

Supporting Materials for the Article

The Reactions of Oxotitanium(IV) Tetraphenylporphyrin with Methyl Methacrylate Radicals: A DFT Study

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Взаимодействие титанилового комплекса мезо-тетрафенилпорфирина с метилметакрилатными радикалами: DFT исследование

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S1. DFT calculations

Table S1 compares the calculated geometric parameters of oxotitanium 2,3,7,8,12,13,17,18-octaethylporphyrin (OEPTi=O) with those found by single crystal X-ray diffraction analysis. As one can see from Table S1, both methods used sufficiently well reproduce its structure: the mean deviation from the experiment does not exceed 2 %. The PBE/3z method more accurately reproduces the metal–extra-ligand bond length and the distance from the metal to the porphyrin ring plane. Furthermore, quantum-chemical calculations by the PBE/3z method are much faster than by the B3LYP/6-31G(d) method, therefore the former approximation was used in this study.

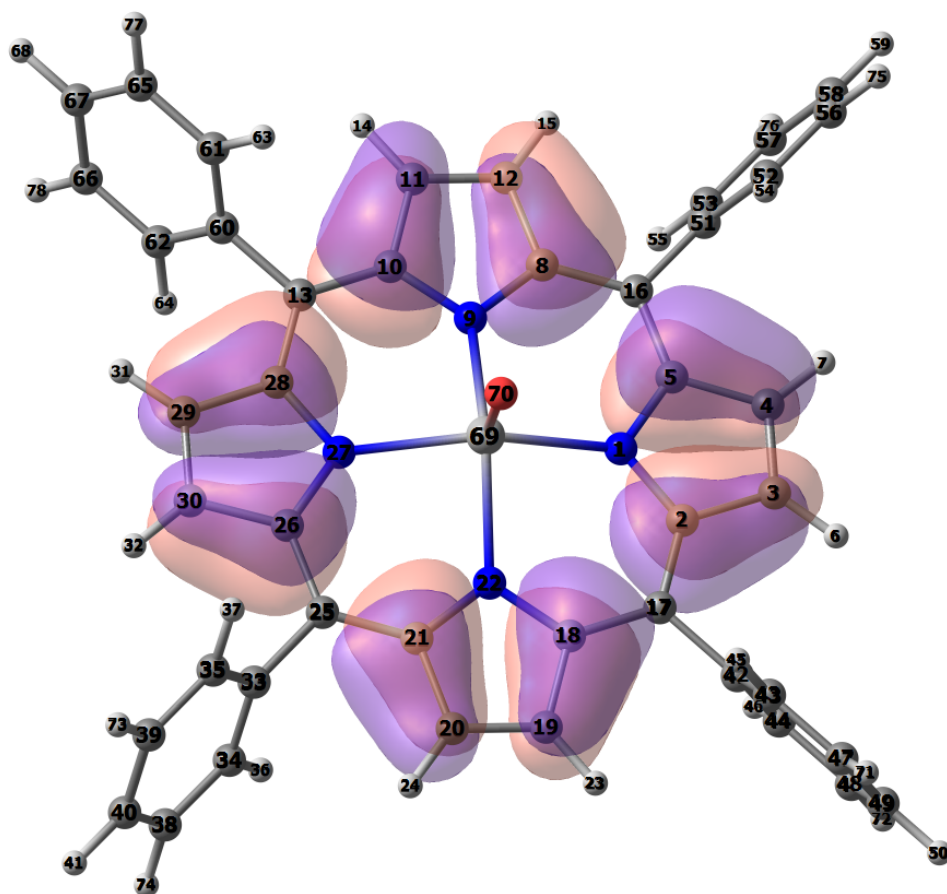
Table S1. Geometric parameters (in Å and deg.) of the OEPTi=O molecule calculated by quantum-chemical methods and found experimentally.

Parameter	B3LYP/6-31G(d)	PBE/3z	Experiment ^[1]
Ti-O	1.614	1.636	1.629
Ti-N	2.132	2.134	2.140
N-C _α	1.375	1.377	1.386
C _α -C _β	1.452	1.453	1.457
C _β -C _β	1.374	1.380	1.365
C _α -C _m	1.395	1.398	1.409
Ti– ring plane	0.536	0.526	0.525
O-Ti-N	106.2	105.9	106.0
N-Ti-N	85.6	85.7	84.8

1. Lecomte C., Protas J., Guillard R. *Comptesrendus de l'Academie des sciences. Ser. C (Chim.)* **1975**, 281, 921–923.

S2. Frontier molecular orbitals of the (TPP)Ti=O molecule, the corresponding energies (in parentheses) and the contributions of each atom to the orbital.

Molecular orbital 175 (occupied, E =-0.23003a.u.) –HOMO

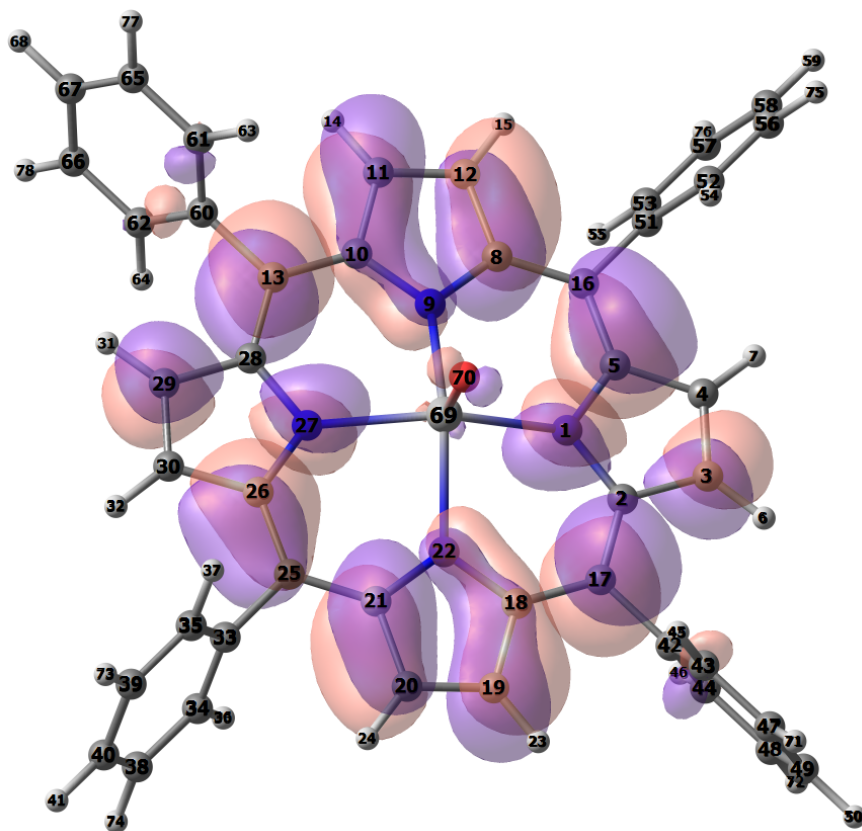


atom	contribution according to Hirshfield, %	atom	contribution according to Becke, %
1	1,19	1	0,84
2	7,20	2	8,12
3	3,05	3	2,93
4	3,09	4	2,98
5	7,14	5	8,06
6	0,24	6	0,06
7	0,24	7	0,06
8	7,21	8	8,13
9	1,20	9	0,84
10	7,15	10	8,07
11	3,09	11	2,98
12	3,06	12	2,93
13	1,88	13	1,27
14	0,24	14	0,06
15	0,24	15	0,06
16	1,88	16	1,27
17	1,88	17	1,27

18	7,14	18	8,05
19	3,09	19	2,98
20	3,05	20	2,93
21	7,20	21	8,12
22	1,19	22	0,84
23	0,24	23	0,06
24	0,24	24	0,06
25	1,88	25	1,27
26	7,14	26	8,06
27	1,19	27	0,84
28	7,21	28	8,13
29	3,06	29	2,93
30	3,09	30	2,98
31	0,24	31	0,06
32	0,24	32	0,06
33	0,20	33	0,10
34	0,09	34	0,07
35	0,11	35	0,08
36	0,06	36	0,01
37	0,06	37	0,01
38	0,11	38	0,12
39	0,10	39	0,11
40	0,03	40	0,02
41	0,00	41	0,00
42	0,20	42	0,10
43	0,11	43	0,08
44	0,09	44	0,07
45	0,06	45	0,01
46	0,06	46	0,01
47	0,10	47	0,11
48	0,11	48	0,12
49	0,03	49	0,02
50	0,00	50	0,00
51	0,20	51	0,10
52	0,11	52	0,08
53	0,09	53	0,07
54	0,06	54	0,01
55	0,06	55	0,01
56	0,10	56	0,11
57	0,11	57	0,12
58	0,03	58	0,02
59	0,00	59	0,00
60	0,20	60	0,10
61	0,11	61	0,08
62	0,09	62	0,07
63	0,07	63	0,01
64	0,07	64	0,01
65	0,10	65	0,11

66	0,10	66	0,12
67	0,03	67	0,02
68	0,00	68	0,00
69	0,70	69	0,58
70	0,01	70	0,00
71	0,01	71	0,00
72	0,01	72	0,00
73	0,01	73	0,00
74	0,01	74	0,00
75	0,01	75	0,00
76	0,01	76	0,00
77	0,01	77	0,00
78	0,01	78	0,00

Molecular orbital 176 (unoccupied, E =-0.00085a.u.) –LUMO

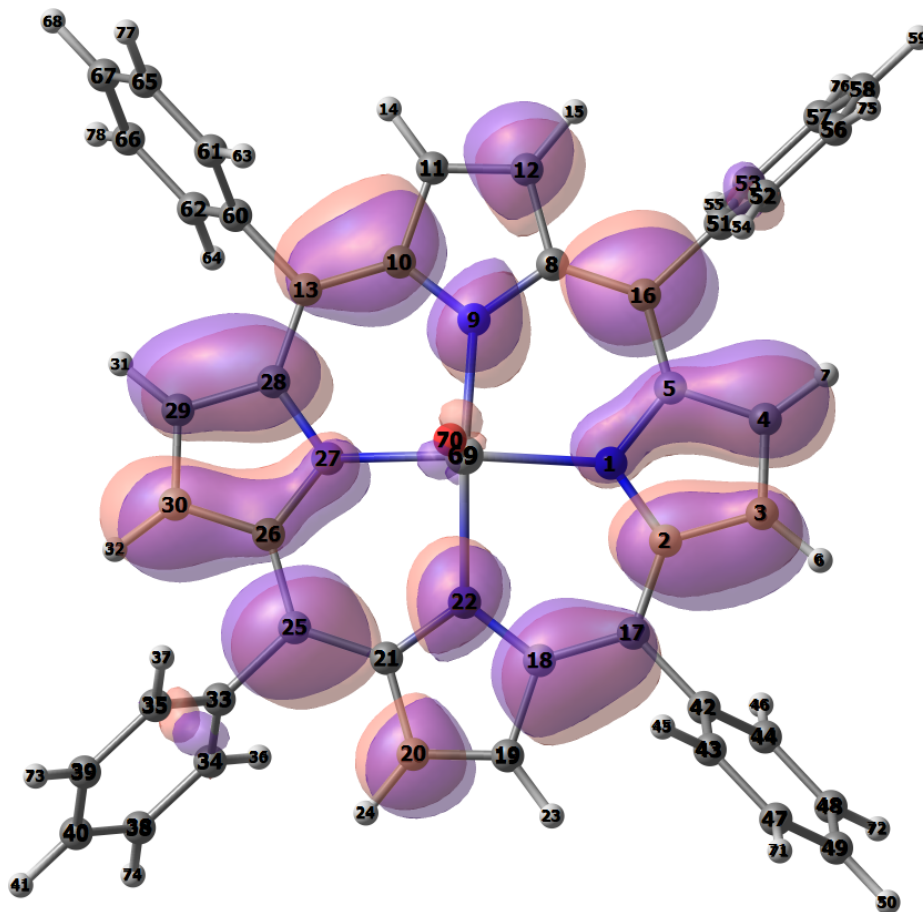


atom	contribution according to Hirshfeld, %	atom	contribution according to Becke, %
1	3,21	1	3,06
2	1,89	2	1,35
3	2,97	3	3,36
4	1,15	4	0,83
5	4,90	5	5,45
6	0,33	6	0,12
7	0,08	7	0,01
8	6,04	8	6,78
9	1,44	9	1,21

10	3,03	10	2,70
11	5,33	11	5,93
12	3,51	12	3,39
13	8,18	13	9,42
14	0,59	14	0,21
15	0,34	15	0,10
16	2,56	16	2,27
17	8,17	17	9,41
18	3,03	18	2,70
19	5,34	19	5,93
20	3,51	20	3,39
21	6,04	21	6,79
22	1,44	22	1,21
23	0,60	23	0,21
24	0,34	24	0,10
25	2,56	25	2,27
26	4,90	26	5,46
27	3,21	27	3,06
28	1,89	28	1,35
29	2,98	29	3,37
30	1,15	30	0,83
31	0,33	31	0,12
32	0,08	32	0,01
33	0,35	33	0,24
34	0,15	34	0,13
35	0,19	35	0,17
36	0,09	36	0,02
37	0,10	37	0,02
38	0,13	38	0,15
39	0,13	39	0,14
40	0,05	40	0,05
41	0,01	41	0,00
42	0,99	42	0,67
43	0,40	43	0,36
44	0,43	44	0,40
45	0,11	45	0,01
46	0,11	46	0,01
47	0,11	47	0,10
48	0,09	48	0,08
49	0,14	49	0,16
50	0,02	50	0,01
51	0,35	51	0,24
52	0,19	52	0,17
53	0,15	53	0,13
54	0,10	54	0,02
55	0,09	55	0,02
56	0,13	56	0,14
57	0,13	57	0,15

58	0,05	58	0,05
59	0,01	59	0,00
60	0,99	60	0,67
61	0,41	61	0,37
62	0,44	62	0,41
63	0,11	63	0,01
64	0,11	64	0,01
65	0,11	65	0,10
66	0,10	66	0,08
67	0,15	67	0,17
68	0,02	68	0,01
69	1,17	69	1,75
70	0,35	70	0,33
71	0,02	71	0,02
72	0,02	72	0,02
73	0,02	73	0,01
74	0,02	74	0,01
75	0,02	75	0,01
76	0,02	76	0,01
77	0,02	77	0,02
78	0,02	78	0,02

