

Supporting Information

The Influence of Branching on the Conformational Space: A Case Study of Tri-secondary-butyl Phosphate using Matrix Isolation Infrared Spectroscopy and DFT Computations

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Table S1. Total number of all possible conformations of TsBP after elimination of a bunch of conformers based on the analysis of DMsBP.

S. No.	Structure	Remarks
$G^\pm(xyz)G^\pm(xyz)G^\pm(xyz)$cluster		
1	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(g^tg^t)$	
2	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(g^tt)$	
3	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(tg^t)$	
4	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(tg^tg^t)$	
5	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(g^tg^t)$	
6	$G^\pm(g^tg^t)G^\pm(g^tt)G^\pm(g^tg^t)$	Identical as 2
7	$G^\pm(g^tg^t)G^\pm(g^tt)G^\pm(g^tg^t)$	
8	$G^\pm(g^tg^t)G^\pm(g^tt)G^\pm(tg^t)$	
9	$G^\pm(g^tg^t)G^\pm(g^tt)G^\pm(tg^tg^t)$	
10	$G^\pm(g^tg^t)G^\pm(g^tt)G^\pm(g^tg^t)$	
11	$G^\pm(g^tg^t)G^\pm(tg^t)G^\pm(g^tg^t)$	Identical as 3
12	$G^\pm(g^tg^t)G^\pm(tg^t)G^\pm(g^tt)$	Identical as 8
13	$G^\pm(g^tg^t)G^\pm(tg^t)G^\pm(tg^t)$	
14	$G^\pm(g^tg^t)G^\pm(tg^t)G^\pm(tg^tg^t)$	
15	$G^\pm(g^tg^t)G^\pm(tg^t)G^\pm(g^tg^t)$	
16	$G^\pm(g^tg^t)G^\pm(tg^tg^t)G^\pm(g^tg^t)$	Identical as 4
17	$G^\pm(g^tg^t)G^\pm(tg^tg^t)G^\pm(g^tt)$	Identical as 9
18	$G^\pm(g^tg^t)G^\pm(tg^tg^t)G^\pm(tg^t)$	Identical as 14
19	$G^\pm(g^tg^t)G^\pm(tg^tg^t)G^\pm(tg^tg^t)$	
20	$G^\pm(g^tg^t)G^\pm(tg^tg^t)G^\pm(g^tg^t)$	
21	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(g^tg^t)$	Identical as 5
22	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(g^tt)$	Identical as 10
23	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(tg^t)$	Identical as 15
24	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(tg^tg^t)$	Identical as 20
25	$G^\pm(g^tg^t)G^\pm(g^tg^t)G^\pm(g^tg^t)$	
26	$G^\pm(g^tt)G^\pm(g^tg^t)G^\pm(g^tg^t)$	
27	$G^\pm(g^tt)G^\pm(g^tg^t)G^\pm(g^tt)$	
28	$G^\pm(g^tt)G^\pm(g^tg^t)G^\pm(tg^t)$	
29	$G^\pm(g^tt)G^\pm(g^tg^t)G^\pm(tg^tg^t)$	
30	$G^\pm(g^tt)G^\pm(g^tg^t)G^\pm(g^tg^t)$	
31	$G^\pm(g^tt)G^\pm(g^tt)G^\pm(g^tg^t)$	Identical as 27
32	$G^\pm(g^tt)G^\pm(g^tt)G^\pm(g^tt)$	
33	$G^\pm(g^tt)G^\pm(g^tt)G^\pm(tg^t)$	
34	$G^\pm(g^tt)G^\pm(g^tt)G^\pm(tg^tg^t)$	
35	$G^\pm(g^tt)G^\pm(g^tt)G^\pm(g^tg^t)$	

