Synthesis of Methyl(*p*-tolyl)(η^1-alkynyl)palladium(IV) Species Pd(OTf)Me(*p*-Tol)(C≡CR)(L_2) (OTf = Triflate; L_2 = Bidentate Ligand; R =Bu^t, $SiMe_3$), and Computational Studies of Selectivity in Reductive Elimination from the '$Pd^{IV}C_{sp3}C_{sp2}C_{sp}$' Kernel in the Complex with L_2 = 1,2-bis(dimethylphosphino)ethane and R = $SiMe_3$

Manab Sharma, Alireza Ariafard, Allan J. Canty, Brian F. Yates*, Michael G. Gardiner and Roderick C. Jones*

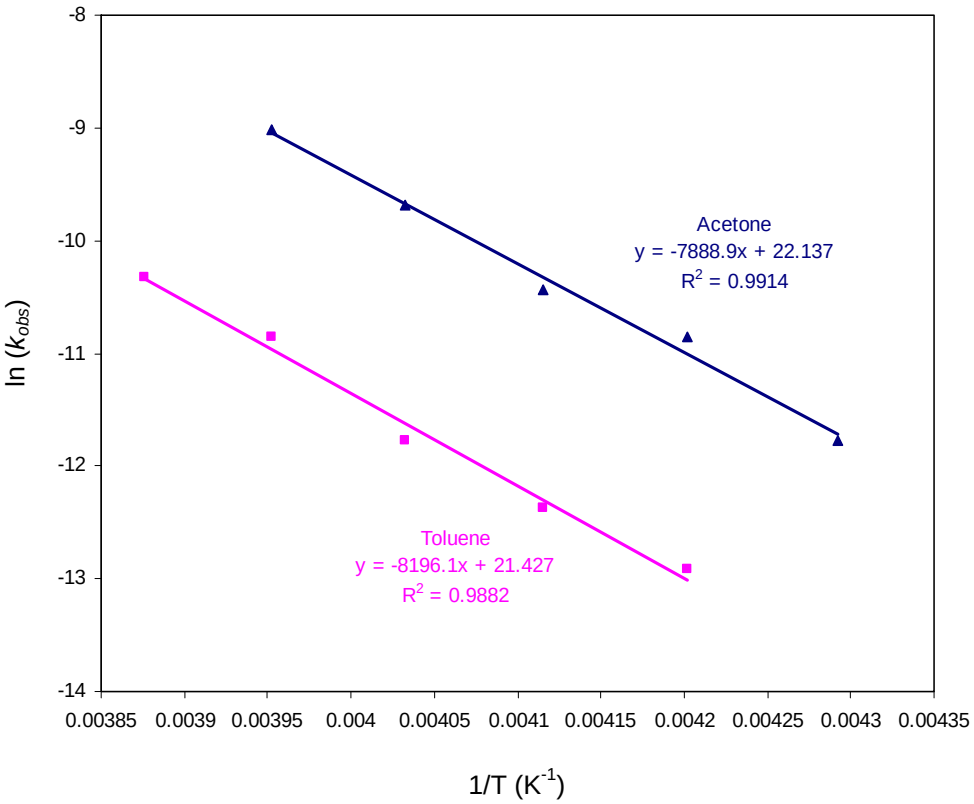


Fig. S1. Arrhenius plot of decomposition study of the three isomer of **4** in acetone (▲), and in toluene (■)

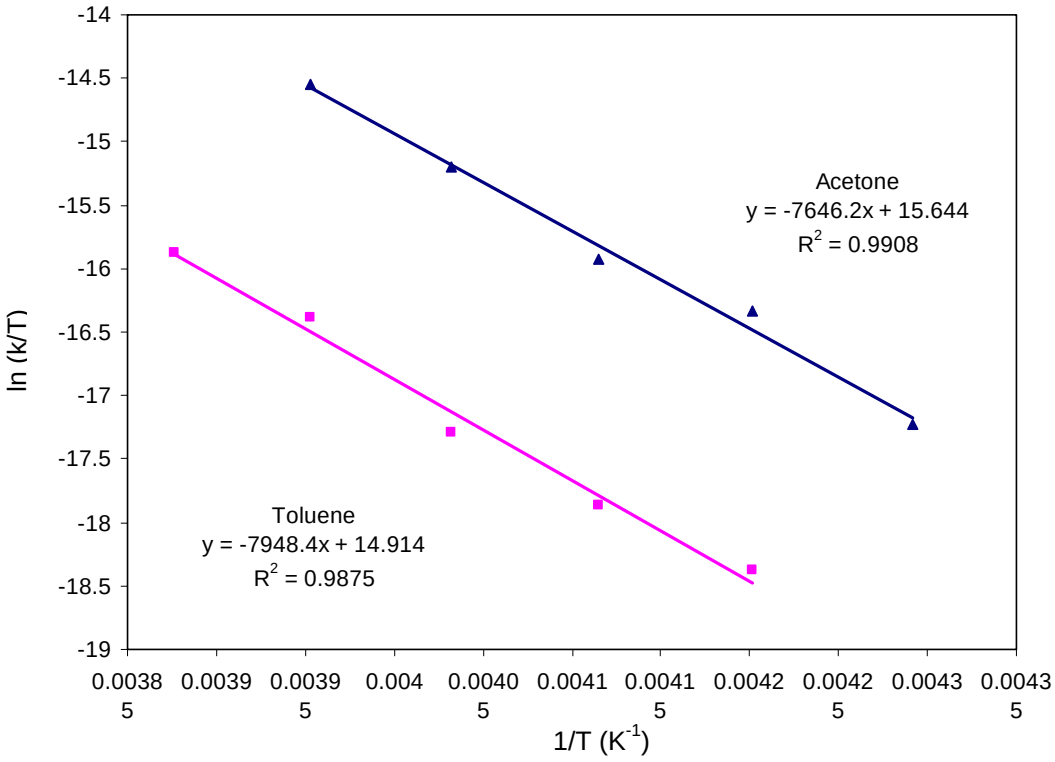


Fig. S2. Eyring plot of decomposition study of the three isomer of **4** in acetone (▲), and in toluene (■).

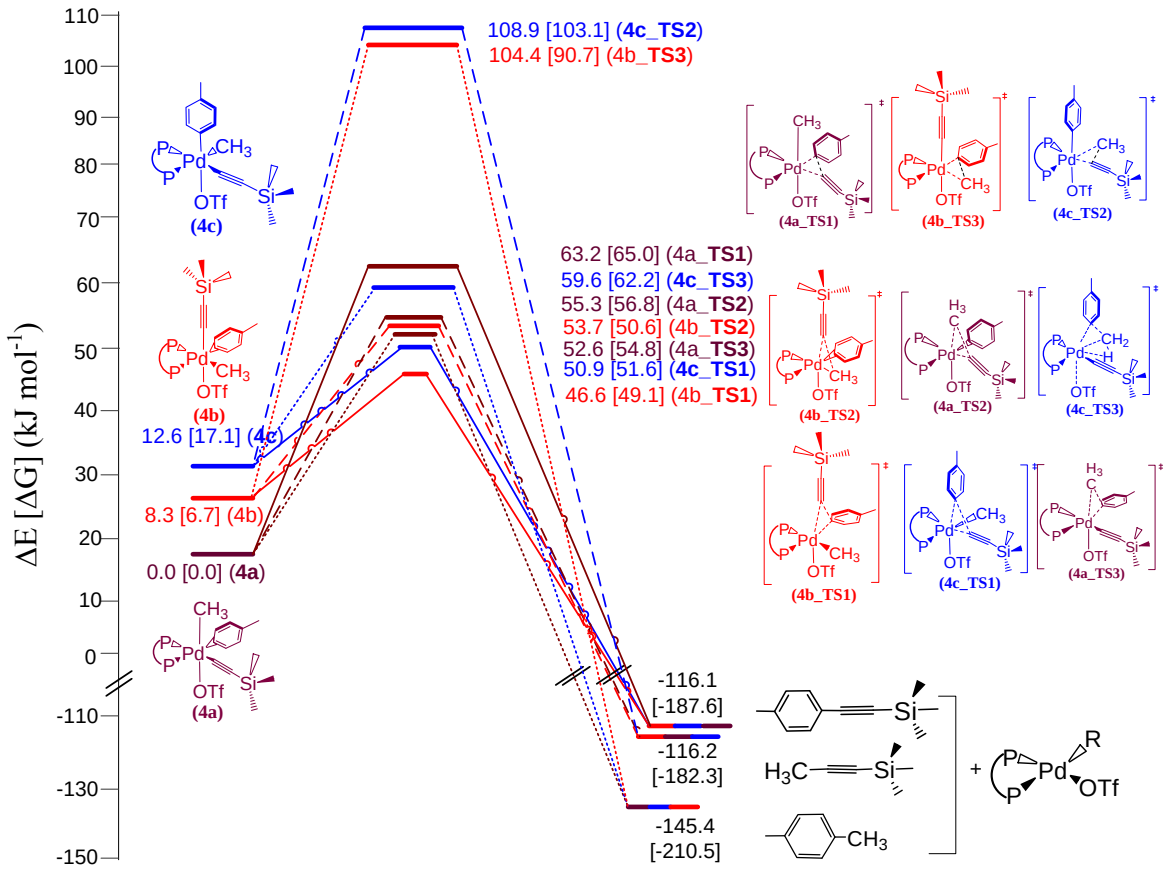


Fig S3: The complete energy profile diagram for non-dissociative pathways along with ΔG in parenthesis with all possible transition states.