Molecular orbital 177 (unoccupied, E =-0.00083a.u.) – LUMO+1



atom	contribution according to	atom	contribution according to
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	Hirshfield, %		Becke, %
1	1,44	1	1,22
2	6,04	2	6,79
3	3,51	3	3,39
4	5,34	4	5,93
5	3,03	5	2,70
6	0,34	6	0,10
7	0,59	7	0,21
8	1,89	8	1,36
9	3,21	9	3,06
10	4,90	10	5,45
11	1,15	11	0,83
12	2,97	12	3,37
13	2,56	13	2,27
14	0,08	14	0,01
15	0,33	15	0,12
16	8,18	16	9,42
17	2,56	17	2,27
18	4,90	18	5,45
19	1,15	19	0,83
20	2,98	20	3,37
21	1,89	21	1,35
22	3,21	22	3,06
23	0,08	23	0,01
24	0,33	24	0,12
25	8,17	25	9,41
26	3,03	26	2,70
27	1,44	27	1,21
28	6,04	28	6,78
29	3,51	29	3,39
30	5,33	30	5,93
31	0,34	31	0,10
32	0,59	32	0,21
33	0,99	33	0,67
34	0,43	34	0,40
35	0,40	35	0,36
36	0,11	36	0,01
37	0,11	37	0,01
38	0,09	38	0,08
39	0,10	39	0,10
40	0,14	40	0,16
41	0,02	41	0,01
42	0,35	42	0,24
43	0,19	43	0,17
44	0,15	44	0,13
45	0,10	45	0,02
46	0,09	46	0,02
47	0,13	47	0,14

48	0,13	48	0,15
49	0,05	49	0,05
50	0,01	50	0,00
51	0,99	51	0,67
52	0,41	52	0,36
53	0,44	53	0,41
54	0,11	54	0,01
55	0,11	55	0,01
56	0,11	56	0,10
57	0,10	57	0,08
58	0,15	58	0,16
59	0,02	59	0,01
60	0,35	60	0,24
61	0,19	61	0,17
62	0,15	62	0,13
63	0,10	63	0,02
64	0,09	64	0,02
65	0,13	65	0,14
66	0,13	66	0,15
67	0,05	67	0,05
68	0,01	68	0,00
69	1,17	69	1,74
70	0,35	70	0,33
71	0,02	71	0,01
72	0,02	72	0,01
73	0,02	73	0,02
74	0,02	74	0,02
75	0,02	75	0,02
76	0,02	76	0,02
77	0,02	77	0,01
78	0,02	78	0,01

S3. Cartesian coordinates and energies of calculated structures

(TPP)Ti=O

7	-5.736658910	-5.324680720	14.773309960
6	-5.295836560	-6.625912930	14.621855160
6	-3.931023550	-6.620701400	14.152746520
6	-3.558100340	-5.313841800	14.012923420
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6	-5.847666550	-0.859429810	14.641765260
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6	-4.704205890	-3.096019680	14.383403240
6	-6.050322240	-7.788560320	14.874733560
6	-7.396305400	-7.798884990	15.290972350
6	-8.183120460	-8.993622430	15.481266070
6	-9.435410250	-8.596117940	15.855907360
6	-9.432707370	-7.153228740	15.885886710
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6	-10.561071000	-4.948965620	16.208218670
7	-9.492850080	-4.127769920	15.900300780
6	-9.954304910	-2.827602530	15.984998660
6	-11.348225600	-2.834612000	16.358802050
6	-11.724469640	-4.141738510	16.486740010
1	-11.962602090	-1.951896700	16.495512050
1	-12.705206220	-4.527435120	16.741453500
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6	-12.255299750	-7.059931490	17.926591520
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6	-9.545703280	0.481566840	17.006975420
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6	-11.133737440	2.152737920	16.261317680
1	-11.621715510	3.118757190	16.394402470
22	-7.443698070	-4.717532940	15.897663480
8	-6.966224800	-4.692964500	17.462341980
1	-4.113970520	-11.722607990	16.486623640
1	-4.260194020	-11.194632890	12.210839140
1	-13.764216560	-7.704894340	19.325217190
1	-14.373754570	-8.860493700	15.217214090
1	-0.312812950	-1.693834450	15.142120240
1	-2.105885100	-0.635490160	11.367548030
1	-9.910048420	2.342498080	18.033074780
1	-12.211574160	1.674669760	14.449855890

E = -2835.507126Hartree

CH₃-CH₂-C'(CH₃)(C(O)OCH₃)

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1	2.157818740	-2.366336610	-0.297573830
1	0.695551750	-1.805701380	-1.143354550
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6	1.274689620	1.899174140	-0.000631640
6	0.506777100	0.645816440	0.233439410
1	1.762996480	2.235693040	0.931594990
1	2.092061600	1.731512220	-0.723494180
1	0.625811380	2.701391500	-0.368022970
6	-0.936096650	0.678061980	0.039592890
8	-1.523117850	-0.550737810	0.265779070
8	-1.589790610	1.669107960	-0.286683530
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E = -385.352320Hartree

Product 1

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7	-9.499845600	-2.164764420	15.813856300
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6	-10.456660080	-0.086808480	16.090562880
6	-9.120053430	0.108242760	15.860426780
6	-11.947300910	-2.127791470	16.238049980
1	-11.211806150	0.668303880	16.277437440
1	-8.587177880	1.051530550	15.822020190
6	-7.185834720	-1.429439480	15.299181060
6	-6.630259190	-6.286773330	14.902727610
6	-7.750934380	-6.911754560	15.528370390
6	-7.858357140	-8.275402880	15.770518550
6	-9.046635220	-8.516823460	16.630574030
6	-9.764647230	-7.176809340	16.490218270
7	-8.899563520	-6.240199330	15.990271220
1	-7.118231750	-9.021131130	15.503871720
1	-9.660509630	-9.368028000	16.312286260
6	-11.134389140	-6.959509070	16.704233220
6	-11.772449390	-5.694831930	16.557633620
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6	-12.143963370	-3.515663080	16.336199440
6	-13.429412530	-4.161767070	16.387314930
6	-13.203274450	-5.503552310	16.524493540
1	-14.385642440	-3.657331290	16.306817110

1	-13.943032440	-6.293705490	16.573461250
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6	-12.817229380	-8.171971410	18.149158950
1	-11.642908970	-9.099208460	15.093482570
1	-12.715453740	-7.377242880	18.889324460
6	-13.082169300	-10.204378630	16.258855450
6	-13.695451980	-9.232016800	18.381814680
6	-13.828280230	-10.255901410	17.439482480
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1	-6.040529780	-6.770921530	12.298324900
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Imaginary Frequency: 370.11i

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1	-13.143303610	-13.113293930	18.204325540
1	-11.961547950	-13.019027390	14.059872390
1	-8.845586630	1.933740740	17.129062230
1	-11.738542700	1.901101990	13.933297940
1	-18.049553390	-4.026853850	20.263249010
1	-19.231539110	-4.754147100	16.182085420
1	-7.319868070	-10.951947230	17.431161170
6	-7.583752230	-10.319861000	18.292190940

1	-8.642529230	-10.509795590	18.521199660
6	-6.732596460	-10.739464670	19.495767910
1	-5.656096850	-10.643602960	19.296913940
1	-6.929626900	-11.793422950	19.736570100
1	-6.961601700	-10.147170760	20.391175960
6	-7.465166680	-8.818656760	17.873645390
6	-8.114724200	-7.917998160	18.929384720
1	-7.956797070	-6.855127590	18.716031410
1	-9.196689470	-8.097685210	18.977259610
1	-7.685947660	-8.113827810	19.919058380
6	-5.959755110	-8.526058120	17.804485570
8	-5.349656310	-7.793530840	18.559418970
8	-5.352070980	-9.288894030	16.849022680
6	-3.906593040	-9.213643930	16.840155570
1	-3.503300320	-9.609540630	17.781812480
1	-3.589059130	-9.831635610	15.994602830
1	-3.575289390	-8.177758010	16.710786180

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Product 4

7	-8.405181860	-9.942109900	15.738482390
6	-7.347065380	-9.087860970	15.681752430
6	-7.797996950	-7.735502750	15.675247750
6	-9.171819090	-7.763883540	15.741198020
6	-9.559383310	-9.138346810	15.786238890
1	-7.162559430	-6.861922260	15.593475290
1	-9.851045560	-6.919438440	15.735348180
6	-11.317440740	-10.930264630	15.809788450
7	-10.492244300	-12.032078240	15.679491770
6	-11.306690190	-13.145724990	15.740885250
6	-12.675474000	-12.733333360	15.906879110
6	-12.681120360	-11.363833510	15.947990040
6	-10.883195440	-14.486709450	15.591413120
1	-13.527163870	-13.401203180	15.967742370
1	-13.538056050	-10.709884970	16.062323500
6	-10.891332290	-9.585292800	15.841219610
6	-5.869449920	-9.450816930	15.609398070
6	-5.589785530	-10.840811800	15.053448880
6	-4.375515350	-11.158666890	14.374321570
6	-4.439798370	-12.486702490	14.027321240
6	-5.701099490	-12.978167020	14.486912940
7	-6.404576980	-11.927078310	15.104552760
1	-3.571046600	-10.462278880	14.165954950
1	-3.700469550	-13.065178870	13.485601570
6	-6.143811400	-14.302861390	14.333451070
6	-7.435044090	-14.784590900	14.645410870
7	-8.511672240	-14.005641470	15.028525190
6	-9.569278170	-14.871394010	15.240664570
6	-9.137511120	-16.224314910	15.010687050
6	-7.821902500	-16.168154760	14.630366160
1	-9.755927020	-17.107508540	15.122060360
1	-7.171855750	-16.998096810	14.377883250
6	-5.160159160	-15.293235690	13.801322060
6	-5.378580570	-15.932229960	12.569034200
6	-4.000026950	-15.607832590	14.529544080
1	-6.273624200	-15.691945930	11.994399660
1	-3.829033450	-15.122418630	15.490831360
6	-4.455445420	-16.856372300	12.074804860
6	-3.084795930	-16.541744700	14.039809410
6	-3.307395670	-17.166451170	12.809264840
1	-2.590005840	-17.892137400	12.424892660
6	-5.270436230	-8.491649520	14.528312770
6	-4.112347040	-7.716173860	14.666051790
6	-5.931300500	-8.468998130	13.284197790
1	-3.539614580	-7.727774310	15.589807720
1	-6.824310600	-9.078926310	13.141157410
6	-3.647877480	-6.927872960	13.603763560
6	-5.468260710	-7.689493940	12.227037870
6	-4.320532660	-6.905072540	12.383722390
1	-3.954862830	-6.289799990	11.560975230

6	-11.955219390	-8.539783730	15.954111420
6	-12.085796700	-7.779361220	17.127902320
6	-12.843102480	-8.303797310	14.891788720
1	-11.402846180	-7.960103530	17.958560700
1	-12.747263690	-8.887369200	13.975500770
6	-13.084500030	-6.809238060	17.237674780
6	-13.834671890	-7.325814610	14.999701380
6	-13.960340670	-6.577359500	16.173328230
1	-14.737349070	-5.817059310	16.258156430
6	-11.906500660	-15.556702600	15.779459140
6	-12.475621210	-15.770809340	17.047000780
6	-12.326672160	-16.362051660	14.706985090
1	-12.150989100	-15.154466390	17.886061800
1	-11.900002790	-16.198587550	13.716752970
6	-13.434258210	-16.768287740	17.237200770
6	-13.290911470	-17.354347190	14.897862160
6	-13.846471030	-17.562556440	16.163428520
1	-14.597271420	-18.339308780	16.311776480
22	-8.383797050	-12.089553740	15.946566690
8	-8.226804880	-12.444861580	17.534197710
1	-2.744667640	-6.332136940	13.743013670
1	-6.004730100	-7.696142330	11.277465980
1	-2.195389440	-16.783606480	14.622843770
1	-4.634069130	-17.335129160	11.111337150
1	-13.178418760	-6.233335300	18.159027710
1	-14.510724280	-7.148198700	14.162546790
1	-13.858474460	-16.926615680	18.229412390
1	-13.611827470	-17.964639090	14.052766410
1	-6.011000630	-11.247222890	17.740453350
6	-6.048687320	-10.212199300	18.096072370
1	-7.103383040	-9.909193190	18.055296160
6	-5.596893220	-10.180702770	19.561367900
1	-4.541883500	-10.466772870	19.679298350
1	-6.197724300	-10.900592030	20.133131660
1	-5.736535670	-9.193372280	20.021647380
6	-5.250827350	-9.291556180	17.133438600
6	-5.357158960	-7.840676770	17.646475250
1	-4.997639500	-7.095796000	16.931265880
1	-6.399804120	-7.608769970	17.894184770
1	-4.755353190	-7.729875610	18.555878390
6	-3.763173660	-9.707866810	17.194305880
8	-2.814859100	-8.939805210	17.228060470
8	-3.608218750	-11.053216760	17.274388600
6	-2.236534770	-11.505301720	17.338838230
1	-1.735024620	-11.081776430	18.218030540
1	-2.296596070	-12.595448540	17.411155620
1	-1.691377440	-11.204987770	16.435122850

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Product 5

7	-8.706281270	-1.699142980	14.927541140
6	-7.403896380	-2.060748630	14.626109750
6	-6.651082880	-0.889578660	14.269273620
6	-7.511541260	0.175377890	14.323692120
6	-8.788450800	-0.331087710	14.756821470
1	-5.603356570	-0.878060510	13.991175340
1	-7.295683090	1.212131930	14.092063160
6	-11.169432930	-0.027046880	15.469928650
7	-11.431919820	-1.333625600	15.830024460
6	-12.711252840	-1.352676060	16.356440680
6	-13.271482450	-0.030363840	16.305264270
6	-12.320872820	0.789500770	15.755230160
6	-13.385210040	-2.501611120	16.832878700
1	-14.268590830	0.240700440	16.633275710
1	-12.395176550	1.854120060	15.564765710
6	-9.940070100	0.460074880	14.970162280
6	-6.904164870	-3.381875950	14.612122810
6	-7.668838420	-4.549139850	14.789831350
6	-7.194198430	-5.880363370	14.575862940
6	-8.277745080	-6.719638010	14.718613010

