

		11	12	13	14	15
11	H	0.000000				
12	H	2.576811	0.000000			
13	H	4.935807	2.406526	0.000000		
14	H	6.332983	4.209384	2.406526	0.000000	
15	H	8.023058	6.869389	6.054666	4.015393	0.000000
16	H	7.175833	6.328545	5.808909	3.979947	2.357170
17	H	2.386423	4.015393	6.054665	6.869389	7.379968
18	H	2.401008	3.979947	5.808909	6.328545	6.928386
19	C	5.125253	5.046433	5.953115	6.000373	5.499494
20	H	6.008642	5.865526	6.656308	6.712319	6.074044
21	H	5.325113	5.618307	6.645477	6.512580	5.493482
22	H	4.244951	4.388004	5.655149	6.123926	6.233021
23	C	5.593450	4.286308	4.245170	4.286308	4.899183
24	H	6.092505	4.400140	3.753125	3.455479	4.399018
25	H	6.415660	5.211515	5.156380	5.211515	5.533738
26	H	4.806491	3.455479	3.753125	4.400140	5.688744
27	C	6.794991	6.000373	5.953115	5.046433	3.430605
28	H	7.498039	6.712319	6.656308	5.865526	4.268582
29	H	7.244682	6.123926	5.655149	4.388004	2.618786
30	H	6.989039	6.512580	6.645477	5.618307	3.340489
		16	17	18	19	20
16	H	0.000000				
17	H	6.928386	0.000000			
18	H	5.751553	2.357170	0.000000		
19	C	6.194782	3.430605	4.896590	0.000000	
20	H	7.059848	4.268582	5.940416	1.099758	0.000000
21	H	6.024577	3.340489	4.633870	1.095391	1.772973
22	H	6.649400	2.618786	4.391044	1.093228	1.769511
23	C	5.916662	4.899183	5.916662	2.505993	2.758292
24	H	5.520938	5.688744	6.373414	3.470476	3.765106
25	H	6.818526	5.533738	6.818526	2.753705	2.547225
26	H	6.373414	4.399018	5.520938	2.762385	3.116943
27	C	4.896590	5.499494	6.194782	2.503450	2.746605
28	H	5.940417	6.074044	7.059848	2.746605	2.530257
29	H	4.391044	6.233021	6.649400	3.470983	3.754991
30	H	4.633871	5.493482	6.024577	2.766173	3.108754
		21	22	23	24	25
21	H	0.000000				
22	H	1.766440	0.000000			
23	C	3.474493	2.759588	0.000000		
24	H	4.334375	3.771532	1.092086	0.000000	
25	H	3.767557	3.103472	1.102278	1.773716	0.000000
26	H	3.774043	2.565545	1.092086	1.762940	1.773716
27	C	2.766173	3.470983	2.505993	2.762385	2.753705
28	H	3.108754	3.754991	2.758292	3.116943	2.547225
29	H	3.780542	4.335048	2.759588	2.565545	3.103472
30	H	2.577176	3.780542	3.474493	3.774043	3.767557
		26	27	28	29	30
26	H	0.000000				
27	C	3.470476	0.000000			
28	H	3.765106	1.099758	0.000000		
29	H	3.771532	1.093228	1.769511	0.000000	
30	H	4.334375	1.095391	1.772973	1.766440	0.000000

Interatomic angles:

P1-C2-C3=120.4058	P1-C2-C4= 93.6487	P1-C3-C4= 92.3012
C2-C3-C4=126.3139	C2-P1-C5= 76.3797	P1-C5-C3= 64.1156
C2-C3-C5= 97.3776	P1-C5-C4= 92.3012	C2-C4-C5= 95.0067
C3-C4-C5=121.2919	C2-P1-C6= 99.9432	C3-P1-C6= 76.3797

C3-C2-C6= 82.6224	P1-C6-C4= 93.6487	C2-C4-C6= 68.4712
C3-C4-C6= 95.0067	P1-C6-C5=120.4058	C2-C6-C5= 82.6224
C3-C5-C6= 97.3776	C4-C5-C6=126.3139	C2-P1-C7=104.0219
C3-P1-C7=100.8561	C3-C2-C7=110.5277	C4-C2-C7= 92.5354
C5-P1-C7=100.8561	C5-C2-C7= 77.0533	C6-P1-C7=104.0219
C2-C6-C7= 61.9341	C3-C6-C7= 77.0533	C4-C6-C7= 92.5354
C5-C6-C7=110.5277	P1-C5-Si8= 68.8219	C2-C5-Si8=102.1139
C3-C5-Si8=128.9755	C4-C5-Si8=157.8761	P1-C6-Si8=119.3675
C2-C6-Si8=149.4872	C3-C6-Si8=160.5933	C4-C6-Si8=144.9924
C5-C6-Si8=119.7011	C7-C6-Si8=119.9687	P1-C6-H9=150.2211
C2-C6-H9=159.4645	C3-C6-H9=139.8767	C4-C6-H9=115.2034
C5-C6-H9= 88.9902	C7-C6-H9=138.5125	C5-Si8-H9= 84.7745
C6-Si8-H9=110.1801	P1-C2-Si10=119.3675	P1-C3-Si10= 68.8219
C3-C2-Si10=119.7011	C4-C2-Si10=144.9924	C4-C3-Si10=157.8761
C5-C2-Si10=160.5933	C5-C3-Si10=128.9755	C6-C2-Si10=149.4872
C6-C3-Si10=102.1139	C7-C2-Si10=119.9687	P1-C2-H11=150.2211
C3-C2-H11= 88.9902	C4-C2-H11=115.2034	C5-C2-H11=139.8767
C6-C2-H11=159.4645	C7-C2-H11=138.5125	C2-Si10-H11=110.1801
C3-Si10-H11= 84.7745	P1-C2-H12=147.3447	P1-C3-H12=151.9227
C2-C3-H12=117.7262	C2-H12-C4= 71.7968	C4-C3-H12=115.7734
C5-C2-H12= 81.574	C5-C3-H12=143.4311	C5-C4-H12=147.2424
C6-C2-H12=109.1589	C6-C3-H12=167.8145	C6-C4-H12=122.0466
C7-C2-H12=127.551	Si10-C2-H12= 93.1561	Si10-C3-H12= 83.5736
C4-H12-Si10=110.2593	C2-H12-H11= 70.5815	C3-H12-H11=105.4299
C4-H12-H11=140.525	Si10-H11-H12= 86.0645	P1-C3-H13=118.5297
C2-C3-H13=152.5753	C2-C4-H13=145.4544	C3-C4-H13=118.7776
P1-C5-H13=118.5297	C2-C5-H13= 82.9434	C3-H13-C5= 69.448
C5-C4-H13=118.7776	C6-C3-H13= 82.9434	C6-C4-H13=145.4544
C6-C5-H13=152.5753	Si8-C5-H13=168.1899	Si10-C3-H13=168.1899
C2-H12-H13= 98.6405	H12-C3-H13= 89.5447	H12-C4-H13= 91.1928
C5-H13-H12= 96.0676	Si10-H12-H13=136.7289	H11-H12-H13=164.1515
C2-C4-H14=122.0466	C3-C4-H14=147.2424	P1-C5-H14=151.9227
C2-C5-H14=167.8145	C3-C5-H14=143.4311	C4-C5-H14=115.7734
P1-C6-H14=147.3447	C2-C6-H14=109.1589	C3-C6-H14= 81.574
C4-H14-C6= 71.7968	C6-C5-H14=117.7262	C7-C6-H14=127.551
C4-H14-Si8=110.2593	Si8-C5-H14= 83.5736	Si8-C6-H14= 93.1561
C4-H14-H9=140.525	C5-H14-H9=105.4299	C6-H14-H9= 70.5815
Si8-H9-H14= 86.0645	H12-C4-H14=164.3143	C3-H13-H14= 96.0676
H13-C4-H14= 91.1928	H13-C5-H14= 89.5447	C6-H14-H13= 98.6405
Si8-H14-H13=136.7289	H9-H14-H13=164.1515	H12-H13-H14=121.9899
P1-C6-H15=103.8053	C2-C6-H15=143.6741	C3-C6-H15=169.3707
C4-C6-H15=157.9492	C5-C6-H15=132.729	C7-C6-H15= 92.5447
C5-Si8-H15=128.4913	C6-Si8-H15=115.9353	C6-H9-H15= 66.6932
H9-Si8-H15=105.2919	H14-C6-H15=106.9366	H14-Si8-H15=129.3742
H14-H9-H15=107.9407	P1-C6-H16=102.0209	C2-C6-H16=121.4852
C3-C6-H16=135.4165	C4-C6-H16=139.9901	C5-C6-H16=126.8808
C7-C6-H16=122.5901	C5-Si8-H16=122.1872	C6-Si8-H16=114.7293
C6-H9-H16= 65.9811	H9-Si8-H16=106.2919	H14-C6-H16=106.2061
H14-Si8-H16=127.0765	H14-H9-H16=106.1179	C6-H16-H15= 65.797
H15-Si8-H16=103.53	H9-H15-H16= 60.8128	P1-C2-H17=103.8053
C3-C2-H17=132.729	C4-C2-H17=157.9492	C5-C2-H17=169.3707
C6-C2-H17=143.6741	C7-C2-H17= 92.5447	C2-Si10-H17=115.9353
C3-Si10-H17=128.4913	C2-H11-H17= 66.6932	H11-Si10-H17=105.2919
H12-C2-H17=106.9366	H12-Si10-H17=129.3742	H12-H11-H17=107.9407
P1-C2-H18=102.0209	C3-C2-H18=126.8808	C4-C2-H18=139.9902
C5-C2-H18=135.4165	C6-C2-H18=121.4852	C7-C2-H18=122.5901
C2-Si10-H18=114.7293	C3-Si10-H18=122.1872	C2-H11-H18= 65.9811
H11-Si10-H18=106.2919	H12-C2-H18=106.2061	H12-Si10-H18=127.0765
H12-H11-H18=106.1179	C2-H18-H17= 65.797	H17-Si10-H18=103.53
H11-H17-H18= 60.8128	C2-P1-C19= 91.638	C3-P1-C19=101.915
C5-P1-C19=126.5033	C6-P1-C19=135.2233	P1-C7-C19=106.9597

