326553	3.608350
C	3.739975	6.685862	3.316456
C	4.878103	6.763989	2.513471
C	6.160142	6.722795	-0.115109
C	6.068971	6.606815	-1.503652
C	4.432007	6.202238	-3.900248
C	3.181505	5.982669	-4.482154
C	0.291029	5.606857	-4.219593
C	-0.860040	5.519253	-3.436053
H	3.241949	-6.798596	4.760351
H	1.148499	-7.205910	3.705394
H	-0.296864	-7.655208	-0.410391
H	-0.075906	-7.492907	1.954587
H	2.614806	-7.356931	-3.678599
H	0.674087	-7.606090	-2.326186
H	6.833706	-6.633606	-2.876638
H	4.710274	-7.030744	-3.876677
H	8.196009	-6.160153	1.244605
H	8.030905	-6.332394	-1.123619
H	5.346990	-6.458306	4.532604
H	7.268517	-6.205373	3.158026
H	-2.192357	6.676364	0.988477
H	-2.399236	6.450468	-1.371990
H	-0.978433	6.988187	2.741590
H	1.127328	7.352292	3.787671
H	3.243886	7.613056	3.560127
H	5.187410	7.748918	2.199998
H	6.134992	7.720188	0.295719
H	5.972719	7.520105	-2.070982

H	4.766018	7.225446	-3.818890
H	2.637021	6.852405	-4.815867
H	0.533742	6.576500	-4.625924
H	-1.423364	6.427351	-3.283441
Pd	-3.370295	-1.927358	-1.064865
Pd	-4.816569	-0.876461	1.028270
Pd	-3.492034	1.407610	2.030702
Pd	-3.815119	0.851024	-0.892149
Pd	-5.294795	-0.711621	-2.827726
Pd	-6.500721	0.555147	-0.480744
Pd	-5.118017	2.826396	0.412728
Pd	-6.327429	-2.485460	-0.826382
Pd	-6.093697	1.064360	2.252229
C	-7.586574	-3.795588	0.654381
C	-8.483353	-3.263352	-0.263161
C	-9.491127	-2.160930	-0.000312
C	-7.440792	-3.396457	2.110724
H	-8.630925	-3.815108	-1.194945
H	-7.090435	-4.730911	0.377875
H	-8.011441	-4.089280	2.749984
H	-6.392256	-3.449128	2.428580
H	-7.800640	-2.381769	2.307186
H	-10.475166	-2.596757	0.235613
H	-9.199976	-1.515874	0.834891
H	-9.617818	-1.530341	-0.888230
H	-4.930554	-2.202372	-1.914849
H	-6.592308	-0.748112	-1.630038

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C	2.656543	-5.932993	4.452655
C	3.226149	-4.641726	4.459776
C	2.295335	-3.507443	4.237453
C	1.073501	-3.736273	3.592916
C	0.715065	-5.123662	3.201152
C	1.421794	-6.170726	3.828938
C	2.790545	-2.131624	4.387152
C	1.917801	-1.051195	4.187350
C	0.637092	-1.281560	3.458782
C	0.313503	-2.580351	3.051232
C	2.462779	0.317710	4.227526
C	1.551341	1.455246	4.007577
C	0.270255	1.209510	3.284401
C	-0.048449	-0.149800	2.878194
C	2.075126	2.755575	4.041737
C	1.210776	3.898076	3.717213
C	-0.016203	3.677917	3.079127
C	-0.412296	2.288256	2.726689
C	-1.279356	2.105372	1.578899
C	-1.597330	3.271261	0.759188
C	-1.544818	4.637118	1.356131
C	-0.750255	4.840345	2.514882
C	-1.387214	0.787140	0.997028
C	-1.563346	0.666269	-0.454412
C	-1.537089	1.860375	-1.261888
C	-1.727345	3.144052	-0.618551
C	-0.839318	1.849076	-2.526612
C	-0.486116	3.153254	-3.150034
C	-1.136080	4.342632	-2.731673
C	-1.789007	4.366196	-1.465738
C	-0.220109	0.686951	-2.976311
C	1.028972	0.800721	-3.780423
C	1.527309	2.094879	-4.069368
C	0.702731	3.237906	-3.918583
C	2.919601	2.278661	-4.204994
C	3.446159	3.589426	-4.188892
C	2.597730	4.695034	-4.437953
C	1.191288	4.515359	-4.299085
C	3.782211	1.178083	-4.008964
C	5.053499	1.401153	-3.434326
C	5.419198	2.713144	-3.066392
C	4.720977	3.810182	-3.608780
C	6.197629	2.906123	-1.906482
C	6.258662	4.190535	-1.331965
C	5.910190	5.324617	-2.107079
C	5.116686	5.129434	-3.275900
C	6.585294	1.782054	-1.147205
C	6.652264	1.891571	0.260091
C	6.346678	3.130398	0.863923
C	6.336359	4.305846	0.079088
C	5.743208	3.146427	2.138952
C	5.132014	4.346102	2.585031
C	5.461158	5.580710	1.965843
C	6.084660	5.559714	0.685721
C	5.498791	1.917603	2.802949
C	4.366505	1.843844	3.760921
C	3.532460	2.959352	3.903825
C	4.008927	4.285241	3.447964
C	1.774215	5.270090	3.765925
C	3.184722	5.431863	3.608724
C	-0.882406	-0.356359	1.733303
C	-0.505666	-0.574227	-2.339223
C	-1.199693	-0.591901	-1.086906
C	3.264425	-0.136462	-4.039193
C	1.870250	-0.331846	-3.914928
C	6.540779	0.501067	-1.733783
C	5.763690	0.307356	-2.897995
C	6.090564	0.715955	2.325508
C	6.682325	0.713418	1.040853
C	3.846213	0.511967	4.112801
C	-1.171012	-1.797950	-0.281438
C	-0.966454	-1.669430	1.153828
C	1.385501	-1.628847	-3.615695
C	0.143357	-1.769400	-2.806869
C	5.405485	-1.005039	-3.268895
C	4.135315	-1.232601	-3.844300
C	7.003437	-0.518698	0.426749
C	6.935940	-0.623262	-0.980895
C	4.731378	-0.651237	3.934894
C	5.855811	-0.528491	2.972499
C	-0.496121	-2.797808	1.884742
C	-0.123009	-2.991340	-2.191292
C	-0.792250	-3.027571	-0.918174
C	3.626942	-2.549567	-3.875837
C	2.237768	-2.754350	-3.739826
C	6.899174	-1.902655	-1.574161
C	6.122224	-2.096737	-2.734895
C	6.452470	-1.714827	2.475563
C	7.050686	-1.700136	1.197971
C	4.247881	-1.928018	4.245931
C	-0.648957	-4.213348	-0.114769
C	-0.504553	-4.107100	1.264745
C	1.771199	-4.055029	-3.421214
C	0.594556	-4.211409	-2.645848
C	5.777245	-3.409571	-3.112307
C	4.505132	-3.641311	-3.694061
C	7.390084	-2.924632	0.579072
C	7.311027	-3.027253	-0.832923
C	5.091506	-3.112141	3.963718
C	6.200460	-2.966890	3.092397
C	-0.080569	-5.310509	2.039787
C	0.302321	-5.468810	-2.057863
C	-0.344043	-5.505897	-0.788131
C	4.012817	-4.966199	-3.776922
C	2.611275	-5.178898	-3.636083
C	7.315547	-4.307055	-1.441541
C	6.525240	-4.504253	-2.612181
C	6.879259	-4.128505	2.638678
C	7.493735	-4.104550	1.354172
C	4.626711	-4.413400	4.296424
C	-0.374364	-6.661044	0.020745
C	-0.240480	-6.564436	1.413975
C	2.068222	-6.459328	-3.400135
C	0.927028	-6.603160	-2.609943
C	6.196464	-5.788244	-3.090015
C	4.948074	-6.017492	-3.672590
C	7.919777	-5.280395	0.700417
C	7.826646	-5.382487	-0.689046

C	5.537791	-5.477049	4.153926
C	6.662253	-5.332441	3.341052
C	-2.039141	5.698202	0.569520
C	-2.164747	5.563380	-0.821081
C	-0.382326	6.120056	2.980890
C	0.859382	6.331501	3.599748
C	3.756958	6.681954	3.306446
C	4.893870	6.755980	2.501428
C	6.172751	6.708882	-0.128629
C	6.081188	6.592089	-1.517043
C	4.443208	6.190220	-3.913345
C	3.191841	5.973599	-4.494551
C	0.300349	5.606427	-4.228621
C	-0.850592	5.522842	-3.444296
H	3.220577	-6.799623	4.762573
H	1.125702	-7.201798	3.707880
H	-0.321786	-7.650634	-0.407457
H	-0.099000	-7.486713	1.957051
H	2.587786	-7.363232	-3.678001
H	0.647222	-7.605865	-2.324237
H	6.809388	-6.651540	-2.879860
H	4.683994	-7.043416	-3.877624
H	8.172709	-6.179086	1.241278
H	8.006675	-6.352699	-1.126629
H	5.326876	-6.465603	4.532734
H	7.247888	-6.219449	3.155954
H	-2.176149	6.687366	0.979770
H	-2.387411	6.459465	-1.380342
H	-0.959510	6.997554	2.731253
H	1.146764	7.356645	3.777732
H	3.264102	7.610809	3.550353
H	5.205500	7.739719	2.186611
H	6.150197	7.706674	0.281302
H	5.987245	7.505161	-2.085093
H	4.780055	7.212578	-3.833060
H	2.649630	6.844411	-4.829191
H	0.545553	6.574953	-4.636150
H	-1.411257	6.432657	-3.292119
Pd	-3.381202	-1.920816	-1.039321
Pd	-4.810283	-0.842155	1.051279
Pd	-3.489407	1.437024	2.037297
Pd	-3.818038	0.871336	-0.890780
Pd	-5.315741	-0.717627	-2.799353
Pd	-6.506243	0.581912	-0.455999
Pd	-5.115699	2.853839	0.418824
Pd	-6.327959	-2.458017	-0.745692
Pd	-6.083061	1.101533	2.276256
C	-7.645721	-3.760240	0.668575
C	-8.466290	-2.743710	0.200949
C	-9.450956	-2.895221	-0.945307
C	-6.984916	-3.778228	2.036668
H	-6.606593	-0.704526	-1.608990
H	-7.662007	-4.715388	0.134857
H	-7.555162	-4.428871	2.719254
H	-5.962516	-4.173544	1.990268
H	-6.944895	-2.774351	2.476095
H	-10.471340	-3.018625	-0.548540
H	-9.219673	-3.772723	-1.561641
H	-9.457090	-2.011425	-1.594040
H	-4.954158	-2.200860	-1.869923
H	-8.586045	-1.853068	0.821005