6	-9.405613980	-5.901037020	15.022946740
7	-9.042986620	-4.595294050	15.073513880
1	-6.174668130	-6.152000640	14.326924770
1	-8.287922610	-7.800522700	14.637730310
6	-10.805560770	-6.463620980	15.216551030
6	-11.771860240	-5.572026530	15.981531990
7	-11.785713990	-4.215148840	15.976404630
6	-12.931699570	-3.825178390	16.689890110
6	-13.600062810	-4.993494550	17.168031760
6	-12.878671780	-6.080174570	16.722580580
1	-14.506066000	-5.002542970	17.762962010
1	-13.091624800	-7.128950120	16.895584460
6	-10.598923930	-7.706243480	16.143402150
6	-11.034184850	-9.020110660	15.932379320
6	-9.922515070	-7.431758410	17.350492530
1	-11.606577890	-9.279992820	15.049263160
1	-9.588653410	-6.413820260	17.558638810
6	-10.781154820	-10.024421990	16.877475930
6	-9.675673360	-8.426353240	18.293416110
6	-10.099503500	-9.738348440	18.058215690
1	-9.905578610	-10.522907600	18.790327690
6	-5.445608260	-3.567634840	14.335429120
6	-4.586982670	-3.982659830	15.366425920
6	-4.911745230	-3.342582780	13.056432690
1	-4.996490910	-4.159341260	16.361553220
1	-5.572844670	-3.028685610	12.247817690
6	-3.222692530	-4.159652920	15.124580150
6	-3.548162530	-3.527718030	12.815219510
6	-2.699222840	-3.933976230	13.848481380
1	-1.634651720	-4.075392260	13.659471120
6	-9.841683470	1.923833330	14.682539360
6	-9.079598560	2.767108710	15.508413160
6	-10.514812310	2.483333300	13.583750690
1	-8.560273750	2.343260140	16.368771210
1	-11.107844020	1.836698220	12.935792290
6	-8.993295080	4.135438640	15.241147300
6	-10.423662430	3.851267880	13.315197450
6	-9.663438250	4.681956000	14.143039790
1	-9.594375650	5.749957350	13.934130130
6	-14.704142440	-2.289213620	17.497904480
6	-14.783313820	-1.566370560	18.700635390
6	-15.886235380	-2.798165130	16.932843410
1	-13.869473070	-1.174171700	19.147910410
1	-15.833472140	-3.352770380	15.995540120
6	-16.015014270	-1.364764930	19.326930220
6	-17.117826860	-2.583640400	17.555180760
6	-17.186285370	-1.869625850	18.755020550
1	-18.148384260	-1.706663070	19.241804760
22	-10.060143930	-2.950007550	15.986343020
8	-9.546296230	-2.968295600	17.538568100
1	-2.567340330	-4.475012380	15.937249020
1	-3.148905650	-3.355750870	11.814961550
1	-9.152077310	-8.173084440	19.215816680
1	-11.131162480	-11.038601280	16.679216360
1	-8.402437110	4.776908290	15.896124880
1	-10.947762610	4.268380140	12.454434550
1	-16.058671900	-0.811797740	20.265927650
1	-18.027992110	-2.974409290	17.098607940
6	-11.407350310	-8.143958230	11.554034000
6	-10.740858970	-7.792244560	12.891300530
1	-11.463945240	-7.281109830	10.877645110
1	-10.819565880	-8.921051450	11.046082660
1	-12.423789470	-8.538447640	11.690799380
1	-10.646589200	-8.704020860	13.489524080
1	-9.715107410	-7.453400760	12.688581890
6	-11.259572550	-5.340689970	12.918781670
6	-11.438494140	-6.659194090	13.699490180
1	-10.199929670	-5.162669750	12.702974450
1	-11.804530370	-5.397499000	11.969985140
1	-11.663924070	-4.481343070	13.463368350

6	-12.966595580	-6.892826440	13.769656800
8	-13.296963240	-8.156398420	14.163736730
8	-13.807441200	-6.070418670	13.463067620
6	-14.720476390	-8.410086460	14.235210790
1	-15.193550600	-7.723004280	14.947812030
1	-15.182109660	-8.277354180	13.248873160
1	-14.813028180	-9.447182410	14.572728120

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Product 6

7	-5.819751430	-6.940496470	15.213112430
6	-5.496110440	-8.119491300	14.577730020
6	-4.226094840	-7.959239660	13.899476170
6	-3.784731240	-6.691941620	14.160313710
6	-4.802135100	-6.039303390	14.951233700
1	-3.740399360	-8.717519330	13.295319950
1	-2.876307760	-6.220159290	13.801828320
6	-6.026234930	-3.979332470	15.614276220
7	-7.266484230	-4.574042140	15.743033560
6	-8.174493850	-3.566969170	15.994903110
6	-7.481033360	-2.301698190	16.049507670
6	-6.153798590	-2.559176630	15.831156960
6	-9.561743540	-3.759128280	16.161942060
1	-7.942718370	-1.341385300	16.250092920
1	-5.337067950	-1.846179500	15.820933110
6	-4.842141690	-4.660584750	15.239565980
6	-6.282893840	-9.284294170	14.581612220
6	-7.437109680	-9.469841200	15.392352060
6	-8.172296930	-10.730494120	15.413119890
6	-9.114436530	-10.650726250	16.364093330
6	-9.059781040	-9.294638340	17.026340080
7	-7.953933380	-8.604858420	16.295419950
1	-7.951177830	-11.581914730	14.778077030
1	-9.815999070	-11.427149600	16.643217090
6	-10.400780650	-8.571448320	16.808012890
6	-10.543692240	-7.220109020	16.534423970
7	-9.544655180	-6.237720380	16.462267240
6	-10.177431120	-5.032119090	16.274137710
6	-11.606899040	-5.244005350	16.175988970
6	-11.831052340	-6.578291380	16.313642860
1	-12.339038620	-4.466584400	15.988523030
1	-12.783460480	-7.092575090	16.261311480
6	-11.671304770	-9.363708870	16.890182840
6	-12.048612420	-10.241778670	15.856424460
6	-12.557174620	-9.200843460	17.971494010
1	-11.398939540	-10.353344840	14.988692970
1	-12.299778900	-8.507894870	18.772391710
6	-13.252966620	-10.946383330	15.915258040
6	-13.758818670	-9.910351090	18.033733790
6	-14.110333730	-10.790893810	17.008052670
1	-15.048844420	-11.343917740	17.054392170
6	-5.844143630	-10.426513020	13.717840970
6	-4.736408290	-11.216546460	14.067523280
6	-6.533439460	-10.729038000	12.531252400
1	-4.190741500	-10.991060440	14.984958620
1	-7.390211060	-10.117710680	12.243486410
6	-4.331338940	-12.280148870	13.256438730
6	-6.130843010	-11.793987510	11.721266580
6	-5.028253730	-12.573918170	12.081266560
1	-4.712867660	-13.404296840	11.448787960
6	-3.588567520	-3.878860480	15.044162110
6	-2.446394730	-4.191992710	15.802836320
6	-3.506066500	-2.837023590	14.103310740
1	-2.503599230	-4.992858440	16.540758530
1	-4.378501330	-2.595711550	13.495409760
6	-1.258741830	-3.477925810	15.631086280
6	-2.315693330	-2.128215310	13.928934730
6	-1.188596420	-2.443918060	14.693409910
1	-0.260504400	-1.887681210	14.557795250
6	-10.436524530	-2.555072730	16.230177320

6	-11.256746170	-2.326895880	17.350593780
6	-10.461978740	-1.618020740	15.180856570
1	-11.235863400	-3.037367590	18.177645150
1	-9.839930850	-1.787279990	14.301405750
6	-12.074262860	-1.197425890	17.419879400
6	-11.283756740	-0.491198840	15.249341900
6	-12.092353340	-0.275537690	16.369022640
1	-12.732150780	0.605874650	16.422680440
22	-7.437182060	-6.554036810	16.497677510
8	-6.872700130	-6.326761520	18.018565030
1	-3.469506370	-12.883000100	13.545787530
1	-6.677299750	-12.010797490	10.802470560
1	-14.422839130	-9.770536270	18.887554100
1	-13.526914670	-11.611518510	15.095393790
1	-0.386282110	-3.728324110	16.235786480
1	-2.266949910	-1.329445900	13.187782240
1	-12.694502950	-1.033334740	18.301942100
1	-11.295969290	0.218906350	14.421499670
1	-9.034066720	-11.588460500	18.715020500
6	-9.445785580	-10.700099820	19.211951650
1	-10.513502300	-10.653164430	18.954387310
6	-9.312926750	-10.884845930	20.728812280
1	-8.263074480	-10.895928280	21.054198150
1	-9.763529540	-11.843938910	21.020303420
1	-9.827339090	-10.093546750	21.288805780
6	-8.734239340	-9.433446680	18.636312420
6	-9.167539840	-8.181031520	19.407794760
1	-8.730870460	-7.268905840	18.986969280
1	-10.260311820	-8.091400420	19.421355720
1	-8.808568410	-8.244190140	20.440368690
6	-7.224568470	-9.644408630	18.889947640
8	-6.574277580	-9.048258510	19.722997420
8	-6.714839080	-10.671927810	18.152103070
6	-5.311929600	-10.932376820	18.385862760
1	-5.142892470	-11.220500030	19.431369960
1	-5.054423100	-11.755700110	17.711616680
1	-4.716128660	-10.038608770	18.161347600

Energy: -3220.824888Hartree

Product 7

7	-5.939691630	-5.262495880	16.057352110
6	-5.479876850	-6.561885280	15.910741220
6	-4.103736500	-6.543710560	15.502457350
6	-3.726226160	-5.226818250	15.405795410
6	-4.871012730	-4.433233740	15.755575440
1	-3.491149560	-7.421086710	15.326781160
1	-2.752704470	-4.833965700	15.133820010
6	-6.039820860	-2.243055840	16.012470710
7	-7.302830050	-2.718268880	16.343891090
6	-8.127589640	-1.604462410	16.419142360
6	-7.367576820	-0.415383180	16.125596600
6	-6.077695800	-0.804809410	15.899346400
6	-9.488372920	-1.625273890	16.751039690
1	-7.769822170	0.591423160	16.100473970
1	-5.227607070	-0.176732320	15.657127730
6	-4.898874590	-3.022928550	15.763581200
6	-6.237281920	-7.723716030	16.167635150
6	-7.587653400	-7.732150050	16.556836490
6	-8.366684910	-8.935076340	16.728553080
6	-9.644901480	-8.552832750	17.016378520
6	-9.666507020	-7.110242980	17.023553670
7	-8.399070290	-6.619475200	16.750453960
1	-7.986264540	-9.944886260	16.622789810
1	-10.502672530	-9.190899040	17.197053180
6	-10.800513450	-6.332697900	17.299106060
6	-10.813590620	-4.921507050	17.274599940
7	-9.732860010	-4.100532950	16.988171000
6	-10.222779950	-2.800449120	17.020293350
6	-11.621430840	-2.813986180	17.349305790
6	-11.989190630	-4.124819160	17.497418410

1	-12.252228520	-1.936290020	17.434081840
1	-12.976329020	-4.515397990	17.717528730
6	-12.075924700	-7.036955490	17.638111800
6	-12.796852700	-7.735807710	16.655686830
6	-12.578729700	-7.010149410	18.949655520
1	-12.419287570	-7.757687350	15.632590710
1	-12.026450940	-6.470648740	19.720208020
6	-13.987631120	-8.392270980	16.977310270
6	-13.767923960	-7.668741140	19.271231340
6	-14.476847900	-8.362103490	18.286065190
1	-15.405867840	-8.875120120	18.536769150
6	-5.551203920	-9.043348660	16.004569700
6	-5.248893920	-9.831709150	17.127452590
6	-5.194596000	-9.518973250	14.732090070
1	-5.523345550	-9.470234670	18.119570000
1	-5.427997660	-8.916756090	13.853182980
6	-4.605722690	-11.063400420	16.981421170
6	-4.554154990	-10.752103980	14.586642860
6	-4.256463190	-11.528111990	15.710398960
1	-3.756071250	-12.490199220	15.596089110
6	-3.614447790	-2.310617340	15.465834100
6	-2.646524160	-2.162957890	16.473055300
6	-3.354654940	-1.786472030	14.190078640
1	-2.843192060	-2.565561830	17.468485820
1	-4.101850380	-1.899134960	13.403277500
6	-1.445086570	-1.500834070	16.205686900
6	-2.151124910	-1.127454460	13.925021410
6	-1.193136170	-0.982360440	14.932239020
1	-0.254581900	-0.466910800	14.725439800
6	-10.209288080	-0.316093540	16.828851940
6	-9.964256540	0.571579960	17.889431570
6	-11.142160220	0.050705080	15.844897390
1	-9.241892420	0.295775750	18.658825990
1	-11.337753870	-0.630093980	15.015521410
6	-10.637534840	1.793452180	17.966013190
6	-11.811164690	1.274845840	15.919346380
6	-11.562467110	2.149643740	16.980777570
1	-12.086258590	3.104280200	17.039231270
22	-7.664470240	-4.653311950	17.094188120
8	-7.067111930	-4.567571720	18.790612330
1	-4.376213550	-11.661366010	17.864377110
1	-4.290162490	-11.108990820	13.590363390
1	-14.140392950	-7.641688330	20.296075820
1	-14.536420060	-8.926473190	16.200652350
1	-0.704119850	-1.389254150	16.998388250
1	-1.962087630	-0.727212230	12.928115750
1	-10.438314210	2.468751290	18.799062890
1	-12.528080520	1.546394570	15.143494150
1	-6.929414930	-6.021104810	20.873864030
6	-6.939815920	-4.957969170	21.150296800
1	-7.995832190	-4.658509110	21.236537380
6	-6.216719420	-4.751588200	22.483959900
1	-5.159379130	-5.048934360	22.425363130
1	-6.685424010	-5.365097570	23.265330920
1	-6.254554710	-3.705742080	22.817443790
6	-6.357397110	-4.169814680	19.955531540
6	-6.485468390	-2.655961450	20.126895410
1	-6.101141160	-2.140334960	19.239478050
1	-7.545516700	-2.402353600	20.260680510
1	-5.915055590	-2.303797930	20.995012810
6	-4.866796850	-4.543921460	19.726287360
8	-3.946930470	-3.749127540	19.663390870
8	-4.715852740	-5.884018430	19.595380710
6	-3.358311080	-6.318849760	19.335040040
1	-2.696175290	-6.011718820	20.154491690
1	-3.412779820	-7.409500180	19.266083190
1	-2.997018770	-5.890363700	18.392310640