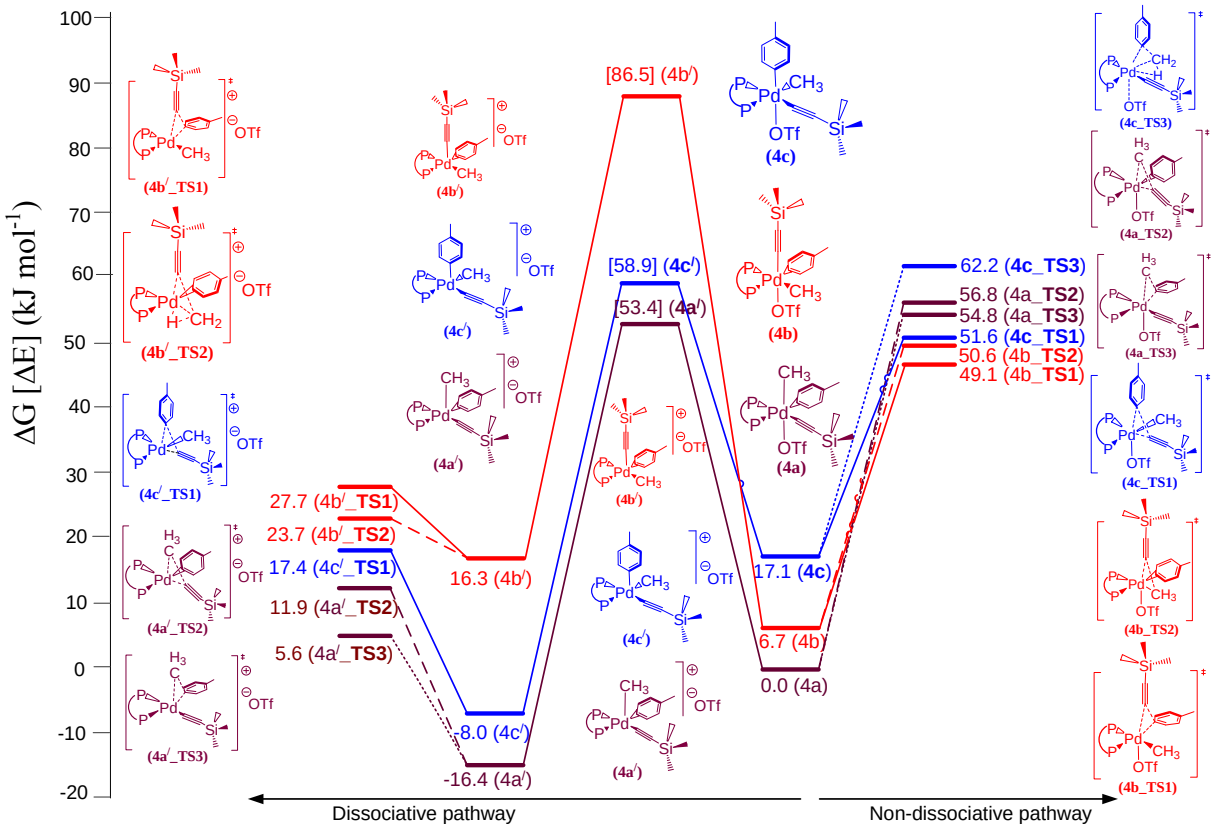
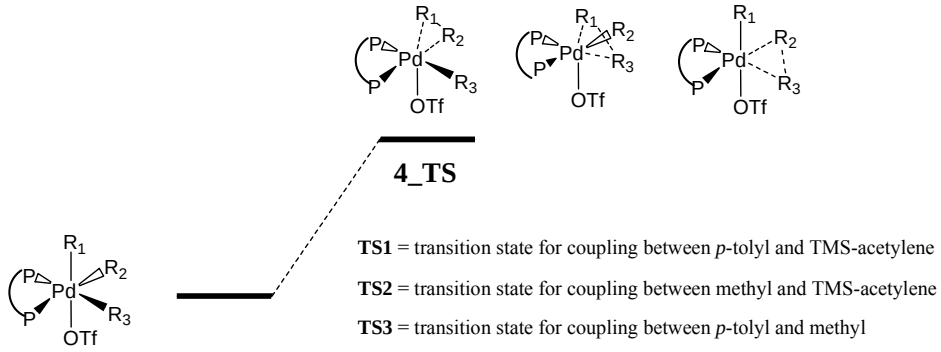


Fig S4: Free energy profile diagram for dissociative and non-dissociative pathways along with ΔE for triflate dissociation

Table S1: The calculated relative energies, ΔE (ΔG) (in kJ mol^{-1}), obtained from various level of DFT methods in acetone for different isomers and transition states (Scheme S1) w. r. t. the most stable isomer 4a



Scheme S1: Possible different hexacoordinated Pd(IV) isomers and the possible transition states

Methods / Complex	B3LYP/BS2 // B3LYP/BS1	M06/BS2 // B3LYP/BS1	B97D/BS2 // B3LYP/BS1	BP86/BS2 // B3LYP/BS1	TPSS/BS2 // B3LYP/BS1	WB97XD/BS2 // B3LYP/BS1	B3LYP-D/BS2 // B3LYP/BS1
4a	0 (0)	0 (0)	0	0 (0)	0	0 (0)	0 (0)
4b	14.0 (14.6)	4.5 (5.1)	12.7 (10.2)	12.7 (13.3)	10.6 (11.2)	10.6 (11.3)	10.0 (7.2)
4c	19.4 (19.7)	11.5 (11.7)	16.1 (9.1)	16.1 (16.4)	14.9 (15.1)	14.0 (14.3)	9.4 (5.1)
4a_TS1	66.4 (62.8)	54.3 (50.7)	60.1 (61.1)	60.1 (56.5)	61.5 (57.8)	70.4 (66.8)	69.3 (65.6)
4a_TS2	65.7(56.5)	34.8 (34.6)	56.0 (52.6)	56.0 (55.7)	56.1 (55.8)	49.0 (48.7)	60.5 (60.2)
4a_TS3	43.5 (39.0)	22.5 (18.0)	40.7 (39.4)	40.7 (36.2)	43.3 (38.8)	35.7 (31.2)	48.2 (43.8)

4b_TS1	57.8 (51.9)	36.1 (30.2)	48.6 (41.9)	48.6 (42.6)	49.8 (43.9)	55.0 (49.1)	55.4 (49.5)
4b_TS2	54.7 (53.6)	25.8 (24.7)	46.6 (45.8)	46.6 (45.5)	51.3 (50.2)	43.2 (42.1)	54.1 (53.1)
4b_TS3	101.2 (98.9)	77.2 (74.9)	101.8 (101.0)	101.8 (99.4)	101.1 (98.8)	97.9 (95.6)	104.9 (102.6)
4b_TS1	56.1 (54.4)	41.0 (39.2)	49.7 (48.0)	50.3 (48.6)	48.4 (46.7)	58.3 (56.6)	58.0 (56.3)
4b_TS2	106.6 (100.8)	86.3 (80.5)	108.8 (103.0)	105.1 (99.3)	105.6 (99.8)	107.8 (102.0)	115.8 (110.0)
4b_TS3	58.6 (59.0)	33.5 (33.9)	55.4 (55.8)	55.9 (56.3)	58.6 (59.0)	48.4 (48.8)	57.5 (57.9)

Transition states that lead to the reductive elimination of experimentally observed major product

Theoretically predicted lowest energy transition states

BS1 : LanL2DZ:6-31G(d)

BS2 : LANL2augmented:6-311+G(2d,p)

Table S2: The calculated relative energies, ΔE (ΔG) (in kJ mol^{-1}), obtained from various level of DFT methods in acetone for different isomers and transition states (Scheme S1) w. r. t. the most stable isomer 4a

Methods / Complex	M06/BS2 // M06/BS1	B3LYP/BS2 // M06/BS1	B97D/BS2 // M06/BS1
4a	0 (0)	0 (0)	0 (0)
4b	1.6 (9.9)	11.9 (20.1)	7.5 (15.8)
4c	14.3 (18.2)	26.4 (30.4)	14.0 (17.9)
4a_TS1	NC	NC	NC
4a_TS2	32.3 (46.6)	53.5 (67.7)	51.6 (65.8)
4a_TS3	25.3 (32.9)	52.4 (60.0)	47.8 (55.5)
4b_TS1	36.4 (44.1)	58.5 (66.2)	50.5 (58.1)
4b_TS2	27.0 (29.9)	53.6 (56.6)	44.1 (47.0)
4b_TS3	NC	NC	NC
4b_TS1	40.2 (50.8)	56.9 (67.5)	50.0 (60.6)
4b_TS2	NC	NC	NC
4b_TS3	39.3 (52.4)	67.0 (80.1)	59.2 (72.3)

Transition states that lead to the reductive elimination of experimentally observed major product

Theoretically predicted lowest energy transition states

BS1 : LanL2DZ:6-31G(d)

BS2 : LANL2augmented:6-311+G(2d,p)

Table S3: Calculated [DFT (B97D/BS2//B97D/BS1)] homolytic C-C bond dissociation energy (kJ mol^{-1}) according to the equation 1 of the various organic products formed during the reductive elimination

$R\text{-}R^{/} \rightarrow R\bullet + \bullet R^{/}$ Eq.1

R	$R^{/}$	
	Tolyl	CH_3
TMS-C≡C	569.2	518.1
CH_3	425.3	

Table S4: Optimized bond lengths around the metal center for six coordinates Pd(IV) intermediates and the transition states