36	$G^\pm(g^\mp tt)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	Identical as 28
37	$G^\pm(g^\mp tt)G^\pm(tg^\pm t)G^\pm(g^\mp tt)$	Identical as 33
38	$G^\pm(g^\mp tt)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	
39	$G^\pm(g^\mp tt)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	
40	$G^\pm(g^\mp tt)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	
41	$G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	Identical as 29
42	$G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)$	Identical as 34
43	$G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)$	Identical as 38
44	$G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
45	$G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
46	$G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	Identical as 30
47	$G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)$	Identical as 35
48	$G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)$	Identical as 40
49	$G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)$	Identical as 45
50	$G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
51	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	
52	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	
53	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	
54	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	
55	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	
56	$G^\pm(tg^\pm t)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	Identical as 52
57	$G^\pm(tg^\pm t)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	
58	$G^\pm(tg^\pm t)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	
59	$G^\pm(tg^\pm t)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	
60	$G^\pm(tg^\pm t)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	
61	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	Identical as 53
62	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(g^\mp tt)$	Identical as 58
63	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	
64	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	
65	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	
66	$G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	Identical as 54
67	$G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)$	Identical as 59
68	$G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)$	Identical as 64
69	$G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
70	$G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
71	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	Identical as 55
72	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)$	Identical as 60
73	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)$	Identical as 65
74	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)$	Identical as 70
75	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	

76	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	
77	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	
78	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	
79	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	
80	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	
81	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\mp)}$	Identical as 77
82	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	
83	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	
84	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	
85	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	
86	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)}$	Identical as 78
87	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(g^\mp tt)}$	Identical as 83
88	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	
89	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	
90	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	
91	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)}$	Identical as 79
92	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)}$	Identical as 84
93	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)}$	Identical as 88
94	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
95	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
96	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)}$	Identical as 80
97	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)}$	Identical as 85
98	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)}$	Identical as 90
99	$\textcolor{blue}{G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)}$	Identical as 95
100	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
101	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	
102	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	
103	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	
104	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	
105	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	
106	$\textcolor{blue}{G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\mp)}$	Identical as 102
107	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	
108	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	
109	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	
110	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	
111	$\textcolor{blue}{G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)}$	Identical as 103
112	$\textcolor{blue}{G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)G^\pm(g^\mp tt)}$	Identical as 108
113	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	
114	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	
115	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	

116	$\mathbf{G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)}$	Identical as 104
117	$\mathbf{G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)}$	Identical as 109
118	$\mathbf{G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)}$	Identical as 114
119	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
120	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
121	$\mathbf{G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)}$	Identical as 105
122	$\mathbf{G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)}$	Identical as 110
123	$\mathbf{G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)}$	Identical as 115
124	$\mathbf{G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)}$	Identical as 120
125	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
T(xyz)G$^\pm$(xyz)G$^\pm$(xyz) cluster		
1	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	
2	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	
3	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	
4	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	
5	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	
6	$\mathbf{T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\mp)}$	Identical as 2
7	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	
8	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	
9	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	
10	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	
11	$\mathbf{T(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)}$	Identical as 3
12	$\mathbf{T(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(g^\mp tt)}$	Identical as 8
13	$T(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	
14	$T(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	
15	$T(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	
16	$\mathbf{T(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)}$	Identical as 4
17	$\mathbf{T(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)}$	Identical as 9
18	$\mathbf{T(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)}$	Identical as 14
19	$T(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
20	$T(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
21	$\mathbf{T(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)}$	Identical as 5
22	$\mathbf{T(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)}$	Identical as 10
23	$\mathbf{T(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)}$	Identical as 15
24	$\mathbf{T(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)}$	Identical as 20
25	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
26	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	
27	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	
28	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	
29	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	