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C	1.866575	5.848521	-4.602067
C	2.612061	4.650369	-4.572632
C	1.848877	3.402584	-4.321435
C	0.600561	3.474045	-3.691345
C	0.046140	4.806639	-3.340450
C	0.605465	5.926380	-3.990824
C	2.534582	2.106827	-4.427730
C	1.821230	0.920231	-4.200586
C	0.508440	0.986814	-3.496337
C	0.002822	2.236912	-3.126531
C	2.553352	-0.358324	-4.194840
C	1.808485	-1.606395	-3.949437
C	0.488070	-1.525694	-3.259307
C	-0.026350	-0.217078	-2.898052
C	2.510164	-2.819909	-3.939849
C	1.809910	-4.064672	-3.596906
C	0.548976	-4.005432	-2.989985
C	-0.047909	-2.678097	-2.681129
C	-0.945594	-2.592252	-1.552425
C	-1.112188	-3.764279	-0.709489
C	-0.860984	-5.125619	-1.266013
C	-0.025066	-5.245384	-2.406919
C	-1.284149	-1.289941	-1.020737
C	-1.440618	-1.153386	0.446362
C	-1.210526	-2.309757	1.267510
C	-1.243889	-3.618785	0.668448
C	-0.553615	-2.165645	2.535117
C	-0.031570	-3.385370	3.206025
C	-0.497350	-4.666593	2.815028
C	-1.132274	-4.815534	1.548101
C	-0.126039	-0.910613	2.969387
C	1.106520	-0.818410	3.799428
C	1.784005	-2.018378	4.130290
C	1.138823	-3.274161	3.998469
C	3.185964	-1.993296	4.286388
C	3.897581	-3.213552	4.316376
C	3.215026	-4.423372	4.589742
C	1.800704	-4.455852	4.423100
C	3.882061	-0.785224	4.063117
C	5.179352	-0.838677	3.505663
C	5.736651	-2.094270	3.183290
C	5.198661	-3.263936	3.755299
C	6.548980	-2.207877	2.036158
C	6.800899	-3.486898	1.502704
C	6.611336	-4.635387	2.310914
C	5.785844	-4.521262	3.468104
C	6.779790	-1.063176	1.244734
C	6.879393	-1.204486	-0.157801
C	6.759406	-2.491855	-0.724602
C	6.908072	-3.632532	0.096399
C	6.176973	-2.631987	-2.001801
C	5.744082	-3.918959	-2.412601
C	6.237539	-5.075312	-1.753039
C	6.842111	-4.927193	-0.472122
C	5.769501	-1.470727	-2.705900
C	4.647555	-1.586439	-3.671577
C	3.979696	-2.812041	-3.783900
C	4.632163	-4.043187	-3.283369
C	2.563146	-5.343481	-3.596789
C	3.979651	-5.299054	-3.415434
C	-0.909354	-0.100067	-1.776091
C	-0.582889	0.271996	2.294290
C	-1.250920	0.152314	1.038867
C	3.178493	0.440713	4.047805
C	1.771954	0.428047	3.908302
C	6.543009	0.215088	1.789881
C	5.729877	0.329654	2.939940
C	6.181602	-0.183542	-2.263314
C	6.751647	-0.058136	-0.975015
C	3.949011	-0.352330	-4.067711
C	-1.415144	1.331877	0.207419
C	-1.171382	1.201987	-1.224533
C	1.107046	1.631892	3.565831
C	-0.130339	1.567694	2.740179
C	5.179944	1.586844	3.264829
C	3.883321	1.645137	3.823258
C	6.886054	1.225106	-0.397258
C	6.782939	1.361371	1.005501
C	4.660385	0.928815	-3.922782
C	5.781428	0.995084	-2.951122
C	-0.844071	2.368172	-1.974110
C	-0.576882	2.718634	2.101443
C	-1.251266	2.625359	0.823025
C	3.189052	2.874770	3.809490

C	1.785909	2.871818	3.660984
C	6.552819	2.639360	1.556919
C	5.737911	2.754147	2.702129
C	6.199302	2.268377	-2.487845
C	6.776228	2.377427	-1.205129
C	4.004718	2.114816	-4.275560
C	-1.247306	3.799182	-0.019362
C	-1.046829	3.677753	-1.390516
C	1.137825	4.080937	3.302729
C	-0.045680	4.042700	2.522063
C	5.200941	4.013964	3.033273
C	3.901652	4.076290	3.597877
C	6.928224	3.655920	-0.621903
C	6.810754	3.788680	0.784894
C	4.670762	3.413923	-4.027025
C	5.780542	3.452939	-3.145865
C	-0.784906	4.908638	-2.193554
C	-0.512381	5.228222	1.897499
C	-1.141303	5.138623	0.621453
C	3.221813	5.317609	3.636513
C	1.804981	5.320358	3.486705
C	6.620331	5.073524	1.351604
C	5.789632	5.189824	2.505157
C	6.283171	4.712042	-2.724097
C	6.875449	4.814635	-1.433202
C	4.029829	4.626166	-4.400823
C	-1.318910	6.255499	-0.221554
C	-1.137831	6.142606	-1.608269
C	1.082590	6.501084	3.215481
C	-0.063554	6.455698	2.420872
C	5.270937	6.426610	2.936845
C	3.995612	6.489949	3.502614
C	7.117924	6.058511	-0.812439
C	6.985599	6.188117	0.571585
C	4.781642	5.811037	-4.289202
C	5.907515	5.851104	-3.466507
C	-1.201272	-6.223690	-0.449533
C	-1.339447	-6.070320	0.937781
C	0.531139	-6.471306	-2.828516
C	1.804467	-6.519709	-3.416774
C	4.717589	-6.446207	-3.067181
C	5.844941	-6.334696	-2.252933
C	7.086742	-6.026851	0.377698
C	6.967634	-5.882479	1.761432
C	5.265996	-5.648448	4.134558
C	3.988014	-5.598954	4.695536
C	1.081328	-5.667864	4.367011
C	-0.054031	-5.774123	3.562737
H	2.305765	6.777787	-4.931838
H	0.166957	6.908488	-3.898483
H	-1.419073	7.253272	0.178325
H	-1.118550	7.060882	-2.175613
H	1.463375	7.478099	3.469742
H	-0.485301	7.398883	2.107924
H	5.754106	7.363002	2.702772
H	3.583288	7.472643	3.671525
H	7.249118	6.967373	-1.378966
H	7.017218	7.186875	0.979820
H	4.437716	6.747686	-4.701101
H	6.361525	6.816718	-3.306691
H	-1.195959	-7.233125	-0.832637
H	-1.433564	-6.973316	1.521687
H	0.078047	-7.415027	-2.564455
H	2.237771	-7.497797	-3.560784
H	4.362599	-7.442403	-3.283184
H	6.287353	-7.254751	-1.904065
H	7.210956	-7.029411	-0.001360
H	6.999849	-6.782129	2.357076
H	5.749769	-6.612460	4.091553
H	3.573264	-6.528531	5.053611
H	1.458359	-6.579723	4.803564
H	-0.471938	-6.760132	3.427539
Pd	-3.550178	1.836507	0.866915
Pd	-4.698862	0.591989	-1.438565
Pd	-3.361838	-1.786205	-1.846545
Pd	-3.768396	-1.045271	0.676992
Pd	-5.474361	0.189125	2.407385
Pd	-6.562419	-0.769006	0.127627
Pd	-5.290349	-3.091039	-0.321940
Pd	-6.281545	1.993675	0.342468
Pd	-6.091424	-1.512822	-2.358859
C	-6.931154	3.848268	0.987907
C	-7.370181	3.911344	2.455758
C	-8.482587	2.925012	2.874120
C	-8.020094	4.115544	-0.059066
H	-7.722176	4.942817	2.652421
H	-6.042242	4.473161	0.820732
H	-8.455219	5.119074	0.100719
H	-7.618772	4.102956	-1.081771
H	-8.848831	3.397670	0.002205
H	-9.406426	3.080908	2.301732
H	-8.155066	1.888298	2.718213
H	-8.725382	3.050696	3.937509
H	-5.182716	1.806430	1.726128
H	-6.490292	3.757193	3.093003

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C	-0.402051	5.966226	3.840634
C	-2.368953	2.181413	4.398714
C	-1.679590	0.981059	4.167588
C	-0.391737	1.018688	3.417214
C	0.118544	2.256079	3.012241
C	-2.429608	-0.286654	4.204021
C	-1.710272	-1.549072	3.954171
C	-0.413988	-1.497345	3.217590
C	0.105543	-0.201040	2.819585
C	-2.429465	-2.752054	3.983890
C	-1.758258	-4.011603	3.636810
C	-0.516932	-3.979259	2.988785
C	0.087785	-2.665233	2.641205
C	0.953641	-2.609485	1.484527
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C	0.821801	-5.144912	1.237666
C	0.020544	-5.235731	2.405884
C	1.289113	-1.318863	0.920107
C	1.403773	-1.206728	-0.550628
C	1.137264	-2.370653	-1.346168
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C	0.448211	-2.235555	-2.597732
C	-0.112851	-3.456989	-3.233187
C	0.346087	-4.739216	-2.837683
C	1.015713	-4.879398	-1.587870
C	0.026176	-0.980778	-3.038554
C	-1.232928	-0.882391	-3.827579
C	-1.937190	-2.076919	-4.119824
C	-1.305825	-3.339888	-3.990299
C	-3.342762	-2.033728	-4.233117
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C	-3.415427	-4.467257	-4.499897
C	-1.997164	-4.517751	-4.377059
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C	-5.294850	-0.839104	-3.409439
C	-5.859633	-2.081700	-3.051639
C	-5.355892	-3.267243	-3.622229
C	-6.637904	-2.166860	-1.878714
C	-6.891313	-3.434225	-1.318778
C	-6.742755	-4.596951	-2.115106
C	-5.951547	-4.511656	-3.298460
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C	-6.886754	-1.127059	0.309054
C	-6.767903	-2.407672	0.891154
C	-6.957646	-3.557838	0.092169

C	-6.149347	-2.537756	2.152348
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C	-6.893032	-4.844914	0.677790
C	-5.704221	-1.372582	2.826516
C	-4.555947	-1.490894	3.760546
C	-3.902858	-2.724518	3.871547
C	-4.587814	-3.952906	3.408921
C	-2.529311	-5.279031	3.678778
C	-3.949911	-5.216267	3.540198
C	0.953356	-0.112997	1.669126
C	0.521357	0.204344	-2.395432
C	1.222312	0.091976	-1.157215
C	-3.293505	0.403091	-4.030428
C	-1.883774	0.371907	-3.933561
C	-6.590372	0.259099	-1.668942
C	-5.811302	0.345203	-2.844757
C	-6.110879	-0.086063	2.377120
C	-6.717867	0.028978	1.104818
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C	1.219150	1.176251	1.091653
C	-1.191560	1.570741	-3.630041
C	0.072583	1.500379	-2.846018
C	-5.253734	1.589452	-3.204688
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C	-6.851775	1.305529	0.512349
C	-6.789944	1.419964	-0.894778
C	-4.525315	1.027589	3.974342
C	-5.673542	1.096327	3.035049
C	0.930341	2.358199	1.832658
C	0.554503	2.653582	-2.237918
C	1.264273	2.568529	-0.978435
C	-3.262084	2.840245	-3.827890
C	-1.855209	2.818962	-3.722526
C	-6.558855	2.686371	-1.471905
C	-5.777687	2.772770	-2.642801
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C	-6.701077	2.467659	1.299253
C	-3.842818	2.208812	4.290144
C	1.300652	3.754186	-0.153259
C	1.135864	3.655830	1.224359
C	-1.178851	4.023594	-3.403277
C	0.028741	3.979320	-2.660619
C	-5.233099	4.019717	-3.008520
C	-3.950680	4.054935	-3.612636
C	-6.852891	3.739647	0.701921
C	-6.776829	3.850338	-0.709612
C	-4.497607	3.513925	4.041859
C	-5.632303	3.556453	3.193140
C	0.916811	4.902008	2.016354
C	0.531361	5.166603	-2.068042
C	1.197587	5.085641	-0.810578
C	-3.254776	5.285521	-3.690306
C	-1.834010	5.269825	-3.584365
C	-6.585791	5.123941	-1.300951
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C	-6.129500	4.816559	2.767734
C	-6.759114	4.909083	1.493841
C	-3.828741	4.722019	4.378214
C	1.417021	6.211454	0.010446
C	1.272668	6.121575	1.403264
C	-1.086933	6.443721	-3.353027
C	0.083195	6.392977	-2.594388
C	-5.265929	6.434262	-2.945841
C	-4.007498	6.470819	-3.550489
C	-7.003021	6.147242	0.862196
C	-6.911494	6.254849	-0.526995
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C	-5.715666	5.960693	3.481440
C	1.121426	-6.259631	0.427732
C	1.221740	-6.128269	-0.965120
C	-0.539204	-6.447256	2.863037
C	-1.793604	-6.468656	3.492127
C	-4.714647	-6.357230	3.231749
C	-5.864076	-6.240833	2.449674
C	-7.178589	-5.953149	-0.147769
C	-7.099704	-5.830612	-1.536481
C	-5.468223	-5.655852	-3.963395
C	-4.207651	-5.633010	-4.564056
C	-1.293312	-5.739095	-4.326066
C	-0.135317	-5.850564	-3.555564
H	-2.058660	6.855861	4.823416
H	0.046987	6.940394	3.719249
H	1.522069	7.201457	-0.407135
H	1.284430	7.047926	1.957473
H	-1.461941	7.422542	-3.608958
H	0.527256	7.334235	-2.307761
H	-5.728554	7.380895	-2.711388
H	-3.586691	7.444844	-3.746490
H	-7.104121	7.066068	1.418721
H	-6.941802	7.247876	-0.949079
H	-4.197056	6.853573	4.658159
H	-6.160221	6.930494	3.320464
H	1.112431	-7.263272	0.825609
H	1.285316	-7.040870	-1.538038
H	-0.108302	-7.401174	2.598653
H	-2.236053	-7.438109	3.664007
H	-4.367998	-7.355304	3.452581
H	-6.330297	-7.159181	2.128378
H	-7.305080	-6.948215	0.249768
H	-7.162929	-6.738252	-2.117350
H	-5.963694	-6.612101	-3.890839
H	-3.817169	-6.573711	-4.920341
H	-1.696246	-6.651324	-4.737933
H	0.272867	-6.840467	-3.419023
Pd	3.551328	1.752392	-1.015907
Pd	4.630085	0.536762	1.350119
Pd	3.344029	-1.880129	1.722073
Pd	3.792353	-1.106895	-0.797412
Pd	5.553596	0.164670	-2.459319
Pd	6.576876	-0.776339	-0.152664
Pd	5.333291	-3.113906	0.225922
Pd	6.246219	1.976137	-0.352440
Pd	6.044107	-1.543315	2.313321
C	6.965291	3.793212	-1.033835
C	8.398208	3.746144	-0.485189
C	9.395648	2.964692	-1.366421
C	6.070113	4.884964	-0.443160
H	8.392865	3.323985	0.539506
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H	6.462126	5.880823	-0.718660
H	5.043626	4.812296	-0.818395
H	6.037926	4.841892	0.654732
H	9.072397	1.924856	-1.502731
H	9.477023	3.423338	-2.361112
H	10.396188	2.953524	-0.915451
H	5.233318	1.785682	-1.806997
H	8.753649	4.784850	-0.353189