Description	Bond length (Å) of complexes								
	4a	4a_TS2	4a_TS3	4b	4b_TS1	4b_TS2	4c	4c_TS1	4c_TS3
Pd-Me	2.11	2.27	2.27	2.14	2.13	2.25	2.14	2.12	2.24
Pd-tol	2.10	2.09	2.15	2.10	2.17	2.10	2.07	2.13	2.15
Pd-Alkyn	2.00	1.99	2.00	1.94	1.97	1.95	1.99	1.99	1.99
Pd-P(trans-Me)	NA	NA	NA	2.49	2.49	2.37	2.47	2.49	2.36
Pd-P (trans-Tol)	2.40	2.37	2.37	2.46	2.42	2.45	NA	NA	NA
Pd-P (trans-alkyn)	2.44	2.42	2.36	NA	NA	NA	2.40	2.38	2.42
C-C (akyn-tolyl)	2.72	2.04	NA	2.88	2.09	NA	2.83	3.01	2.16
C-C (alkyn-Me)	2.92	2.98	2.15	2.75	NA	2.08	2.86	2.11	3.03
Pd-H (agostic)	NA	2.41	2.43	NA	NA	2.37	NA	NA	2.35
Pd-O	2.30	2.61	2.54	2.21	2.28	2.40	2.30	2.39	2.58

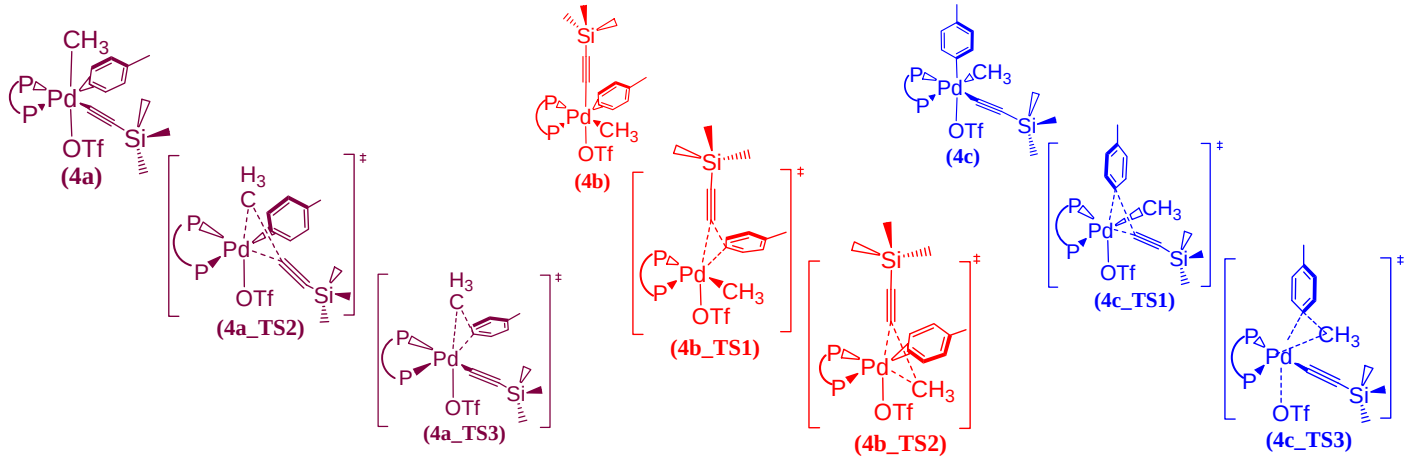
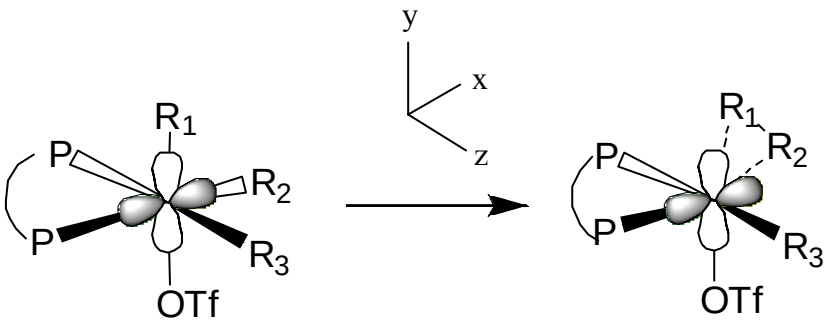
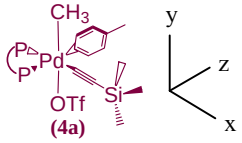
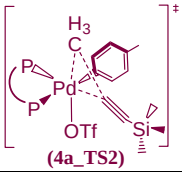
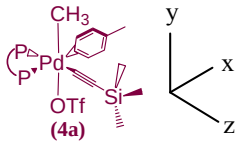
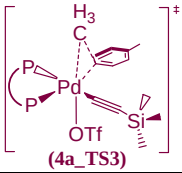
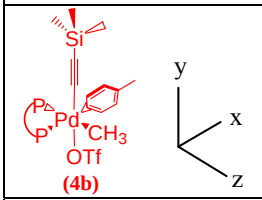
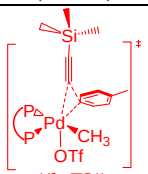
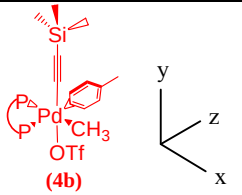
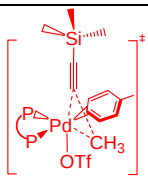
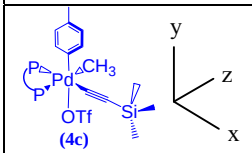
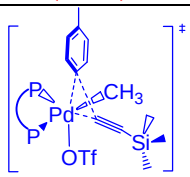
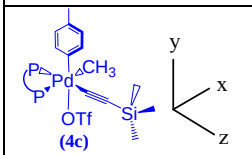
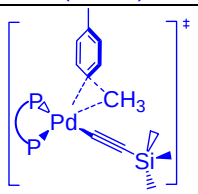


Table S5: NBO population analysis along the $\mathbf{d_{x^2-y^2}}$ orbital



Parent complexes (**4**) Transition states

Complex	Electron density along $d_{x^2-y^2}$	Transition state	Electron density along $d_{x^2-y^2}$
 **(4a)**	1.53	 **(4a_TS2)**	1.74
 **(4a)**	1.55	 **(4a_TS3)**	1.83
 **(4b)**	1.52	 **(4b_TS1)**	1.64
 **(4b)**	1.49	 **(4b_TS2)**	1.71
 **(4c)**	1.50	 **(4c_TS1)**	1.64
 **(4c)**	1.57	 **(4c_TS3)**	1.80

Optimized coordinates of various molecules from different level of theory:

Complex : **1** (optimized by B97D/BS1)
E (BS1) = -1358.4519966 au
Δ H (BS1) = 0.380766 au
Δ G(BS1) = 0.298692 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.330572	2.226204	-0.071492
2	6	0	-3.242908	1.149823	0.564161
3	15	0	-2.756721	-0.576670	-0.026909
4	6	0	-3.801443	-1.688422	1.031939
5	6	0	-3.592595	-0.686869	-1.684862
6	15	0	-0.524575	1.708002	0.074948
7	6	0	-0.004957	2.346974	1.737040
8	6	0	0.382777	2.813302	-1.104723
9	1	0	-2.512606	3.214312	0.384520
10	1	0	-2.549091	2.314026	-1.149306
11	1	0	-4.305857	1.360019	0.353360
12	1	0	-3.114099	1.150107	1.659906
13	1	0	-3.629170	-2.731827	0.727001
14	1	0	-4.875834	-1.455667	0.944772
15	1	0	-3.486462	-1.583527	2.081333
16	1	0	-3.141229	0.054488	-2.361501
17	1	0	-4.679000	-0.508702	-1.615221
18	1	0	-3.411857	-1.686267	-2.108933
19	1	0	1.037588	2.036902	1.905027
20	1	0	-0.087880	3.444343	1.811027
21	1	0	-0.628849	1.876805	2.512651
22	1	0	-0.004153	2.650155	-2.122575
23	1	0	0.287667	3.879653	-0.841361
24	1	0	1.442829	2.516390	-1.090599
25	46	0	-0.415878	-0.631121	-0.058801
26	6	0	-0.187971	-2.738981	-0.045356
27	1	0	-1.150635	-3.263798	0.074064
28	1	0	0.282227	-3.037512	-0.996437
29	1	0	0.486439	-3.004721	0.783841
30	6	0	1.659748	-0.543183	-0.064361
31	6	0	2.380593	-0.162541	-1.219293
32	6	0	2.406558	-0.755709	1.115623
33	6	0	3.777772	-0.004041	-1.195902
34	1	0	1.845713	0.019791	-2.156392
35	6	0	3.802976	-0.589280	1.142276
36	1	0	1.892434	-1.058538	2.032461
37	6	0	4.513036	-0.214201	-0.013718
38	1	0	4.307422	0.288172	-2.109134
39	1	0	4.352607	-0.756833	2.074799
40	6	0	6.023440	-0.074582	0.003739
41	1	0	6.387659	0.219200	1.002018
42	1	0	6.520154	-1.026936	-0.257958
43	1	0	6.365093	0.680565	-0.723538

Complex : **4a** (optimized by B97D/BS1)