30	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\mp})G^{\pm}(g^{\mp}tg^{\pm})$	
31	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\mp})$	Identical as 27
32	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tt)$	
33	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}t)$	
34	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})$	
35	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})$	
36	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}t)G^{\pm}(g^{\mp}tg^{\mp})$	Identical as 28
37	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}t)G^{\pm}(g^{\mp}tt)$	Identical as 33
38	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}t)G^{\pm}(tg^{\pm}t)$	
39	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}t)G^{\pm}(tg^{\pm}g^{\pm})$	
40	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}t)G^{\pm}(g^{\mp}tg^{\pm})$	
41	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(g^{\mp}tg^{\mp})$	Identical as 29
42	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(g^{\mp}tt)$	Identical as 34
43	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(tg^{\pm}t)$	Identical as 39
44	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(tg^{\pm}g^{\pm})$	
45	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(g^{\mp}tg^{\pm})$	
46	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\mp})$	Identical as 30
47	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)$	Identical as 35
48	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)$	Identical as 40
49	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}g^{\pm})$	Identical as 45
50	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\pm})$	
51	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\mp})G^{\pm}(g^{\mp}tg^{\mp})$	
52	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\mp})G^{\pm}(g^{\mp}tt)$	
53	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\mp})G^{\pm}(tg^{\pm}t)$	
54	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\mp})G^{\pm}(tg^{\pm}g^{\pm})$	
55	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\mp})G^{\pm}(g^{\mp}tg^{\pm})$	
56	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\mp})$	Identical as 52
57	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tt)$	
58	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}t)$	
59	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})$	
60	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})$	
61	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)G^{\pm}(g^{\mp}tg^{\mp})$	Identical as 53
62	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)G^{\pm}(g^{\mp}tt)$	Identical as 58
63	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)G^{\pm}(tg^{\pm}t)$	
64	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)G^{\pm}(tg^{\pm}g^{\pm})$	
65	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)G^{\pm}(g^{\mp}tg^{\pm})$	
66	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(g^{\mp}tg^{\mp})$	Identical as 54
67	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(g^{\mp}tt)$	Identical as 59
68	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(tg^{\pm}t)$	Identical as 64
69	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(tg^{\pm}g^{\pm})$	

70	$T(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
71	$\textcolor{blue}{T(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)}$	Identical as 55
72	$\textcolor{blue}{T(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)}$	Identical as 60
73	$\textcolor{blue}{T(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)}$	Identical as 65
74	$\textcolor{blue}{T(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)}$	Identical as 70
75	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	

Table S2. Further reduction in the total conformations of $G^\pm(xyz)G^\pm(xyz)G^\pm(xyz)$ cluster of TsBP after elimination of a bunch of conformers.

S. No.	Structure	Remarks
1	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	
2	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	
3	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	
4	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	
5	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	
6	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	
7	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	
8	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	
9	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	
10	$G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	
11	$G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	
12	$G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	
13	$G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
14	$G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
15	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
16	$\textcolor{blue}{G^\pm(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)}$	Same as 2
17	$\textcolor{blue}{G^\pm(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)}$	Same as 6
18	$\textcolor{blue}{G^\pm(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)}$	Same as 7
19	$\textcolor{blue}{G^\pm(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)}$	Same as 8
20	$\textcolor{blue}{G^\pm(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)}$	Same as 9
21	$G^\pm(g^\mp tt)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	
22	$G^\pm(g^\mp tt)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	
23	$G^\pm(g^\mp tt)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	
24	$G^\pm(g^\mp tt)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	
25	$G^\pm(g^\mp tt)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	
26	$G^\pm(g^\mp tt)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	
27	$G^\pm(g^\mp tt)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	
28	$G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
29	$G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
30	$G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
31	$\textcolor{blue}{G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)}$	Same as 3
32	$\textcolor{blue}{G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)}$	Same as 7
33	$\textcolor{blue}{G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)}$	Same as 10
34	$\textcolor{blue}{G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)}$	Same as 11
35	$\textcolor{blue}{G^\pm(tg^\pm t)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)}$	Same as 12