C2-C7-C19=	91.9267	C6-C7-C19=	143.2147	P1-C7-H20=	135.0047
C2-C7-H20=	116.2701	C6-C7-H20=	171.367	P1-C19-H20=	151.8729
C7-C19-H20=	110.5741	C2-P1-H21=	100.6479	C3-P1-H21=	117.6534
C5-P1-H21=	147.8766	C6-P1-H21=	148.8902	P1-C7-H21=	90.2167
C2-C7-H21=	91.2675	C6-C7-H21=	125.1612	P1-C19-H21=	85.5504
C7-C19-H21=	111.5997	P1-H21-H20=	105.5984	C7-H20-H21=	66.3455
H20-C19-H21=	107.7391	P1-C2-H22=	73.8039	C3-C2-H22=	121.9227
C4-C2-H22=	121.4244	C5-C2-H22=	117.3077	C6-C2-H22=	104.8153
P1-C7-H22=	94.1526	C2-H22-C7=	68.5458	C6-C7-H22=	124.4363
Si10-C2-H22=	81.7515	H11-C2-H22=	95.5395	H12-C2-H22=	117.1097
C2-H17-H22=	66.1722	C7-H22-H17=	121.9962	Si10-H17-H22=	101.7137
H11-H17-H22=	115.9354	H18-C2-H22=	98.3592	H18-H17-H22=	123.7946
P1-C19-H22=	90.9461	C2-H22-C19=	103.1068	C7-C19-H22=	111.5293
H17-H22-C19=	130.4634	C2-H22-H20=	134.4327	C7-H20-H22=	66.3066
H17-H22-H20=	152.6453	H20-C19-H22=	107.587	P1-H21-H22=	75.8116
C2-H22-H21=	100.7886	C7-H22-H21=	66.2715	H17-H22-H21=	97.3308
H21-C19-H22=	107.6276	H20-H22-H21=	60.187	C2-P1-C23=	85.9945
C3-P1-C23=	75.3904	C5-P1-C23=	75.3904	C6-P1-C23=	85.9945
P1-C7-C23=	114.371	C2-C7-C23=	89.8774	C6-C7-C23=	89.8774
P1-C19-C23=	66.7391	C19-C7-C23=	109.5798	P1-C23-H20=	84.1514
H20-C7-C23=	94.3653	H20-C19-C23=	91.234	H21-P1-C23=	72.4908
H21-C7-C23=	137.2978	H21-C19-C23=	146.7679	H21-H20-C23=	97.7592
P1-C23-H22=	64.3046	C2-H22-C23=	71.3065	H22-C7-C23=	94.148
H17-H22-C23=	131.2434	H22-C19-C23=	91.466	H22-H20-C23=	71.3353
H21-H22-C23=	97.8791	P1-C5-H24=	67.0575	C2-C5-H24=	77.6098
C3-C5-H24=	83.1348	C4-C5-H24=	86.3268	P1-C6-H24=	79.3003
C2-C6-H24=	79.6641	C3-C6-H24=	74.2546	C4-C6-H24=	70.0263
C6-C5-H24=	77.4837	P1-C7-H24=	98.8243	C2-C7-H24=	89.0336
C5-H24-C7=	93.1961	C6-H24-C7=	70.0151	Si8-C5-H24=	96.1773
Si8-C6-H24=	124.1054	H9-C6-H24=	116.1966	H13-C5-H24=	95.3337
H14-C5-H24=	112.779	H14-C6-H24=	84.8764	H15-C6-H24=	99.7605
H16-C6-H24=	148.771	C19-C7-H24=	137.36	H20-C7-H24=	119.3555
H21-C7-H24=	165.0781	H22-C7-H24=	119.3724	P1-C23-H24=	90.5231
C5-H24-C23=	117.0093	C6-H24-C23=	104.0589	C7-C23-H24=	111.3874
C19-C23-H24=	146.6379	H20-C23-H24=	153.1523	H22-C23-H24=	153.9797
P1-C7-H25=	142.6449	C2-C7-H25=	114.5885	C6-C7-H25=	114.5885
P1-C19-H25=	89.3461	C19-C7-H25=	94.1022	H20-C7-H25=	71.5159
C19-H20-H25=	88.8246	H21-C7-H25=	119.1796	H21-C19-H25=	153.7734
H21-H20-H25=	120.3415	H22-C7-H25=	90.603	H22-C19-H25=	98.1495
H22-H20-H25=	90.0764	P1-C23-H25=	147.8142	C7-C23-H25=	110.5508
C19-C23-H25=	90.9114	H20-H25-C23=	89.0286	H22-C23-H25=	97.5676
C5-H24-H25=	153.2372	C6-H24-H25=	135.8978	C7-H25-H24=	66.0823
C19-H25-H24=	97.7378	H20-H25-H24=	120.1726	H24-C23-H25=	107.8604
P1-C2-H26=	79.3003	P1-C3-H26=	67.0575	C2-C3-H26=	77.4837
C4-C2-H26=	70.0263	C4-C3-H26=	86.3268	C5-C2-H26=	74.2546
C5-C3-H26=	83.1348	C6-C2-H26=	79.6641	C6-C3-H26=	77.6098
P1-C7-H26=	98.8243	C2-H26-C7=	70.0151	C3-H26-C7=	93.1961
C6-C7-H26=	89.0336	Si10-C2-H26=	124.1054	Si10-C3-H26=	96.1773
H11-C2-H26=	116.1966	H12-C2-H26=	84.8764	H12-C3-H26=	112.779
H13-C3-H26=	95.3337	H17-C2-H26=	99.7604	H18-C2-H26=	148.771
P1-C19-H26=	68.6128	C2-H26-C19=	73.5773	C3-H26-C19=	101.3502
C19-C7-H26=	94.4021	H20-C7-H26=	91.2208	H20-C19-H26=	98.2809
H21-C7-H26=	119.3899	H21-C19-H26=	153.4321	C2-H26-H22=	65.601
C3-H26-H22=	91.344	H22-C7-H26=	71.9217	H17-H22-H26=	116.0988
C19-H22-H26=	88.5045	H20-H22-H26=	90.0135	H21-H22-H26=	120.0671
P1-C23-H26=	90.5231	C2-H26-C23=	104.0589	C3-H26-C23=	117.0093
C7-C23-H26=	111.3874	C19-C23-H26=	91.6554	H20-C23-H26=	98.731
H22-H26-C23=	88.3705	C2-H26-H24=	100.3359	C3-H26-H24=	96.8652
C5-H24-H26=	96.8652	C6-H24-H26=	100.3359	C7-H24-H26=	66.1703
C19-H26-H24=	97.7028	H22-H26-H24=	120.0847	H24-C23-H26=	107.6355
C2-H26-H25=	135.8978	C3-H26-H25=	153.2372	C7-H25-H26=	66.0823