E (BS1) = -2804.8386756 au
Δ H (BS1) = 0.548523 au
Δ G(BS1) = 0.430022 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.266092	-2.181177	-2.111721
2	6	0	0.960982	-2.459728	-2.895865
3	15	0	-0.528100	-1.798205	-1.965198
4	6	0	-1.903202	-1.724037	-3.196042
5	6	0	-1.013615	-3.114102	-0.773445
6	15	0	2.388543	-0.376529	-1.635850
7	6	0	3.012173	0.422790	-3.186131
8	6	0	3.801502	-0.192888	-0.471041
9	1	0	3.146720	-2.471656	-2.709304
10	1	0	2.277915	-2.744134	-1.168120
11	1	0	0.855175	-3.540202	-3.089216
12	1	0	0.979321	-1.947980	-3.873788
13	1	0	-2.770209	-1.268739	-2.693213
14	1	0	-2.171504	-2.723506	-3.573715
15	1	0	-1.612284	-1.081159	-4.040347
16	1	0	-0.143606	-3.366597	-0.153360
17	1	0	-1.386758	-4.006497	-1.302484
18	1	0	-1.792180	-2.705808	-0.114423
19	1	0	3.082589	1.510543	-3.042689
20	1	0	4.010390	0.027830	-3.432716
21	1	0	2.327271	0.216652	-4.021520
22	1	0	3.619499	-0.777726	0.438238
23	1	0	4.737459	-0.518043	-0.953760
24	1	0	3.868708	0.869738	-0.194363
25	46	0	0.187161	0.306902	-0.955203
26	6	0	-0.214980	1.478143	-2.660326
27	1	0	0.709438	1.525747	-3.243870
28	1	0	-1.027277	0.983708	-3.202536
29	1	0	-0.519321	2.463870	-2.300087
30	6	0	0.943101	2.033912	-0.037557
31	6	0	0.732552	2.154612	1.345287
32	6	0	1.700043	2.999788	-0.713853
33	6	0	1.304807	3.230359	2.041011
34	1	0	0.145784	1.408193	1.875864
35	6	0	2.272251	4.072756	-0.002761
36	1	0	1.850354	2.941837	-1.793994
37	6	0	2.084616	4.203202	1.383401
38	1	0	1.144076	3.309779	3.119916
39	1	0	2.869027	4.817347	-0.538171
40	6	0	2.689036	5.360050	2.155036
41	1	0	3.342580	5.970946	1.512583
42	1	0	1.904537	6.020381	2.564032
43	1	0	3.286848	5.000605	3.009597
44	6	0	-1.710398	0.751374	-0.508481
45	6	0	-2.915253	0.908129	-0.273582
46	14	0	-4.675791	1.075298	0.211896
47	6	0	-5.322903	2.804678	-0.260221
48	1	0	-4.754110	3.594194	0.258588
49	1	0	-5.230685	2.982911	-1.344884
50	1	0	-6.387023	2.917370	0.012278
51	6	0	-5.700246	-0.249093	-0.708409

52	1	0	-5.620499	-0.126924	-1.802384
53	1	0	-5.354250	-1.265855	-0.455480
54	1	0	-6.769222	-0.181167	-0.440457
55	6	0	-4.837541	0.811810	2.090869
56	1	0	-5.891323	0.872892	2.414852
57	1	0	-4.445606	-0.175989	2.385336
58	1	0	-4.265249	1.574581	2.644467
59	8	0	2.226957	-0.682458	2.479942
60	16	0	1.284889	-1.583866	1.781385
61	8	0	1.889514	-2.723197	1.027474
62	8	0	0.167686	-0.885598	1.014234
63	6	0	0.245135	-2.403335	3.132694
64	9	0	1.040154	-3.117123	3.953396
65	9	0	-0.405180	-1.470512	3.854078
66	9	0	-0.664752	-3.237850	2.577980

Complex : **4b** (optimized by B97D/BS1)
E (BS1) = -2804.8454315 au
Δ H (BS1) = 0.550117 au
Δ G(BS1) = 0.426057 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.084233	-2.018770	2.487808
2	6	0	0.638787	-2.913151	1.453418
3	15	0	0.082046	-2.555732	-0.297966
4	6	0	1.324261	-3.440755	-1.340763
5	6	0	-1.497230	-3.481489	-0.532973
6	15	0	0.121819	-0.210381	2.052510
7	6	0	1.787131	0.215390	2.736350
8	6	0	-1.032558	0.743057	3.133321
9	1	0	0.308908	-2.215538	3.499754
10	1	0	-1.164664	-2.218525	2.487261
11	1	0	0.491341	-3.980077	1.692613
12	1	0	1.722722	-2.709916	1.460705
13	1	0	1.006857	-3.397725	-2.393741
14	1	0	1.431286	-4.495532	-1.039710
15	1	0	2.284006	-2.914019	-1.239790
16	1	0	-2.244595	-3.092395	0.170201
17	1	0	-1.343977	-4.562422	-0.379190
18	1	0	-1.866517	-3.300830	-1.553035
19	1	0	1.941993	1.299466	2.636133
20	1	0	1.852997	-0.065963	3.799890
21	1	0	2.563204	-0.294019	2.150081
22	1	0	-2.056428	0.378009	2.991105
23	1	0	-0.735529	0.654424	4.191109
24	1	0	-0.991629	1.797654	2.822548
25	46	0	0.096454	-0.094698	-0.436268
26	6	0	0.213386	-0.026013	-2.570369
27	1	0	0.886953	-0.815108	-2.922832
28	1	0	-0.833212	-0.193022	-2.856926
29	1	0	0.576644	0.969364	-2.843508
30	6	0	0.168391	2.004121	-0.375227
31	6	0	-0.938759	2.694336	-0.891504
32	6	0	1.230936	2.714619	0.202194

33	6	0	-0.985637	4.095473	-0.799432
34	1	0	-1.770323	2.152837	-1.337576
35	6	0	1.167288	4.117704	0.288225
36	1	0	2.109893	2.187224	0.570460
37	6	0	0.061526	4.829348	-0.209888
38	1	0	-1.861095	4.623458	-1.188549
39	1	0	1.997178	4.665124	0.745471
40	6	0	0.005234	6.343129	-0.142818
41	1	0	0.725538	6.737885	0.591068
42	1	0	0.245592	6.795331	-1.121666
43	1	0	-1.001491	6.693525	0.138159
44	6	0	2.034351	-0.185606	-0.514377
45	6	0	3.262003	-0.336384	-0.509769
46	14	0	5.088528	-0.493310	-0.443521
47	6	0	5.759576	0.671675	0.908306
48	1	0	5.495147	1.720198	0.691533
49	1	0	5.343071	0.418616	1.898105
50	1	0	6.859314	0.607089	0.978791
51	6	0	5.537538	-2.296132	-0.006675
52	1	0	5.117584	-2.586171	0.971794
53	1	0	5.149114	-3.000528	-0.761780
54	1	0	6.632008	-2.429621	0.045237
55	6	0	5.836791	-0.031478	-2.131665
56	1	0	6.937458	-0.115501	-2.115466
57	1	0	5.457537	-0.692196	-2.929065
58	1	0	5.578526	1.004878	-2.405449
59	8	0	-3.508191	1.216121	0.845767
60	16	0	-3.175023	-0.126017	0.329789
61	8	0	-3.015561	-1.215970	1.335280
62	8	0	-2.092355	-0.144457	-0.759939
63	6	0	-4.639864	-0.671669	-0.735628
64	9	0	-5.747120	-0.752163	0.025599
65	9	0	-4.851806	0.210790	-1.729910
66	9	0	-4.394849	-1.888132	-1.275793

Complex : **4c** (optimized by B97D/BS1)
E (BS1) = -2804.8386328 au
Δ H (BS1) = 0.550433 au
Δ G(BS1) = 0.426664 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.262115	-2.163587	-2.133138
2	6	0	0.952668	-2.446583	-2.908272
3	15	0	-0.532498	-1.796028	-1.963919
4	6	0	-1.917168	-1.725305	-3.184367
5	6	0	-1.001252	-3.118705	-0.772830
6	15	0	2.378343	-0.359903	-1.651922
7	6	0	2.984785	0.447581	-3.204909
8	6	0	3.800213	-0.173064	-0.498378
9	1	0	3.139760	-2.447036	-2.738427
10	1	0	2.284062	-2.729676	-1.191642
11	1	0	0.850996	-3.526975	-3.104249
12	1	0	0.960912	-1.931623	-3.884585
13	1	0	-2.782032	-1.272540	-2.675584