36	$G^\pm(tg^\pm t)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	Same as 22
37	$G^\pm(tg^\pm t)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	Same as 25
38	$G^\pm(tg^\pm t)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	Same as 26
39	$G^\pm(tg^\pm t)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	Same as 27
40	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	
41	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	
42	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	
43	$G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
44	$G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
45	$G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
46	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	Same as 4
47	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	Same as 8
48	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	Same as 11
49	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	Same as 13
50	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	Same as 14
51	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	Same as 23
52	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	Same as 26
53	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	Same as 28
54	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	Same as 29
55	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	
56	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	
57	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	
58	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
59	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
60	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
61	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	Same as 5
62	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	Same as 9
63	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	Same as 12
64	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	Same as 14
65	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	Same as 15
66	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	Same as 24
67	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	Same as 27
68	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	Same as 29
69	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	Same as 30
70	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	Same as 41
71	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	Same as 44
72	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	Same as 45
73	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	Same as 59
74	$G^\pm(g^\mp tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	Same as 60
75	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	

Table S3. Further reduction in the total conformations of $G^\pm(xyz)G^\pm(xyz)G^\pm(xyz)$ and $T(xyz)G^\pm(xyz)G^\pm(xyz)$ clusters of TsBP after elimination of a bunch of conformers due to steric hindrance during optimization.

S. No.	Structure	Remarks
$G^\pm(xyz)G^\pm(xyz)G^\pm(xyz)$ cluster		
1	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)$	
2	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tt)$	
3	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)G^\pm(tg^\pm t)$	
4	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)G^\pm(tg^\pm g^\pm)$	
5	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)$	
6	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tt)G^\pm(g^\pm tt)$	
7	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tt)G^\pm(tg^\pm t)$	
8	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)$	
9	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tt)G^\pm(g^\pm tg^\pm)$	
10	$G^\pm(g^\pm tg^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	optimized to $G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tt)G^\pm(tg^\pm t)$ (Conf. 7)
11	$G^\pm(g^\pm tg^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	optimized to $G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)$ (Conf. 8)
12	$G^\pm(g^\pm tg^\pm)G^\pm(tg^\pm t)G^\pm(g^\pm tg^\pm)$	optimized to $G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tt)G^\pm(g^\pm tg^\pm)$ (Conf. 9)
13	$G^\pm(g^\pm tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
14	$G^\pm(g^\pm tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\pm tg^\pm)$	optimized to $G^\pm(g^\pm tg^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$ (Conf. 13)
15	$G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)$	
16	$G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(g^\pm tt)$	
17	$G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(tg^\pm t)$	
18	$G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)$	
19	$G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(g^\pm tg^\pm)$	optimized to $G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(tg^\pm t)$ (Conf. 17)
20	$G^\pm(g^\pm tt)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	optimized to $G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(tg^\pm t)$ (Conf. 17)
21	$G^\pm(g^\pm tt)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	optimized to $G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)$ (Conf. 18)
22	$G^\pm(g^\pm tt)G^\pm(tg^\pm t)G^\pm(g^\pm tg^\pm)$	optimized to $G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)$ (Conf. 18)
23	$G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
24	$G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)G^\pm(g^\pm tg^\pm)$	
25	$G^\pm(g^\pm tt)G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)$	
26	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	optimized to $G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(tg^\pm t)$ (Conf. 17)
27	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	optimized to $G^\pm(g^\pm tt)G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)$ (Conf. 18)
28	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(g^\pm tg^\pm)$	
29	$G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	optimized to $G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$ (Conf. 23)
30	$G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)G^\pm(g^\pm tg^\pm)$	optimized to $G^\pm(g^\pm tt)G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)$ (Conf. 25)
31	$G^\pm(tg^\pm t)G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)$	optimized to $G^\pm(g^\pm tt)G^\pm(g^\pm tg^\pm)G^\pm(g^\pm tg^\pm)$ (Conf. 25)
32	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	optimized to $G^\pm(tg^\pm g^\pm)G^\pm(g^\pm tt)G^\pm(g^\pm tt)$ (Conf. 18)
33	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	optimized to $G^\pm(tg^\pm g^\pm)G^\pm(g^\pm tt)G^\pm(tg^\pm g^\pm)$ (Conf. 23)
34	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm t)G^\pm(g^\pm tg^\pm)$	optimized to $G^\pm(tg^\pm g^\pm)G^\pm(g^\pm tt)G^\pm(g^\pm tg^\pm)$ (Conf. 25)