C19-H25-H26= 71.5088	H20-H25-H26= 90.513	H22-H26-H25= 89.3922
H25-C23-H26=107.8604	H25-H24-H26= 60.2008	C2-P1-C27=135.2233
C3-P1-C27=126.5033	C5-P1-C27=101.915	C6-P1-C27= 91.638
P1-C7-C27=106.9597	C2-C7-C27=143.2147	C6-C7-C27= 91.9267
P1-C27-C19= 63.586	C19-C7-C27=109.2527	P1-C27-H20= 86.75
H20-C7-C27= 93.7232	H20-C19-C27= 90.6983	P1-C27-H21= 63.565
H21-C7-C27= 94.2708	H21-C19-C27= 91.9285	H21-H20-C27= 71.8394
H22-C7-C27=136.9583	H22-C19-C27=146.8982	H22-H20-C27= 98.1185
H22-H21-C27= 97.5007	P1-C27-C23= 66.7391	C23-C7-C27=109.5798
C19-C27-C23= 60.0336	H20-C27-C23= 63.1584	H21-C27-C23= 82.2915
H22-C23-C27= 82.3232	P1-C27-H24= 68.6128	C5-H24-C27=101.3502
C6-H24-C27= 73.5773	H24-C7-C27= 94.4021	C19-C27-H24= 82.2972
H20-C27-H24= 86.2268	H21-C27-H24=103.2561	H24-C23-C27= 91.6554
P1-C27-H25= 89.3461	H25-C7-C27= 94.1022	C19-C27-H25= 62.9634
H25-H20-C27= 62.5539	H21-C27-H25= 86.0851	H25-C23-C27= 90.9114
H24-H25-C27= 71.5088	H26-C7-C27=137.36	H26-C19-C27= 82.2972
H26-C23-C27=146.6379	H26-H24-C27= 97.7028	H26-H25-C27= 97.7378
P1-C7-H28=135.0047	C2-C7-H28=171.367	C6-C7-H28=116.2701
P1-C19-H28= 86.75	C19-C7-H28= 93.7232	H20-C7-H28= 70.9462
C19-H20-H28= 89.3017	H21-C7-H28= 90.7037	H21-C19-H28= 98.8008
H21-H20-H28= 90.7581	H22-C7-H28=118.5934	H22-C19-H28=153.2147
H22-H20-H28=120.6618	P1-C23-H28= 84.1514	C23-C7-H28= 94.3653
C23-C19-H28= 63.1584	H20-H28-C23= 62.6991	H22-C23-H28= 85.7675
H24-C7-H28= 91.2208	H24-C23-H28= 98.731	H25-C7-H28= 71.5159
C19-H28-H25= 62.5539	H20-H28-H25= 60.2201	C23-H25-H28= 89.0286
H24-H25-H28= 90.513	H26-C7-H28=119.3555	H26-C19-H28= 86.2268
H26-C23-H28=153.1523	H26-H25-H28=120.1726	P1-C27-H28=151.8729
C7-C27-H28=110.5741	C19-C27-H28= 90.6983	H20-H28-C27= 89.3017
H21-C27-H28= 97.5857	C23-C27-H28= 91.234	H24-C27-H28= 98.2809
H25-H28-C27= 88.8246	P1-C6-H29= 73.8039	C2-C6-H29=104.8153
C3-C6-H29=117.3077	C4-C6-H29=121.4244	C5-C6-H29=121.9227
P1-C7-H29= 94.1526	C2-C7-H29=124.4363	C6-H29-C7= 68.5458
Si8-C6-H29= 81.7515	H9-C6-H29= 95.5395	H14-C6-H29=117.1097
C6-H15-H29= 66.1722	C7-H29-H15=121.9962	Si8-H15-H29=101.7137
H9-H15-H29=115.9354	H16-C6-H29= 98.3592	H16-H15-H29=123.7946
C19-C7-H29=136.9583	H20-C7-H29=118.5934	H21-C7-H29=119.4871
H22-C7-H29=164.6506	P1-C23-H29= 64.3046	C6-H29-C23= 71.3065
C23-C7-H29= 94.148	H15-H29-C23=131.2434	C19-C23-H29= 82.3232
H20-C23-H29= 85.7675	H22-C23-H29=103.525	C5-H24-H29= 91.344
C6-H24-H29= 65.601	H24-C7-H29= 71.9217	H15-H29-H24=116.0988
C23-H24-H29= 88.3705	H25-C7-H29= 90.603	H25-C23-H29= 97.5676
H25-H24-H29= 89.3922	H26-C7-H29=119.3724	H26-C23-H29=153.9797
H26-H24-H29=120.0847	P1-C27-H29= 90.9461	C6-H29-C27=103.1068
C7-C27-H29=111.5293	H15-H29-C27=130.4634	C19-C27-H29=146.8982
H20-C27-H29=153.2147	H21-C27-H29=154.2087	C23-C27-H29= 91.466
H24-H29-C27= 88.5045	H25-C27-H29= 98.1495	C6-H29-H28=134.4327
C7-H28-H29= 66.3066	H15-H29-H28=152.6453	C19-H28-H29= 98.1185
H20-H28-H29=120.6618	C23-H28-H29= 71.3353	H24-H29-H28= 90.0135
H25-H28-H29= 90.0764	H28-C27-H29=107.587	C2-P1-H30=148.8902
C3-P1-H30=147.8766	C5-P1-H30=117.6534	C6-P1-H30=100.6479
P1-C7-H30= 90.2167	C2-C7-H30=125.1612	C6-C7-H30= 91.2675
P1-C19-H30= 63.565	C19-C7-H30= 94.2708	H20-C7-H30= 90.7037
H20-C19-H30= 97.5857	P1-H30-H21= 63.9975	H21-C7-H30= 72.1006
C19-H21-H30= 88.0715	H20-H21-H30= 89.2419	H22-C7-H30=119.4871
H22-C19-H30=154.2087	H22-H21-H30=119.8397	C23-P1-H30= 72.4908
C23-C7-H30=137.2978	C23-C19-H30= 82.2915	H24-C7-H30=119.3899
H25-C7-H30=119.1796	H25-C19-H30= 86.0851	H26-C7-H30=165.0781
H26-C19-H30=103.2561	P1-C27-H30= 85.5504	C7-C27-H30=111.5997
C19-C27-H30= 91.9285	H20-C27-H30= 98.8008	H21-H30-C27= 88.0715
C23-C27-H30=146.7679	H24-C27-H30=153.4321	H25-C27-H30=153.7734
P1-H30-H28=105.5984	C7-H28-H30= 66.3455	C19-H28-H30= 71.8394

H20-H28-H30= 90.7581	H21-H30-H28= 89.2419	C23-H28-H30= 97.7592
H25-H28-H30=120.3415	H28-C27-H30=107.7391	P1-H30-H29= 75.8116
C6-H29-H30=100.7886	C7-H29-H30= 66.2715	H15-H29-H30= 97.3308
C19-H30-H29= 97.5007	H21-H30-H29=119.8397	C23-H29-H30= 97.8791
H24-H29-H30=120.0671	H29-C27-H30=107.6276	H28-H29-H30= 60.187

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
P 1	0.82315	9.99814	4.13312	0.04558	14.17685
C 2	-0.97660	1.99909	4.95121	0.02630	6.97660
C 3	-0.15193	1.99907	4.12870	0.02416	6.15193
C 4	-0.39180	1.99910	4.36432	0.02838	6.39180
C 5	-0.15193	1.99907	4.12870	0.02416	6.15193
C 6	-0.97660	1.99909	4.95121	0.02630	6.97660
C 7	-0.38394	1.99925	4.35815	0.02654	6.38394
Si 8	0.91294	9.99825	3.05772	0.03108	13.08706
H 9	-0.19652	0.00000	1.19525	0.00127	1.19652
Si 10	0.91294	9.99825	3.05772	0.03108	13.08706
H 11	-0.19652	0.00000	1.19525	0.00127	1.19652
H 12	0.17627	0.00000	0.82237	0.00136	0.82373
H 13	0.17752	0.00000	0.82018	0.00230	0.82248
H 14	0.17627	0.00000	0.82237	0.00136	0.82373
H 15	-0.20092	0.00000	1.19921	0.00171	1.20092
H 16	-0.18890	0.00000	1.18710	0.00180	1.18890
H 17	-0.20092	0.00000	1.19921	0.00171	1.20092
H 18	-0.18890	0.00000	1.18710	0.00180	1.18890
C 19	-0.56929	1.99930	4.55485	0.01514	6.56929
H 20	0.17723	0.00000	0.82118	0.00159	0.82277
H 21	0.19558	0.00000	0.80345	0.00097	0.80442
H 22	0.20399	0.00000	0.79501	0.00101	0.79601
C 23	-0.57048	1.99929	4.55469	0.01650	6.57048
H 24	0.20730	0.00000	0.79175	0.00094	0.79270
H 25	0.16727	0.00000	0.83082	0.00191	0.83273
H 26	0.20730	0.00000	0.79175	0.00094	0.79270
C 27	-0.56929	1.99930	4.55485	0.01514	6.56929
H 28	0.17723	0.00000	0.82118	0.00159	0.82277
H 29	0.20399	0.00000	0.79501	0.00101	0.79601
H 30	0.19558	0.00000	0.80345	0.00097	0.80442
=====					
* Total *	-1.00000	47.98721	67.67692	0.33586	116.00000

Table 25 : Distances, angles and NBO charges in pentadienyl anion.

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	3.386322	0.000000			
3	C	3.251504	1.375447	0.000000		
4	C	2.557804	2.557801	1.417183	0.000000	
5	C	1.375466	3.251520	2.563386	1.417183	0.000000
6	H	1.087767	4.454021	4.323875	3.497686	2.138790
7	H	1.082264	2.830819	3.143971	2.936084	2.169149
8	H	4.454026	1.087757	2.138721	3.497636	4.323867
9	H	2.830826	1.082232	2.169096	2.936061	3.143984
10	H	4.308125	2.080936	1.096127	2.104665	3.460212
11	H	3.451232	3.451251	2.124972	1.090195	2.124935
12	H	2.080948	4.308149	3.460235	2.104694	1.096129
		6	7	8	9	10
6	H	0.000000				
7	H	1.844896	0.000000			
8	H	5.508956	3.812471	0.000000		
9	H	3.812459	2.020569	1.844910	0.000000	
10	H	5.363763	4.239791	2.370751	3.079786	0.000000
11	H	4.257029	3.977431	4.256993	3.977418	2.312830
12	H	2.370833	3.079833	5.363759	4.239807	4.202118
		11	12			
11	H	0.000000				
12	H	2.312814	0.000000			

Interatomic angles:

C1-C4-C2= 82.8989	C1-C4-C3=106.1909	C2-C3-C4=132.6654
C1-C5-C3=107.4058	C2-C3-C5=107.4073	C1-C5-C4=132.6638
C2-C4-C5=106.1919	C3-C4-C5=129.4839	C4-C1-H6=144.1116
C5-C1-H6=120.0684	C3-C5-H6=133.5191	C4-C5-H6=158.7771
C1-H7-C2=111.8688	C3-C2-H7= 89.8467	C4-C1-H7= 99.4282
C4-C2-H7= 65.8041	C3-C4-H7= 84.8677	C5-C1-H7=123.4714
C2-H7-C5= 79.9346	C3-C5-H7= 82.8114	C4-C5-H7=108.0694
H6-C1-H7=116.4602	C2-H7-H6=143.7287	C4-H7-H6= 91.1085
C5-H6-H7= 65.4982	C3-C2-H8=120.0643	C4-C2-H8=144.1069
C4-C3-H8=158.7805	C5-C3-H8=133.5225	H7-C2-H8=150.089
C1-H9-C2=111.8697	C1-H9-C3= 79.9348	C3-C2-H9=123.4706
C4-C1-H9= 65.8034	C4-C2-H9= 99.428	C4-C3-H9=108.0709
C5-C1-H9= 89.8466	C5-C3-H9= 82.8128	C5-C4-H9= 84.8691
H6-C1-H9=150.085	C1-H7-H9=129.1215	C2-H9-H7=129.1234
C3-H9-H7= 97.1885	C4-H9-H7= 69.8741	C5-H7-H9= 97.1873
H6-H7-H9=160.9814	C1-H9-H8=143.7275	H8-C2-H9=116.4651
C3-H8-H9= 65.4977	C4-H9-H8= 91.1071	H7-H9-H8=160.9812
C2-C3-H10=114.2187	C1-C4-H10=134.8106	C2-H10-C4= 75.3351
C4-C3-H10=113.1159	C5-C3-H10=138.374	C5-C4-H10=158.1036
H7-C2-H10=118.5573	H7-C4-H10=113.4874	H8-C2-H10= 91.3537
H8-C3-H10= 88.1035	C4-H10-H8=102.6381	H9-C2-H10=152.1812
H9-C3-H10=138.8132	H9-C4-H10= 73.2344	H9-H8-H10= 93.0204
C2-C3-H11=160.3099	C1-C4-H11=138.5494	C2-C4-H11=138.5517
C3-C4-H11=115.2597	C1-C5-H11=160.3097	C3-H11-C5= 74.1935
C5-C4-H11=115.2564	H6-C5-H11=173.577	H7-C4-H11=159.8726
H7-C5-H11=135.7153	H8-C3-H11=173.575	H9-C3-H11=135.7154
H9-C4-H11=159.8744	C2-H10-H11=103.4056	H10-C3-H11= 85.4714
H10-C4-H11= 86.64	C5-H11-H10=102.3872	H8-H10-H11=130.7086
C1-H12-C4= 75.3343	C2-C4-H12=134.8107	C3-C4-H12=158.1027
C1-C5-H12=114.218	C3-C5-H12=138.3762	C4-C5-H12=113.1182
H6-C1-H12= 91.3577	C4-H12-H6=102.6365	H6-C5-H12= 88.1047
H7-C1-H12=152.1821	H7-C4-H12= 73.235	H7-C5-H12=138.8124
H7-H6-H12= 93.02	H9-C1-H12=118.5573	H9-C4-H12=113.488

H10-C4-H12=173.2776 C1-H12-H11=103.405 C3-H11-H12=102.3875
 H11-C4-H12= 86.6376 H11-C5-H12= 85.4723 H6-H12-H11=130.7072
 H10-H11-H12=130.5812

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
C 1	-0.68938	1.99931	4.64420	0.04587	6.68938
C 2	-0.68937	1.99931	4.64419	0.04587	6.68937
C 3	-0.24315	1.99924	4.22434	0.01958	6.24315
C 4	-0.48932	1.99919	4.45424	0.03589	6.48932
C 5	-0.24316	1.99924	4.22434	0.01958	6.24316
H 6	0.18749	0.00000	0.81157	0.00094	0.81251
H 7	0.19746	0.00000	0.80136	0.00118	0.80254
H 8	0.18749	0.00000	0.81157	0.00094	0.81251
H 9	0.19746	0.00000	0.80136	0.00118	0.80254
H 10	0.19354	0.00000	0.80456	0.00190	0.80646
H 11	0.19740	0.00000	0.80129	0.00131	0.80260
H 12	0.19354	0.00000	0.80456	0.00190	0.80646
=====					
* Total *	-1.00000	9.99628	27.82758	0.17614	38.00000

Table 26 : Distances, angles and NBO charges in cyclopentadienyl anion.

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.516895	0.000000			
3	C	2.490173	1.372106	0.000000		
4	C	2.884342	2.449515	1.423548	0.000000	
5	C	2.490174	2.798089	2.412022	1.423548	0.000000
6	C	1.516895	2.465411	2.798088	2.449514	1.372106
7	H	1.100982	2.169912	3.379769	3.897013	3.379770
8	H	1.124823	2.186097	3.007162	3.315740	3.007162
9	H	2.263337	1.089673	2.147268	3.438117	3.873002
10	H	3.484301	2.127229	1.093596	2.171475	3.387341
11	H	3.971401	3.424330	2.186260	1.087185	2.186260
12	H	3.484302	3.876950	3.387342	2.171476	1.093596
13	H	2.263336	3.436092	3.873001	3.438117	2.147267
		6	7	8	9	10
6	C	0.000000				
7	H	2.169913	0.000000			
8	H	2.186096	1.760346	0.000000		
9	H	3.436092	2.499555	2.814866	0.000000	
10	H	3.876948	4.279388	3.949032	2.460767	0.000000
11	H	3.424329	4.978957	4.351464	4.322837	2.499896
12	H	2.127230	4.279389	3.949032	4.940629	4.261208
13	H	1.089673	2.499556	2.814864	4.307331	4.940628
		11	12	13		
11	H	0.000000				
12	H	2.499897	0.000000			
13	H	4.322837	2.460767	0.000000		

Interatomic angles:

C1-C2-C3=118.9875	C1-C2-C4= 90.1413	C1-C3-C4= 90.7433
C2-C3-C4=122.3608	C2-C1-C5= 84.8919	C1-C3-C5= 61.0329
C2-C3-C5= 91.1148	C1-C5-C4= 90.7433	C2-C4-C5= 88.3788
C3-C4-C5=115.814	C2-C1-C6=108.7114	C3-C1-C6= 84.8919
C3-C2-C6= 88.8852	C1-C6-C4= 90.1414	C2-C4-C6= 60.4298
C3-C4-C6= 88.3787	C1-C6-C5=118.9876	C2-C6-C5= 88.8853
C3-C5-C6= 91.1147	C4-C5-C6=122.3607	C2-C1-H7=110.9703
C3-C1-H7=136.9923	C3-C2-H7=144.2329	C4-C1-H7=152.9236
C4-C2-H7=114.9135	C5-C1-H7=136.9924	C5-C2-H7= 84.7317
C6-C1-H7=110.9704	C2-H7-C6= 69.2343	C3-C6-H7= 84.7317
C4-C6-H7=114.9135	C5-C6-H7=144.233	C2-C1-H8=110.8185
C3-C1-H8=106.3484	C3-C2-H8=113.3875	C4-C1-H8=102.5458
C4-C2-H8= 91.1503	C4-C3-H8= 89.4955	C5-C1-H8=106.3483
C5-C2-H8= 73.0564	C5-C3-H8= 66.3564	C4-C5-H8= 89.4955
C6-C1-H8=110.8184	C2-H8-C6= 68.6497	C3-C6-H8= 73.0564
C4-C6-H8= 91.1503	C5-C6-H8=113.3875	H7-C1-H8=104.5307
C2-H7-H8= 66.6468	C3-H8-H7= 86.1059	C5-H8-H7= 86.106
C6-H7-H8= 66.6468	C1-C2-H9=119.6288	C1-H9-C3= 68.6893
C3-C2-H9=121.013	C4-C1-H9= 82.8661	C4-C2-H9=150.2154
C4-C3-H9=147.9801	C5-C1-H9=109.0355	C5-C2-H9=168.8768
C5-C3-H9=116.1888	C6-C1-H9=129.6671	C6-C2-H9=147.6903
C6-C3-H9= 86.9788	H7-C1-H9= 88.9988	H7-C2-H9= 94.2672
C3-H9-H7= 93.0134	C6-H7-H9= 94.4965	H8-C1-H9=107.5524
H8-C2-H9=114.2539	C3-H9-H8= 73.2137	C5-H8-H9= 83.3301
C6-H8-H9= 85.8261	H8-H7-H9= 80.6935	C1-C2-H10=145.433
C1-C3-H10=150.5654	C2-C3-H10=118.8154	C1-C4-H10= 85.9057