Energy: -3220.881668Hartree

TS2

7	1.458124170	-0.622988870	-1.269583570
6	1.928895470	-1.920810390	-1.369786450
6	3.313254440	-1.900459230	-1.760180770
6	3.674891560	-0.587041190	-1.906702890
6	2.519591360	0.209121200	-1.593857080
1	3.934858690	-2.777157280	-1.904380620
1	4.643302040	-0.192639620	-2.192756320
6	1.351715680	2.397166370	-1.353322690
7	0.115071140	1.924962220	-0.933089400
6	-0.703749080	3.035891550	-0.798633170
6	0.038298850	4.225763300	-1.134241250
6	1.304927320	3.834615650	-1.463833460
6	-2.059848070	3.012440980	-0.433339360
1	-0.363748260	5.232666430	-1.129205870
1	2.134741310	4.460604790	-1.772064340
6	2.482116560	1.615826230	-1.640574270
6	1.167770350	-3.086708690	-1.140349690
6	-0.201089220	-3.101453190	-0.820126290
6	-0.992249840	-4.303707690	-0.706787290
6	-2.275565610	-3.921439660	-0.441794660
6	-2.288624330	-2.479060780	-0.391306170
7	-1.013883870	-1.994384620	-0.624152660
1	-0.612920060	-5.311995150	-0.829295610
1	-3.141986280	-4.557860400	-0.301348140
6	-3.423087300	-1.700088770	-0.112686180
6	-3.428388270	-0.289771410	-0.077590130
7	-2.344632890	0.534432620	-0.327602740
6	-2.811515370	1.837814020	-0.219262560
6	-4.209896110	1.821315660	0.118462490
6	-4.593710200	0.509721680	0.191793180
1	-4.826859300	2.700192190	0.266804220
1	-5.583410370	0.119586200	0.400928450
6	-4.709805910	-2.409134280	0.172050600
6	-5.426277320	-3.041859230	-0.856958040
6	-5.224464120	-2.454526920	1.478282370
1	-5.037566720	-3.009228200	-1.875628720
1	-4.673452060	-1.968674210	2.284580600
6	-6.626858180	-3.703422550	-0.586091880
6	-6.423642960	-3.118161200	1.748637770
6	-7.129281350	-3.744460870	0.717350470
1	-8.065797860	-4.261657310	0.928410360
6	1.863275510	-4.405566110	-1.267314870
6	2.117864480	-5.183125370	-0.125243720
6	2.272529550	-4.892045720	-2.519631100
1	1.804389550	-4.811628560	0.851334750
1	2.075282270	-4.298793130	-3.413371270
6	2.766433800	-6.415781300	-0.233373120
6	2.918053210	-6.126451470	-2.626907770
6	3.168165380	-6.891924730	-1.484509800
1	3.672686750	-7.854932880	-1.569140500
6	3.752198190	2.327065680	-1.993982950
6	4.764016680	2.462713270	-1.028868630
6	3.952727380	2.862429070	-3.275599160
1	4.604613730	2.046480990	-0.032827250
1	3.170560800	2.757707250	-4.028968500
6	5.952601500	3.125667470	-1.346228390
6	5.144609250	3.521393850	-3.589379140
6	6.147404600	3.655508150	-2.625225310
1	7.076873870	4.170870540	-2.870035180
6	-2.757497440	4.327586290	-0.286600200
6	-2.427936210	5.192338120	0.770443970
6	-3.744534560	4.728612970	-1.202376460
1	-1.661965500	4.890818440	1.486123530
1	-4.003471330	4.068452140	-2.030992120
6	-3.072477120	6.423738590	0.911101360
6	-4.384904790	5.962272890	-1.063653230
6	-4.052679640	6.813260520	-0.005753150
1	-4.554036870	7.775535370	0.102534620
22	-0.285998200	-0.028606070	-0.248956450
8	0.097683160	-0.093774530	1.408978010

1	2.959314620	-7.005186310	0.663904280
1	3.223362560	-6.492475070	-3.607941730
1	-6.806110800	-3.147939600	2.769676340
1	-7.172430120	-4.186111370	-1.397901310
1	6.729968760	3.228877610	-0.587863870
1	5.289301610	3.929728000	-4.590424980
1	-2.807644650	7.080192200	1.740893790
1	-5.144133840	6.260679320	-1.787622270
1	0.518857330	-1.170466770	3.785937940
6	0.483317920	-0.092312090	3.985555030
1	-0.576269470	0.204101970	3.986387200
6	1.106923640	0.199487540	5.363911080
1	2.154555940	-0.128730740	5.403760060
1	0.556178850	-0.340392050	6.147118760
1	1.071816420	1.270171700	5.609297000
6	1.168523100	0.640326200	2.862393810
6	0.898416930	2.104393550	2.711225330
1	1.350119980	2.499401190	1.795131320
1	-0.184205550	2.289532580	2.706311480
1	1.332936710	2.662783490	3.559043170
6	2.502728530	0.189491400	2.415739410
8	3.301816550	0.867922530	1.771144480
8	2.761514980	-1.108240480	2.780472460
6	4.026001460	-1.617018600	2.310511090
1	4.856897890	-1.016704950	2.704395390
1	4.082211920	-2.644941530	2.683644270
1	4.064312700	-1.599820810	1.212954270

Energy = -3220.848309

Imaginary Frequency: 550.52i

TS3

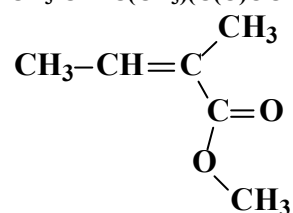
7	1.584087400	-0.912187350	-1.620671830
6	1.903636440	-2.167990520	-2.106504580
6	3.275279830	-2.184223520	-2.544822280
6	3.785679560	-0.935051100	-2.321616990
6	2.730905770	-0.141224300	-1.748604490
1	3.782993780	-3.040707750	-2.973680740
1	4.786201440	-0.578283960	-2.539302650
6	1.798616260	2.040837540	-0.989682230
7	0.527618220	1.600990550	-0.653594470
6	-0.196796090	2.731271040	-0.300581750
6	0.641724360	3.897845520	-0.423956450
6	1.873255700	3.471271090	-0.832897330
6	-1.545986450	2.760331260	0.095041000
1	0.325926710	4.913837300	-0.217062150
1	2.753091300	4.074639300	-1.027104220
6	2.849094080	1.229855690	-1.449233980
6	1.040962130	-3.282209340	-2.147330560
6	-0.276373590	-3.274375760	-1.657836790
6	-1.167675680	-4.408074550	-1.685116880
6	-2.330819310	-4.021549400	-1.082665660
6	-2.180648630	-2.635508130	-0.713105160
7	-0.913136020	-2.196523390	-1.068447200
1	-0.932430580	-5.376064260	-2.112937900
1	-3.222362520	-4.616689140	-0.920378200
6	-3.194751970	-1.859013510	-0.124488550
6	-3.105126010	-0.475069760	0.127902120
7	-1.996595650	0.319962500	-0.115528830
6	-2.370017770	1.620474410	0.189658540
6	-3.735933430	1.634059070	0.641648060
6	-4.188602540	0.342224510	0.603993240
1	-4.279343140	2.518321900	0.954242170
1	-5.175001690	-0.021953590	0.868866500
6	-4.484389490	-2.535665530	0.223966460
6	-5.395146770	-2.919253420	-0.773627510
6	-4.806274200	-2.790061410	1.567045570
1	-5.157302070	-2.720454860	-1.819380060
1	-4.104185850	-2.495715080	2.348199700
6	-6.598447220	-3.543515710	-0.435204160
6	-6.007989780	-3.417845160	1.903988140

6	-6.908191510	-3.795990870	0.904038500
1	-7.847068760	-4.284147370	1.167129000
6	1.569655580	-4.556726560	-2.723633800
6	1.819185210	-5.666238090	-1.898559880
6	1.828230990	-4.668711410	-4.099974440
1	1.628730180	-5.586979710	-0.827551760
1	1.635259370	-3.814584870	-4.750339230
6	2.314491330	-6.856504100	-2.436466180
6	2.319767840	-5.860832710	-4.637368750
6	2.565292260	-6.958462030	-3.807658410
1	2.950493060	-7.888221300	-4.227440260
6	4.184273540	1.872624780	-1.668200450
6	5.219399400	1.676297990	-0.739958080
6	4.427588240	2.674282760	-2.794507380
1	5.037099590	1.053723720	0.137075010
1	3.630553640	2.829231680	-3.522923070
6	6.468899950	2.271046090	-0.933050370
6	5.678275400	3.267073510	-2.987296860
6	6.702228860	3.068104880	-2.057219140
1	7.677728330	3.531380710	-2.208191760
6	-2.152115410	4.087229490	0.428258920
6	-1.750989800	4.794682210	1.574689220
6	-3.135380040	4.644534830	-0.407060720
1	-0.990305960	4.375115360	2.237054560
1	-3.448073900	4.102482590	-1.300644970
6	-2.328053770	6.032129940	1.873895440
6	-3.704596450	5.883924110	-0.106056700
6	-3.303502370	6.581236460	1.037111430
1	-3.749645070	7.547889250	1.273902000
22	-0.031091070	-0.408515440	-0.328050600
8	0.490083030	-0.825457760	1.248214030
1	2.507927800	-7.706062370	-1.780392570
1	2.508888800	-5.932300790	-5.709156070
1	-6.240354280	-3.612585700	2.951626370
1	-7.297260520	-3.831014420	-1.221674560
1	7.262019700	2.111165450	-0.201606730
1	5.852866510	3.884646910	-3.869125040
1	-2.010861300	6.565979340	2.770633490
1	-4.461581430	6.305989320	-0.768318550
6	0.289389170	-1.308506780	4.366185160
6	0.918816880	-0.089074900	3.712005130
1	-0.792357670	-1.360736720	4.182150920
1	0.736846840	-2.229350180	3.969960040
1	0.441638670	-1.301856070	5.458594000
1	2.013425070	-0.109172030	3.659286120
1	0.688839180	-0.359912410	2.408995030
6	-1.074848680	1.379164670	4.296782560
6	0.355937090	1.198758330	3.893265190
1	-1.749381330	0.843064120	3.608325620
1	-1.260556120	0.960255140	5.299605530
1	-1.344200140	2.440301340	4.303519350
6	1.112316380	2.416665550	3.597938890
8	2.417952160	2.169931870	3.237455700
8	0.662356060	3.566034240	3.663385250
6	3.190675010	3.353876750	2.961076900
1	2.747857300	3.924339910	2.134146690
1	3.243453860	3.999152710	3.848315230
1	4.188236830	2.992917420	2.688617130

Energy = -3220.841946

Imaginary Frequency: 1755.86i

CH₃-CH=C(CH₃)(C(O)OCH₃)



6	-0.258974940	-2.608996200	0.775686800
6	0.201473020	-1.264753640	0.311754210
1	-1.330376830	-2.650541080	1.000950640
1	-0.036317590	-3.372664000	0.012896350
1	0.296008580	-2.911666180	1.678437530
1	1.265771630	-1.187131560	0.079340560
6	-2.021503360	-0.030273170	0.409406480
6	-0.544187600	-0.149818380	0.150277130
1	-2.548523880	0.284776530	-0.502366940
1	-2.455921200	-0.973148650	0.758267090
1	-2.219607040	0.748298700	1.159661200
6	0.086551510	1.117534630	-0.326694070
8	1.430105540	1.014274700	-0.563953980
8	-0.532900960	2.158052750	-0.493825350
6	2.045386060	2.236239640	-1.026845080
1	1.591058800	2.564157690	-1.970657550
1	1.929311050	3.033948930	-0.281925960
1	3.102647210	1.991709290	-1.170409060

Energy: -384.779228

(TPP)TiOH

7	1.899472390	-0.474459920	-0.561593520
6	2.447059700	-1.749451900	-0.613635230
6	3.781014810	-1.680302000	-1.156613230
6	4.025814330	-0.369807260	-1.464046970
6	2.858871220	0.381776010	-1.087188860
1	4.443663230	-2.527208630	-1.294601100
1	4.923629010	0.050353420	-1.903901270
6	1.548045120	2.490265650	-0.908364480
7	0.366820220	1.961300620	-0.400966220
6	-0.512695390	3.026505880	-0.294890320
6	0.126175520	4.237546840	-0.738643080
6	1.402919560	3.908081010	-1.102916230
6	-1.846472780	2.955784940	0.154138670
1	-0.344800270	5.213160580	-0.780489520
1	2.171796450	4.567062360	-1.490303680
6	2.715359220	1.769397500	-1.232064230
6	1.805370050	-2.942439740	-0.230249200
6	0.478116010	-3.027525980	0.240625510
6	-0.200947590	-4.256153560	0.554950340
6	-1.474115520	-3.926935950	0.943171080
6	-1.587242540	-2.498037410	0.861705260
7	-0.382339040	-1.957533680	0.433360830
1	0.236393280	-5.246200300	0.492162760
1	-2.262534180	-4.599779820	1.261747170
6	-2.735909940	-1.756170000	1.193390510
6	-2.853680500	-0.360104370	1.066943240
7	-1.878139290	0.513728260	0.598141450
6	-2.473012260	1.764196190	0.554631380
6	-3.836108600	1.675514770	1.016446550
6	-4.069486250	0.367496030	1.331968510
1	-4.528816970	2.507014560	1.080614030
1	-4.991417040	-0.071153800	1.697108270
6	-3.925515550	-2.511008350	1.699546850
6	-4.696156060	-3.305157730	0.835082450
6	-4.290621570	-2.436339520	3.053601600
1	-4.422726840	-3.366726890	-0.219012040
1	-3.696322910	-1.823103360	3.732242680
6	-5.806238350	-4.005877870	1.313483510
6	-5.398862070	-3.140045830	3.531569350
6	-6.160820070	-3.926486120	2.663070830
1	-7.026858250	-4.474315270	3.035854870
6	2.568843350	-4.222665010	-0.371063310
6	3.022245370	-4.912219820	0.765578990
6	2.840912070	-4.763539910	-1.638525620
1	2.816135570	-4.502000540	1.755171940
1	2.488974710	-4.239632900	-2.528085920
6	3.732552310	-6.108536150	0.638542690
6	3.548459610	-5.961518720	-1.765238670
6	3.997751190	-6.637654400	-0.627528950