14	1	0	-2.185060	-2.725398	-3.560714
15	1	0	-1.634381	-1.081230	-4.030514
16	1	0	-0.125202	-3.367473	-0.159758
17	1	0	-1.372319	-4.011861	-1.302050
18	1	0	-1.777581	-2.717795	-0.106693
19	1	0	3.052512	1.535103	-3.058344
20	1	0	3.982146	0.057096	-3.461765
21	1	0	2.292987	0.241762	-4.034648
22	1	0	3.631284	-0.767087	0.407479
23	1	0	4.734428	-0.486633	-0.992037
24	1	0	3.861198	0.887809	-0.213761
25	46	0	0.179023	0.309507	-0.952087
26	6	0	-0.242067	1.485094	-2.649547
27	1	0	0.679739	1.547790	-3.235814
28	1	0	-1.049896	0.983749	-3.192119
29	1	0	-0.557207	2.465095	-2.283050
30	6	0	0.932269	2.037753	-0.034507
31	6	0	0.729226	2.154107	1.349866
32	6	0	1.679015	3.009851	-0.713077
33	6	0	1.299303	3.231498	2.044696
34	1	0	0.148905	1.403685	1.881861
35	6	0	2.249277	4.084493	-0.002830
36	1	0	1.821668	2.956444	-1.794469
37	6	0	2.070278	4.209954	1.384863
38	1	0	1.143346	3.308189	3.124508
39	1	0	2.837272	4.834576	-0.540268
40	6	0	2.681221	5.362578	2.157516
41	1	0	3.246393	6.034574	1.492602
42	1	0	1.904191	5.960231	2.664362
43	1	0	3.369696	4.998486	2.939363
44	6	0	-1.718014	0.742169	-0.490754
45	6	0	-2.922237	0.892883	-0.248758
46	14	0	-4.683810	1.055497	0.234000
47	6	0	-5.206984	2.887055	0.198543
48	1	0	-4.596747	3.484544	0.896037
49	1	0	-5.082417	3.317907	-0.809069
50	1	0	-6.266161	3.001251	0.488869
51	6	0	-5.757987	0.069200	-1.000475
52	1	0	-5.641501	0.454028	-2.028047
53	1	0	-5.478962	-0.998509	-1.005529
54	1	0	-6.827950	0.134936	-0.736101
55	6	0	-4.923391	0.346476	1.986014
56	1	0	-5.977574	0.420034	2.306239
57	1	0	-4.627578	-0.715185	2.026466
58	1	0	-4.305159	0.891146	2.718712
59	8	0	2.245987	-0.672991	2.465455
60	16	0	1.306847	-1.579872	1.770166
61	8	0	1.916074	-2.710278	1.006477
62	8	0	0.177319	-0.888652	1.014498
63	6	0	0.285581	-2.415562	3.125629
64	9	0	1.093757	-3.127425	3.935148
65	9	0	-0.366021	-1.492410	3.858097
66	9	0	-0.622054	-3.254465	2.573930

Complex : **4a_TS1** (optimized by B97D/BS1)
E (BS1) = -2804.8204698 au
Δ H (BS1) = 0.548993 au
Δ G(BS1) = 0.427332 au

Imaginary frequency = -330.7i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.412974	0.663074	-1.942827
2	6	0	2.796562	-0.382467	-2.907705
3	15	0	1.382252	-1.322884	-2.107610
4	6	0	0.533351	-2.159879	-3.525189
5	6	0	2.172214	-2.700415	-1.167136
6	15	0	2.115885	1.803698	-1.219270
7	6	0	1.921867	3.112197	-2.523500
8	6	0	2.970768	2.715170	0.144310
9	1	0	4.189594	1.248860	-2.463220
10	1	0	3.871667	0.159207	-1.081260
11	1	0	3.576256	-1.079334	-3.258269
12	1	0	2.379325	0.117154	-3.799042
13	1	0	-0.283063	-2.776859	-3.119169
14	1	0	1.222111	-2.799373	-4.101006
15	1	0	0.091739	-1.404284	-4.191801
16	1	0	2.883348	-2.274137	-0.447829
17	1	0	2.682681	-3.400820	-1.848898
18	1	0	1.393617	-3.227805	-0.597960
19	1	0	1.167027	3.844964	-2.199212
20	1	0	2.877505	3.632441	-2.698097
21	1	0	1.580753	2.659735	-3.465024
22	1	0	3.311903	1.998985	0.901218
23	1	0	3.825564	3.289588	-0.249585
24	1	0	2.250006	3.401003	0.614504
25	46	0	0.121348	0.384869	-0.870120
26	6	0	-0.599196	1.098835	-2.704717
27	1	0	-0.691243	2.184477	-2.602383
28	1	0	0.115106	0.836211	-3.495785
29	1	0	-1.569399	0.615665	-2.862727
30	6	0	-1.385694	1.522228	0.210207
31	6	0	-1.121693	1.666826	1.587900
32	6	0	-2.276858	2.411707	-0.421122
33	6	0	-1.730247	2.706299	2.304437
34	1	0	-0.443646	0.985327	2.092097
35	6	0	-2.880966	3.440498	0.315007
36	1	0	-2.535170	2.286686	-1.471500
37	6	0	-2.618279	3.609942	1.687862
38	1	0	-1.502979	2.815025	3.368536
39	1	0	-3.575386	4.120178	-0.187473
40	6	0	-3.294127	4.705850	2.486211
41	1	0	-2.604104	5.146902	3.224082
42	1	0	-3.661247	5.511173	1.830170
43	1	0	-4.161794	4.313771	3.046781
44	6	0	-1.694614	-0.360244	-0.456150
45	6	0	-2.692863	-1.100211	-0.419009
46	14	0	-4.197926	-2.132966	-0.257533
47	6	0	-4.680227	-2.807646	-1.977369
48	1	0	-4.866257	-1.986085	-2.689691
49	1	0	-3.880781	-3.442252	-2.396086
50	1	0	-5.599014	-3.417009	-1.918103
51	6	0	-3.844093	-3.584734	0.923997
52	1	0	-3.028170	-4.219000	0.539022
53	1	0	-3.539760	-3.216995	1.917887

54	1	0	-4.737696	-4.220155	1.053996
55	6	0	-5.628421	-1.074201	0.426398
56	1	0	-6.547943	-1.675263	0.538851
57	1	0	-5.371143	-0.655590	1.413458
58	1	0	-5.853489	-0.229503	-0.246041
59	8	0	1.971785	0.747880	2.740056
60	16	0	2.091437	-0.416763	1.833512
61	8	0	3.363835	-0.523216	1.059472
62	8	0	0.842754	-0.710507	1.004809
63	6	0	2.080258	-1.950191	2.942369
64	9	0	3.119292	-1.900743	3.798797
65	9	0	0.934596	-2.012554	3.646014
66	9	0	2.192416	-3.068752	2.189521

Complex : **4a_TS2** (optimized by B97D/BS1)
E (BS1) = -2804.8207785 au
Δ H (BS1) = 0.548595 au
Δ G(BS1) = 0.427249 au
Imaginary frequency = -378.5i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.094112	-3.076703	-0.051268
2	6	0	1.187867	-3.529531	-1.219104
3	15	0	-0.135952	-2.248949	-1.616986
4	6	0	-0.301911	-2.342273	-3.462679
5	6	0	-1.737652	-2.918511	-1.004926
6	15	0	2.666326	-1.316701	-0.289793
7	6	0	3.928260	-1.391517	-1.645881
8	6	0	3.615060	-0.845138	1.212651
9	1	0	2.954532	-3.758131	0.061271
10	1	0	1.511106	-3.076666	0.880598
11	1	0	0.708397	-4.489621	-0.971375
12	1	0	1.780921	-3.678897	-2.137143
13	1	0	-1.111060	-1.664879	-3.775860
14	1	0	-0.540585	-3.364432	-3.798239
15	1	0	0.634712	-2.011355	-3.936724
16	1	0	-1.657911	-3.060360	0.081183
17	1	0	-1.976641	-3.871335	-1.505561
18	1	0	-2.522616	-2.177667	-1.213216
19	1	0	4.295303	-0.372452	-1.841621
20	1	0	4.780398	-2.035964	-1.375014
21	1	0	3.458839	-1.775795	-2.564372
22	1	0	2.916275	-0.841357	2.059015
23	1	0	4.446475	-1.545483	1.393449
24	1	0	4.004138	0.173493	1.069529
25	46	0	0.711392	-0.108017	-0.861160
26	6	0	0.479305	0.986665	-2.839029
27	1	0	1.475047	0.565223	-3.042103
28	1	0	-0.246649	0.629559	-3.569343
29	1	0	0.531078	2.071489	-2.747944
30	6	0	1.687275	1.611213	-0.184518
31	6	0	1.262942	2.163822	1.034847

32	6	0	2.740732	2.205391	-0.892293
33	6	0	1.903447	3.310302	1.532440
34	1	0	0.455387	1.696711	1.595627
35	6	0	3.379689	3.351027	-0.378903
36	1	0	3.076996	1.789350	-1.846571
37	6	0	2.969149	3.920261	0.838890
38	1	0	1.568553	3.736730	2.482579
39	1	0	4.206635	3.804405	-0.933791
40	6	0	3.635694	5.167030	1.387283
41	1	0	3.855590	5.062991	2.462693
42	1	0	4.580097	5.380265	0.861836
43	1	0	2.983088	6.050801	1.274095
44	6	0	-0.950288	0.855110	-1.383420
45	6	0	-2.107690	1.305931	-1.354931
46	14	0	-3.836270	1.868780	-1.042848
47	6	0	-4.978173	0.346076	-0.983811
48	1	0	-4.949997	-0.213368	-1.934469
49	1	0	-4.672463	-0.335946	-0.175310
50	1	0	-6.024535	0.646628	-0.801073
51	6	0	-3.879493	2.799628	0.613396
52	1	0	-3.483675	2.169678	1.424233
53	1	0	-3.263879	3.713258	0.566441
54	1	0	-4.911071	3.094913	0.872854
55	6	0	-4.373745	3.019085	-2.466044
56	1	0	-5.408574	3.369487	-2.307503
57	1	0	-3.722897	3.906836	-2.531232
58	1	0	-4.339487	2.501699	-3.439651
59	8	0	-0.042570	-1.471469	3.993588
60	16	0	-0.380237	-1.572148	2.557588
61	8	0	-0.663853	-2.938413	2.022249
62	8	0	0.516478	-0.747921	1.659585
63	6	0	-2.027177	-0.650858	2.386651
64	9	0	-2.952323	-1.137451	3.236009
65	9	0	-1.857755	0.669991	2.644758
66	9	0	-2.514860	-0.766369	1.121093