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C	-1.737981	5.165660	-2.881342
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C	-0.677616	5.449183	-3.741999
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C	-2.134204	2.562065	-0.124714
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C	-1.218424	1.567710	1.970217
C	-1.139594	0.287252	1.339373
C	-1.396287	0.187034	-0.075992
C	-0.475431	-0.801272	2.006811
C	0.380443	-0.521838	3.122977

C	0.524853	0.848270	3.558821
C	-0.344188	1.835160	3.075729
C	1.263873	-1.562998	3.604859
C	2.550191	-1.167213	4.248048
C	2.889124	0.266930	4.307758
C	1.804697	1.261186	4.203482
C	1.105153	-2.877046	3.157324
C	2.066122	-3.924734	3.587856
C	3.287675	-3.538648	4.153481
C	3.585930	-2.110167	4.331181
C	1.885858	-5.334652	3.156459
C	2.785598	-6.285997	3.681430
C	4.017023	-5.888584	4.225414
C	4.389593	-4.527545	4.253019
C	4.980778	-1.685117	4.088138
C	5.963912	-2.719245	3.690568
C	5.723828	-4.085979	3.997972
C	0.254431	-3.171243	2.033691
C	0.388725	-4.441787	1.357429
C	1.039189	-5.596002	2.046300
C	5.243808	-0.340631	3.798083
C	4.214657	0.670379	4.094290
C	-0.414162	-2.094872	1.379718
C	4.502418	2.075920	3.761393
C	3.527386	3.048519	4.014228
C	2.131426	2.624189	4.250828
C	1.085094	3.633263	4.034137
C	-0.139404	3.252399	3.469722
C	3.766017	4.444930	3.582693
C	2.797209	5.448862	3.852782
C	1.442331	5.071926	4.102126
C	0.371605	5.988406	4.044547
C	-0.867212	5.612843	3.503372
C	-1.077997	4.307578	3.009896
C	-1.935060	4.020922	1.914022
C	-2.839046	4.921687	-0.176900
C	-2.626563	5.025623	1.205687
C	-0.685896	-2.199764	-0.039605
C	-0.968454	-0.992742	-0.786308
C	-0.415078	-0.842531	-2.106215
C	-0.368079	0.465988	-2.696747
C	0.780398	0.794158	-3.585539
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C	0.360973	-1.911623	-2.669914
C	1.501233	-1.559726	-3.561021
C	1.766326	-0.194069	-3.832984
C	3.103954	0.213573	-4.039900
C	3.422807	1.589610	-3.983136
C	2.395091	2.554337	-4.067540
C	2.722375	3.928066	-4.027029
C	1.703635	4.901418	-4.163080
C	4.686232	1.981185	-3.486204
C	4.881430	3.319917	-3.085293
C	3.990883	4.317720	-3.527989
C	4.212194	5.669370	-3.164374
C	3.343393	6.638143	-3.704544
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C	4.139259	-0.745166	-3.953421
C	5.400543	-0.348977	-3.454363
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C	6.412961	1.257267	-1.934465
C	6.313292	2.509807	-1.295696
C	5.708137	3.587979	-1.974750
C	5.623694	4.846992	-1.349087
C	5.054489	5.941594	-2.046257
C	6.471970	2.581008	0.106687
C	6.036074	3.739247	0.785550
C	5.792285	4.925359	0.056595
C	5.407528	6.106543	0.735031
C	5.262147	7.282438	-0.031543
C	5.081875	7.199799	-1.413700
C	7.025703	0.180475	-1.262389
C	7.185633	0.246818	0.140082
C	6.735654	1.395502	0.830047
C	6.253228	1.266828	2.153409
C	5.531174	2.349739	2.725898
C	5.539222	3.622493	2.100741
C	4.796034	4.701743	2.643187
C	4.890447	5.991512	2.056902
C	3.153917	6.779991	3.565616
C	4.200832	7.050218	2.684178
C	6.256566	-0.019164	2.760347
C	0.336925	-3.173697	-2.076083
C	-0.199749	-3.342798	-0.752993
C	3.830442	-2.122064	-4.010099
C	2.500549	-2.538744	-3.789683
C	7.133222	-1.068839	-1.908431
C	6.308577	-1.337887	-3.020346
C	6.980176	-1.085342	2.168607
C	7.466754	-0.938837	0.852495
C	0.164146	-4.519748	-0.016584
C	2.258769	-3.904003	-3.490624
C	1.185633	-4.258239	-2.634363
C	6.134961	-2.673774	-3.432488
C	4.871759	-3.074536	-3.936615
C	7.933979	-2.076881	0.156751
C	7.762244	-2.142807	-1.249248
C	6.965796	-2.380467	2.746362
C	1.131515	-5.561212	-2.076368
C	0.599964	-5.731704	-0.764642
C	4.576201	-4.455057	-4.043558
C	3.236938	-4.881210	-3.811502
C	7.910126	-3.385689	-1.913657
C	7.072095	-3.659599	-3.034679
C	7.770355	-3.411163	2.192663
C	8.271323	-3.252595	0.868991
C	0.795421	-6.904983	-0.006650
C	1.015640	-6.837264	1.377162
C	2.910815	-6.235233	-3.586807
C	1.871261	-6.572158	-2.718812
C	6.902574	-4.961222	-3.546559
C	5.661966	-5.356053	-4.051885
C	8.814595	-4.328201	0.134496
C	8.630814	-4.396454	-1.248050
C	6.767375	-4.995224	3.741321
C	7.789895	-4.656454	2.854946
Pd	-4.123946	2.210706	0.847028
Pd	-6.661452	1.403787	1.571556
Pd	-6.242269	2.165074	-0.983234
Pd	-6.741978	-0.372914	-0.367967
Pd	-5.796248	-3.044506	0.145926
C	-7.713179	-3.914139	1.130248
C	-8.888970	-2.959110	1.006952
Pd	-4.147411	0.428583	-1.122814
Pd	-5.424603	-1.561635	-2.370232
Pd	-3.102768	-2.211433	-0.637025
Pd	-4.704972	-0.611096	1.368998
C	-6.713063	-3.816637	2.090757
H	-6.695747	-2.990637	2.799614
H	4.725024	-6.671499	4.451254
H	2.636287	-7.344696	3.532113
H	0.955960	-7.861676	-0.480262
H	1.326883	-7.747049	1.868087
H	3.535634	-7.041868	-3.937790
H	1.768560	-7.613183	-2.452381
H	7.650620	-5.728757	-3.418318
H	5.537927	-6.402313	-4.284999
H	9.239164	-5.195854	0.615154
H	8.918699	-5.312938	-1.740335
H	6.735342	-6.016124	4.090565
H	8.483325	-5.438665	2.587989
H	-2.855108	5.977737	1.659833
H	-3.210122	5.803860	-0.675799
H	-1.586248	6.400864	3.338676
H	0.516594	7.038628	4.247653
H	2.550383	7.615794	3.885627
H	4.338893	8.079448	2.391602
H	5.124929	8.251337	0.422945
H	4.811236	8.107059	-1.932207
H	3.531217	7.696167	-3.602460
H	1.407497	7.046211	-4.459171
H	-0.611490	6.456903	-4.121943
H	-2.416937	5.973354	-2.654261
H	-7.811068	-4.853859	0.578081
H	-6.054009	-4.655808	2.307483
C	-10.188571	-3.580767	1.582188
H	-8.662221	-2.020583	1.530156
H	-9.055806	-2.705724	-0.049910

H	-4.685429	-2.745756	-1.265879
H	-11.031131	-2.886280	1.468434
H	-10.445914	-4.512725	1.060539
H	-10.073033	-3.810385	2.649109
H	-4.138373	-2.114279	0.831820