35	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
36	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
37	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
38	$G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	optimized to $G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$ (Conf. 35)
T(xyz)G$^\pm$(xyz)G$^\pm$(xyz)cluster		
1	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	
2	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	
3	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	optimized to $T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$ (Conf. 2)
4	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	optimized to $T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$ (Conf. 5)
5	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	
6	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	
7	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	
8	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	optimized to $T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$ (Conf. 9)
9	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	
10	$T(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	optimized to $T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$ (Conf. 7)
11	$T(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	optimized to $T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$ (Conf. 9)
12	$T(g^\mp tg^\mp)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	optimized to $T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$ (Conf. 9)
13	$T(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	optimized to $T(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$ (Conf. 15)
14	$T(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
15	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
16	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	
17	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	
18	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	
19	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	optimized to $T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$ (Conf. 20)
20	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	
21	$T(g^\mp tt)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	
22	$T(g^\mp tt)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	
23	$T(g^\mp tt)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	
24	$T(g^\mp tt)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	
25	$T(g^\mp tt)G^\pm(tg^\pm t)G^\pm(tg^\pm t)$	optimized to $T(g^\mp tt)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$ (Conf. 22)
26	$T(g^\mp tt)G^\pm(tg^\pm t)G^\pm(tg^\pm g^\pm)$	optimized to $T(g^\mp tt)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$ (Conf. 23)
27	$T(g^\mp tt)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	
28	$T(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	
29	$T(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	
30	$T(g^\mp tt)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	
31	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	
32	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	
33	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	
34	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	
35	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	

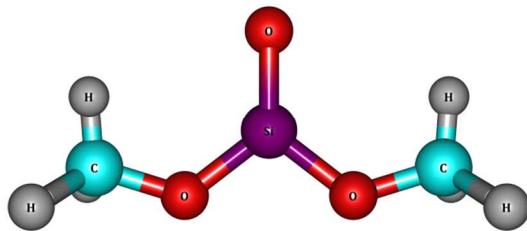
36	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tt)$	
37	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}t)$	
38	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})$	
39	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})$	
40	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)G^{\pm}(tg^{\pm}t)$	optimized to $T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}t)$ (Conf. 37)
41	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)G^{\pm}(tg^{\pm}g^{\pm})$	optimized to $T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})$ (Conf. 39)
42	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)G^{\pm}(g^{\mp}tg^{\pm})$	
43	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(tg^{\pm}g^{\pm})$	optimized to $T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}g^{\pm})$ (Conf.44)
44	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(g^{\mp}tg^{\pm})$	
45	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\pm})$	

Table S4. The population of TsBP calculated using relative free energy at 298 K using B3LYP/6-311++G(d,p) basis set.