C2-H10-C4= 69.4675	C4-C3-H10=118.6508	C5-C2-H10= 85.7591
C5-C3-H10=147.7214	C5-C4-H10=139.9466	C6-C2-H10=114.9671
C6-C3-H10=168.9006	C6-C4-H10=113.9316	H7-C2-H10=169.5795
H8-C2-H10=132.561	H8-C3-H10=144.5186	C1-H9-H10= 94.9558
H9-C2-H10= 94.2416	H9-C3-H10= 93.0351	C4-H10-H9= 95.6383
H7-H9-H10=119.2455	H8-H9-H10= 96.6988	C1-C3-H11=116.1066
C2-C3-H11=147.5649	C1-C4-H11=178.9756	C2-C4-H11=148.5545
C3-C4-H11=120.5059	C1-C5-H11=116.1066	C2-C5-H11= 85.8613
C3-H11-C5= 66.9581	C5-C4-H11=120.506	C6-C3-H11= 85.8613
C6-C4-H11=148.5546	C6-C5-H11=147.5648	H8-C3-H11=112.8808
H8-C5-H11=112.8808	H9-C3-H11=171.9488	C2-H10-H11= 95.1324
H10-C3-H11= 93.2825	H10-C4-H11= 94.2779	C5-H11-H10= 92.3325
H9-H10-H11=121.2469	C1-C4-H12= 85.9057	C2-C4-H12=113.9316
C3-C4-H12=139.9466	C1-C5-H12=150.5654	C2-C5-H12=168.9006
C3-C5-H12=147.7214	C4-C5-H12=118.6508	C1-C6-H12=145.4331
C2-C6-H12=114.9671	C3-C6-H12= 85.7591	C4-H12-C6= 69.4674
C6-C5-H12=118.8154	H7-C6-H12=169.5795	H8-C5-H12=144.5186
H8-C6-H12=132.561	H10-C4-H12=157.7319	C3-H11-H12= 92.3325
H11-C4-H12= 94.2779	H11-C5-H12= 93.2825	C6-H12-H11= 95.1324
H10-H11-H12=116.9204	C2-C1-H13=129.6672	C3-C1-H13=109.0355
C4-C1-H13= 82.8661	C1-H13-C5= 68.6893	C2-C5-H13= 86.9788
C3-C5-H13=116.1888	C4-C5-H13=147.9801	C1-C6-H13=119.6287
C2-C6-H13=147.6903	C3-C6-H13=168.8768	C4-C6-H13=150.2154
C5-C6-H13=121.013	H7-C1-H13= 88.9989	C2-H7-H13= 94.4965
C5-H13-H7= 93.0134	H7-C6-H13= 94.2672	H8-C1-H13=107.5524
C2-H8-H13= 85.8261	C3-H8-H13= 83.3301	C5-H13-H8= 73.2138
H8-C6-H13=114.2538	H8-H7-H13= 80.6934	H9-C1-H13=144.1814
H9-H7-H13=118.9978	H9-H8-H13= 99.8326	H11-C5-H13=171.9488
C1-H13-H12= 94.9559	C4-H12-H13= 95.6382	H12-C5-H13= 93.0351
H12-C6-H13= 94.2416	H7-H13-H12=119.2456	H8-H13-H12= 96.6989
H11-H12-H13=121.2468		

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
C 1	-0.41737	1.99930	4.39580	0.02227	6.41737
C 2	-0.36375	1.99917	4.32662	0.03796	6.36375
C 3	-0.22307	1.99911	4.19965	0.02432	6.22307
C 4	-0.49038	1.99915	4.44548	0.04575	6.49038
C 5	-0.22307	1.99911	4.19965	0.02432	6.22307
C 6	-0.36375	1.99917	4.32662	0.03796	6.36375
H 7	0.16362	0.00000	0.83375	0.00263	0.83638
H 8	0.11129	0.00000	0.87908	0.00963	0.88871
H 9	0.15932	0.00000	0.83887	0.00181	0.84068
H 10	0.16058	0.00000	0.83708	0.00233	0.83942
H 11	0.16669	0.00000	0.83132	0.00199	0.83331
H 12	0.16058	0.00000	0.83708	0.00233	0.83942
H 13	0.15932	0.00000	0.83887	0.00181	0.84068
=====					
* Total *	-1.00000	11.99501	31.78988	0.21511	44.00000

Table 27 : Distances, angles and NBO charges in Me-P(CH=CH₂)₂

Distance matrix (angstroms):

		1	2	3	4	5
1	P	0.000000				
2	C	1.841096	0.000000			
3	C	2.792612	1.332772	0.000000		
4	C	2.792615	3.918202	4.845202	0.000000	
5	C	1.841098	2.801929	3.918172	1.332772	0.000000
6	H	3.809151	2.117871	1.086897	5.714378	4.762939
7	H	3.809153	4.762965	5.714369	1.086897	2.117870
8	H	2.959865	2.116766	1.086606	5.015482	4.283069
9	H	2.959870	4.283119	5.015513	1.086606	2.116766
10	H	2.545613	1.091756	2.096570	4.223889	2.994550
11	H	2.545612	2.994516	4.223821	2.096571	1.091756
12	C	1.867755	2.811810	3.914603	3.914569	2.811807
13	H	2.454940	3.065475	3.909076	4.883786	3.788606
14	H	2.504812	2.929595	4.155617	4.155584	2.929591
15	H	2.454938	3.788607	4.883812	3.909016	3.065467
		6	7	8	9	10
6	H	0.000000				
7	H	6.495646	0.000000			
8	H	1.847593	5.962750	0.000000		
9	H	5.962793	1.847593	4.948091	0.000000	
10	H	2.441578	4.897646	3.077435	4.816830	0.000000
11	H	4.897576	2.441577	4.816750	3.077436	2.774980
12	C	4.753525	4.753492	4.279457	4.279407	3.005966
13	H	4.683390	5.781358	4.192104	5.130886	3.344760
14	H	4.824440	4.824406	4.755561	4.755516	2.708490
15	H	5.781385	4.683333	5.130927	4.192012	4.012011
		11	12	13	14	15
11	H	0.000000				
12	C	3.005993	0.000000			
13	H	4.012032	1.092278	0.000000		
14	H	2.708516	1.094047	1.775564	0.000000	
15	H	3.344801	1.092278	1.768935	1.775564	0.000000

Interatomic angles:

P1-C2-C3=122.444	C2-P1-C4=113.8874	C3-P1-C4=120.3396
C2-P1-C5= 99.0943	C3-P1-C5=113.886	C3-C2-C5=140.0437
P1-C5-C4=122.4441	C2-C5-C4=140.0465	P1-C2-H6=148.2951
P1-C3-H6=155.6285	C2-C3-H6=121.8249	C5-C2-H6=150.6948
P1-C4-H7=155.6284	P1-C5-H7=148.2953	C2-C5-H7=150.6973
C5-C4-H7=121.8248	P1-C2-H8= 96.5601	P1-C3-H8= 87.9359
C2-C3-H8=121.7402	C4-P1-H8=121.3289	C5-P1-H8=124.6346
C5-C2-H8=120.4593	P1-H8-H6=102.3282	C2-H8-H6= 64.1625
H6-C3-H8=116.4349	C2-P1-H9=124.6372	C3-P1-H9=121.3301
P1-C4-H9= 87.936	P1-C5-H9= 96.5603	C2-C5-H9=120.4617
C5-C4-H9=121.7402	P1-H9-H7=102.3281	H7-C4-H9=116.4349
C5-H9-H7= 64.1625	H8-P1-H9=113.4117	P1-C2-H10=118.1822
P1-H10-C3= 73.2453	C3-C2-H10=119.373	C4-P1-H10=104.5105
C5-P1-H10= 84.4751	C5-C2-H10= 89.2938	C3-H10-C5= 99.1148
C4-C5-H10=152.7719	P1-H10-H6= 99.5773	H6-C2-H10= 93.5209
H6-C3-H10= 94.8377	C5-H10-H6=122.0371	H7-C5-H10=146.1506
H8-P1-H10= 67.4854	H8-C2-H10=145.2575	H8-C3-H10=148.7272
H8-H6-H10= 90.6078	H9-P1-H10=121.8895	H9-C5-H10=140.2982
C2-P1-H11= 84.4739	C3-P1-H11=104.5083	C3-C2-H11=152.7673
P1-H11-C4= 73.2454	C2-H11-C4= 99.117	P1-C5-H11=118.182
C2-C5-H11= 89.2919	C4-C5-H11=119.373	H6-C2-H11=146.1476
P1-H11-H7= 99.5774	C2-H11-H7=122.0396	H7-C4-H11= 94.8377