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C	-1.140692	6.034231	4.276960
C	-1.963712	4.890159	4.352998
C	-1.303749	3.583114	4.110355
C	-0.100607	3.541646	3.395799
C	0.515554	4.816880	2.948158
C	0.077374	5.999091	3.580617
C	-2.064289	2.343359	4.322151
C	-1.447732	1.101490	4.105736
C	-0.183995	1.047156	3.316157
C	0.374889	2.243165	2.852849
C	-2.261432	-0.122290	4.206752
C	-1.618536	-1.428654	3.975387
C	-0.342940	-1.470426	3.202359
C	0.231632	-0.214623	2.745938
C	-2.399005	-2.589284	4.067650
C	-1.806703	-3.893635	3.744640
C	-0.583268	-3.949590	3.064488
C	0.081394	-2.681775	2.657192
C	0.915843	-2.711468	1.473599
C	0.929760	-3.925788	0.672055
C	0.626962	-5.240408	1.308658
C	-0.133763	-5.251201	2.506774
C	1.297603	-1.456342	0.849077
C	1.324438	-1.394658	-0.627895
C	0.968134	-2.564518	-1.370645
C	0.958926	-3.846719	-0.716500
C	0.247596	-2.430282	-2.604372
C	-0.398154	-3.637755	-3.182544
C	0.003457	-4.930671	-2.760092
C	0.708433	-5.069446	-1.529598
C	-0.118304	-1.168380	-3.070789
C	-1.393663	-1.024178	-3.825118
C	-2.171508	-2.186268	-4.057246
C	-1.606214	-3.477931	-3.906751
C	-3.575737	-2.068911	-4.126664
C	-4.368999	-3.236068	-4.055313
C	-3.789454	-4.501609	-4.313820
C	-2.372856	-4.626914	-4.233679
C	-4.172042	-0.806430	-3.916565
C	-5.430648	-0.744576	-3.277246
C	-6.049066	-1.942992	-2.862023
C	-5.630685	-3.170783	-3.411791
C	-6.788035	-1.950667	-1.660933
C	-7.088230	-3.185219	-1.052831
C	-7.032124	-4.377195	-1.817056
C	-6.280980	-4.370380	-3.029183
C	-6.886891	-0.760254	-0.910569
C	-6.899234	-0.835027	0.500552
C	-6.826389	-2.102622	1.117800
C	-7.107170	-3.263683	0.362747
C	-6.167866	-2.229058	2.358960
C	-5.794116	-3.524465	2.800178
C	-6.407301	-4.670492	2.229092
C	-7.088205	-4.534679	0.985570
C	-5.637314	-1.070330	2.980092
C	-4.462773	-1.222823	3.875561
C	-3.871883	-2.485847	4.002481
C	-4.636643	-3.688653	3.602469
C	-2.643157	-5.115316	3.850497
C	-4.062311	-4.980069	3.752748
C	1.047571	-0.206072	1.569944
C	0.464828	0.006060	-2.482551
C	1.207370	-0.110280	-1.270290
C	-3.387241	0.366166	-4.001572
C	-1.978687	0.260178	-3.948656
C	-6.602101	0.474116	-1.529075
C	-5.862028	0.482475	-2.732867
C	-5.992555	0.222548	2.505902
C	-6.639659	0.333007	1.253153
C	-3.659003	-0.024773	4.168279
C	1.541970	1.092681	-0.514864
C	1.364452	1.046218	0.941919
C	-1.212697	1.427286	-3.704242
C	0.071859	1.311310	-2.959004
C	-5.250749	1.682838	-3.149991
C	-3.992522	1.625604	-3.790197
C	-6.727210	1.597046	0.626065
C	-6.710564	1.666509	-0.785256
C	-4.292256	1.295253	4.010102
C	-5.469473	1.398333	3.110808
C	1.152201	2.265666	1.647148
C	0.639570	2.454993	-2.409578
C	1.407748	2.372656	-1.184351
C	-3.216996	2.802371	-3.877359
C	-1.810606	2.706517	-3.816550
C	-6.432132	2.900721	-1.409384
C	-5.689585	2.909326	-2.608211
C	-5.832451	2.676968	2.616953
C	-6.486111	2.771908	1.370419
C	-3.537537	2.446699	4.264967
C	1.523366	3.580467	-0.394789
C	1.400009	3.533135	0.988614
C	-1.059468	3.881067	-3.560841
C	0.169731	3.793746	-2.858828
C	-5.091263	4.112864	-3.030993
C	-3.830995	4.059075	-3.678744
C	-6.590987	4.032211	0.739092
C	-6.559306	4.096935	-0.676980
C	-4.131619	3.777231	4.000283
C	-5.292923	3.856134	3.191148
C	1.272409	4.812645	1.747054
C	0.757537	4.970488	-2.326704
C	1.463304	4.894604	-1.091051
C	-3.072756	5.246351	-3.819672
C	-1.652080	5.155220	-3.762503
C	-6.320431	5.340070	-1.314077
C	-5.562176	5.348640	-2.522081
C	-5.737921	5.128295	2.744501
C	-6.406421	5.217585	1.490364
C	-3.388313	4.956809	4.275680
C	1.766057	6.032942	-0.315227
C	1.666952	5.993196	1.083578
C	-0.834208	6.292601	-3.599035
C	0.358363	6.201757	-2.880444
C	-4.990338	6.526283	-3.042993
C	-3.754494	6.475116	-3.691671
C	-6.605143	6.448166	0.828745
C	-6.556754	6.509561	-0.565422
C	-4.066047	6.185078	4.158523
C	-5.239149	6.268587	3.408288
C	0.830211	-6.393344	0.522890
C	0.874847	-6.308824	-0.876461
C	-0.743117	-6.415363	3.020049
C	-1.977870	-6.348524	3.683760
C	-4.896467	-6.086872	3.505404
C	-6.065988	-5.931873	2.760524
C	-7.464541	-5.649307	0.206326
C	-7.432861	-5.571902	-1.187531
C	-5.884001	-5.558600	-3.673643
C	-4.645516	-5.623185	-4.315721
C	-1.735486	-5.883331	-4.164237
C	-0.561135	-6.035191	-3.426044
H	-1.493989	7.004739	4.590782
H	0.572042	6.943932	3.413453
H	1.905657	7.003034	-0.767804
H	1.746164	6.934057	1.606900
H	-1.164141	7.281571	-3.877068
H	0.864331	7.125598	-2.643807
H	-5.391743	7.503644	-2.822310
H	-3.288620	7.418113	-3.932350

H	-6.636422	7.387182	1.359265
H	-6.547937	7.489889	-1.017167
H	-3.634248	7.112018	4.504370
H	-5.638027	7.255732	3.233519
H	0.784554	-7.382737	0.952799
H	0.865415	-7.240233	-1.421904
H	-0.371905	-7.399184	2.775078
H	-2.466075	-7.286505	3.900542
H	-4.595352	-7.095320	3.744940
H	-6.591157	-6.832902	2.484325
H	-7.628975	-6.623801	0.639370
H	-7.567024	-6.491240	-1.737135
H	-6.427752	-6.483467	-3.554588
H	-4.318983	-6.594123	-4.654810
H	-2.200811	-6.784134	-4.533374
H	-0.203636	-7.041622	-3.270092
Pd	3.607702	1.492025	-1.175960
Pd	4.473348	0.334928	1.174862
Pd	3.273819	-2.134587	1.575504
Pd	3.783015	-1.301402	-1.033958
Pd	5.582753	0.035594	-2.477692
Pd	6.649608	-0.969602	-0.280543
Pd	5.301608	-3.235335	0.006328
Pd	6.251332	1.654274	-0.327805
Pd	5.927807	-1.629404	2.181844
C	6.483183	4.910110	-0.432890
C	8.011964	4.885566	-0.201532
C	8.466106	3.855414	0.853676
C	5.659701	5.399012	0.776310
H	8.345550	5.890691	0.100771
H	6.257425	5.540546	-1.306097
H	5.939086	6.426932	1.047657
H	4.587276	5.386142	0.546930
H	5.814617	4.761633	1.655559
H	8.072414	4.087638	1.851002
H	8.112101	2.840458	0.583835
H	9.560868	3.809835	0.923096
H	6.143488	3.886642	-0.711742
H	8.512222	4.663267	-1.155990

TS *cis*-but-2-ene/$Pd_9(H_2)$/nanotube → pre-*cis*/$Pd_9(H)$/nanotube

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C	-1.294581	5.981580	4.374499
C	-2.097089	4.821602	4.427462
C	-1.410018	3.529981	4.177892
C	-0.198514	3.519628	3.476541
C	0.397883	4.811411	3.049248
C	-0.068598	5.977514	3.691095
C	-2.149656	2.273650	4.366014
C	-1.507399	1.046030	4.141824
C	-0.236520	1.025365	3.362123
C	0.305545	2.237154	2.921551
C	-2.299736	-0.193896	4.218444
C	-1.630507	-1.484979	3.975847
C	-0.350412	-1.491962	3.209457
C	0.203971	-0.221284	2.775532
C	-2.390190	-2.661265	4.044439
C	-1.771470	-3.949625	3.706226
C	-0.545132	-3.972595	3.029925
C	0.096766	-2.687018	2.643685
C	0.934852	-2.683123	1.464715
C	0.988541	-3.886038	0.650682
C	0.704368	-5.215065	1.266260
C	-0.066880	-5.257300	2.457077
C	1.300321	-1.413933	0.865785
C	1.361030	-1.330784	-0.609941
C	1.034067	-2.497645	-1.374404
C	1.040689	-3.788387	-0.736430
C	0.317072	-2.360904	-2.610601
C	-0.301223	-3.573097	-3.209448
C	0.123642	-4.863280	-2.802053
C	0.821854	-5.004677	-1.568062
C	-0.072738	-1.100570	-3.063412
C	-1.345971	-0.971982	-3.824648
C	-2.097730	-2.146037	-4.078578
C	-1.507451	-3.427848	-3.940263
C	-3.503228	-2.055559	-4.160059
C	-4.273392	-3.239045	-4.110551
C	-3.666268	-4.489394	-4.379754
C	-2.248089	-4.587417	-4.288918
C	-4.126652	-0.807782	-3.940062
C	-5.391525	-0.779053	-3.311026
C	-5.988998	-1.994799	-2.915896
C	-5.541523	-3.206994	-3.477392
C	-6.737062	-2.032421	-1.721040
C	-7.017647	-3.280322	-1.131114
C	-6.931376	-4.461180	-1.909764
C	-6.170669	-4.424067	-3.115360
C	-6.865560	-0.853819	-0.956601
C	-6.887928	-0.946752	0.453327
C	-6.796235	-2.220410	1.055309
C	-7.047674	-3.377049	0.283166
C	-6.147442	-2.349813	2.301313
C	-5.754300	-3.643391	2.730689
C	-6.340055	-4.793536	2.139243
C	-7.010305	-4.655223	0.890267
C	-5.644598	-1.189141	2.941796
C	-4.476701	-1.330792	3.847814
C	-3.864031	-2.584228	3.965764
C	-4.602371	-3.796004	3.543089
C	-2.584929	-5.188283	3.789530
C	-4.005411	-5.078330	3.682568
C	1.024796	-0.182707	1.603003
C	0.478714	0.077366	-2.453635
C	1.209066	-0.038491	-1.233126
C	-3.364819	0.381266	-4.003417
C	-1.955207	0.302272	-3.938552
C	-6.600684	0.393739	-1.557218
C	-5.851750	0.432238	-2.754938
C	-6.019260	0.102620	2.479902
C	-6.657279	0.216426	1.222753
C	-3.698454	-0.121688	4.164182
C	1.483229	1.157569	-0.454911
C	1.318554	1.085472	0.993987
C	-1.214840	1.481071	-3.672793
C	0.064233	1.379934	-2.917112
C	-5.261296	1.649850	-3.151871
C	-3.996745	1.625918	-3.781640
C	-6.764297	1.486362	0.610908
C	-6.738589	1.574124	-0.799266
C	-4.354140	1.188309	4.014279
C	-5.523955	1.280416	3.104074
C	1.089111	2.290087	1.719901
C	0.602491	2.526234	-2.344676
C	1.346562	2.438316	-1.104985
C	-3.243762	2.819008	-3.846066
C	-1.836441	2.750066	-3.772979
C	-6.480468	2.821529	-1.405628
C	-5.729044	2.860337	-2.598326
C	-5.906534	2.558034	2.622570
C	-6.551847	2.656088	1.371911
C	-3.623897	2.350404	4.291426
C	1.447320	3.636932	-0.302717
C	1.319937	3.568708	1.080640
C	-1.110926	3.935574	-3.492096
C	0.112644	3.861956	-2.778470
C	-5.151359	4.080947	-3.000509
C	-3.884162	4.060692	-3.636526
C	-6.676946	3.921994	0.755781
C	-6.637033	4.005428	-0.659106
C	-4.239772	3.672907	4.035750
C	-5.394488	3.739982	3.216029
C	1.165168	4.835743	1.854601
C	0.672317	5.041124	-2.221815
C	1.370684	4.959251	-0.981820
C	-3.147978	5.264526	-3.753107
C	-1.726456	5.200709	-3.680592
C	-6.418822	5.261144	-1.278642