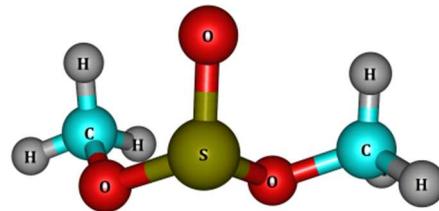
S. No.	Structure	Free energy (Hartrees)	Relative free energy (kcal/mol)	Population at 298 K ^a
$G^\pm(xyz)G^\pm(xyz)G^\pm(xyz)$ cluster				
1	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	-1115.827535	0	17.1
2	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	-1115.827340	0.12	13.9
3	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)$	-1115.827224	0.19	12.3
4	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	-1115.826987	0.34	9.6
5	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	-1115.826824	0.45	8.1
6	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	-1115.826748	0.49	7.4
7	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	-1115.824119	2.14	0.5
8	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	-1115.825569	1.23	2.1
9	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	-1115.824805	1.71	1.0
10	$G^\pm(g^\mp tt)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	-1115.824392	1.97	0.6
11	$G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	-1115.822965	2.87	0.1
12	$G^\pm(g^\mp tt)G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)$	-1115.822718	3.02	0.1
13	$G^\pm(tg^\pm t)G^\pm(tg^\pm t)G^\pm(g^\mp tg^\pm)$	-1115.825869	1.04	2.9
14	$G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	-1115.826677	0.53	6.9
15	$G^\pm(g^\mp tt)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	-1115.823451	2.56	0.2
16	$G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	-1115.824194	2.10	0.5
17	$G+(g^\mp tt)G+(tg^\pm g^\pm)G+(tg^\pm g^\pm)$	-1115.824138	2.13	0.5
18	$G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)G^\pm(g^\mp tg^\pm)$	-1115.826662	0.55	6.8
19	$G^\pm(g^\mp tt)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	-1115.823394	2.60	0.2
20	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)$	-1115.823263	2.68	0.2
21	$G^\pm(tg^\pm g^\pm)G^\pm(tg^\pm g^\pm)G^\pm(g^\mp tg^\pm)$	-1115.818634	5.58	0.0
$T(xyz)G^\pm(xyz)G^\pm(xyz)$ cluster				
22	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	-1115.821757	3.62	0.1
23	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	-1115.823720	2.39	0.9
24	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	-1115.822548	3.12	0.3
25	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	-1115.822721	3.02	0.3
26	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	-1115.822130	3.39	0.2
27	$T(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	-1115.822464	3.18	0.2
28	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tt)$	-1115.820070	4.68	0.0
29	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\mp)$	-1115.820845	4.20	0.0
30	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(tg^\pm t)$	-1115.822670	3.05	0.3
31	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	-1115.823751	2.37	0.9
32	$T(g^\mp tt)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	-1115.823284	2.67	0.6
33	$T(g^\mp tt)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	-1115.822489	3.17	0.2
34	$T(g^\mp tt)G^\pm(g^\mp tt)G^\pm(tg^\pm t)$	-1115.823540	2.51	0.7
35	$T(g^\mp tg^\mp)G^\pm(g^\mp tt)G^\pm(g^\mp tg^\pm)$	-1115.823360	2.62	0.6
36	$T(g^\mp tg^\pm)G^\pm(g^\mp tg^\mp)G^\pm(g^\mp tg^\pm)$	-1115.821617	3.71	0.1
37	$T(g^\mp tg^\pm)G^\pm(g^\mp tt)G^\pm(g^\mp tt)$	-1115.823059	2.81	0.4

38	$T(g^{\mp}tg^{\mp})G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}t)$	-1115.823058	2.81	0.4
39	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})$	-1115.822068	3.43	0.2
40	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}t)G^{\pm}(g^{\mp}tg^{\pm})$	-1115.820829	4.21	0.0
41	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}t)$	-1115.821382	3.86	0.1
42	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\mp})G^{\pm}(tg^{\pm}g^{\pm})$	-1115.822241	3.32	0.2
43	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})$	-1115.823022	2.83	0.4
44	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})$	-1115.822979	2.86	0.4
45	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}t)G^{\pm}(g^{\mp}tg^{\pm})$	-1115.822096	3.41	0.2
46	$T(g^{\mp}tg^{\mp})G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\pm})$	-1115.821896	3.54	0.1
47	$T(g^{\mp}tt)G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\pm})$	-1115.822887	2.92	0.4
48	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})$	-1115.822330	3.26	0.2
49	$T(g^{\mp}tg^{\mp})G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(g^{\mp}tg^{\pm})$	-1115.821713	3.65	0.1
50	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(g^{\mp}tg^{\pm})$	-1115.820719	4.28	0.0
51	$T(g^{\mp}tt)G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(tg^{\pm}g^{\pm})$	-1115.820726	4.27	0.0
52	$T(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\pm})G^{\pm}(g^{\mp}tg^{\pm})$	-1115.818401	5.73	0.0
53	$T(g^{\mp}tg^{\pm})G^{\pm}(tg^{\pm}g^{\pm})G^{\pm}(tg^{\pm}g^{\pm})$	-1115.819684	4.93	0.0

^apopulation was calculated using Maxwell-Boltzmann equation based on the relative free energy with respect to the ground state structure



Dimethoxy silanone



Dimethyl sulphite

Figure S1. The structures of dimethyl silanone and dimethyl sulphite optimized at B3LYP level of theory using 6-311++G(d,p) basis set.