1	4.550872410	-7.572124490	-0.727035610
6	3.880189060	2.532014720	-1.782454350
6	5.023013620	2.749807700	-0.995871720
6	3.856549440	3.036764030	-3.092791860
1	5.048973310	2.363535990	0.023863530
1	2.974782750	2.870325900	-3.712846690
6	6.114267820	3.457625240	-1.506043280
6	4.950082760	3.740276870	-3.603806300
6	6.081837690	3.954213740	-2.811967900
1	6.934216670	4.505071790	-3.210873060
6	-2.632583450	4.226127010	0.220954360
6	-2.333526200	5.200015160	1.188523060
6	-3.682187850	4.472562940	-0.679674650
1	-1.522675140	5.016873030	1.894735790
1	-3.920216750	3.725732360	-1.438224260
6	-3.066491410	6.387304510	1.255119180
6	-4.413204730	5.661436420	-0.614016980
6	-4.108601710	6.622602400	0.353773300
1	-4.679974880	7.549981400	0.405148230
22	0.201584230	0.056574710	0.560918020
8	0.824413920	0.195126990	2.269949330
1	4.080634300	-6.627788880	1.532345290
1	3.746555980	-6.369166740	-2.757335870
1	-5.666238620	-3.074196320	4.586942450
1	-6.397596270	-4.613744190	0.627596450
1	6.991898530	3.622325730	-0.879730190
1	4.917560400	4.120994160	-4.625381280
1	-2.823771160	7.129767500	2.016421980
1	-5.221796470	5.837969950	-1.324485790
1	1.446877260	-0.387101570	2.731319200

Energy: -2836.085003

TS4

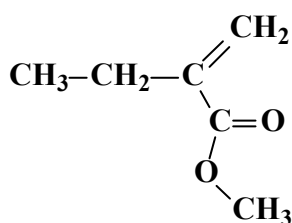
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6	3.384696400	-0.330241530	-1.788254550
6	2.241023340	0.473722340	-1.435930090
1	3.613453280	-2.521163170	-1.863957100
1	4.350575530	0.062538650	-2.084516500
6	1.086937040	2.666551160	-1.184935540
7	-0.175941450	2.187196660	-0.869954590
6	-0.985240960	3.297749580	-0.694763090
6	-0.213572020	4.493955150	-0.900251600
6	1.065309780	4.105558740	-1.195592200
6	-2.365406240	3.271202580	-0.414151820
1	-0.599261440	5.504826950	-0.829126950
1	1.919978770	4.739305070	-1.402331940
6	2.224573950	1.880238980	-1.453757080
6	0.866944050	-2.815203980	-1.065505740
6	-0.511194720	-2.828309030	-0.777092030
6	-1.293145690	-4.028300920	-0.637843600
6	-2.589049280	-3.644273800	-0.429239370
6	-2.613152490	-2.204477130	-0.442529190
7	-1.333997960	-1.717602450	-0.650720010
1	-0.901873050	-5.037547470	-0.702259760
1	-3.454445370	-4.281463540	-0.286806760
6	-3.773283700	-1.425670050	-0.259447100
6	-3.782553450	-0.020418170	-0.245366300
7	-2.674371130	0.797601360	-0.379690350
6	-3.139067390	2.102816810	-0.298161300
6	-4.567713410	2.094075290	-0.102296190
6	-4.966419950	0.787986810	-0.087947600
1	-5.188368410	2.977776540	-0.005931080
1	-5.974733460	0.403309190	0.015513660
6	-5.072320890	-2.137432010	-0.054389440
6	-5.677059270	-2.849023730	-1.103932530
6	-5.713171250	-2.106072890	1.195582470
1	-5.190623980	-2.876621730	-2.079811830
1	-5.248644170	-1.561355040	2.018447490

6	-6.892616130	-3.509309480	-0.908874710
6	-6.926637590	-2.770006610	1.390550160
6	-7.521157310	-3.472932800	0.338954300
1	-8.469263190	-3.989693520	0.490978050
6	1.563031180	-4.136397660	-1.188710010
6	1.941007400	-4.846715420	-0.038261780
6	1.849400600	-4.685499600	-2.448399620
1	1.723376700	-4.425580790	0.944152370
1	1.557456470	-4.141162770	-3.347490810
6	2.592324880	-6.078201090	-0.145907640
6	2.499636730	-5.917833990	-2.554827470
6	2.873313990	-6.617631210	-1.404254290
1	3.381034230	-7.579045200	-1.487892380
6	3.498303140	2.588524650	-1.792188650
6	4.581179670	2.566377490	-0.896498630
6	3.629209780	3.284067620	-3.005834410
1	4.485069820	2.027682150	0.048013110
1	2.793681300	3.299940200	-3.707048310
6	5.767378590	3.233767390	-1.214486080
6	4.819537090	3.943782200	-3.320746550
6	5.891996230	3.922341340	-2.424495800
1	6.820221380	4.440173150	-2.668814460
6	-3.058951200	4.589216790	-0.256624370
6	-2.876922690	5.348486620	0.910528970
6	-3.893209650	5.092445920	-1.267682550
1	-2.230471380	4.964544750	1.700714710
1	-4.036734200	4.512247540	-2.180119790
6	-3.518407880	6.579992060	1.064686850
6	-4.531214810	6.325960590	-1.113927380
6	-4.346994810	7.072933130	0.052854510
1	-4.846116360	8.035007960	0.172559130
22	-0.627690550	0.243227760	-0.199347440
8	-0.333660500	0.259885120	1.489953480
1	2.882374840	-6.616203070	0.757370100
1	2.712630670	-6.332667560	-3.540769050
1	-7.407411130	-2.739724790	2.369095240
1	-7.351272060	-4.051671770	-1.736572560
1	6.598045260	3.215402240	-0.507577190
1	4.908928570	4.474056960	-4.269744000
1	-3.370278930	7.155088850	1.979460230
1	-5.172657290	6.705025420	-1.910428000
6	2.786106190	-1.866953980	5.301727380
6	2.043246750	-1.707506130	3.958974050
1	2.567215940	-1.025909170	5.974240750
1	2.475671770	-2.794982170	5.803314610
1	3.871875090	-1.909741430	5.145531430
1	2.272200910	-2.576315330	3.324057220
1	0.958185600	-1.709695560	4.141791290
6	1.540142130	0.677046950	3.253950840
6	2.402847230	-0.436903010	3.238799650
1	0.604700150	0.432706610	2.290642000
1	0.825476000	0.735744750	4.083531660
1	1.956585760	1.630405540	2.917503750
6	3.633907560	-0.348516320	2.450278520
8	4.330358980	-1.541428580	2.432730110
8	4.042476390	0.654930370	1.862486460
6	5.562026710	-1.497994960	1.688385480
1	5.369252540	-1.272081870	0.630928510
1	6.235382810	-0.732095100	2.096272250
1	6.002825170	-2.494825280	1.794396840

Energy = -3220.841857

Imaginary Frequency: 1718.48i

CH₃-CH₂-C(=CH₂)(C(O)OCH₃)



6	-0.427881300	-0.887077480	1.947667800
6	-1.289898500	-0.467514240	0.744109420
1	-0.378139960	-0.081192860	2.693100950
1	-0.854006110	-1.775876840	2.433870050
1	0.596599470	-1.130877580	1.637467070
1	-1.351847630	-1.306095920	0.034858630
1	-2.314394680	-0.256358820	1.085000210
6	-1.341722940	1.968274580	0.135172310
6	-0.767662110	0.758317030	0.031618280
1	-2.238446770	2.115406410	0.737413830
1	-0.919253690	2.827471610	-0.384373580
6	0.453317420	0.660809930	-0.838723050
8	0.859361650	-0.637151090	-0.984400720
8	1.024297230	1.596634180	-1.371926240
6	2.024980690	-0.806672950	-1.823224110
1	1.825469170	-0.434471040	-2.836000970
1	2.880042320	-0.260062880	-1.405824430
1	2.219185740	-1.883562030	-1.835805430

Energy: -384.773043

Product 8 – (TPP)Ti(OR)(R)

7	-6.012918020	-5.329025580	16.050846430
6	-5.643025260	-6.645925490	15.940297230
6	-4.267427170	-6.700256530	15.490010400
6	-3.837484060	-5.409943000	15.337413000
6	-4.939813250	-4.543382950	15.697162280
1	-3.698701620	-7.607386480	15.318513320
1	-2.858587840	-5.073162540	15.014429200
6	-5.980462230	-2.255278570	15.980472400
7	-7.249281600	-2.630379230	16.361595050
6	-7.994182620	-1.495677810	16.566226760
6	-7.161237530	-0.342988880	16.293019320
6	-5.922052150	-0.809238580	15.946772290
6	-9.353119620	-1.462396830	16.968027850
1	-7.481536630	0.691030980	16.355859690
1	-5.048293730	-0.225158530	15.679722600
6	-4.907211380	-3.127750530	15.677560080
6	-6.457647280	-7.761607910	16.255336930
6	-7.797165620	-7.715830380	16.715452220
6	-8.613715760	-8.868608070	17.027264040
6	-9.841584270	-8.408054790	17.420273070
6	-9.806947920	-6.964915520	17.337389290
7	-8.555058570	-6.580048990	16.911706500
1	-8.292471060	-9.901612980	16.954908560
1	-10.696609980	-8.997091980	17.732877410
6	-10.882981050	-6.097343660	17.647788460
6	-10.860138240	-4.683733200	17.574191910
7	-9.784781080	-3.909589530	17.197106000
6	-10.168828370	-2.585516680	17.249775680
6	-11.549239130	-2.525441500	17.679516650
6	-11.975816790	-3.811560170	17.869587720
1	-12.121549040	-1.614925460	17.818053040
1	-12.960994550	-4.139271830	18.182207380
6	-12.164550890	-6.734238120	18.088117410
6	-12.955395720	-7.456850300	17.179343790
6	-12.601892810	-6.620073890	19.418236990
1	-12.628425510	-7.546325990	16.142626650
1	-11.993968020	-6.063913760	20.132955390
6	-14.152572320	-8.048413110	17.589834930
6	-13.797376340	-7.214917470	19.828918390
6	-14.577267750	-7.930471300	18.916156470

1	-15.511225530	-8.393192370	19.236570140
6	-5.844198040	-9.115129510	16.081194970
6	-5.570299950	-9.930618090	17.192292610
6	-5.526779560	-9.594956310	14.799040600
1	-5.810445870	-9.565830140	18.191992780
1	-5.735362850	-8.968912620	13.930455550
6	-4.994677630	-11.192616190	17.025593120
6	-4.953764810	-10.858270930	14.633735340
6	-4.685172780	-11.661373850	15.745722640
1	-4.236971470	-12.646915000	15.615753170
6	-3.594656550	-2.492110790	15.331586220
6	-2.558173670	-2.466218150	16.279684880
6	-3.378763810	-1.915943910	14.070091110
1	-2.726006180	-2.906346570	17.264232500
1	-4.177965760	-1.937722160	13.328019760
6	-1.331997630	-1.873011320	15.967929860
6	-2.149688160	-1.327580110	13.760164100
6	-1.123299190	-1.303530200	14.708426980
1	-0.164983010	-0.842480540	14.466824210
6	-9.985192620	-0.111715430	17.103665730
6	-9.617317040	0.751846190	18.148717120
6	-10.955704120	0.318654660	16.183630640
1	-8.865604440	0.427065790	18.869383510
1	-11.242855410	-0.341889840	15.364449140
6	-10.207747880	2.011970010	18.272469120
6	-11.543215280	1.580134500	16.306492600
6	-11.172210130	2.430644780	17.351699360
1	-11.631556740	3.414959400	17.447600520
22	-7.879022210	-4.608530650	16.667852590
8	-7.268956510	-4.518753130	18.403336620
1	-4.784730880	-11.810503980	17.899680440
1	-4.718971490	-11.216972170	13.630758300
1	-14.118851620	-7.120425390	20.866898130
1	-14.757000900	-8.600498450	16.869056420
1	-0.537468230	-1.854329720	16.715106010
1	-1.994554870	-0.888093810	12.774036300
1	-9.913827280	2.667669910	19.093042700
1	-12.290860560	1.900512210	15.579822030
1	-7.363250030	-6.099522470	20.397784750
6	-7.314650920	-5.054221160	20.731008430
1	-8.349556090	-4.680057540	20.765609550
6	-6.672510670	-4.971647850	22.118464560
1	-5.635126000	-5.336876220	22.110001040
1	-7.231423550	-5.595060120	22.829917040
1	-6.667203480	-3.946307510	22.512410740
6	-6.601801080	-4.250395830	19.616534060
6	-6.623832040	-2.742323040	19.884846670
1	-6.125022930	-2.202472240	19.073198110
1	-7.668557790	-2.411409690	19.954786520
1	-6.104247100	-2.498801790	20.820278110
6	-5.126181350	-4.716291040	19.449076470
8	-4.165916080	-3.975340330	19.344213470
8	-5.035324750	-6.069720810	19.419202360
6	-3.690719920	-6.580535630	19.246465010
1	-3.049133210	-6.247356190	20.072299590
1	-3.791892000	-7.670199680	19.249557170
1	-3.269526790	-6.234198190	18.295025450
8	-8.380591410	-4.629984850	14.821083140
6	-8.221611110	-4.868513460	13.528446900
8	-7.807477930	-6.161713380	13.212794310
6	-8.426214670	-3.955362110	12.536719360
6	-8.870406450	-7.124328110	13.327700990
1	-8.418190820	-8.112623920	13.180258940
1	-9.342693230	-7.080550310	14.319890840
1	-9.633765710	-6.951346160	12.549971540
6	-8.846724730	-2.543234310	12.855385580
1	-9.804418510	-2.340097900	12.340102120
1	-9.042922490	-2.459038170	13.931844960
6	-7.831298020	-1.468223510	12.429385780
1	-7.654675340	-1.482292810	11.344393190