C	-5.651436	5.300416	-2.480178
C	-5.859819	5.008958	2.781037
C	-6.521072	5.101077	1.523225
C	-3.521690	4.862746	4.333391
C	1.652592	6.091093	-0.188616
C	1.545253	6.031074	1.209161
C	-0.933409	6.351463	-3.489339
C	0.253313	6.272977	-2.759372
C	-5.098692	6.495840	-2.980716
C	-3.855396	6.477760	-3.616724
C	-6.740218	6.335778	0.875877
C	-6.684016	6.415952	-0.517039
C	-4.220738	6.079632	4.222939
C	-5.388044	6.150309	3.462479
C	0.941098	-6.353197	0.468355
C	1.003865	-6.249142	-0.928992
C	-0.656568	-6.440089	2.950223
C	-1.895447	-6.406181	3.608747
C	-4.816359	-6.197269	3.413914
C	-5.980954	-6.054810	2.659084
C	-7.356932	-5.767097	0.093424
C	-7.313648	-5.671483	-1.298960
C	-5.744610	-5.595875	-3.771353
C	-4.499654	-5.627645	-4.403354
C	-1.585901	-5.831550	-4.231607
C	-0.413806	-5.969693	-3.487090
H	-1.669227	6.941472	4.696063
H	0.410122	6.933260	3.540128
H	1.779643	7.069255	-0.627403
H	1.604337	6.966190	1.745425
H	-1.280424	7.338156	-3.754315
H	0.737354	7.202987	-2.502070
H	-5.522082	7.462019	-2.751937
H	-3.406030	7.432850	-3.840530
H	-6.794295	7.267120	1.417947
H	-6.692064	7.401912	-0.956382
H	-3.809597	7.010354	4.583433
H	-5.803308	7.131993	3.295430
H	0.909539	-7.348953	0.884574
H	1.019608	-7.173165	-1.486764
H	-0.265484	-7.413090	2.693346
H	-2.366927	-7.356283	3.809142
H	-4.498699	-7.202791	3.644282
H	-6.486429	-6.961979	2.366721
H	-7.506001	-6.750144	0.512435
H	-7.424210	-6.586317	-1.861190
H	-6.270783	-6.532800	-3.668795
H	-4.150859	-6.587498	-4.751776
H	-2.030062	-6.736346	-4.616679
H	-0.036768	-6.970684	-3.342410
Pd	3.572085	1.620688	-1.256058
Pd	4.546983	0.450704	1.166949
Pd	3.326507	-2.005223	1.608168
Pd	3.786291	-1.237676	-0.950282
Pd	5.601220	0.081928	-2.541540
Pd	6.555284	-0.839775	-0.225093
Pd	5.355476	-3.192285	0.133596
Pd	6.261462	1.899386	-0.328208
Pd	5.992008	-1.565798	2.235155
C	7.221562	3.791157	-0.939221
C	7.826695	3.541000	0.332600
C	6.202312	4.888446	-1.193081
C	7.542749	4.379173	1.573946
H	8.811429	3.072991	0.306174
H	7.779834	3.458691	-1.815844
H	5.495861	5.008609	-0.364545
H	5.624675	4.672074	-2.097167
H	6.713528	5.854453	-1.341742
H	7.868646	3.863442	2.483061
H	6.479498	4.614241	1.679553
H	8.095000	5.328485	1.505087
H	5.252207	1.738465	-1.941576
H	7.198879	2.042793	0.958227

1
A

Frequencies -- -672.0079
Red. masses -- 1.1948
Frc consts -- 0.3179
IR Inten -- 0.0000

Atom	AN	X	Y	Z
1	6	0.00	0.00	0.00
2	6	0.00	0.00	0.00
3	6	0.00	0.00	0.00
4	6	0.00	0.00	0.00
5	6	0.00	0.00	0.00
6	6	0.00	0.00	0.00
7	6	0.00	0.00	0.00
8	6	0.00	0.00	0.00
9	6	0.00	0.00	0.00
10	6	0.00	0.00	0.00
11	6	0.00	0.00	0.00
12	6	0.00	0.00	0.00
13	6	0.00	0.00	0.00
14	6	0.00	0.00	0.00
15	6	0.00	0.00	0.00
16	6	0.00	0.00	0.00
17	6	0.00	0.00	0.00
18	6	0.00	0.00	0.00
19	6	0.00	0.00	0.00
20	6	0.00	0.00	0.00
21	6	0.00	0.00	0.00
22	6	0.00	0.00	0.00
23	6	0.00	0.00	0.00
24	6	0.00	0.00	0.00
25	6	0.00	0.00	0.00
26	6	0.00	0.00	0.00
27	6	0.00	0.00	0.00
28	6	0.00	0.00	0.00
29	6	0.00	0.00	0.00
30	6	0.00	0.00	0.00
31	6	0.00	0.00	0.00
32	6	0.00	0.00	0.00
33	6	0.00	0.00	0.00
34	6	0.00	0.00	0.00
35	6	0.00	0.00	0.00
36	6	0.00	0.00	0.00
37	6	0.00	0.00	0.00
38	6	0.00	0.00	0.00
39	6	0.00	0.00	0.00
40	6	0.00	0.00	0.00
41	6	0.00	0.00	0.00
42	6	0.00	0.00	0.00
43	6	0.00	0.00	0.00
44	6	0.00	0.00	0.00
45	6	0.00	0.00	0.00
46	6	0.00	0.00	0.00
47	6	0.00	0.00	0.00
48	6	0.00	0.00	0.00
49	6	0.00	0.00	0.00
50	6	0.00	0.00	0.00
51	6	0.00	0.00	0.00
52	6	0.00	0.00	0.00
53	6	0.00	0.00	0.00
54	6	0.00	0.00	0.00
55	6	0.00	0.00	0.00
56	6	0.00	0.00	0.00
57	6	0.00	0.00	0.00
58	6	0.00	0.00	0.00
59	6	0.00	0.00	0.00
60	6	0.00	0.00	0.00
61	6	0.00	0.00	0.00
62	6	0.00	0.00	0.00
63	6	0.00	0.00	0.00
64	6	0.00	0.00	0.00
65	6	0.00	0.00	0.00
66	6	0.00	0.00	0.00
67	6	0.00	0.00	0.00
68	6	0.00	0.00	0.00
69	6	0.00	0.00	0.00
70	6	0.00	0.00	0.00
71	6	0.00	0.00	0.00
72	6	0.00	0.00	0.00
73	6	0.00	0.00	0.00
74	6	0.00	0.00	0.00
75	6	0.00	0.00	0.00
76	6	0.00	0.00	0.00
77	6	0.00	0.00	0.00
78	6	0.00	0.00	0.00
79	6	0.00	0.00	0.00
80	6	0.00	0.00	0.00
81	6	0.00	0.00	0.00
82	6	0.00	0.00	0.00
83	6	0.00	0.00	0.00
84	6	0.00	0.00	0.00
85	6	0.00	0.00	0.00
86	6	0.00	0.00	0.00
87	6	0.00	0.00	0.00
88	6	0.00	0.00	0.00
89	6	0.00	0.00	0.00
90	6	0.00	0.00	0.00
91	6	0.00	0.00	0.00
92	6	0.00	0.00	0.00
93	6	0.00	0.00	0.00
94	6	0.00	0.00	0.00
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96	6	0.00	0.00	0.00
97	6	0.00	0.00	0.00
98	6	0.00	0.00	0.00
99	6	0.00	0.00	0.00
100	6	0.00	0.00	0.00
101	6	0.00	0.00	0.00
102	6	0.00	0.00	0.00
103	6	0.00	0.00	0.00
104	6	0.00	0.00	0.00
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106	6	0.00	0.00	0.00
107	6	0.00	0.00	0.00
108	6	0.00	0.00	0.00
109	6	0.00	0.00	0.00
110	6	0.00	0.00	0.00

111	6	0.00	0.00	0.00
112	6	0.00	0.00	0.00
113	6	0.00	0.00	0.00
114	6	0.00	0.00	0.00
115	6	0.00	0.00	0.00
116	6	0.00	0.00	0.00
117	6	0.00	0.00	0.00
118	6	0.00	0.00	0.00
119	6	0.00	0.00	0.00
120	6	0.00	0.00	0.00
121	6	0.00	0.00	0.00
122	6	0.00	0.00	0.00
123	6	0.00	0.00	0.00
124	6	0.00	0.00	0.00
125	6	0.00	0.00	0.00
126	6	0.00	0.00	0.00
127	6	0.00	0.00	0.00
128	6	0.00	0.00	0.00
129	6	0.00	0.00	0.00
130	6	0.00	0.00	0.00
131	6	0.00	0.00	0.00
132	6	0.00	0.00	0.00
133	1	0.00	0.00	0.00
134	1	0.00	0.00	0.00
135	1	0.00	0.00	0.00
136	1	0.00	0.00	0.00
137	1	0.00	0.00	0.00
138	1	0.00	0.00	0.00
139	1	0.00	0.00	0.00
140	1	0.00	0.00	0.00
141	1	0.00	0.00	0.00
142	1	0.00	0.00	0.00
143	1	0.00	0.00	0.00
144	1	0.00	0.00	0.00
145	1	0.00	0.00	0.00
146	1	0.00	0.00	0.00
147	1	0.00	0.00	0.00
148	1	0.00	0.00	0.00
149	1	0.00	0.00	0.00
150	1	0.00	0.00	0.00
151	1	0.00	0.00	0.00
152	1	0.00	0.00	0.00
153	1	0.00	0.00	0.00
154	1	0.00	0.00	0.00
155	1	0.00	0.00	0.00
156	1	0.00	0.00	0.00
157	46	0.00	0.00	0.00
158	46	0.00	0.00	0.00
159	46	0.00	0.00	0.00
160	46	0.00	0.00	0.00
161	46	0.00	0.00	0.00
162	46	0.00	0.00	0.00
163	46	0.00	0.00	0.00
164	46	0.00	0.00	0.01
165	46	0.00	0.00	0.00
166	6	0.03	0.05	0.00
167	6	0.01	0.08	-0.07
168	6	0.00	0.00	-0.01
169	6	-0.01	-0.02	-0.01
170	1	-0.12	-0.18	0.03
171	1	-0.04	-0.04	-0.01
172	1	0.00	0.00	0.00
173	1	-0.01	-0.01	0.00
174	1	-0.02	0.01	-0.02
175	1	-0.01	-0.06	-0.03
176	1	0.00	0.00	0.00
177	1	0.00	-0.02	0.03
178	1	-0.03	0.03	-0.07
179	1	-0.44	-0.82	0.25

TS pre-*trans*/Pd$_9$(H)/nanotube → *trans*-but-2-ene/Pd$_9$(H$_2$)/nanotube

179

C	-1.405353	5.950416	4.433999
C	-2.198295	4.783214	4.468920
C	-1.497632	3.499751	4.215107
C	-0.279235	3.505840	3.525750
C	0.310143	4.806329	3.115582
C	-0.172674	5.962762	3.762858
C	-2.228160	2.235566	4.385101
C	-1.573109	1.015520	4.156685
C	-0.294555	1.012505	3.389370
C	0.241283	2.232611	2.964700
C	-2.355326	-0.231751	4.214955
C	-1.672535	-1.514840	3.967943
C	-0.384953	-1.504177	3.214191
C	0.162722	-0.225260	2.796715
C	-2.422596	-2.698164	4.019092
C	-1.789449	-3.978191	3.676077
C	-0.556406	-3.984821	3.011734
C	0.078046	-2.690541	2.642625
C	0.927482	-2.669274	1.472370
C	1.000704	-3.864837	0.649323
C	0.721759	-5.201463	1.250743
C	-0.061226	-5.260456	2.433126
C	1.289607	-1.392209	0.888972
C	1.367198	-1.296023	-0.586072
C	1.056028	-2.459355	-1.363853
C	1.066814	-3.755143	-0.736383
C	0.348624	-2.318039	-2.605059
C	-0.253456	-3.530370	-3.220023
C	0.178800	-4.820277	-2.819616
C	0.866434	-4.966175	-1.580246
C	-0.048047	-1.057269	-3.050672
C	-1.315007	-0.933259	-3.823015
C	-2.053957	-2.111540	-4.094305
C	-1.453895	-3.389325	-3.961115
C	-3.459302	-2.032483	-4.189117
C	-4.219616	-3.222915	-4.157330
C	-3.598997	-4.465667	-4.430889
C	-2.180973	-4.552226	-4.326831
C	-4.095706	-0.792021	-3.965018
C	-5.367066	-0.779462	-3.348674
C	-5.957948	-2.003584	-2.969848
C	-5.494317	-3.207106	-3.536878
C	-6.717695	-2.057726	-1.783027
C	-6.993403	-3.312942	-1.206472
C	-6.889085	-4.486374	-1.994089
C	-6.116532	-4.432548	-3.191492
C	-6.864034	-0.886792	-1.010052
C	-6.899656	-0.991879	0.398749
C	-6.802938	-2.269779	0.990884
C	-7.036714	-3.421925	0.206568
C	-6.165319	-2.404219	2.242110
C	-5.765166	-3.697985	2.664393
C	-6.335127	-4.848037	2.057543
C	-6.994295	-4.704847	0.803234
C	-5.678836	-1.244775	2.897278
C	-4.518624	-1.384117	3.813468
C	-3.896229	-2.633177	3.926751
C	-4.619874	-3.847607	3.486669
C	-2.592865	-5.224484	3.740983
C	-4.013151	-5.125881	3.621102
C	0.995321	-0.169667	1.633066
C	0.487415	0.120311	-2.425944
C	1.207930	0.000719	-1.199864
C	-3.343620	0.404012	-4.010727
C	-1.934104	0.336599	-3.932345
C	-6.603921	0.368040	-1.597462
C	-5.843341	0.423091	-2.787166
C	-6.060122	0.047616	2.442612
C	-6.686677	0.166650	1.180194
C	-3.754030	-0.171126	4.147669
C	1.462821	1.192478	-0.408495
C	1.283675	1.106346	1.037733
C	-1.206626	1.519439	-3.649530
C	0.066001	1.422994	-2.882396
C	-5.259471	1.649030	-3.167880
C	-3.988501	1.641262	-3.784997
C	-6.798558	1.440782	0.578010
C	-6.759568	1.540732	-0.831046
C	-4.419595	1.134409	4.002475
C	-5.581175	1.224253	3.081562
C	1.036316	2.302595	1.771433
C	0.588815	2.569160	-2.295320
C	1.320989	2.477304	-1.048834
C	-3.245291	2.841265	-3.831946
C	-1.838205	2.783818	-3.745425
C	-6.506148	2.795399	-1.424278
C	-5.743190	2.850735	-2.608972
C	-5.970004	2.502605	2.607061
C	-6.603739	2.605774	1.350904
C	-3.702210	2.300309	4.296661
C	1.402859	3.669875	-0.235651
C	1.262296	3.588681	1.145640
C	-1.125800	3.973141	-3.447726
C	0.091376	3.904157	-2.722771
C	-5.172091	4.079603	-2.995094
C	-3.898508	4.075586	-3.618543
C	-6.733599	3.875758	0.744217
C	-6.680332	3.971541	-0.669447
C	-4.326975	3.619617	4.046107
C	-5.474066	3.683795	3.215521