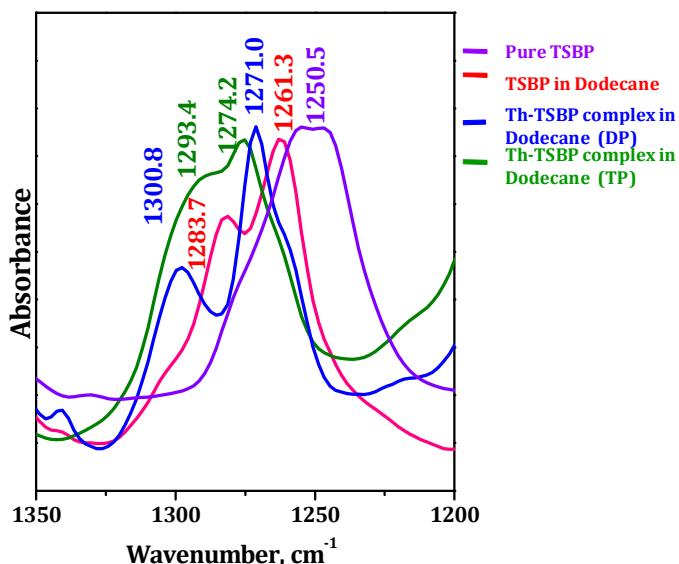


Figure S2. The infrared spectra of $\text{Th}(\text{NO}_3)_4\text{-TsBP}$ complex in dodecane.

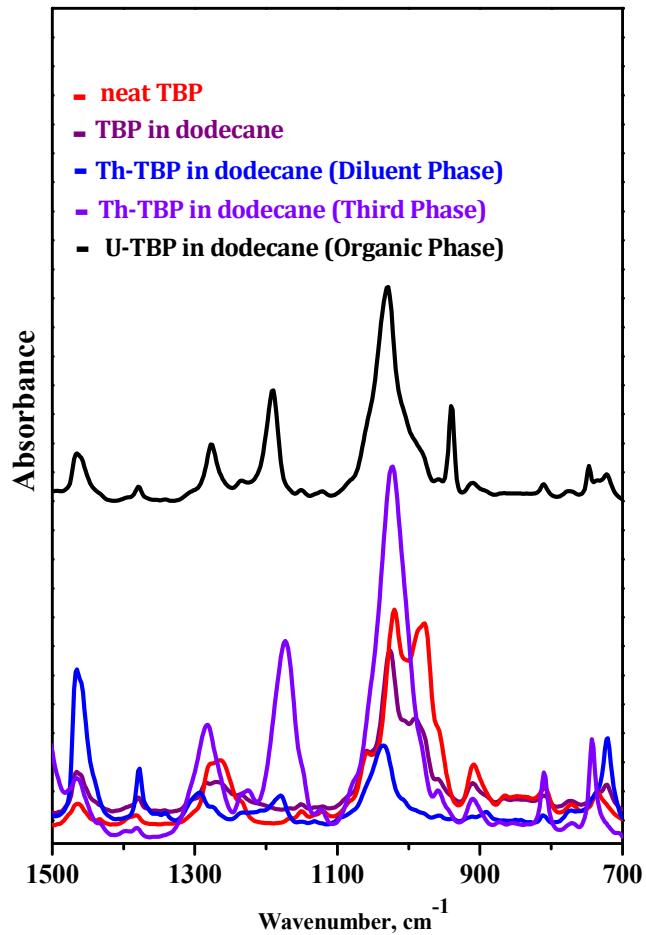


Figure S3. The infrared spectra of Th and U-TBP system in dodecane.