1	-6.865657460	-1.621957290	12.930355830
1	-8.191816270	-0.463789850	12.694070060
6	-8.264757220	-4.320245940	11.087295050
1	-7.461025050	-3.734125150	10.610883470
1	-8.022034680	-5.380593090	10.960318570
1	-9.186441000	-4.096193220	10.522123300

Energy: -3606.251231Hartree

Product 9 – (TPP)Ti(OH)(R)

7	1.949277580	-0.798630550	0.169488260
6	2.320080300	-2.119176870	0.097771140
6	3.698773270	-2.184596220	-0.342093440
6	4.123772860	-0.899804710	-0.543177650
6	3.018751870	-0.023756440	-0.209563950
1	4.268291180	-3.095762590	-0.486643160
1	5.098902490	-0.575329490	-0.888529730
6	1.966976170	2.263008200	0.060060640
7	0.698069950	1.886720750	0.442616640
6	-0.029016430	3.022445260	0.701419550
6	0.811655070	4.175736480	0.461485920
6	2.039542760	3.709634390	0.077963470
6	-1.382527400	3.057560200	1.117628420
1	0.504840840	5.209511630	0.576082750
1	2.916801710	4.295271870	-0.173080700
6	3.040934850	1.394097400	-0.260431530
6	1.499168570	-3.230587830	0.416060040
6	0.145440330	-3.188917530	0.834127290
6	-0.663793200	-4.344446150	1.157484770
6	-1.905775950	-3.890183130	1.511126480
6	-1.884691640	-2.448556820	1.395980580
7	-0.634166370	-2.059618560	0.979288280
1	-0.325868000	-5.374124740	1.123930930
1	-2.758481780	-4.481239420	1.826246640
6	-2.961754310	-1.578258180	1.696070670
6	-2.921730100	-0.164686240	1.644754100
7	-1.829508910	0.608050170	1.300934020
6	-2.205186290	1.936456690	1.376782270
6	-3.588865800	1.999101470	1.785953740
6	-4.031162570	0.712661660	1.938831150
1	-4.154734740	2.912047790	1.935067170
1	-5.024705570	0.388413740	2.227426300
6	-4.250181220	-2.211763690	2.117289620
6	-5.015525540	-2.954480660	1.202584040
6	-4.717364200	-2.080002040	3.435900440
1	-4.664400300	-3.058532060	0.175155780
1	-4.126713130	-1.512175260	4.155768230
6	-6.217972540	-3.547044730	1.595491110
6	-5.918010130	-2.676227060	3.828650970
6	-6.673012280	-3.410740590	2.909936290
1	-7.610876190	-3.874734750	3.216804430
6	2.126272440	-4.584749760	0.289901000
6	2.411652060	-5.354328450	1.429876610
6	2.445392660	-5.108047730	-0.974372590
1	2.173662560	-4.954458830	2.416442070
1	2.231253950	-4.515393300	-1.864741140
6	3.000150720	-6.615535670	1.308590710
6	3.030509510	-6.370982490	-1.094327770
6	3.310109830	-7.129004110	0.046193460
1	3.768335910	-8.113991030	-0.048228800
6	4.330642170	2.034017210	-0.670603340
6	5.466390260	1.950949710	0.152761420
6	4.432216150	2.729881170	-1.886919470
1	5.399219830	1.417863180	1.101888340
1	3.560840360	2.791600720	-2.539624430
6	6.668984200	2.550723920	-0.228121920
6	5.636598330	3.325034930	-2.269604120
6	6.758820690	3.239220820	-1.441088080
1	7.698314250	3.705619270	-1.739192680
6	-2.000579250	4.410823240	1.296247840
6	-1.669048610	5.207931690	2.403788080

6	-2.919291180	4.907321000	0.357283610
1	-0.958843400	4.828877490	3.139809250
1	-3.179261180	4.296852510	-0.508604520
6	-2.244664860	6.470301070	2.569152830
6	-3.492459390	6.170784560	0.522346880
6	-3.157605280	6.956024670	1.628982300
1	-3.605781630	7.941726630	1.757928210
22	0.041224750	-0.092031320	0.722446720
8	0.729954860	-0.072290950	2.459216020
1	3.219785640	-7.197163080	2.204763610
1	3.267238460	-6.764155580	-2.083852800
1	-6.262418840	-2.569053110	4.857992630
1	-6.802553580	-4.114572510	0.870356210
1	7.537943260	2.481706900	0.427436440
1	5.697833280	3.855220380	-3.220767460
1	-1.979989070	7.074788950	3.437569540
1	-4.200969800	6.543352090	-0.218501520
8	-0.372631730	-0.155862100	-1.142808470
6	-0.152530330	-0.367230530	-2.431896550
8	0.292634600	-1.644976860	-2.758079200
6	-0.336343980	0.564390640	-3.411141290
6	-0.744273490	-2.637427720	-2.646134380
1	-0.267137730	-3.610441610	-2.813770970
1	-1.207742030	-2.620220120	-1.649253780
1	-1.519022840	-2.472117150	-3.414095180
6	-0.800228660	1.960131210	-3.080405050
1	-1.762737110	2.135007470	-3.597363390
1	-1.003894010	2.029504830	-2.004462780
6	0.177750650	3.072668040	-3.495861250
1	0.363312850	3.069034240	-4.579338080
1	1.143912510	2.954158830	-2.986494600
1	-0.222298420	4.061591670	-3.230015210
6	-0.126455110	0.228514550	-4.861162170
1	0.699780000	0.815648000	-5.295908590
1	0.110241340	-0.831386390	-5.001916600
1	-1.025367590	0.475461990	-5.452490020
1	1.677895860	-0.148654570	2.651532400

Energy: -3221.456482

(TPP)Ti(OR)(H)

7	1.417912870	-0.732769780	-1.200492640
6	1.790893840	-2.040813730	-1.346070970
6	3.158428550	-2.091203410	-1.818772780
6	3.581343580	-0.798459310	-1.966704330
6	2.482140540	0.057347990	-1.576937790
1	3.721751870	-2.996888000	-2.014750830
1	4.550407930	-0.453318860	-2.309328480
6	1.436382920	2.338161550	-1.303048710
7	0.187183100	1.962349730	-0.866629910
6	-0.559470610	3.094708940	-0.698888140
6	0.250347350	4.249002710	-1.032855540
6	1.483650380	3.783124150	-1.394234150
6	-1.923090930	3.130660110	-0.312012000
1	-0.083822790	5.279988450	-1.001649650
1	2.344999820	4.363704860	-1.704491640
6	2.508969690	1.470753870	-1.615638580
6	0.966414220	-3.163923000	-1.083195710
6	-0.382626680	-3.110209800	-0.673995400
6	-1.229796000	-4.262161830	-0.485567700
6	-2.474318360	-3.805497420	-0.144523280
6	-2.415806160	-2.364802800	-0.131725470
7	-1.129354370	-1.965989370	-0.438083050
1	-0.917286950	-5.293119360	-0.608368070
1	-3.357860490	-4.396237020	0.070129230
6	-3.502734500	-1.511575880	0.160410100
6	-3.451852810	-0.098716650	0.159555000
7	-2.343932540	0.673465120	-0.122135340
6	-2.733754600	2.002824580	-0.059259160
6	-4.127872140	2.058191010	0.307253280
6	-4.571365430	0.768952200	0.429967570

1	-4.701444210	2.967807220	0.444821040
1	-5.572851100	0.436504090	0.679511020
6	-4.813250290	-2.152638340	0.495713290
6	-5.573230680	-2.796993820	-0.494617960
6	-5.308144860	-2.121272120	1.810184120
1	-5.201125480	-2.821584280	-1.519622760
1	-4.723786140	-1.627011390	2.587465350
6	-6.796000640	-3.394147110	-0.177864070
6	-6.530000460	-2.720178800	2.126432710
6	-7.278309600	-3.358486330	1.133453120
1	-8.232459080	-3.825199730	1.380154470
6	1.573026290	-4.518652030	-1.271788600
6	1.835051370	-5.343121430	-0.164437450
6	1.893409520	-4.992719130	-2.554923940
1	1.589099680	-4.983526500	0.835758030
1	1.686317890	-4.364460200	-3.422085000
6	2.404724790	-6.607237540	-0.335794810
6	2.460429090	-6.258039310	-2.725319570
6	2.719360040	-7.069123540	-1.616859540
1	3.162434670	-8.056436470	-1.750795080
6	3.811802400	2.109596210	-1.992986790
6	4.863414170	2.146453380	-1.061275390
6	4.001285160	2.686441320	-3.258627040
1	4.716953640	1.708194970	-0.072558170
1	3.188521300	2.661493450	-3.985675210
6	6.080077770	2.746352290	-1.396611550
6	5.221270500	3.281443170	-3.591147560
6	6.263741700	3.313722130	-2.660931440
1	7.214948020	3.779847390	-2.920323540
6	-2.555852480	4.480031010	-0.180160820
6	-2.167858030	5.351806500	0.851342540
6	-3.540927750	4.906382330	-1.086942660
1	-1.403691330	5.031519810	1.560735780
1	-3.841827570	4.242135770	-1.897897210
6	-2.753805240	6.613686830	0.976212540
6	-4.123419660	6.169964320	-0.963227600
6	-3.733471280	7.027422470	0.069316430
1	-4.189191400	8.013368260	0.165595830
22	-0.391989350	-0.019947440	-0.373237630
8	0.359462320	0.164821650	1.317397410
1	2.604717280	-7.232466130	0.535362390
1	2.696515990	-6.612682700	-3.729345920
1	-6.896433040	-2.690246730	3.153341270
1	-7.375378530	-3.885790340	-0.960323480
1	6.886885730	2.772345180	-0.662950330
1	5.356180930	3.720005730	-4.580650510
1	-2.444242640	7.274795760	1.786621010
1	-4.882016990	6.486761270	-1.680009910
1	0.434744750	-1.105419990	3.499682280
6	0.581804720	-0.032723060	3.684859450
1	-0.418447370	0.414269120	3.794312500
6	1.400385640	0.174530680	4.962080870
1	2.404316850	-0.267356840	4.879845390
1	0.900197990	-0.308318300	5.812924550
1	1.519795220	1.237883810	5.210146510
6	1.189713500	0.572322950	2.394417950
6	1.264051080	2.099656580	2.455845140
1	1.701531170	2.505050310	1.537721220
1	0.247620800	2.497160520	2.577942410
1	1.884671140	2.431991800	3.297423880
6	2.609223600	-0.005598170	2.151704200
8	3.616351980	0.655298060	1.969961860
8	2.597647650	-1.362119760	2.171850570
6	3.887727220	-1.981811760	1.950566620
1	4.596548610	-1.673919100	2.730067270
1	3.703030730	-3.059444330	1.998545600
1	4.283906520	-1.700733010	0.967302900
1	-0.639625470	0.120790400	-2.085583860

Energy: -3221.418533

(TPP)Ti(OH)(H)			
7	1.923166860	-0.698944970	-0.450816880
6	2.269957080	-2.014149110	-0.604022490
6	3.626690340	-2.086811090	-1.118621340
6	4.056977510	-0.802033410	-1.292123340
6	2.973681770	0.070052610	-0.869862060
1	4.167624820	-3.000978230	-1.336451020
1	5.012568230	-0.472016870	-1.683996360
6	1.892730550	2.340376900	-0.629482220
7	0.628006110	1.960670580	-0.210064960
6	-0.110453220	3.102870660	-0.018566340
6	0.710742600	4.250687220	-0.320099030
6	1.943525250	3.782564630	-0.687574550
6	-1.468910470	3.154118610	0.382034010
1	0.388871480	5.284178170	-0.253802030
1	2.811001730	4.366758940	-0.972655910
6	2.976115950	1.485944870	-0.941825150
6	1.429378410	-3.120908470	-0.330736920
6	0.081440380	-3.068140790	0.092086190
6	-0.738780310	-4.227252340	0.352673710
6	-1.976074130	-3.776528450	0.726598680
6	-1.938127860	-2.333695240	0.682711060
7	-0.681745960	-1.931102800	0.303525810
1	-0.411507980	-5.257022590	0.263664170
1	-2.837366040	-4.371654890	1.008816300
6	-3.025169560	-1.475288180	0.989947620
6	-2.979466680	-0.066893430	0.962141660
7	-1.864238510	0.710826410	0.681873780
6	-2.274594640	2.037355710	0.675234820
6	-3.676271380	2.091040060	1.007034520
6	-4.109774280	0.803460040	1.173247710
1	-4.263194380	2.999646030	1.084331920
1	-5.115979910	0.472085140	1.404519340
6	-4.325344050	-2.114962480	1.359342450
6	-5.063145010	-2.846611590	0.413210080
6	-4.834745010	-1.994801230	2.663584820
1	-4.681056230	-2.940527460	-0.604003760
1	-4.265946470	-1.435441590	3.407412340
6	-6.278587980	-3.439924650	0.762354980
6	-6.048500960	-2.591700780	3.012420680
6	-6.775230330	-3.315472560	2.062966080
1	-7.723534810	-3.780008160	2.334999780
6	2.026172890	-4.482864430	-0.520902270
6	2.388784680	-5.264318390	0.587980910
6	2.236623980	-4.998818300	-1.809704160
1	2.229873770	-4.870701610	1.592808150
1	1.955569370	-4.399723450	-2.676684700
6	2.949882870	-6.531687710	0.411867700
6	2.794659350	-6.267752720	-1.984403620
6	3.153847930	-7.037824300	-0.874763050
1	3.590283940	-8.027629950	-1.012061700
6	4.243018890	2.132591120	-1.406642560
6	5.402635100	2.081287470	-0.614937660
6	4.301284460	2.793462980	-2.645236550
1	5.367731820	1.573356580	0.349584480
1	3.409423090	2.831304150	-3.271679890
6	6.587625590	2.680910310	-1.047649940
6	5.488643630	3.387438140	-3.079404590
6	6.635224200	3.335056000	-2.281833470
1	7.561135420	3.800775680	-2.620694200
6	-2.100467920	4.508920890	0.486167030
6	-1.822663400	5.341870620	1.582076190
6	-2.976319380	4.971615390	-0.509068170
1	-1.145129670	4.989635390	2.361063060
1	-3.194554010	4.333016140	-1.366048320
6	-2.408362900	6.606590410	1.680923560
6	-3.560592320	6.237030960	-0.410004180
6	-3.278868520	7.058296760	0.685171350
1	-3.735268710	8.045649550	0.762120890
22	0.056776430	0.026906270	0.350282660