H7-C5-H11=	93.5209	H8-P1-H11=	121.8862	H8-C2-H11=	140.295
H9-P1-H11=	67.4853	H9-C4-H11=	148.7273	H9-C5-H11=	145.2575
H9-H7-H11=	90.6078	H10-P1-H11=	66.0564	C2-H10-H11=	90.7062
C3-H10-H11=	119.5835	C4-H11-H10=	119.5867	C5-H11-H10=	90.7081
H6-H10-H11=	139.6332	H7-H11-H10=	139.6377	C2-P1-C12=	98.5976
C3-P1-C12=	112.7668	C3-C2-C12=	138.8256	C4-P1-C12=	112.7651
C5-P1-C12=	98.5974	C2-C5-C12=	60.1162	C4-C5-C12=	138.8228
H6-C2-C12=	148.9571	H7-C5-C12=	148.9545	H8-P1-C12=	123.2635
H8-C2-C12=	119.8603	H9-P1-C12=	123.2606	H9-C5-C12=	119.858
H10-P1-C12=	84.3704	H10-C2-C12=	89.4179	C3-H10-C12=	98.6362
H10-C5-C12=	62.2626	H6-H10-C12=	121.177	H11-P1-C12=	84.3714
H11-C2-C12=	62.2637	C4-H11-C12=	98.6341	H11-C5-C12=	89.4196
H7-H11-C12=	121.1745	H11-H10-C12=	62.5116	C2-P1-H13=	89.8781
C3-P1-H13=	96.0934	C4-P1-H13=	136.988	C5-P1-H13=	123.1049
H8-P1-H13=	101.0532	H9-P1-H13=	142.558	H10-P1-H13=	83.9401
H11-P1-H13=	106.69	P1-C12-H13=	109.2491	C2-C12-H13=	92.7788
C5-C12-H13=	148.8017	H10-C12-H13=	98.3933	H11-C12-H13=	153.3152
C2-P1-H14=	83.268	C3-P1-H14=	103.2074	C3-C2-H14=	152.2421
C4-P1-H14=	103.2062	C5-P1-H14=	83.2678	C2-C5-H14=	61.4314
C4-C5-H14=	152.2384	H6-C2-H14=	145.3432	H7-C5-H14=	145.3409
H8-P1-H14=	120.746	H8-C2-H14=	140.3697	H9-P1-H14=	120.7439
H9-C5-H14=	140.3669	H10-P1-H14=	64.8569	C2-H10-H14=	90.5298
C3-H10-H14=	119.1825	C5-H14-H10=	64.0227	H6-H10-H14=	138.9751
H11-P1-H14=	64.8576	C2-H14-H11=	64.0215	C4-H11-H14=	119.1798
C5-H11-H14=	90.5281	H7-H11-H14=	138.9714	H10-H14-H11=	61.6306
P1-C12-H14=	112.875	C2-C12-H14=	85.1453	C5-C12-H14=	85.1452
H10-H14-C12=	94.8686	H11-H14-C12=	94.8687	P1-H13-H14=	70.5334
C2-H14-H13=	77.0126	C5-H14-H13=	104.5775	H10-H14-H13=	94.1669
H11-H14-H13=	125.6637	H13-C12-H14=	108.6077	C2-P1-H15=	123.1051
C3-P1-H15=	136.9899	C4-P1-H15=	96.0914	C5-P1-H15=	89.8779
H8-P1-H15=	142.5611	H9-P1-H15=	101.0501	H10-P1-H15=	106.6892
H11-P1-H15=	83.9414	P1-C12-H15=	109.249	C2-C12-H15=	148.8014
C5-C12-H15=	92.7785	H10-C12-H15=	153.3161	H11-C12-H15=	98.3941
P1-H15-H13=	68.8826	H13-C12-H15=	108.1423	P1-H15-H14=	70.5335
C2-H14-H15=	104.5774	C5-H14-H15=	77.0125	H10-H14-H15=	125.6639
H11-H14-H15=	94.1676	H14-C12-H15=	108.6077	H13-H15-H14=	60.1234

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
P 1	0.74859	9.99833	4.19949	0.05359	14.25141
C 2	-0.49290	1.99914	4.46811	0.02565	6.49290
C 3	-0.33028	1.99916	4.31117	0.01996	6.33028
C 4	-0.33029	1.99916	4.31117	0.01996	6.33029
C 5	-0.49289	1.99914	4.46811	0.02565	6.49289
H 6	0.18573	0.00000	0.81288	0.00139	0.81427
H 7	0.18573	0.00000	0.81288	0.00139	0.81427
H 8	0.18688	0.00000	0.81119	0.00193	0.81312
H 9	0.18688	0.00000	0.81119	0.00193	0.81312
H 10	0.19293	0.00000	0.80435	0.00272	0.80707
H 11	0.19293	0.00000	0.80435	0.00272	0.80707
C 12	-0.87884	1.99938	4.86540	0.01405	6.87884
H 13	0.22054	0.00000	0.77864	0.00081	0.77946
H 14	0.20444	0.00000	0.79327	0.00229	0.79556
H 15	0.22055	0.00000	0.77864	0.00081	0.77945
* Total *	0.00000	19.99431	33.83086	0.17483	54.00000

Table 28 : Distances, angles and NBO charges in *t*-Bu-P(CH=CH₂)₂.

Distance matrix (angstroms):

		1	2	3	4	5
1	P	0.000000				
2	C	1.840393	0.000000			
3	C	2.787833	1.333616	0.000000		
4	C	2.787833	3.947799	4.952731	0.000000	
5	C	1.840392	2.787669	3.947796	1.333616	0.000000
6	H	3.805597	2.118486	1.087081	5.813697	4.779832
7	H	3.805597	4.779834	5.813695	1.087081	2.118486
8	H	2.952912	2.118241	1.086624	5.178791	4.349487
9	H	2.952912	4.349493	5.178795	1.086624	2.118241
10	H	2.553999	1.090469	2.091232	4.180493	2.926493
11	H	2.553999	2.926489	4.180486	2.091231	1.090469
12	C	1.921270	2.921574	3.934924	3.934926	2.921578
13	C	2.783943	3.345101	3.922663	5.274593	4.264773
14	H	3.781321	4.332398	4.930636	6.071977	5.083099
15	H	2.922385	3.724745	4.078192	5.415883	4.584985
16	H	3.012593	2.925521	3.284401	5.685838	4.547902
17	C	2.912787	3.258945	4.420286	4.420397	3.259033
18	H	3.142738	3.599005	4.886975	3.887677	2.831513
19	H	3.878692	4.266077	5.339460	5.339541	4.266138
20	H	3.142742	2.831426	3.887523	4.887144	3.599163
21	C	2.783937	4.264755	5.274614	3.922557	3.344996
22	H	3.012586	4.547829	5.685808	3.284298	2.925382
23	H	2.922375	4.585007	5.415965	4.077997	3.724591
24	H	3.781317	5.083088	6.072003	4.930543	4.332313
		6	7	8	9	10
6	H	0.000000				
7	H	6.585725	0.000000			
8	H	1.847367	6.124174	0.000000		
9	H	6.124180	1.847367	5.176770	0.000000	
10	H	2.433607	4.831778	3.073784	4.810839	0.000000
11	H	4.831771	2.433607	4.810830	3.073783	2.645661
12	C	4.803933	4.803938	4.214338	4.214337	3.237680
13	C	4.709942	6.222325	4.013434	5.394823	3.827835
14	H	5.633065	6.959143	5.056551	6.220485	4.666679
15	H	4.955255	6.437558	3.871561	5.316350	4.438985
16	H	3.905023	6.625199	3.485700	5.887782	3.355920
17	C	5.052088	5.052220	5.011765	5.011864	3.042750
18	H	5.513585	4.328977	5.536351	4.635302	3.229661
19	H	5.925393	5.925494	5.888586	5.888658	4.041462
20	H	4.328803	5.513795	4.635141	5.536481	2.397200
21	C	6.222336	4.709813	5.394882	4.013365	4.614527
22	H	6.625144	3.904880	5.887808	3.485686	4.771581
23	H	6.437638	4.955030	5.316476	3.871388	5.146707
24	H	6.959161	5.632947	6.220545	5.056485	5.337188
		11	12	13	14	15
11	H	0.000000				
12	C	3.237689	0.000000			
13	C	4.614589	1.538008	0.000000		
14	H	5.337238	2.172932	1.096020	0.000000	
15	H	5.146731	2.191820	1.093969	1.767026	0.000000
16	H	4.771721	2.194952	1.093129	1.766593	1.767345
17	C	3.042846	1.535124	2.514087	2.754397	3.480821
18	H	2.397246	2.194316	3.483971	3.762011	4.348063
19	H	4.041530	2.171246	2.754324	2.539467	3.762080
20	H	3.229877	2.194313	2.773510	3.108499	3.790062
21	C	3.827704	1.538008	2.510650	2.750886	2.763217

22	H	3.355711	2.194951	3.480641	3.761580	3.778590
23	H	4.438822	2.191820	2.763221	3.102437	2.564521
24	H	4.666572	2.172932	2.750884	2.535642	3.102428
		16	17	18	19	20
16	H	0.000000				
17	C	2.776559	0.000000			
18	H	3.794556	1.093000	0.000000		
19	H	3.114746	1.096748	1.760716	0.000000	
20	H	2.587852	1.093001	1.770722	1.760718	0.000000
21	C	3.480641	2.514088	2.773519	2.754321	3.483969
22	H	4.349445	2.776556	2.587857	3.114737	3.794554
23	H	3.778592	3.480821	3.790068	3.762080	4.348061
24	H	3.761580	2.754400	3.108512	2.539468	3.762011
		21	22	23	24	
21	C	0.000000				
22	H	1.093129	0.000000			
23	H	1.093969	1.767345	0.000000		
24	H	1.096020	1.766593	1.767027	0.000000	

Interatomic angles:

P1-C2-C3=122.0715	C2-P1-C4=115.552	C3-P1-C4=125.3148
C2-P1-C5= 98.4635	C3-P1-C5=115.5519	C3-C2-C5=144.2648
P1-C5-C4=122.0715	C2-C5-C4=144.2651	P1-C2-H6=147.927
P1-C3-H6=155.8063	C2-C3-H6=121.7954	C5-C2-H6=153.6898
P1-C4-H7=155.8063	P1-C5-H7=147.9269	C2-C5-H7=153.69
C5-C4-H7=121.7954	P1-C2-H8= 96.227	P1-C3-H8= 87.7953
C2-C3-H8=121.8092	C4-P1-H8=128.8513	C5-P1-H8=128.8049
C5-C2-H8=124.3282	P1-H8-H6=102.4393	C2-H8-H6= 64.1556
H6-C3-H8=116.3951	C2-P1-H9=128.8053	C3-P1-H9=128.8515
P1-C4-H9= 87.7953	P1-C5-H9= 96.227	C2-C5-H9=124.3285
C5-C4-H9=121.8092	P1-H9-H7=102.4393	H7-C4-H9=116.3951
C5-H9-H7= 64.1556	H8-P1-H9=122.4587	P1-C2-H10=119.0134
P1-H10-C3= 72.9942	C3-C2-H10=118.8989	C4-P1-H10=102.9102
C5-P1-H10= 81.7706	C5-C2-H10= 86.2667	C3-H10-C5=102.4917
C4-C5-H10=156.0512	P1-H10-H6= 99.4324	H6-C2-H10= 93.0439
H6-C3-H10= 94.6356	C5-H10-H6=125.9386	H7-C5-H10=146.1168
H8-P1-H10= 67.4084	H8-C2-H10=144.7371	H8-C3-H10=148.9638
H8-H6-H10= 90.7197	H9-P1-H10=121.5913	H9-C5-H10=144.4955
C2-P1-H11= 81.7704	C3-P1-H11=102.9099	C3-C2-H11=156.0506
P1-H11-C4= 72.9942	C2-H11-C4=102.492	P1-C5-H11=119.9135
C2-C5-H11= 86.2666	C4-C5-H11=118.8989	H6-C2-H11=146.1165
P1-H11-H7= 99.4324	C2-H11-H7=125.9389	H7-C4-H11= 94.6356
H7-C5-H11= 93.0438	H8-P1-H11=121.5909	H8-C2-H11=144.4951
H9-P1-H11= 67.4084	H9-C4-H11=148.9638	H9-C5-H11=144.7371
H9-H7-H11= 90.7197	H10-P1-H11= 62.389	C2-H10-H11= 93.7333
C3-H10-H11=123.477	C4-H11-H10=123.4774	C5-H11-H10= 93.7335
H6-H10-H11=144.0479	H7-H11-H10=144.0485	C2-P1-C12=101.892
C3-P1-C12=112.0428	C3-C2-C12=131.5592	C4-P1-C12=112.0429
C5-P1-C12=101.8923	C5-C2-C12= 61.505	C4-C5-C12=131.559
H6-C2-C12=144.3137	H7-C5-C12=144.3137	H8-P1-C12=118.1301
H8-C2-C12=112.5078	H9-P1-C12=118.13	H9-C5-C12=112.5076
H10-P1-C12= 91.5671	H10-C2-C12= 96.8309	H10-C5-C12= 67.233
H11-P1-C12= 91.5674	H11-C2-C12= 67.2334	H11-C5-C12= 96.8312
C2-P1-C13= 90.2925	C3-P1-C13= 89.5014	C4-P1-C13=142.4048
C5-P1-C13=133.479	H8-P1-C13= 88.7371	H9-P1-C13=140.2129
H10-P1-C13= 91.5275	H11-P1-C13=119.5868	P1-C12-C13=106.6528
C2-C12-C13= 91.8406	C5-C12-C13=144.1817	P1-C12-H14=134.8202
C2-C12-H14=115.732	C5-C12-H14=172.2444	P1-C13-H14=151.1828
C12-C13-H14=110.033	C2-P1-H15=100.4247	C3-P1-H15= 91.1229
C4-P1-H15=143.0367	C5-P1-H15=147.725	H8-P1-H15= 82.4388

H9-P1-H15=129.6095	H10-P1-H15=108.115	H11-P1-H15=139.9429
P1-C12-H15= 90.306	C2-C12-H15= 92.39	C5-C12-H15=126.8593
P1-C13-H15= 86.1708	C12-C13-H15=111.6563	P1-H15-H14=104.7855
C12-H14-H15= 66.6801	H14-C13-H15=107.5815	P1-C2-H16= 74.5424
C3-P1-H16= 68.8506	C3-C2-H16= 93.3067	C4-P1-H16=157.1674
C5-P1-H16=137.8469	C5-C2-H16=105.481	H6-C2-H16=100.2353
H8-P1-H16= 71.5004	H8-C2-H16= 85.8565	H9-P1-H16=161.4812
H10-P1-H16= 73.6323	H10-C2-H16=103.7304	H11-P1-H16=117.7739
H11-C2-H16=109.2536	P1-C12-H16= 93.8522	C2-C12-H16= 68.047
C5-C12-H16=124.8562	P1-C13-H16= 91.2281	C2-H16-C13=102.9754
C12-C13-H16=111.9597	P1-H16-H14=101.3887	C2-H16-H14=133.3096
C12-H14-H16= 66.7981	H14-C13-H16=107.6032	P1-H15-H16= 75.4899
C2-H16-H15=102.2356	C12-H15-H16= 66.3346	H15-C13-H16=107.8171
H15-H14-H16= 60.02	C2-P1-C17= 83.3012	C3-P1-C17=101.661
C4-P1-C17=101.6645	C5-P1-C17= 83.3042	H8-P1-C17=117.3896
H9-P1-C17=117.3933	H10-P1-C17= 67.2699	H11-P1-C17= 67.2724
P1-C12-C17=114.3961	C2-C12-C17= 88.2657	C5-C12-C17= 88.2692
P1-C13-C17= 66.4782	C13-C12-C17=109.7873	P1-C17-H14= 83.6574
H14-C12-C17= 94.371	H14-C13-C17= 90.6738	H15-P1-C17= 73.2425
H15-C12-C17=137.4242	H15-C13-C17=146.7231	H15-H14-C17= 98.311
P1-C17-H16= 63.8927	C2-H16-C17= 69.6586	H16-C12-C17= 94.5522
H16-C13-C17= 92.0198	H16-H14-C17= 72.0558	H15-H16-C17= 97.5136
P1-C5-H18= 81.5711	C2-C5-H18= 79.6519	C4-C5-H18=134.7618
H7-C5-H18=121.3106	H9-C5-H18=138.4813	H10-C5-H18= 68.213
P1-H11-H18= 78.731	C2-H11-H18= 84.4447	C4-H11-H18=119.8734
C5-H11-H18=101.9389	H7-H11-H18=127.3012	H10-H11-H18= 79.4816
P1-C12-H18= 99.3544	C2-C12-H18= 88.2222	C5-H18-C12= 69.7704
H11-H18-C12= 89.5688	C13-C12-H18=137.2633	H14-C12-H18=118.9507
H15-C12-H18=164.8906	H16-C12-H18=119.6531	P1-C17-H18= 91.7804
C5-H18-C17=103.1597	H11-H18-C17=116.2465	C12-C17-H18=112.1229
C13-C17-H18=147.2613	H14-C17-H18=153.1371	H16-C17-H18=154.8626
P1-C12-H19=142.7222	C2-C12-H19=112.9624	C5-C12-H19=112.9648
P1-C13-H19= 88.9076	C13-C12-H19= 94.3495	H14-C12-H19= 71.5449
C13-H14-H19= 89.3428	H15-C12-H19=119.141	H15-C13-H19=153.0151
H15-H14-H19=120.7004	H16-C12-H19= 91.0191	H16-C13-H19= 98.7921
H16-H14-H19= 90.8423	P1-C17-H19=146.9776	C12-C17-H19=110.0573
C13-C17-H19= 90.6526	H14-H19-C17= 89.3309	H16-C17-H19= 97.4483
C5-H18-H19=135.259	H11-H18-H19=152.4874	C12-H19-H18= 66.903
C13-H19-H18= 98.6075	H14-H19-H18=120.9847	H18-C17-H19=107.0414
P1-C2-H20= 81.5737	C3-C2-H20=134.7561	C5-C2-H20= 79.6576
H6-C2-H20=121.3061	H8-C2-H20=138.4761	P1-H10-H20= 78.7319
C2-H10-H20=101.936	C3-H10-H20=119.8676	C5-H10-H20= 84.4501
H6-H10-H20=127.2941	H11-C2-H20= 68.2194	H11-H10-H20= 79.4888
P1-C12-H20= 99.3547	C2-H20-C12= 69.772	C5-C12-H20= 88.2272
H10-H20-C12= 89.5697	P1-C13-H20= 68.8738	C2-H20-C13= 73.2758
H10-H20-C13= 95.2356	C13-C12-H20= 94.3493	H14-C12-H20= 90.7578
H14-C13-H20= 97.2681	H15-C12-H20=119.5604	H15-C13-H20=154.463
P1-H16-H20= 67.7823	C2-H20-H16= 65.164	H10-H20-H16= 84.5363
H16-C12-H20= 72.2554	C13-H16-H20= 87.9788	H14-H16-H20= 89.0283
H15-H16-H20=119.7866	P1-C17-H20= 91.7806	C2-H20-C17=103.1593
H10-H20-C17=116.2426	C12-C17-H20=112.1226	C13-C17-H20= 91.8464
H14-C17-H20= 98.4176	H16-H20-C17= 88.1528	C2-H20-H18=100.3435
C5-H18-H20=100.347	H10-H20-H18=100.5109	H11-H18-H20=100.5188
C12-H20-H18= 66.2042	C13-H20-H18= 97.6658	H16-H20-H18=119.8835
H18-C17-H20=108.1974	C2-H20-H19=135.2605	H10-H20-H19=152.4845
C12-H19-H20= 66.9028	C13-H19-H20= 72.0195	H14-H19-H20= 90.7288
H16-H20-H19= 89.3998	H19-C17-H20=107.0415	H18-H19-H20= 60.3763
C2-P1-C21=133.4781	C3-P1-C21=142.4065	C4-P1-C21= 89.4985
C5-P1-C21= 90.2888	H8-P1-C21=140.2167	H9-P1-C21= 88.7353
H10-P1-C21=119.5843	H11-P1-C21= 91.5236	P1-C12-C21=106.6525
C2-C12-C21=144.1804	C5-C12-C21= 91.8359	P1-C21-C13= 63.1976