C	1.088847	4.847616	1.928823
C	0.634991	5.083432	-2.150711
C	1.321257	4.997220	-0.904301
C	-3.171708	5.286640	-3.717842
C	-1.750462	5.234451	-3.631883
C	-6.466775	5.234286	-1.276193
C	-5.687854	5.290295	-2.469617
C	-5.945992	4.952405	2.786609
C	-6.595497	5.049567	1.523067
C	-3.622192	4.812973	4.360954
C	1.584773	6.124766	-0.098766
C	1.464282	6.051809	1.297293
C	-0.969368	6.390365	-3.423417
C	0.210683	6.316056	-2.682311
C	-5.140559	6.494599	-2.954613
C	-3.890943	6.492558	-3.578375
C	-6.818799	6.287812	0.883957
C	-6.749442	6.380288	-0.507604
C	-4.330590	6.024736	4.253785
C	-5.490861	6.091906	3.482318
C	0.976646	-6.330745	0.445880
C	1.052745	-6.214383	-0.949819
C	-0.645492	-6.452433	2.910367
C	-1.891077	-6.434809	3.556762
C	-4.811699	-6.249431	3.335104
C	-5.970137	-6.110564	2.570192
C	-7.323404	-5.812830	-0.006351
C	-7.267037	-5.705033	-1.397376
C	-5.673693	-5.595072	-3.852865
C	-4.422188	-5.610807	-4.472415
C	-1.508536	-5.791033	-4.273653
C	-0.342435	-5.925395	-3.519109
H	-1.791426	6.904222	4.760128
H	0.299308	6.923829	3.625044
H	1.707117	7.107785	-0.527930
H	1.509529	6.982828	1.841961
H	-1.322296	7.376188	-3.683784
H	0.684071	7.248028	-2.412591
H	-5.574552	7.455143	-2.722005
H	-3.447705	7.453330	-3.789732
H	-6.886250	7.214026	1.433265
H	-6.761577	7.369841	-0.938697
H	-3.931079	6.955843	4.626169
H	-5.912899	7.071393	3.319398
H	0.949498	-7.330213	0.853421
H	1.082029	-7.133491	-1.515120
H	-0.243412	-7.419815	2.649284
H	-2.356220	-7.390609	3.744466
H	-4.487545	-7.254110	3.560036
H	-6.464846	-7.019521	2.265234
H	-7.468161	-6.800632	0.402878
H	-7.364080	-6.615967	-1.968368
H	-6.192719	-6.537320	-3.763493
H	-4.061601	-6.564656	-4.825287
H	-1.941049	-6.696308	-4.670670
H	0.041959	-6.924282	-3.379305
Pd	3.558793	1.681619	-1.191581
Pd	4.542011	0.494491	1.213898
Pd	3.320164	-1.965356	1.641064
Pd	3.767385	-1.184162	-0.911401
Pd	5.576274	0.151401	-2.504791
Pd	6.530077	-0.796251	-0.199721
Pd	5.341725	-3.154838	0.155801
Pd	6.254449	1.948346	-0.274890
Pd	5.990852	-1.538559	2.257074
C	7.227971	3.821844	-0.907270
C	8.035009	3.414189	0.198472
C	6.236770	4.969543	-0.815626
H	7.899383	3.970967	1.128256
C	9.409033	2.783475	0.004814
H	7.597161	3.585205	-1.906723
H	5.828371	5.072157	0.197363
H	5.399684	4.826001	-1.507158
H	6.731612	5.918439	-1.080599
H	5.233205	1.803142	-1.879170
H	7.216323	2.117358	0.996475
H	10.164717	3.579064	-0.075670
H	9.685343	2.139271	0.845991
H	9.444950	2.183900	-0.911165

1
A

Frequencies -- -679.4889
Red. masses -- 1.1943
Frc consts -- 0.3249
IR Inten -- 0.0000

Atom	AN	X	Y	Z
1	6	0.00	0.00	0.00
2	6	0.00	0.00	0.00
3	6	0.00	0.00	0.00
4	6	0.00	0.00	0.00
5	6	0.00	0.00	0.00
6	6	0.00	0.00	0.00
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8	6	0.00	0.00	0.00
9	6	0.00	0.00	0.00
10	6	0.00	0.00	0.00
11	6	0.00	0.00	0.00
12	6	0.00	0.00	0.00
13	6	0.00	0.00	0.00
14	6	0.00	0.00	0.00
15	6	0.00	0.00	0.00
16	6	0.00	0.00	0.00
17	6	0.00	0.00	0.00
18	6	0.00	0.00	0.00
19	6	0.00	0.00	0.00
20	6	0.00	0.00	0.00
21	6	0.00	0.00	0.00
22	6	0.00	0.00	0.00
23	6	0.00	0.00	0.00
24	6	0.00	0.00	0.00
25	6	0.00	0.00	0.00
26	6	0.00	0.00	0.00
27	6	0.00	0.00	0.00
28	6	0.00	0.00	0.00
29	6	0.00	0.00	0.00
30	6	0.00	0.00	0.00
31	6	0.00	0.00	0.00
32	6	0.00	0.00	0.00
33	6	0.00	0.00	0.00
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35	6	0.00	0.00	0.00
36	6	0.00	0.00	0.00
37	6	0.00	0.00	0.00
38	6	0.00	0.00	0.00
39	6	0.00	0.00	0.00
40	6	0.00	0.00	0.00
41	6	0.00	0.00	0.00
42	6	0.00	0.00	0.00
43	6	0.00	0.00	0.00
44	6	0.00	0.00	0.00
45	6	0.00	0.00	0.00
46	6	0.00	0.00	0.00
47	6	0.00	0.00	0.00
48	6	0.00	0.00	0.00
49	6	0.00	0.00	0.00
50	6	0.00	0.00	0.00
51	6	0.00	0.00	0.00
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56	6	0.00	0.00	0.00
57	6	0.00	0.00	0.00
58	6	0.00	0.00	0.00
59	6	0.00	0.00	0.00
60	6	0.00	0.00	0.00
61	6	0.00	0.00	0.00
62	6	0.00	0.00	0.00
63	6	0.00	0.00	0.00
64	6	0.00	0.00	0.00
65	6	0.00	0.00	0.00
66	6	0.00	0.00	0.00
67	6	0.00	0.00	0.00
68	6	0.00	0.00	0.00
69	6	0.00	0.00	0.00
70	6	0.00	0.00	0.00
71	6	0.00	0.00	0.00
72	6	0.00	0.00	0.00
73	6	0.00	0.00	0.00
74	6	0.00	0.00	0.00
75	6	0.00	0.00	0.00
76	6	0.00	0.00	0.00
77	6	0.00	0.00	0.00
78	6	0.00	0.00	0.00
79	6	0.00	0.00	0.00
80	6	0.00	0.00	0.00
81	6	0.00	0.00	0.00
82	6	0.00	0.00	0.00
83	6	0.00	0.00	0.00
84	6	0.00	0.00	0.00
85	6	0.00	0.00	0.00
86	6	0.00	0.00	0.00
87	6	0.00	0.00	0.00
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89	6	0.00	0.00	0.00
90	6	0.00	0.00	0.00
91	6	0.00	0.00	0.00
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95	6	0.00	0.00	0.00
96	6	0.00	0.00	0.00
97	6	0.00	0.00	0.00
98	6	0.00	0.00	0.00
99	6	0.00	0.00	0.00
100	6	0.00	0.00	0.00
101	6	0.00	0.00	0.00

102	6	0.00	0.00	0.00
103	6	0.00	0.00	0.00
104	6	0.00	0.00	0.00
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106	6	0.00	0.00	0.00
107	6	0.00	0.00	0.00
108	6	0.00	0.00	0.00
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110	6	0.00	0.00	0.00
111	6	0.00	0.00	0.00
112	6	0.00	0.00	0.00
113	6	0.00	0.00	0.00
114	6	0.00	0.00	0.00
115	6	0.00	0.00	0.00
116	6	0.00	0.00	0.00
117	6	0.00	0.00	0.00
118	6	0.00	0.00	0.00
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123	6	0.00	0.00	0.00
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125	6	0.00	0.00	0.00
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127	6	0.00	0.00	0.00
128	6	0.00	0.00	0.00
129	6	0.00	0.00	0.00
130	6	0.00	0.00	0.00
131	6	0.00	0.00	0.00
132	6	0.00	0.00	0.00
133	1	0.00	0.00	0.00
134	1	0.00	0.00	0.00
135	1	0.00	0.00	0.00
136	1	0.00	0.00	0.00
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143	1	0.00	0.00	0.00
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145	1	0.00	0.00	0.00
146	1	0.00	0.00	0.00
147	1	0.00	0.00	0.00
148	1	0.00	0.00	0.00
149	1	0.00	0.00	0.00
150	1	0.00	0.00	0.00
151	1	0.00	0.00	0.00
152	1	0.00	0.00	0.00
153	1	0.00	0.00	0.00
154	1	0.00	0.00	0.00
155	1	0.00	0.00	0.00
156	1	0.00	0.00	0.00
157	46	0.00	0.00	0.00
158	46	0.00	0.00	0.00
159	46	0.00	0.00	0.00
160	46	0.00	0.00	0.00
161	46	0.00	0.00	0.00
162	46	0.00	0.00	0.00
163	46	0.00	0.00	0.00
164	46	0.00	0.00	-0.01
165	46	0.00	0.00	0.00
166	6	-0.04	-0.04	0.01
167	6	-0.02	-0.07	0.08
168	6	0.01	0.00	0.00
169	1	0.14	0.19	-0.04
170	6	0.02	0.01	0.00
171	1	0.03	0.00	0.02
172	1	-0.01	0.00	0.00
173	1	0.01	0.02	-0.01
174	1	0.03	-0.01	0.01
175	1	0.02	-0.03	0.07
176	1	0.55	0.71	-0.33
177	1	-0.01	0.02	-0.04
178	1	0.07	0.02	-0.01
179	1	-0.02	0.00	0.01