Complex : **4a_TS3** (optimized by B97D/BS1)
E (BS1) = -2804.8165134 au
Δ H (BS1) = 0.547937 au
Δ G(BS1) = 0.427471 au
Imaginary frequency = -335.2i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.466940	-3.433260	0.298873
2	6	0	0.053172	-3.913745	-0.076572
3	15	0	-1.146112	-2.471197	-0.131993
4	6	0	-2.506138	-3.045441	-1.241182
5	6	0	-1.910339	-2.329992	1.531665
6	15	0	1.976508	-1.972641	-0.753888
7	6	0	2.655814	-2.773097	-2.287172
8	6	0	3.426931	-1.255292	0.123943
9	1	0	2.203106	-4.248168	0.194278
10	1	0	1.482599	-3.063286	1.333496
11	1	0	-0.304066	-4.677795	0.633549

12	1	0	0.048389	-4.364186	-1.083715
13	1	0	-3.246757	-2.235941	-1.298088
14	1	0	-2.972382	-3.967600	-0.857425
15	1	0	-2.104695	-3.228009	-2.249737
16	1	0	-1.116754	-2.249345	2.284960
17	1	0	-2.550779	-3.206285	1.725369
18	1	0	-2.500416	-1.404705	1.557666
19	1	0	2.997375	-2.013917	-3.005750
20	1	0	3.501974	-3.435109	-2.040990
21	1	0	1.861313	-3.365939	-2.766441
22	1	0	3.101623	-1.007354	1.141853
23	1	0	4.258940	-1.977884	0.149201
24	1	0	3.738849	-0.330001	-0.378661
25	46	0	0.028928	-0.646005	-1.041408
26	6	0	-0.004897	-0.421006	-3.303864
27	1	0	0.936468	-0.597619	-3.828157
28	1	0	-0.619277	-1.333471	-3.287592
29	1	0	-0.583714	0.401474	-3.725898
30	6	0	0.960504	1.017695	-2.043525
31	6	0	0.291420	2.242998	-1.857826
32	6	0	2.340056	1.026622	-2.319220
33	6	0	1.019946	3.439495	-1.849004
34	1	0	-0.783222	2.254234	-1.683657
35	6	0	3.058219	2.229967	-2.313106
36	1	0	2.862304	0.097970	-2.547570
37	6	0	2.412416	3.455846	-2.062618
38	1	0	0.493453	4.380927	-1.670966
39	1	0	4.133434	2.218295	-2.511862
40	6	0	3.189529	4.754397	-2.016494
41	1	0	4.161250	4.659959	-2.526117
42	1	0	2.626196	5.575243	-2.489035
43	1	0	3.387466	5.053465	-0.972031
44	6	0	-1.805639	0.152109	-0.959239
45	6	0	-2.935459	0.598614	-0.715195
46	14	0	-4.427145	1.395104	0.006333
47	6	0	-5.997417	0.817800	-0.910291
48	1	0	-5.965823	1.094903	-1.977546
49	1	0	-6.114886	-0.277863	-0.850852
50	1	0	-6.900326	1.275274	-0.469401
51	6	0	-4.506555	0.880051	1.839009
52	1	0	-4.760510	-0.189399	1.940691
53	1	0	-3.528249	1.039390	2.321442
54	1	0	-5.268555	1.458768	2.389770
55	6	0	-4.254747	3.286613	-0.137222
56	1	0	-5.122972	3.801236	0.310301
57	1	0	-3.347759	3.630600	0.387104
58	1	0	-4.178385	3.604148	-1.190928
59	8	0	1.023510	-1.311473	2.628012
60	16	0	0.589714	0.104186	2.374960
61	8	0	-0.759568	0.463160	2.871325
62	8	0	0.934553	0.591272	0.988828
63	6	0	1.796736	1.113904	3.425264
64	9	0	1.653797	0.816426	4.733821
65	9	0	3.076648	0.836502	3.062556
66	9	0	1.585319	2.435299	3.257515

Complex : **4b_TS1** (optimized by B97D/BS1)
E (BS1) = -2804.8278961 au
Δ H (BS1) = 0.548786 au
Δ G(BS1) = 0.427617 au

Imaginary frequency = -290.2i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.657328	-2.332629	2.298988
2	6	0	-0.147171	-3.152846	1.096995
3	15	0	-0.642765	-2.367040	-0.529872
4	6	0	0.548669	-3.107640	-1.733585
5	6	0	-2.261001	-3.145747	-0.976434
6	15	0	-0.082548	-0.559891	2.159276
7	6	0	1.614916	-0.612716	2.902997
8	6	0	-1.102489	0.365959	3.394250
9	1	0	-0.299378	-2.770251	3.246156
10	1	0	-1.755220	-2.305162	2.315120
11	1	0	-0.513568	-4.192087	1.142913
12	1	0	0.955152	-3.183891	1.093260
13	1	0	0.250295	-2.824197	-2.754112
14	1	0	0.575742	-4.206600	-1.656043
15	1	0	1.542744	-2.683091	-1.527899
16	1	0	-3.013310	-2.864192	-0.229750
17	1	0	-2.149016	-4.241128	-1.029109
18	1	0	-2.587814	-2.764334	-1.953219
19	1	0	2.045357	0.399152	2.921823
20	1	0	1.588288	-1.019906	3.926986
21	1	0	2.259213	-1.229388	2.261472
22	1	0	-2.159490	0.284574	3.109185
23	1	0	-0.953190	-0.041705	4.407511
24	1	0	-0.818472	1.428609	3.382930
25	46	0	-0.116668	-0.018361	-0.268149
26	6	0	-0.354680	0.165887	-2.381203
27	1	0	-1.180652	-0.485378	-2.688808
28	1	0	-0.622829	1.220065	-2.506789
29	1	0	0.592302	-0.096603	-2.867723
30	6	0	1.084279	1.792654	-0.222093
31	6	0	1.472698	2.466288	-1.396067
32	6	0	1.116197	2.489584	1.000078
33	6	0	1.843819	3.815111	-1.348479
34	1	0	1.507409	1.934596	-2.344738
35	6	0	1.481840	3.843883	1.035482
36	1	0	0.839362	2.001178	1.930975
37	6	0	1.845907	4.532470	-0.135318
38	1	0	2.143116	4.319704	-2.271338
39	1	0	1.478633	4.373181	1.992293
40	6	0	2.209509	6.002112	-0.100402
41	1	0	1.340566	6.629266	-0.368342
42	1	0	2.541877	6.309016	0.903699
43	1	0	3.012773	6.232863	-0.818688
44	6	0	1.842559	-0.146627	-0.364257
45	6	0	2.995339	-0.607391	-0.413844
46	14	0	4.711775	-1.242986	-0.440920
47	6	0	4.995926	-2.304396	1.121636
48	1	0	4.844780	-1.711967	2.039864
49	1	0	4.301513	-3.161507	1.155078
50	1	0	6.024044	-2.705556	1.146520
51	6	0	4.956901	-2.325895	-1.991521
52	1	0	4.261907	-3.182704	-1.994232

53	1	0	4.777501	-1.746259	-2.912486
54	1	0	5.984980	-2.725363	-2.037827
55	6	0	5.945986	0.206726	-0.460431
56	1	0	6.987811	-0.158323	-0.476711
57	1	0	5.793787	0.843104	-1.347977
58	1	0	5.821591	0.843363	0.431347
59	8	0	-4.130890	1.460200	1.330543
60	16	0	-3.370519	0.510091	0.494514
61	8	0	-3.191730	-0.869537	1.039748
62	8	0	-2.092533	1.098612	-0.090430
63	6	0	-4.414100	0.250723	-1.061893
64	9	0	-5.567974	-0.377931	-0.759811
65	9	0	-4.694857	1.428392	-1.647969
66	9	0	-3.736432	-0.519059	-1.958351

Complex : **4b_TS2** (optimized by B97D/BS1)
E (BS1) = -2804.8229999 au
Δ H (BS1) = 0.548433 au
Δ G(BS1) = 0.425464 au
Imaginary frequency = -346.7i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.341503	-1.621226	2.963289
2	6	0	0.391324	-2.727483	2.173240
3	15	0	0.050434	-2.604690	0.329876
4	6	0	1.394008	-3.623234	-0.432134
5	6	0	-1.495004	-3.578167	0.063526
6	15	0	0.061629	0.062464	2.263188
7	6	0	1.751358	0.485104	2.866775
8	6	0	-1.103358	1.248586	3.046509
9	1	0	-0.085787	-1.672213	4.035341
10	1	0	-1.431592	-1.731883	2.858688
11	1	0	0.102726	-3.724264	2.546899
12	1	0	1.482771	-2.627430	2.297644
13	1	0	1.180297	-3.746151	-1.505142
14	1	0	1.466067	-4.618809	0.034829
15	1	0	2.344661	-3.080050	-0.332787
16	1	0	-2.332693	-3.092886	0.581187
17	1	0	-1.363199	-4.613970	0.417520
18	1	0	-1.732047	-3.583460	-1.009159
19	1	0	1.980410	1.508003	2.533375
20	1	0	1.832013	0.421844	3.963752
21	1	0	2.475524	-0.192586	2.390491
22	1	0	-2.105651	1.035983	2.649481
23	1	0	-1.092064	1.160144	4.144868
24	1	0	-0.818229	2.266518	2.746081
25	46	0	0.074476	-0.191633	-0.092002
26	6	0	0.427223	-0.242869	-2.316898
27	1	0	0.839453	-1.152013	-2.759369
28	1	0	-0.671227	-0.239315	-2.374300
29	1	0	0.841069	0.677310	-2.732745
30	6	0	0.076322	1.905357	-0.088202
31	6	0	-1.182356	2.528107	-0.094896
32	6	0	1.246682	2.677634	-0.043233