8	1.030640340	-0.101337790	1.930180220
1	3.229371440	-7.124379500	1.283743760
1	2.947041510	-6.656124870	-2.992126160
1	-6.425361130	-2.493392740	4.031216380
1	-6.841403690	-3.998261860	0.013265320
1	7.476069360	2.638161940	-0.416461780
1	5.517945500	3.890277550	-4.046795720
1	-2.184849990	7.239592750	2.540552610
1	-4.236242690	6.582641650	-1.193372640
1	1.949764860	-0.409268270	2.007425410
1	-0.044678960	-0.172068040	-1.357982470
Energy:		-2836.624833	

S4. Atomic partitions of spin density of the calculated open-shell structures

Product 1

atom	spin
1 N	0.0504
2 C	-0.0093
3 C	0.0101
4 C	-0.0095
5 C	0.0146
6 H	0.0006
7 H	-0.0006
8 C	0.0131
9 N	0.0055
10 C	0.0361
11 C	0.0069
12 C	0.0258
13 C	-0.0087
14 H	0.0004
15 H	0.0015
16 C	0.0519
17 C	0.1008
18 C	0.0020
19 C	0.3079
20 C	0.0254
21 C	0.0176
22 N	0.0738
23 H	0.0189
24 H	0.0157
25 C	0.0417
26 C	0.0122
27 N	0.0009
28 C	0.0353
29 C	0.0056
30 C	0.0263
31 H	0.0003
32 H	0.0016
33 C	0.0033
34 C	0.0045
35 C	0.0036
36 H	0.0014
37 H	0.0002
38 C	-0.0000
39 C	-0.0001
40 C	0.0029
41 H	0.0002
42 C	0.0059
43 C	0.0049
44 C	0.0048
45 H	0.0010
46 H	0.0006
47 C	0.0003
48 C	0.0009
49 C	0.0016
50 H	0.0001
51 C	0.0034
52 C	0.0040
53 C	0.0035
54 H	0.0007
55 H	0.0003
56 C	0.0005
57 C	0.0001
58 C	0.0023
59 H	0.0002
60 C	0.0003
61 C	-0.0009
62 C	-0.0008
63 H	0.0003
64 H	0.0004

65	C	0.0008
66	C	0.0008
67	C	-0.0008
68	H	-0.0000
69	Ti	0.0050
70	O	0.0077
71	H	0.0002
72	H	0.0002
73	H	0.0001
74	H	-0.0000
75	H	0.0001
76	H	0.0001
77	H	0.0000
78	H	0.0000
79	H	0.0006
80	C	0.0037
81	H	0.0006
82	C	0.0022
83	H	0.0002
84	H	0.0010
85	H	0.0001
86	C	0.0396
87	C	0.0027
88	H	0.0020
89	H	0.0008
90	H	0.0009
91	C	0.0047
92	O	0.0015
93	O	0.0004
94	C	0.0000
95	H	0.0000
96	H	0.0001
97	H	-0.0001
total		1.0000

TS1

atom	spin
1	N 0.0282
2	C -0.0048
3	C 0.0039
4	C -0.0051
5	C 0.0062
6	H 0.0002
7	H -0.0003
8	C 0.0055
9	N 0.0037
10	C 0.0197
11	C 0.0024
12	C 0.0142
13	C -0.0064
14	H 0.0001
15	H 0.0009
16	C 0.0310
17	C 0.0535
18	C 0.0025
19	C 0.1894
20	C -0.0056
21	C 0.0147
22	N 0.0489
23	H 0.0130
24	H 0.0082
25	C 0.0172
26	C 0.0082
27	N -0.0019
28	C 0.0200
29	C 0.0044
30	C 0.0148
31	H 0.0003
32	H 0.0010
33	C 0.0024

34	C	0.0028
35	C	0.0026
36	H	0.0012
37	H	0.0002
38	C	0.0000
39	C	-0.0001
40	C	0.0018
41	H	0.0001
42	C	0.0034
43	C	0.0033
44	C	0.0028
45	H	0.0010
46	H	0.0004
47	C	0.0002
48	C	0.0006
49	C	0.0011
50	H	0.0001
51	C	0.0020
52	C	0.0024
53	C	0.0021
54	H	0.0004
55	H	0.0002
56	C	0.0003
57	C	0.0000
58	C	0.0013
59	H	0.0001
60	C	0.0001
61	C	-0.0006
62	C	-0.0005
63	H	0.0001
64	H	0.0002
65	C	0.0004
66	C	0.0005
67	C	-0.0005
68	H	-0.0000
69	Ti	0.0037
70	O	0.0034
71	H	0.0001
72	H	0.0001
73	H	0.0000
74	H	-0.0000
75	H	0.0001
76	H	0.0001
77	H	0.0000
78	H	0.0000
79	H	0.0045
80	C	0.0160
81	H	0.0039
82	C	0.0194
83	H	0.0013
84	H	0.0045
85	H	0.0011
86	C	0.2642
87	C	0.0174
88	H	0.0046
89	H	0.0047
90	H	0.0179
91	C	0.0457
92	O	0.0452
93	O	0.0182
94	C	0.0013
95	H	0.0007
96	H	0.0002
97	H	0.0012
total		1.0000

Product 2

atom	spin
1 N	0.0024
2 C	0.0122

3	C	0.0270
4	C	0.0057
5	C	0.0361
6	H	0.0017
7	H	0.0002
8	C	0.0371
9	N	0.0026
10	C	0.0142
11	C	0.0267
12	C	0.0079
13	C	0.0471
14	H	0.0015
15	H	0.0004
16	C	-0.0094
17	C	0.0494
18	C	0.0174
19	C	0.0246
20	C	0.3009
21	C	0.0009
22	N	0.0761
23	H	0.0170
24	H	0.0185
25	C	0.1020
26	C	-0.0097
27	N	0.0504
28	C	0.0154
29	C	-0.0099
30	C	0.0107
31	H	-0.0006
32	H	0.0007
33	C	0.0059
34	C	0.0048
35	C	0.0049
36	H	0.0010
37	H	0.0006
38	C	0.0001
39	C	0.0008
40	C	0.0015
41	H	0.0001
42	C	0.0037
43	C	0.0053
44	C	0.0041
45	H	0.0015
46	H	0.0002
47	C	0.0000
48	C	-0.0001
49	C	0.0033
50	H	0.0003
51	C	0.0003
52	C	-0.0009
53	C	-0.0009
54	H	0.0004
55	H	0.0004
56	C	0.0008
57	C	0.0008
58	C	-0.0009
59	H	-0.0000
60	C	0.0031
61	C	0.0035
62	C	0.0038
63	H	0.0003
64	H	0.0006
65	C	0.0001
66	C	0.0005
67	C	0.0024
68	H	0.0002
69	Ti	0.0015
70	O	0.0111
71	H	-0.0000
72	H	0.0001

73	H	0.0002
74	H	0.0003
75	H	0.0000
76	H	0.0000
77	H	0.0001
78	H	0.0001
79	H	0.0007
80	C	0.0037
81	H	0.0007
82	C	0.0019
83	H	0.0001
84	H	0.0009
85	H	0.0001
86	C	0.0369
87	C	0.0025
88	H	0.0020
89	H	0.0007
90	H	0.0009
91	C	0.0044
92	O	0.0012
93	O	0.0002
94	C	0.0000
95	H	0.0000
96	H	0.0001
97	H	-0.0001
total		1.0000

Product 3

atom	spin
1 N	0.0020
2 C	0.0114
3 C	0.0267
4 C	0.0050
5 C	0.0360
6 H	0.0016
7 H	0.0002
8 C	0.0363
9 N	0.0041
10 C	0.0149
11 C	0.0259
12 C	0.0086
13 C	0.0485
14 H	0.0015
15 H	0.0005
16 C	-0.0092
17 C	0.0460
18 C	0.0179
19 C	0.0244
20 C	0.2971
21 C	0.0024
22 N	0.0753
23 H	0.0179
24 H	0.0173
25 C	0.0999
26 C	-0.0091
27 N	0.0494
28 C	0.0162
29 C	-0.0095
30 C	0.0109
31 H	-0.0006
32 H	0.0007
33 C	0.0055
34 C	0.0063
35 C	0.0053
36 H	0.0017
37 H	0.0002
38 C	0.0004
39 C	0.0010
40 C	0.0031
41 H	0.0002

42	C	0.0036
43	C	0.0035
44	C	0.0040
45	H	0.0002
46	H	0.0012
47	C	-0.0002
48	C	-0.0000
49	C	0.0023
50	H	0.0002
51	C	0.0003
52	C	-0.0008
53	C	-0.0008
54	H	0.0003
55	H	0.0004
56	C	0.0008
57	C	0.0008
58	C	-0.0008
59	H	-0.0000
60	C	0.0033
61	C	0.0025
62	C	0.0028
63	H	0.0004
64	H	0.0005
65	C	0.0004
66	C	0.0007
67	C	0.0009
68	H	0.0001
69	Ti	0.0054
70	O	0.0083
71	H	0.0001
72	H	-0.0000
73	H	0.0002
74	H	0.0001
75	H	0.0000
76	H	0.0000
77	H	0.0001
78	H	0.0001
79	H	0.0006
80	C	0.0052
81	H	0.0042
82	C	0.0007
83	H	0.0005
84	H	0.0004
85	H	0.0000
86	C	0.0374
87	C	0.0024
88	H	0.0009
89	H	0.0010
90	H	0.0010
91	C	0.0039
92	O	0.0063
93	O	0.0007
94	C	0.0002
95	H	0.0000
96	H	0.0000
97	H	0.0001
total		1.0001

Product 4

atom	spin
1 N	0.0051
2 C	0.0716
3 C	0.0200
4 C	0.0421
5 C	0.0359
6 H	0.0008
7 H	0.0023
8 C	0.0386
9 N	0.0472
10 C	-0.0021

11	C	0.0275
12	C	-0.0073
13	C	0.1448
14	H	0.0016
15	H	-0.0006
16	C	0.0636
17	C	0.0090
18	C	0.0729
19	C	0.0229
20	C	0.0393
21	C	0.0401
22	N	0.0044
23	H	0.0010
24	H	0.0021
25	C	0.0579
26	C	0.0434
27	N	0.0447
28	C	-0.0022
29	C	0.0318
30	C	-0.0076
31	H	0.0019
32	H	-0.0006
33	C	0.0041
34	C	0.0045
35	C	0.0043
36	H	0.0010
37	H	0.0005
38	C	0.0010
39	C	0.0006
40	C	0.0030
41	H	0.0002
42	C	0.0069
43	C	0.0005
44	C	0.0029
45	H	0.0001
46	H	0.0017
47	C	0.0002
48	C	0.0001
49	C	-0.0001
50	H	0.0000
51	C	0.0044
52	C	0.0041
53	C	0.0043
54	H	0.0005
55	H	0.0009
56	C	0.0006
57	C	0.0011
58	C	0.0024
59	H	0.0002
60	C	0.0083
61	C	0.0104
62	C	0.0100
63	H	0.0009
64	H	0.0007
65	C	-0.0002
66	C	-0.0003
67	C	0.0066
68	H	0.0005
69	Ti	0.0178
70	O	0.0059
71	H	0.0001
72	H	0.0000
73	H	0.0002
74	H	0.0001
75	H	0.0002
76	H	0.0001
77	H	0.0002
78	H	0.0002
79	H	0.0003
80	C	0.0010

81	H	0.0007
82	C	0.0005
83	H	0.0001
84	H	0.0002
85	H	0.0000
86	C	0.0219
87	C	0.0025
88	H	0.0003
89	H	0.0009
90	H	0.0005
91	C	0.0032
92	O	0.0032
93	O	0.0008
94	C	0.0003
95	H	0.0000
96	H	0.0000
97	H	0.0000
total		1.0000

Product 5

atom	spin
1 N	0.0478
2 C	0.0402
3 C	-0.0075
4 C	0.0286
5 C	-0.0020
6 H	-0.0006
7 H	0.0017
8 C	-0.0021
9 N	0.0467
10 C	0.0417
11 C	-0.0077
12 C	0.0300
13 C	0.0584
14 H	-0.0006
15 H	0.0018
16 C	0.1497
17 C	0.0629
18 C	0.0387
19 C	0.0432
20 C	0.0232
21 C	0.0719
22 N	0.0045
23 H	0.0025
24 H	0.0010
25 C	0.0089
26 C	0.0710
27 N	0.0034
28 C	0.0381
29 C	0.0450
30 C	0.0212
31 H	0.0025
32 H	0.0010
33 C	0.0057
34 C	0.0002
35 C	0.0029
36 H	0.0000
37 H	0.0016
38 C	0.0002
39 C	0.0001
40 C	-0.0001
41 H	0.0000
42 C	0.0044
43 C	0.0034
44 C	0.0037
45 H	0.0006
46 H	0.0007
47 C	0.0006
48 C	0.0011
49 C	0.0016