TS pre-*cis*/$Pd_9(H)$/nanotube → but-1-ene/$Pd_9(H_2)$/nanotube

179

C	-1.576039	-5.924287	-3.946433
C	-0.834009	-4.911508	-3.308943
C	-1.162761	-3.567414	-3.620280
C	-2.429398	-3.263519	-4.179754
C	-3.333941	-4.321613	-4.456287
C	-2.812669	-5.630617	-4.522670
C	0.001903	-5.179484	-2.185846
C	0.462070	-4.031232	-1.355312
C	0.489743	-2.712730	-1.935295
C	-0.345153	-2.453993	-3.072985
C	0.611712	-4.191265	0.017095
C	0.816382	-3.028855	0.868362
C	1.207092	-1.776598	0.251521
C	1.006647	-1.622231	-1.187209
C	1.213055	-0.565407	1.066175
C	0.547903	-0.558715	2.330230
C	-0.087219	-1.778047	2.799580
C	0.149202	-2.992403	2.154442
C	0.331946	0.706467	3.000070
C	-0.821078	0.832403	3.937324
C	-1.730497	-0.317562	4.089216
C	-1.248361	-1.663027	3.728096
C	0.955243	1.866997	2.531015
C	0.666918	3.173194	3.179829
C	-0.439905	3.285956	4.029927
C	-1.286040	2.110893	4.278906
C	1.346213	4.410026	2.716806
C	1.099340	5.591190	3.446948
C	-0.023464	5.699529	4.282072
C	-0.939114	4.632434	4.405084
C	-2.738794	2.348774	4.409763
C	-3.230985	3.739161	4.277906
C	-2.350158	4.831229	4.505187
C	1.607851	1.885665	1.248729
C	1.855520	3.160549	0.609398
C	1.945688	4.403654	1.430408
C	-3.625507	1.284389	4.206724
C	-3.106756	-0.093458	4.229623
C	1.639687	0.682056	0.457355
C	-4.050899	-1.198057	3.992778
C	-3.572479	-2.514060	3.992615
C	-2.119192	-2.752791	3.869221
C	-1.698059	-4.086578	3.419453
C	-0.578746	-4.215446	2.587022
C	-4.491737	-3.620979	3.643664
C	-4.029375	-4.964911	3.666582
C	-2.628591	-5.232229	3.577298
C	-2.110812	-6.509202	3.271926
C	-0.981270	-6.649692	2.450817
C	-0.331293	-5.518156	1.915624
C	0.268726	-5.507453	0.628746
C	0.133431	-6.464516	-1.617243
C	0.258010	-6.626085	-0.229178
C	1.527541	0.811423	-1.015081
C	0.975913	-0.307743	-1.756509
C	0.112501	-0.059272	-2.869663
C	-0.642987	-1.141647	-3.436370
C	-1.980793	-0.845711	-4.018972
C	-2.885972	-1.921056	-4.201923
C	-0.210645	1.297628	-3.235117
C	-1.557411	1.568598	-3.811692
C	-2.453548	0.489358	-4.011692
C	-3.841897	0.721059	-3.882243
C	-4.716342	-0.381527	-3.748435
C	-4.270948	-1.677939	-4.087443
C	-5.154343	-2.773835	-3.964536
C	-4.731748	-4.069161	-4.349427
C	-5.873490	-0.245528	-2.948923
C	-6.542512	-1.406842	-2.507528
C	-6.313188	-2.634458	-3.159665
C	-7.017857	-3.792394	-2.746378
C	-6.818186	-4.973568	-3.487979
C	-5.682019	-5.110276	-4.288499
C	-4.296061	2.015152	-3.540883
C	-5.454239	2.146719	-2.742356
C	-6.116599	0.982835	-2.300526
C	-6.693591	0.972603	-1.010560
C	-7.009340	-0.264578	-0.413125
C	-7.118674	-1.416281	-1.220377
C	-7.451593	-2.651667	-0.631351
C	-7.604772	-3.800497	-1.446754
C	-6.846724	-0.415055	0.982574
C	-6.814687	-1.715946	1.530081
C	-7.296808	-2.805271	0.769697
C	-7.318629	-4.104987	1.330015
C	-7.892462	-5.138773	0.559637
C	-8.030842	-4.988667	-0.821696
C	-6.594166	2.127409	-0.208359
C	-6.433579	1.982399	1.188141
C	-6.384462	0.683124	1.743258

C	-5.595864	0.448553	2.893682
C	-5.307777	-0.894340	3.262879
C	-6.019501	-1.966634	2.668095
C	-5.718369	-3.311846	3.003079
C	-6.503914	-4.366761	2.468477
C	-4.989501	-5.977901	3.482398
C	-6.221435	-5.679876	2.899524
C	-4.891146	1.539331	3.473214
C	0.517080	2.353296	-2.696318
C	1.404578	2.132235	-1.580103
C	-3.429625	3.122265	-3.673083
C	-2.041370	2.899620	-3.790151
C	-6.285890	3.365394	-0.810605
C	-5.705426	3.375345	-2.095768
C	-5.191140	2.869853	3.085588
C	-5.988882	3.089325	1.942968
C	1.762413	3.275632	-0.775383
C	-1.158183	3.986594	-3.572625
C	0.129209	3.750995	-3.026638
C	-5.055208	4.543608	-2.540452
C	-3.894123	4.415221	-3.344086
C	-6.057095	4.386651	1.386175
C	-6.205618	4.526121	-0.016994
C	-4.472662	3.964125	3.631742
C	0.887577	4.838366	-2.523089
C	1.735159	4.628815	-1.397446
C	-3.049330	5.536901	-3.524869
C	-1.646673	5.317398	-3.643723
C	-5.937117	5.777072	-0.626359
C	-5.341359	5.786051	-1.922083
C	-4.848788	5.292892	3.301884
C	-5.665423	5.508499	2.155375
C	2.253504	5.689846	-0.625702
C	2.353096	5.579963	0.768862
C	-0.711423	6.366685	-3.528503
C	0.543726	6.129701	-2.966879
C	-4.730655	6.935925	-2.460655
C	-3.592339	6.812068	-3.260400
C	-5.835010	6.786150	1.580559
C	-5.964916	6.919712	0.196718
C	-2.916326	6.119934	4.524756
C	-4.161684	6.347389	3.938808
Pd	3.185563	-2.687056	0.883968
Pd	5.151622	-1.667281	2.571801
Pd	5.822409	-3.252452	0.472285
Pd	6.555468	-0.683180	0.545889
Pd	5.644400	1.888865	-0.062194
C	6.778369	3.613291	0.947969
H	7.649961	3.221534	1.467400
Pd	4.530657	-1.645739	-1.228788
Pd	6.408193	0.017235	-2.116909
Pd	3.648397	0.919016	-1.823487
Pd	3.872509	0.086697	0.870439
C	6.790862	3.728852	-0.473631
C	5.953014	4.758574	-1.213733
H	-0.243141	6.679589	4.677440
H	1.661196	6.494492	3.262650
H	2.423194	6.667161	-1.051411
H	2.591880	6.479704	1.315721
H	-0.976601	7.395228	-3.718357
H	1.159611	6.990416	-2.754573
H	-5.009107	7.931130	-2.148928
H	-3.071983	7.722070	-3.516139
H	-5.709977	7.693809	2.150370
H	-5.924860	7.918906	-0.209802
H	-2.357987	6.985395	4.847831
H	-4.482704	7.374234	3.857905
H	0.172979	-7.630697	0.157390
H	-0.030913	-7.358738	-2.198936
H	-0.741004	-7.647299	2.114860
H	-2.656372	-7.410209	3.507767
H	-4.759139	-7.020433	3.640704
H	-6.860268	-6.514528	2.656288
H	-8.090468	-6.117627	0.968015
H	-8.318241	-5.861741	-1.387738
H	-7.426253	-5.852867	-3.338607
H	-5.492266	-6.086001	-4.708474
H	-3.401563	-6.465771	-4.869078
H	-1.297419	-6.965032	-3.882044
H	6.150610	4.289235	1.527656
H	7.668648	3.356890	-1.004272
H	5.400583	1.429701	-1.995923
H	5.784915	2.285964	1.473166
C	6.733220	6.081450	-1.436020
H	5.645977	4.353323	-2.185463
H	5.036531	4.963889	-0.645981
H	6.113351	6.802252	-1.984786
H	7.023027	6.536737	-0.480039
H	7.646640	5.907935	-2.020139

1
A

Frequencies -- -717.7170
Red. masses -- 1.1230
Frc consts -- 0.3408
IR Inten -- 0.0000

Atom	AN	X	Y	Z
1	6	0.00	0.00	0.00
2	6	0.00	0.00	0.00
3	6	0.00	0.00	0.00
4	6	0.00	0.00	0.00
5	6	0.00	0.00	0.00
6	6	0.00	0.00	0.00
7	6	0.00	0.00	0.00
8	6	0.00	0.00	0.00
9	6	0.00	0.00	0.00
10	6	0.00	0.00	0.00
11	6	0.00	0.00	0.00
12	6	0.00	0.00	0.00
13	6	0.00	0.00	0.00
14	6	0.00	0.00	0.00
15	6	0.00	0.00	0.00
16	6	0.00	0.00	0.00
17	6	0.00	0.00	0.00
18	6	0.00	0.00	0.00
19	6	0.00	0.00	0.00
20	6	0.00	0.00	0.00
21	6	0.00	0.00	0.00
22	6	0.00	0.00	0.00
23	6	0.00	0.00	0.00
24	6	0.00	0.00	0.00
25	6	0.00	0.00	0.00
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34	6	0.00	0.00	0.00
35	6	0.00	0.00	0.00
36	6	0.00	0.00	0.00
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39	6	0.00	0.00	0.00
40	6	0.00	0.00	0.00
41	6	0.00	0.00	0.00
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44	6	0.00	0.00	0.00
45	6	0.00	0.00	0.00
46	6	0.00	0.00	0.00
47	6	0.00	0.00	0.00
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49	6	0.00	0.00	0.00
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51	6	0.00	0.00	0.00
52	6	0.00	0.00	0.00
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55	6	0.00	0.00	0.00
56	6	0.00	0.00	0.00
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58	6	0.00	0.00	0.00
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61	6	0.00	0.00	0.00
62	6	0.00	0.00	0.00
63	6	0.00	0.00	0.00
64	6	0.00	0.00	0.00
65	6	0.00	0.00	0.00
66	6	0.00	0.00	0.00
67	6	0.00	0.00	0.00
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69	6	0.00	0.00	0.00
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71	6	0.00	0.00	0.00
72	6	0.00	0.00	0.00
73	6	0.00	0.00	0.00
74	6	0.00	0.00	0.00
75	6	0.00	0.00	0.00
76	6	0.00	0.00	0.00
77	6	0.00	0.00	0.00
78	6	0.00	0.00	0.00
79	6	0.00	0.00	0.00
80	6	0.00	0.00	0.00
81	6	0.00	0.00	0.00
82	6	0.00	0.00	0.00
83	6	0.00	0.00	0.00
84	6	0.00	0.00	0.00

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92	6	0.00	0.00	0.00
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96	6	0.00	0.00	0.00
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125	6	0.00	0.00	0.00
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127	6	0.00	0.00	0.00
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133	46	0.00	0.00	0.00
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136	46	0.00	0.00	0.00
137	46	0.00	0.00	-0.01
138	6	-0.03	-0.04	0.07
139	1	0.09	0.15	0.01
140	46	0.00	0.00	0.00
141	46	0.00	0.00	0.00
142	46	0.00	0.00	0.00
143	46	0.00	0.00	0.00
144	6	-0.03	-0.04	0.00
145	6	0.00	0.00	0.00
146	1	0.00	0.00	0.00
147	1	0.00	0.00	0.00
148	1	0.00	0.00	0.00
149	1	0.00	0.00	0.00
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161	1	0.00	0.00	0.00
162	1	0.00	0.00	0.00
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164	1	0.00	0.00	0.00
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167	1	0.00	0.00	0.00
168	1	0.00	0.00	0.00
169	1	0.00	0.00	0.00
170	1	0.12	0.17	0.01
171	1	0.01	0.01	0.03
172	1	0.00	-0.01	0.07
173	1	0.58	0.75	-0.11
174	6	0.00	0.00	0.00
175	1	0.00	0.00	0.00
176	1	0.00	0.00	0.00
177	1	0.00	0.00	0.00
178	1	0.00	0.00	0.00
179	1	0.00	0.00	0.00