33	6	0	-1.256610	3.932025	-0.089024
34	1	0	-2.098765	1.942331	-0.075389
35	6	0	1.152515	4.081426	-0.029284
36	1	0	2.223737	2.194069	-0.029089
37	6	0	-0.096233	4.729574	-0.058845
38	1	0	-2.240569	4.409403	-0.096739
39	1	0	2.067865	4.680141	0.003865
40	6	0	-0.192261	6.242521	-0.080674
41	1	0	-1.089119	6.594018	0.454335
42	1	0	0.693079	6.707287	0.381978
43	1	0	-0.260550	6.620898	-1.116316
44	6	0	1.881741	-0.271600	-0.830412
45	6	0	3.118722	-0.355981	-0.888880
46	14	0	4.948131	-0.407137	-0.829426
47	6	0	5.558906	0.827638	0.490483
48	1	0	5.229280	1.853706	0.255243
49	1	0	5.165469	0.570789	1.488754
50	1	0	6.661066	0.833058	0.552518
51	6	0	5.506973	-2.169018	-0.353914
52	1	0	5.118765	-2.457182	0.638101
53	1	0	5.150625	-2.914235	-1.085034
54	1	0	6.608052	-2.236184	-0.315478
55	6	0	5.673403	0.060084	-2.527423
56	1	0	6.777095	0.041860	-2.505001
57	1	0	5.338855	-0.640414	-3.310704
58	1	0	5.357558	1.073290	-2.826954
59	8	0	-4.389903	0.821846	0.406229
60	16	0	-3.718951	-0.465316	0.110658
61	8	0	-4.435982	-1.727449	0.412632
62	8	0	-2.267137	-0.499006	0.566969
63	6	0	-3.529813	-0.472201	-1.772580
64	9	0	-4.725830	-0.549958	-2.379447
65	9	0	-2.902856	0.654918	-2.197714
66	9	0	-2.775812	-1.535507	-2.177768

Complex : **4b_TS3** (optimized by B97D/BS1)
E (BS1) = -2804.8137356 au
Δ H (BS1) = 0.548234 au
Δ G(BS1) = 0.421429 au
Imaginary frequency = -399.5i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.011659	-1.831471	2.568888
2	6	0	0.732148	-2.712330	1.534866
3	15	0	0.134157	-2.476095	-0.218378
4	6	0	1.334881	-3.465617	-1.218886
5	6	0	-1.446543	-3.418962	-0.366006
6	15	0	0.031887	-0.005107	2.129766
7	6	0	1.691718	0.549071	2.754781
8	6	0	-1.140453	0.744816	3.363152
9	1	0	0.422116	-2.000778	3.569647
10	1	0	-1.076309	-2.103915	2.606700
11	1	0	0.652992	-3.778191	1.810539

12	1	0	1.800651	-2.446520	1.502685
13	1	0	1.002635	-3.480418	-2.268320
14	1	0	1.397487	-4.501237	-0.845692
15	1	0	2.316803	-2.978312	-1.162392
16	1	0	-2.179281	-3.012588	0.340987
17	1	0	-1.267527	-4.489606	-0.171964
18	1	0	-1.845398	-3.288448	-1.382082
19	1	0	1.784563	1.632992	2.583015
20	1	0	1.823635	0.336421	3.829022
21	1	0	2.476511	0.053198	2.166824
22	1	0	-2.154440	0.383922	3.147382
23	1	0	-0.855882	0.489614	4.398272
24	1	0	-1.125717	1.838759	3.241054
25	46	0	0.041472	-0.085276	-0.527101
26	6	0	0.125524	0.873135	-2.639931
27	1	0	-0.301562	-0.093794	-2.941504
28	1	0	-0.503671	1.677007	-3.023158
29	1	0	1.174069	0.966887	-2.928856
30	6	0	0.188324	2.039181	-0.901258
31	6	0	-0.984335	2.778385	-0.629926
32	6	0	1.440968	2.679147	-0.816340
33	6	0	-0.887074	4.111845	-0.220841
34	1	0	-1.959849	2.307846	-0.708364
35	6	0	1.519182	4.020014	-0.408122
36	1	0	2.349932	2.125490	-1.047152
37	6	0	0.362819	4.758667	-0.099669
38	1	0	-1.803367	4.661777	0.011268
39	1	0	2.499170	4.499680	-0.330186
40	6	0	0.442984	6.211315	0.321091
41	1	0	1.478802	6.504509	0.552988
42	1	0	0.075645	6.878614	-0.478826
43	1	0	-0.179261	6.403938	1.211135
44	6	0	1.959453	-0.314795	-0.506165
45	6	0	3.183728	-0.494220	-0.448161
46	14	0	4.995888	-0.759805	-0.362303
47	6	0	5.700437	0.201237	1.125644
48	1	0	5.499646	1.281297	1.028197
49	1	0	5.248454	-0.137057	2.073313
50	1	0	6.793098	0.065447	1.205018
51	6	0	5.336915	-2.624196	-0.136494
52	1	0	4.866984	-3.008594	0.784880
53	1	0	4.943059	-3.209915	-0.984365
54	1	0	6.420863	-2.821134	-0.067707
55	6	0	5.812328	-0.148088	-1.970386
56	1	0	6.904488	-0.307551	-1.945661
57	1	0	5.411246	-0.681755	-2.848236
58	1	0	5.631097	0.929237	-2.121743
59	8	0	-3.590640	1.230832	0.709515
60	16	0	-3.199108	-0.119448	0.252302
61	8	0	-2.973915	-1.144908	1.308823
62	8	0	-2.138294	-0.131042	-0.862125
63	6	0	-4.659971	-0.783868	-0.750271
64	9	0	-5.742535	-0.885981	0.043468
65	9	0	-4.942361	0.041362	-1.775835
66	9	0	-4.366460	-2.009416	-1.243300

Complex : **4c_TS1** (optimized by B97D/BS1)
E (BS1) = -2804.8230676 au
Δ H (BS1) = 0.548590 au
Δ G(BS1) = 0.426939 au

Imaginary frequency = -282.2i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.692569	-2.286099	2.552745
2	6	0	-0.017814	-3.408114	1.729722
3	15	0	0.123335	-2.928007	-0.081163
4	6	0	1.505765	-3.959063	-0.745894
5	6	0	-1.413502	-3.578461	-0.867387
6	15	0	0.233009	-0.672607	2.323639
7	6	0	1.613101	-0.813462	3.566311
8	6	0	-0.838290	0.646811	3.034064
9	1	0	-0.740973	-2.564984	3.618883
10	1	0	-1.713984	-2.103514	2.189032
11	1	0	-0.574367	-4.355563	1.826830
12	1	0	1.008058	-3.589292	2.094340
13	1	0	1.576366	-3.793014	-1.831874
14	1	0	1.359700	-5.033656	-0.550547
15	1	0	2.446073	-3.617707	-0.287075
16	1	0	-2.270618	-3.041707	-0.440902
17	1	0	-1.517169	-4.664543	-0.712204
18	1	0	-1.383945	-3.360965	-1.945229
19	1	0	2.228730	0.098470	3.538549
20	1	0	1.205840	-0.937613	4.583129
21	1	0	2.255866	-1.675013	3.328386
22	1	0	-1.769568	0.698291	2.454831
23	1	0	-1.054837	0.457274	4.098077
24	1	0	-0.312497	1.606984	2.926476
25	46	0	0.439322	-0.569988	-0.155534
26	6	0	0.045965	-0.634902	-2.241018
27	1	0	0.779991	-1.281099	-2.739398
28	1	0	-0.980203	-1.010282	-2.310178
29	1	0	0.107538	0.408213	-2.567767
30	6	0	2.464241	-0.050775	-0.543147
31	6	0	2.963592	0.194752	-1.837062
32	6	0	3.367841	-0.357932	0.490147
33	6	0	4.336961	0.086702	-2.090141
34	1	0	2.293079	0.487491	-2.640558
35	6	0	4.741320	-0.470409	0.217334
36	1	0	3.012774	-0.507715	1.504305
37	6	0	5.252368	-0.254230	-1.073917
38	1	0	4.703853	0.280831	-3.101916
39	1	0	5.425905	-0.723223	1.032027
40	6	0	6.736597	-0.349640	-1.362696
41	1	0	6.932659	-0.970208	-2.253156
42	1	0	7.168964	0.646781	-1.560974
43	1	0	7.281368	-0.787659	-0.511824
44	6	0	0.948329	1.355689	-0.119854
45	6	0	0.844801	2.586341	0.001943
46	14	0	0.171777	4.297200	0.147977
47	6	0	-1.147825	4.276996	1.522798
48	1	0	-1.918822	3.520286	1.304451
49	1	0	-0.703968	4.041694	2.505510
50	1	0	-1.644356	5.259742	1.606886
51	6	0	1.568414	5.515559	0.596151
52	1	0	2.050439	5.240383	1.549596
53	1	0	2.349149	5.534898	-0.182658