50	H	0.0001
51	C	0.0089
52	C	0.0089
53	C	0.0088
54	H	0.0008
55	H	0.0009
56	C	0.0001
57	C	0.0000
58	C	0.0043
59	H	0.0003
60	C	0.0041
61	C	0.0045
62	C	0.0043
63	H	0.0010
64	H	0.0005
65	C	0.0010
66	C	0.0004
67	C	0.0029
68	H	0.0002
69	Ti	0.0133
70	O	0.0065
71	H	0.0002
72	H	0.0002
73	H	0.0001
74	H	0.0001
75	H	0.0003
76	H	0.0002
77	H	0.0001
78	H	0.0002
79	C	0.0009
80	C	0.0028
81	H	0.0000
82	H	0.0006
83	H	0.0002
84	H	0.0002
85	H	0.0009
86	C	0.0012
87	C	0.0223
88	H	0.0007
89	H	0.0003
90	H	0.0004
91	C	0.0030
92	O	0.0003
93	O	0.0011
94	C	0.0001
95	H	-0.0000
96	H	-0.0000
97	H	-0.0000
total		1.0000

Product 6

atom	spin
1 N	0.0030
2 C	0.0249
3 C	0.0428
4 C	0.0115
5 C	0.0618
6 H	0.0025
7 H	0.0006
8 C	0.0617
9 N	0.0015
10 C	0.0290
11 C	0.0414
12 C	0.0146
13 C	0.0601
14 H	0.0023
15 H	0.0007
16 C	-0.0134
17 C	0.0675
18 C	0.0370

19	C	0.0035
20	C	0.0191
21	C	0.0162
22	N	0.0750
23	H	0.0003
24	H	0.0010
25	C	0.1568
26	C	-0.0041
27	N	0.0674
28	C	0.0398
29	C	-0.0078
30	C	0.0256
31	H	-0.0005
32	H	0.0015
33	C	0.0087
34	C	0.0125
35	C	0.0097
36	H	0.0016
37	H	0.0005
38	C	0.0007
39	C	-0.0002
40	C	0.0071
41	H	0.0005
42	C	0.0050
43	C	0.0031
44	C	0.0039
45	H	0.0004
46	H	0.0011
47	C	0.0009
48	C	0.0013
49	C	0.0009
50	H	0.0001
51	C	0.0006
52	C	-0.0014
53	C	-0.0014
54	H	0.0008
55	H	0.0006
56	C	0.0011
57	C	0.0012
58	C	-0.0015
59	H	-0.0001
60	C	0.0042
61	C	0.0055
62	C	0.0053
63	H	0.0012
64	H	0.0005
65	C	0.0009
66	C	0.0002
67	C	0.0041
68	H	0.0003
69	Ti	0.0053
70	O	0.0123
71	H	0.0002
72	H	0.0002
73	H	0.0002
74	H	0.0003
75	H	0.0000
76	H	0.0001
77	H	0.0001
78	H	0.0002
79	H	0.0003
80	C	0.0020
81	H	0.0005
82	C	0.0015
83	H	0.0001
84	H	0.0005
85	H	0.0001
86	C	0.0377
87	C	0.0035
88	H	0.0006

89	H	0.0015
90	H	0.0007
91	C	0.0029
92	O	0.0052
93	O	0.0004
94	C	0.0003
95	H	-0.0000
96	H	0.0001
97	H	0.0001
total		1.0000

Product 7

atom	spin
1 N	0.0083
2 C	0.0252
3 C	0.0123
4 C	0.0245
5 C	0.0139
6 H	0.0010
7 H	0.0018
8 C	0.0067
9 N	0.0186
10 C	0.0191
11 C	-0.0003
12 C	0.0110
13 C	0.0119
14 H	0.0001
15 H	0.0008
16 C	0.0202
17 C	0.0068
18 C	0.0145
19 C	-0.0000
20 C	0.0075
21 C	0.0087
22 N	0.0205
23 H	-0.0000
24 H	0.0006
25 C	0.0367
26 C	0.0117
27 N	0.0085
28 C	0.0201
29 C	0.0079
30 C	0.0168
31 H	0.0005
32 H	0.0013
33 C	0.0025
34 C	0.0022
35 C	0.0020
36 H	0.0004
37 H	0.0003
38 C	0.0001
39 C	0.0003
40 C	0.0010
41 H	0.0001
42 C	0.0008
43 C	0.0004
44 C	0.0002
45 H	0.0002
46 H	0.0003
47 C	0.0003
48 C	0.0004
49 C	0.0000
50 H	0.0000
51 C	0.0012
52 C	0.0006
53 C	0.0009
54 H	0.0002
55 H	0.0001
56 C	0.0001
57 C	0.0002

58	C	0.0001
59	H	0.0000
60	C	0.0011
61	C	0.0009
62	C	0.0003
63	H	0.0002
64	H	0.0002
65	C	0.0004
66	C	0.0004
67	C	0.0003
68	H	0.0000
69	Ti	0.6571
70	O	-0.0104
71	H	0.0000
72	H	0.0000
73	H	0.0001
74	H	0.0000
75	H	0.0000
76	H	0.0001
77	H	0.0001
78	H	0.0000
79	H	-0.0000
80	C	-0.0006
81	H	-0.0000
82	C	-0.0002
83	H	0.0000
84	H	-0.0001
85	H	-0.0000
86	C	-0.0014
87	C	-0.0004
88	H	0.0001
89	H	0.0001
90	H	-0.0002
91	C	-0.0004
92	O	-0.0003
93	O	-0.0001
94	C	0.0001
95	H	-0.0000
96	H	0.0001
97	H	0.0002
total		1.0001

TS2

atom	spin
1	N 0.0010
2	C 0.0171
3	C 0.0036
4	C 0.0189
5	C 0.0046
6	H 0.0003
7	H 0.0015
8	C 0.0045
9	N 0.0031
10	C 0.0162
11	C 0.0012
12	C 0.0114
13	C 0.0029
14	H 0.0001
15	H 0.0009
16	C 0.0125
17	C 0.0092
18	C 0.0095
19	C -0.0005
20	C 0.0064
21	C 0.0043
22	N 0.0135
23	H -0.0001
24	H 0.0005
25	C 0.0303
26	C 0.0067

27	N	0.0033
28	C	0.0133
29	C	0.0050
30	C	0.0126
31	H	0.0003
32	H	0.0009
33	C	0.0020
34	C	0.0018
35	C	0.0016
36	H	0.0003
37	H	0.0003
38	C	0.0001
39	C	0.0001
40	C	0.0007
41	H	0.0001
42	C	0.0008
43	C	0.0006
44	C	0.0003
45	H	0.0003
46	H	0.0001
47	C	0.0002
48	C	0.0002
49	C	0.0002
50	H	0.0000
51	C	0.0008
52	C	0.0005
53	C	0.0006
54	H	0.0004
55	H	0.0001
56	C	0.0001
57	C	0.0001
58	C	0.0001
59	H	0.0000
60	C	0.0004
61	C	0.0001
62	C	-0.0000
63	H	0.0001
64	H	0.0002
65	C	0.0002
66	C	0.0002
67	C	-0.0000
68	H	0.0000
69	Ti	0.2577
70	O	0.0284
71	H	0.0000
72	H	0.0000
73	H	0.0001
74	H	0.0001
75	H	0.0000
76	H	0.0000
77	H	0.0000
78	H	0.0000
79	H	0.0046
80	C	0.0119
81	H	0.0042
82	C	0.0128
83	H	0.0016
84	H	0.0034
85	H	0.0010
86	C	0.2448
87	C	0.0154
88	H	0.0031
89	H	0.0058
90	H	0.0157
91	C	0.0645
92	O	0.0710
93	O	0.0215
94	C	0.0011
95	H	0.0007
96	H	0.0001

97 H	0.0016
total	1.0000

TS3

atom	spin
1 N	0.0040
2 C	0.0050
3 C	0.0088
4 C	0.0031
5 C	0.0099
6 H	0.0006
7 H	0.0002
8 C	0.0111
9 N	0.0042
10 C	0.0028
11 C	0.0069
12 C	0.0008
13 C	0.0083
14 H	0.0005
15 H	0.0001
16 C	0.0020
17 C	0.0234
18 C	0.0033
19 C	0.0050
20 C	-0.0009
21 C	0.0076
22 N	0.0107
23 H	0.0005
24 H	-0.0001
25 C	0.0041
26 C	0.0134
27 N	0.0020
28 C	0.0044
29 C	0.0142
30 C	0.0026
31 H	0.0010
32 H	0.0002
33 C	0.0004
34 C	0.0002
35 C	0.0001
36 H	0.0001
37 H	0.0003
38 C	0.0002
39 C	0.0002
40 C	0.0000
41 H	0.0000
42 C	0.0015
43 C	0.0016
44 C	0.0013
45 H	0.0002
46 H	0.0002
47 C	0.0001
48 C	0.0000
49 C	0.0008
50 H	0.0001
51 C	0.0003
52 C	0.0000
53 C	0.0001
54 H	0.0001
55 H	0.0001
56 C	0.0002
57 C	0.0002
58 C	-0.0000
59 H	0.0000
60 C	0.0005
61 C	0.0008
62 C	0.0003
63 H	0.0010
64 H	0.0002
65 C	0.0001

66	C	0.0001
67	C	0.0002
68	H	0.0000
69	Ti	0.2637
70	O	0.0056
71	H	0.0001
72	H	0.0000
73	H	0.0000
74	H	0.0000
75	H	0.0000
76	H	0.0000
77	H	0.0000
78	H	0.0000
79	C	0.0095
80	C	0.0547
81	H	0.0010
82	H	0.0003
83	H	0.0060
84	H	0.0099
85	H	0.0363
86	C	0.0183
87	C	0.2193
88	H	0.0130
89	H	0.0125
90	H	0.0017
91	C	0.0666
92	O	0.0218
93	O	0.0846
94	C	0.0013
95	H	0.0011
96	H	0.0012
97	H	0.0001
total		0.9999

(TPP)TiOH

atom	spin
1 N	0.0164
2 C	0.0047
3 C	0.0177
4 C	-0.0007
5 C	0.0242
6 H	0.0014
7 H	0.0001
8 C	0.0213
9 N	0.0117
10 C	0.0070
11 C	0.0169
12 C	0.0015
13 C	0.0418
14 H	0.0014
15 H	0.0001
16 C	0.0025
17 C	0.0260
18 C	0.0084
19 C	0.0240
20 C	0.0051
21 C	0.0271
22 N	0.0113
23 H	0.0018
24 H	0.0006
25 C	0.0003
26 C	0.0188
27 N	0.0170

28 C	0.0057
29 C	0.0128
30 C	-0.0021
31 H	0.0010
32 H	-0.0001
33 C	0.0004
34 C	-0.0001
35 C	-0.0001
36 H	0.0003
37 H	0.0002
38 C	0.0004
39 C	0.0004
40 C	-0.0001
41 H	-0.0000
42 C	0.0016
43 C	0.0011
44 C	0.0014
45 H	0.0003
46 H	0.0002
47 C	-0.0000
48 C	0.0001
49 C	0.0005
50 H	0.0000
51 C	0.0006
52 C	0.0002
53 C	-0.0001
54 H	0.0002
55 H	0.0002
56 C	0.0005
57 C	0.0005
58 C	-0.0000
59 H	0.0000
60 C	0.0028
61 C	0.0025
62 C	0.0024
63 H	0.0003
64 H	0.0004
65 C	0.0002
66 C	-0.0000
67 C	0.0012
68 H	0.0001
69 Ti	0.6650
70 O	-0.0103
71 H	0.0000
72 H	0.0001
73 H	0.0000
74 H	0.0000
75 H	0.0000
76 H	0.0000
77 H	0.0001
78 H	0.0000
79 H	0.0005
total	1.0000

TS4

atomspin

1 N	0.0038
2 C	0.0127

3	C	0.0004
4	C	0.0083
5	C	0.0021
6	H	0.0001
7	H	0.0006
8	C	0.0040
9	N	0.0023
10	C	0.0128
11	C	0.0030
12	C	0.0119
13	C	0.0040
14	H	0.0002
15	H	0.0009
16	C	0.0050
17	C	0.0018
18	C	0.0102
19	C	0.0023
20	C	0.0088
21	C	0.0045
22	N	0.0040
23	H	0.0002
24	H	0.0006
25	C	0.0224
26	C	0.0033
27	N	0.0098
28	C	0.0074
29	C	-0.0008
30	C	0.0049
31	H	-0.0001
32	H	0.0005
33	C	0.0014
34	C	0.0013
35	C	0.0015
36	H	0.0002
37	H	0.0001
38	C	0.0000
39	C	0.0001
40	C	0.0008
41	H	0.0001
42	C	0.0003
43	C	0.0000
44	C	0.0000
45	H	0.0002
46	H	0.0001
47	C	0.0002
48	C	0.0002
49	C	-0.0000
50	H	-0.0000
51	C	0.0004
52	C	0.0004
53	C	0.0002
54	H	0.0007
55	H	0.0001
56	C	0.0001
57	C	0.0001
58	C	0.0001
59	H	0.0000
60	C	0.0004
61	C	0.0001
62	C	0.0002
63	H	0.0001
64	H	0.0001
65	C	0.0002
66	C	0.0002
67	C	0.0000
68	H	0.0000
69	Ti	0.2723
70	O	0.0058
71	H	0.0000
72	H	0.0000

73	H	0.0001
74	H	0.0000
75	H	0.0000
76	H	0.0000
77	H	0.0000
78	H	0.0000
79	C	0.0158
80	C	0.0153
81	H	0.0013
82	H	0.0033
83	H	0.0018
84	H	0.0074
85	H	0.0030
86	C	0.0600
87	C	0.2185
88	H	0.0361
89	H	0.0126
90	H	0.0098
91	C	0.0680
92	O	0.0270
93	O	0.0760
94	C	0.0014
95	H	0.0016
96	H	0.0011
97	H	0.0001
total		1.0000

S5. Energy characteristics of possible reactions of (TPP)Ti=O with methyl methacrylate radicals