TS pre-*cis*/Pd$_9$(H)/nanotube → *n*-butane/Pd$_9$/nanotube

179

C	-1.783989	5.837892	4.607963
C	-2.532578	4.641586	4.583006
C	-1.774211	3.392043	4.325966
C	-0.531665	3.460957	3.685087
C	0.023828	4.792485	3.331521
C	-0.527495	5.913154	3.987035
C	-2.461693	2.097718	4.436720
C	-1.752010	0.909257	4.204952
C	-0.445642	0.973149	3.489008
C	0.058276	2.222596	3.114560
C	-2.487270	-0.367103	4.202724
C	-1.746441	-1.616889	3.953319
C	-0.430623	-1.539508	3.253696
C	0.084464	-0.231323	2.888494
C	-2.452123	-2.828239	3.947002
C	-1.757397	-4.074938	3.601180
C	-0.498917	-4.019480	2.988981
C	0.100426	-2.693947	2.676402
C	0.997351	-2.612385	1.545731
C	1.152231	-3.785034	0.700139
C	0.897611	-5.145225	1.257933
C	0.068394	-5.261581	2.403881
C	1.343338	-1.310263	1.012343
C	1.492930	-1.173427	-0.460237
C	1.244085	-2.331824	-1.280061
C	1.272987	-3.639761	-0.679829
C	0.573952	-2.184198	-2.540367
C	0.042093	-3.402010	-3.207124
C	0.506525	-4.684929	-2.820351
C	1.149957	-4.836389	-1.558182
C	0.148187	-0.927377	-2.970653
C	-1.091682	-0.831146	-3.789276
C	-1.774242	-2.028564	-4.119051
C	-1.132432	-3.286445	-3.992395
C	-3.176429	-1.998686	-4.270708
C	-3.892252	-3.216481	-4.299474
C	-3.214760	-4.428404	-4.576215
C	-1.799916	-4.465615	-4.415382
C	-3.867498	-0.788423	-4.044337
C	-5.163074	-0.837737	-3.482808
C	-5.723073	-2.091696	-3.158631
C	-5.191351	-3.262851	-3.733574
C	-6.529308	-2.203310	-2.007032
C	-6.781236	-3.481850	-1.472325
C	-6.600099	-4.630589	-2.282118
C	-5.780994	-4.518483	-3.444007
C	-6.751740	-1.058221	-1.213736
C	-6.841825	-1.199796	0.189419
C	-6.721028	-2.487710	0.754922
C	-6.878559	-3.627705	-0.065324
C	-6.129925	-2.629793	2.027937
C	-5.697692	-3.917956	2.435556
C	-6.198433	-5.072816	1.778890
C	-6.811641	-4.922735	0.502276
C	-5.714893	-1.469911	2.729749
C	-4.587489	-1.588942	3.688745
C	-3.922457	-2.816211	3.797339
C	-4.581069	-4.045354	3.299925
C	-2.514577	-5.351502	3.604665
C	-3.931655	-5.303033	3.428878
C	0.965068	-0.116033	1.764245
C	0.619358	0.254987	-2.302195
C	1.303454	0.134191	-1.054489
C	-3.159455	0.434960	-4.029994
C	-1.752754	0.417327	-3.894599
C	-6.514522	0.219617	-1.759871
C	-5.707107	0.332151	-2.914101
C	-6.126686	-0.181553	2.290408
C	-6.705265	-0.054117	1.006114
C	-3.883648	-0.357157	4.081867
C	1.481383	1.314290	-0.224292
C	1.227386	1.183940	1.211220
C	-1.081574	1.618821	-3.556582
C	0.165342	1.551225	-2.744598
C	-5.153963	1.587641	-3.240499
C	-3.859016	1.641646	-3.803007
C	-6.840208	1.229750	0.429783
C	-6.746028	1.366310	-0.973565
C	-4.592744	0.925781	3.941409
C	-5.719207	0.995600	2.976222
C	0.898597	2.351572	1.958356
C	0.621269	2.702775	-2.111929

C	1.306105	2.609987	-0.840717
C	-3.160215	2.868764	-3.791533
C	-1.756362	2.861038	-3.649621
C	-6.514892	2.643843	-1.525773
C	-5.705243	2.756524	-2.674858
C	-6.136846	2.270202	2.516264
C	-6.721763	2.381422	1.237339
C	-3.932615	2.109730	4.291882
C	1.303439	3.783219	0.004494
C	1.102421	3.661667	1.375289
C	-1.101518	4.068607	-3.298621
C	0.088918	4.027963	-2.528660
C	-5.164991	4.014597	-3.007569
C	-3.867726	4.072623	-3.577307
C	-6.873865	3.660608	0.655568
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C	-4.597005	3.410772	4.047784
C	-5.711350	3.453266	3.172503
C	0.848014	4.893074	2.179741
C	0.563298	5.212883	-1.908628
C	1.198687	5.122540	-0.635975
C	-3.184001	5.311687	-3.619791
C	-1.766123	5.309977	-3.479457
C	-6.572927	5.078077	-1.319095
C	-5.747226	5.192177	-2.476432
C	-6.213131	4.713952	2.754244
C	-6.812715	4.818845	1.466892
C	-3.951238	4.621156	4.419052
C	1.381138	6.238919	0.206522
C	1.202872	6.126274	1.593715
C	-1.037852	6.488854	-3.215690
C	0.114274	6.441037	-2.429925
C	-5.226139	6.427345	-2.909898
C	-3.953260	6.486546	-3.481704
C	-7.055135	6.063727	0.847947
C	-6.930467	6.193463	-0.536776
C	-4.700466	5.808107	4.311914
C	-5.830440	5.851625	3.495101
C	1.227649	-6.244649	0.439070
C	1.356281	-6.091946	-0.949211
C	-0.489175	-6.485623	2.829190
C	-1.760139	-6.530019	3.422692
C	-4.674480	-6.448078	3.084005
C	-5.806002	-6.333353	2.275968
C	-7.065241	-6.021485	-0.346101
C	-6.956023	-5.876890	-1.730627
C	-5.267762	-5.647040	-4.113251
C	-3.991991	-5.601438	-4.679521
C	-1.084076	-5.679965	-4.364103
C	0.055218	-5.790528	-3.566056
H	-2.218491	6.767960	4.941674
H	-0.087125	6.894204	3.892219
H	1.482238	7.236441	-0.193782
H	1.187837	7.044462	2.161304
H	-1.417298	7.466700	-3.468728
H	0.541328	7.383209	-2.121029
H	-5.705023	7.365296	-2.673236
H	-3.538587	7.467923	-3.652364
H	-7.180216	6.972849	1.415417
H	-6.961338	7.192400	-0.944657
H	-4.351825	6.743719	4.722200
H	-6.282578	6.818565	3.338028
H	1.220705	-7.254077	0.822140
H	1.441880	-6.995469	-1.533610
H	-0.039766	-7.430822	2.564098
H	-2.195662	-7.506720	3.569396
H	-4.321196	-7.445299	3.297981
H	-6.252852	-7.252182	1.929525
H	-7.189062	-7.023872	0.033482
H	-6.994925	-6.776216	-2.326403
H	-5.754343	-6.609551	-4.068253
H	-3.581679	-6.532285	-5.039410
H	-1.465987	-6.590195	-4.799785
H	0.471117	-6.777836	-3.434302
Pd	3.595795	1.929798	-0.721367
Pd	4.649387	0.478714	1.445923
Pd	3.384981	-1.897845	1.821709
Pd	3.717954	-1.086404	-0.745689
Pd	5.340500	0.405880	-2.355104
Pd	6.526922	-0.786554	-0.295764
Pd	5.280279	-3.172071	0.161847
Pd	6.289628	1.908527	-0.223841
Pd	6.133616	-1.597568	2.183976
C	6.403338	4.111335	-0.612067
C	7.833816	4.151695	-0.027026
C	6.301194	4.591811	-2.074112
C	7.022904	3.710819	-3.114463
H	5.171736	3.044619	-0.676395
H	5.742675	4.706545	0.030556
H	8.543064	3.509913	-0.565378
H	7.853905	3.880889	1.036573
H	8.215332	5.185902	-0.105801
H	5.241250	4.674739	-2.349728
H	6.722281	5.612454	-2.117858
H	6.892913	4.120562	-4.124758
H	6.607442	2.690382	-3.100686
H	8.100398	3.640027	-2.916616

1
A

Frequencies -- -800.3138
Red. masses -- 1.1284
Frc consts -- 0.4258
IR Inten -- 0.0000

Atom	AN	X	Y	Z
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3	6	0.00	0.00	0.00
4	6	0.00	0.00	0.00
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31	6	0.00	0.00	0.00
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91	6	0.00	0.00	0.00
92	6	0.00	0.00	0.00
93	6	0.00	0.00	0.00
94	6	0.00	0.00	0.00
95	6	0.00	0.00	0.00
96	6	0.00	0.00	0.00
97	6	0.00	0.00	0.00
98	6	0.00	0.00	0.00
99	6	0.00	0.00	0.00
100	6	0.00	0.00	0.00
101	6	0.00	0.00	0.00
102	6	0.00	0.00	0.00
103	6	0.00	0.00	0.00
104	6	0.00	0.00	0.00
105	6	0.00	0.00	0.00
106	6	0.00	0.00	0.00
107	6	0.00	0.00	0.00
108	6	0.00	0.00	0.00
109	6	0.00	0.00	0.00
110	6	0.00	0.00	0.00
111	6	0.00	0.00	0.00
112	6	0.00	0.00	0.00
113	6	0.00	0.00	0.00
114	6	0.00	0.00	0.00
115	6	0.00	0.00	0.00
116	6	0.00	0.00	0.00
117	6	0.00	0.00	0.00
118	6	0.00	0.00	0.00
119	6	0.00	0.00	0.00
120	6	0.00	0.00	0.00
121	6	0.00	0.00	0.00
122	6	0.00	0.00	0.00
123	6	0.00	0.00	0.00
124	6	0.00	0.00	0.00
125	6	0.00	0.00	0.00
126	6	0.00	0.00	0.00
127	6	0.00	0.00	0.00
128	6	0.00	0.00	0.00
129	6	0.00	0.00	0.00
130	6	0.00	0.00	0.00
131	6	0.00	0.00	0.00
132	6	0.00	0.00	0.00
133	1	0.00	0.00	0.00
134	1	0.00	0.00	0.00
135	1	0.00	0.00	0.00
136	1	0.00	0.00	0.00
137	1	0.00	0.00	0.00
138	1	0.00	0.00	0.00
139	1	0.00	0.00	0.00
140	1	0.00	0.00	0.00
141	1	0.00	0.00	0.00
142	1	0.00	0.00	0.00
143	1	0.00	0.00	0.00
144	1	0.00	0.00	0.00
145	1	0.00	0.00	0.00
146	1	0.00	0.00	0.00
147	1	0.00	0.00	0.00
148	1	0.00	0.00	0.00
149	1	0.00	0.00	0.00
150	1	0.00	0.00	0.00
151	1	0.00	0.00	0.00
152	1	0.00	0.00	0.00
153	1	0.00	0.00	0.00
154	1	0.00	0.00	0.00
155	1	0.00	0.00	0.00
156	1	0.00	0.00	0.00
157	46	0.00	0.00	0.00
158	46	0.00	0.00	0.00
159	46	0.00	0.00	0.00
160	46	0.00	0.00	0.00
161	46	0.00	0.00	0.00
162	46	0.00	0.00	0.00
163	46	0.00	0.00	0.00
164	46	0.00	-0.02	0.00
165	46	0.00	0.00	0.00
166	6	-0.07	0.03	-0.01
167	6	-0.02	-0.01	0.00
168	6	0.00	0.03	-0.02
169	6	0.00	0.00	0.00
170	1	0.71	0.64	0.08
171	1	0.09	0.25	-0.03
172	1	-0.03	-0.02	0.00
173	1	-0.01	-0.01	0.00
174	1	-0.04	-0.01	-0.02
175	1	0.01	0.04	-0.04
176	1	0.02	0.02	-0.03
177	1	0.00	-0.01	0.00
178	1	0.00	0.00	0.01
179	1	0.00	0.00	0.00