C13-C12-C21=109.4127	P1-C21-H14= 86.1843	H14-C12-C21= 94.1205
H14-C13-C21= 90.6533	P1-C21-H15= 63.5812	H15-C12-C21= 93.9619
H15-C13-C21= 91.4108	H15-H14-C21= 71.6887	H16-P1-C21= 73.6882
H16-C12-C21=136.9217	H16-C13-C21=147.2533	H16-H14-C21= 98.4405
H16-H15-C21= 97.9803	P1-C21-C17= 66.4782	C17-C12-C21=109.7874
C17-C13-C21= 60.0452	H14-C21-C17= 62.8989	H15-C21-C17= 82.3903
H16-C17-C21= 82.1158	P1-C21-H18= 68.8737	C5-H18-C21= 73.2717
H11-H18-C21= 95.23	H18-C12-C21= 94.3496	C13-C21-H18= 82.3343
H14-C21-H18= 85.8396	H15-C21-H18=103.4989	H18-C17-C21= 91.8469
P1-C21-H19= 88.9077	H19-C12-C21= 94.3494	C13-C21-H19= 62.8859
H19-H14-C21= 62.5988	H15-C21-H19= 85.9751	H19-C17-C21= 90.6524
H18-H19-C21= 72.0199	H20-C12-C21=137.2634	H20-C13-C21= 82.3344
H20-C17-C21=147.261	H20-H18-C21= 97.6655	H20-H19-C21= 98.6075
C2-P1-H22=137.8421	C3-P1-H22=157.165	C4-P1-H22= 68.8483
P1-C5-H22= 74.5459	C2-C5-H22=105.4822	C4-C5-H22= 93.3079
H7-C5-H22=100.2344	H8-P1-H22=161.4851	H9-P1-H22= 71.5002
H9-C5-H22= 85.8596	H10-P1-H22=117.7685	H10-C5-H22=109.2526
H11-P1-H22= 73.627	H11-C5-H22=103.7256	P1-C12-H22= 93.8519
C2-C12-H22=124.8528	C5-C12-H22= 68.043	C13-P1-H22= 73.6882
C13-C12-H22=136.9217	H14-C12-H22=118.9002	H15-P1-H22= 79.0712
H15-C12-H22=118.9393	H16-P1-H22= 92.4195	H16-C12-H22=164.4306
P1-C17-H22= 63.8926	C5-H22-C17= 69.6629	C17-C12-H22= 94.5521
C13-C17-H22= 82.1159	H14-C17-H22= 85.7013	H16-C17-H22=103.1172
P1-H22-H18= 67.7822	C5-H18-H22= 65.1591	H11-H18-H22= 84.5288
H18-C12-H22= 72.2555	C17-H18-H22= 88.1524	H19-C12-H22= 91.0188
H19-C17-H22= 97.448	H19-H18-H22= 89.3993	H20-C12-H22=119.6532
H20-C17-H22=154.8628	H20-H18-H22=119.8832	P1-C21-H22= 91.228
C5-H22-C21=102.977	C12-C21-H22=111.9596	C13-C21-H22=147.2532
H14-C21-H22=153.6051	H15-C21-H22=154.3863	C17-C21-H22= 92.0195
H18-H22-C21= 87.979	H19-C21-H22= 98.7917	C2-P1-H23=147.7278
C3-P1-H23=143.0425	C4-P1-H23= 91.1175	C5-P1-H23=100.4188
H8-P1-H23=129.6156	H9-P1-H23= 82.4345	H10-P1-H23=139.942
H11-P1-H23=108.1094	P1-C12-H23= 90.3056	C2-C12-H23=126.8606
C5-C12-H23= 92.3847	P1-C13-H23= 63.5808	C13-C12-H23= 93.9621
H14-C12-H23= 90.598	H14-C13-H23= 97.4795	P1-H23-H15= 63.9746
H15-C12-H23= 71.6089	C13-H15-H23= 88.5892	H14-H15-H23= 89.532
H16-P1-H23= 79.0713	H16-C12-H23=118.9394	H16-C13-H23=154.386
H16-H15-H23=120.3296	C17-P1-H23= 73.2427	C17-C12-H23=137.4242
C17-C13-H23= 82.3902	H18-C12-H23=119.5606	H19-C12-H23=119.141
H19-C13-H23= 85.975	H20-C12-H23=164.8907	H20-C13-H23=103.4989
P1-C21-H23= 86.1706	C12-C21-H23=111.6563	C13-C21-H23= 91.411
H14-C21-H23= 98.2243	H15-H23-C21= 88.589	C17-C21-H23=146.7231
H18-C21-H23=154.4626	H19-C21-H23=153.0155	P1-H23-H22= 75.4899
C5-H22-H23=102.2343	C12-H23-H22= 66.3346	C13-H23-H22= 97.9801
H15-H23-H22=120.3296	C17-H22-H23= 97.5137	H18-H22-H23=119.7866
H22-C21-H23=107.817	P1-C12-H24=134.8198	C2-C12-H24=172.2421
C5-C12-H24=115.7281	P1-C13-H24= 86.1841	C13-C12-H24= 94.1204
H14-C12-H24= 71.3887	C13-H14-H24= 89.3467	H15-C12-H24= 90.5976
H15-C13-H24= 98.2238	H15-H14-H24= 90.468	H16-C12-H24=118.9002
H16-C13-H24=153.6055	H16-H14-H24=120.888	P1-C17-H24= 83.6573
C17-C12-H24= 94.3712	C17-C13-H24= 62.899	C17-H14-H24= 62.5943
H16-C17-H24= 85.7012	H18-C12-H24= 90.7582	H18-C17-H24= 98.4182
H19-C12-H24= 71.545	C13-H24-H19= 62.5988	H19-H14-H24= 60.0498
C17-H19-H24= 89.3311	H18-H19-H24= 90.7293	H20-C12-H24=118.9509
H20-C13-H24= 85.8398	H20-C17-H24=153.1365	H20-H19-H24=120.9846
P1-C21-H24=151.183	C12-C21-H24=110.0331	C13-C21-H24= 90.6532
H14-H24-C21= 89.3468	H15-C21-H24= 97.4792	C17-C21-H24= 90.674
H18-C21-H24= 97.2684	H19-H24-C21= 89.3426	P1-H22-H24=101.3888
C5-H22-H24=133.3127	C12-H24-H22= 66.7981	C13-H24-H22= 98.4406
H14-H24-H22=120.888	C17-H24-H22= 72.0556	H18-H22-H24= 89.0287
H19-H24-H22= 90.8419	H22-C21-H24=107.6031	P1-H23-H24=104.7857

C12-H24-H23= 66.6801 C13-H24-H23= 71.6889 H14-H24-H23= 90.4684
H15-H23-H24= 89.5316 C17-H24-H23= 98.3108 H19-H24-H23=120.7003
H23-C21-H24=107.5816 H22-H24-H23= 60.02

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
P 1	0.78386	9.99819	4.17131	0.04665	14.21614
C 2	-0.50259	1.99913	4.47860	0.02486	6.50259
C 3	-0.32636	1.99916	4.30787	0.01933	6.32636
C 4	-0.32636	1.99916	4.30787	0.01932	6.32636
C 5	-0.50259	1.99913	4.47860	0.02486	6.50259
H 6	0.18572	0.00000	0.81304	0.00124	0.81428
H 7	0.18572	0.00000	0.81304	0.00124	0.81428
H 8	0.18671	0.00000	0.81163	0.00166	0.81329
H 9	0.18671	0.00000	0.81163	0.00166	0.81329
H 10	0.19350	0.00000	0.80355	0.00295	0.80650
H 11	0.19350	0.00000	0.80355	0.00295	0.80650
C 12	-0.35467	1.99925	4.33316	0.02226	6.35467
C 13	-0.57289	1.99930	4.55779	0.01580	6.57289
H 14	0.19824	0.00000	0.80058	0.00118	0.80176
H 15	0.20458	0.00000	0.79459	0.00083	0.79542
H 16	0.20561	0.00000	0.79359	0.00080	0.79439
C 17	-0.56935	1.99929	4.55465	0.01540	6.56935
H 18	0.19852	0.00000	0.80065	0.00083	0.80148
H 19	0.19808	0.00000	0.80052	0.00139	0.80192
H 20	0.19852	0.00000	0.80065	0.00083	0.80148
C 21	-0.57289	1.99930	4.55779	0.01580	6.57289
H 22	0.20562	0.00000	0.79358	0.00080	0.79438
H 23	0.20458	0.00000	0.79459	0.00083	0.79542
H 24	0.19824	0.00000	0.80058	0.00118	0.80176
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* Total *	0.00000	25.99191	51.78346	0.22463	78.00000