54	1	0	1.171576	6.540299	0.702685
55	6	0	-0.629390	4.758195	-1.511986
56	1	0	-1.110376	5.750724	-1.462156
57	1	0	0.112656	4.778327	-2.327788
58	1	0	-1.397066	4.008949	-1.763738
59	8	0	-2.340541	1.365417	-1.307204
60	16	0	-2.879257	0.494471	-0.240328
61	8	0	-3.613401	1.131746	0.880682
62	8	0	-1.919160	-0.598360	0.240291
63	6	0	-4.147486	-0.608644	-1.115667
64	9	0	-5.202006	0.104254	-1.549787
65	9	0	-3.571649	-1.221884	-2.184314
66	9	0	-4.592822	-1.579246	-0.277887

Complex : **4c_TS2** (optimized by B97D/BS1)
E (BS1) = -2804.8072325 au
Δ H (BS1) = 0.548012 au
Δ G(BS1) = 0.424424 au
Imaginary frequency = -449.4i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.428550	-2.333824	2.453420
2	6	0	1.380957	-3.103816	1.509697
3	15	0	1.027266	-2.737192	-0.293651
4	6	0	2.411370	-3.640160	-1.145660
5	6	0	-0.461593	-3.775885	-0.653295
6	15	0	0.535435	-0.489533	2.153484
7	6	0	2.091580	-0.054376	3.080721
8	6	0	-0.785148	0.229069	3.236562
9	1	0	0.669536	-2.565130	3.505326
10	1	0	-0.616873	-2.617623	2.266885
11	1	0	1.301883	-4.190353	1.686235
12	1	0	2.429112	-2.813395	1.696350
13	1	0	2.271984	-3.588182	-2.236834
14	1	0	2.431636	-4.699233	-0.840493
15	1	0	3.370549	-3.165521	-0.893132
16	1	0	-1.283607	-3.450062	-0.001823
17	1	0	-0.239333	-4.843455	-0.489175
18	1	0	-0.777560	-3.613654	-1.693787
19	1	0	2.186510	1.038686	3.156340
20	1	0	2.062882	-0.480011	4.097835
21	1	0	2.972267	-0.431700	2.542111
22	1	0	-1.757852	-0.170662	2.924117
23	1	0	-0.596307	-0.010011	4.296601
24	1	0	-0.799922	1.320627	3.100146
25	46	0	0.576830	-0.299353	-0.431574
26	6	0	0.387058	0.634680	-2.550252
27	1	0	0.752235	-0.353472	-2.867088
28	1	0	-0.648692	0.777180	-2.859889
29	1	0	1.082161	1.407784	-2.879561
30	6	0	2.550934	0.200979	-0.489746
31	6	0	3.058309	1.234258	0.313902
32	6	0	3.393547	-0.428963	-1.418220
33	6	0	4.417279	1.579219	0.233718

34	1	0	2.393300	1.780329	0.978470
35	6	0	4.753146	-0.074079	-1.489104
36	1	0	2.999686	-1.184514	-2.096475
37	6	0	5.289760	0.924615	-0.657301
38	1	0	4.799879	2.386299	0.864979
39	1	0	5.400468	-0.578534	-2.212182
40	6	0	6.761015	1.285245	-0.713971
41	1	0	7.329165	0.772933	0.083047
42	1	0	7.206593	0.993004	-1.677842
43	1	0	6.911912	2.368146	-0.577341
44	6	0	0.084941	1.584769	-0.826405
45	6	0	-0.364802	2.724961	-0.617978
46	14	0	-1.388684	4.133461	-0.033105
47	6	0	-1.617559	3.946079	1.851787
48	1	0	-2.124673	2.990300	2.060236
49	1	0	-0.648274	3.950213	2.379703
50	1	0	-2.233031	4.763462	2.266896
51	6	0	-0.539551	5.794048	-0.427187
52	1	0	0.451047	5.862732	0.053582
53	1	0	-0.395506	5.921774	-1.513251
54	1	0	-1.148895	6.640961	-0.065999
55	6	0	-3.085724	4.019681	-0.885965
56	1	0	-3.776324	4.792495	-0.505237
57	1	0	-3.001465	4.146459	-1.978343
58	1	0	-3.525678	3.029243	-0.686742
59	8	0	-2.991079	0.571727	0.684596
60	16	0	-2.690210	-0.796876	0.211150
61	8	0	-2.616264	-1.862889	1.252815
62	8	0	-1.567482	-0.902813	-0.823664
63	6	0	-4.145753	-1.294627	-0.889375
64	9	0	-5.277802	-1.329441	-0.159589
65	9	0	-4.299676	-0.406062	-1.891254
66	9	0	-3.932508	-2.519375	-1.420906

Complex : **4c_TS3** (optimized by B97D/BS1)
E (BS1) = -2804.8176458 au
Δ H (BS1) = 0.549148 au
Δ G(BS1) = 0.427687 au
Imaginary frequency = -316.4i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.253373	-1.853725	2.746996
2	6	0	1.186971	-2.813917	1.985747
3	15	0	0.937910	-2.675550	0.131140
4	6	0	2.244160	-3.832300	-0.510891
5	6	0	-0.621518	-3.606250	-0.187275
6	15	0	0.375721	-0.131853	2.042207
7	6	0	1.951212	0.575460	2.699055
8	6	0	-0.959323	0.864269	2.810597
9	1	0	0.492646	-1.843987	3.823657
10	1	0	-0.798119	-2.147479	2.618840
11	1	0	1.017928	-3.856438	2.304399
12	1	0	2.244232	-2.568593	2.183601

13	1	0	2.214486	-3.862257	-1.610819
14	1	0	2.051786	-4.846365	-0.124950
15	1	0	3.241638	-3.501513	-0.189794
16	1	0	-1.423120	-3.168477	0.420787
17	1	0	-0.477525	-4.671294	0.059063
18	1	0	-0.910381	-3.489659	-1.239865
19	1	0	2.055734	1.586646	2.280474
20	1	0	1.946467	0.620484	3.800506
21	1	0	2.801855	-0.025667	2.347232
22	1	0	-1.926165	0.456799	2.490953
23	1	0	-0.865653	0.831308	3.908569
24	1	0	-0.865258	1.894164	2.444479
25	46	0	0.716087	-0.302694	-0.285067
26	6	0	1.160532	-0.056320	-2.466762
27	1	0	1.669307	-0.891337	-2.954318
28	1	0	0.063681	-0.143850	-2.537313
29	1	0	1.479080	0.919772	-2.835889
30	6	0	2.704349	0.144854	-0.964766
31	6	0	3.182701	1.434655	-0.650283
32	6	0	3.635812	-0.876592	-1.225159
33	6	0	4.560705	1.647751	-0.494937
34	1	0	2.482962	2.255874	-0.510686
35	6	0	5.011370	-0.646829	-1.065352
36	1	0	3.296951	-1.838847	-1.596151
37	6	0	5.499922	0.614449	-0.679853
38	1	0	4.910716	2.649435	-0.229881
39	1	0	5.714540	-1.459465	-1.269506
40	6	0	6.981894	0.855609	-0.478575
41	1	0	7.585865	0.163254	-1.086292
42	1	0	7.259195	1.886584	-0.750081
43	1	0	7.271673	0.706026	0.577283
44	6	0	0.165077	1.607300	-0.213152
45	6	0	-0.324434	2.741576	-0.146285
46	14	0	-1.461440	4.190702	-0.111184
47	6	0	-2.385102	4.174403	1.556288
48	1	0	-2.943064	3.229784	1.659671
49	1	0	-1.695866	4.267603	2.413261
50	1	0	-3.106879	5.007779	1.615196
51	6	0	-0.470707	5.811547	-0.287395
52	1	0	0.260374	5.928364	0.530838
53	1	0	0.083754	5.839444	-1.240674
54	1	0	-1.143684	6.686527	-0.263978
55	6	0	-2.708483	3.992411	-1.529798
56	1	0	-3.467860	4.793987	-1.516699
57	1	0	-2.207325	4.011105	-2.512094
58	1	0	-3.218113	3.021272	-1.423185
59	8	0	-3.339070	0.692313	0.067028
60	16	0	-2.816085	-0.687548	-0.064757
61	8	0	-2.615237	-1.427789	1.226702
62	8	0	-1.678987	-0.883040	-1.040509
63	6	0	-4.194219	-1.667414	-0.914489
64	9	0	-5.320016	-1.646513	-0.171781
65	9	0	-4.466405	-1.147370	-2.128874
66	9	0	-3.813821	-2.960848	-1.078132

Complex : **Pd(dmpe)(OTf)(*p*-Tol)** (optimized by B97D/BS1)
E (BS1) = -2279.737343 au
Δ H (BS1) = 0.380447 au
Δ G(BS1) = 0.282661 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.468533	3.693005	0.782238
2	6	0	0.794431	3.749182	-0.107649
3	15	0	1.606913	2.053856	-0.177458
4	6	0	2.876954	2.201811	-1.516145
5	6	0	2.585906	1.965185	1.389806
6	15	0	-1.569333	2.245539	0.303430
7	6	0	-2.650058	2.891102	-1.048492
8	6	0	-2.704627	2.009385	1.736053
9	1	0	-1.037276	4.636935	0.732650
10	1	0	-0.182034	3.532231	1.834716
11	1	0	1.493142	4.518758	0.261308
12	1	0	0.517739	4.015587	-1.141544
13	1	0	3.414450	1.246318	-1.581315
14	1	0	3.592048	3.014687	-1.308848
15	1	0	2.374258	2.388038	-2.477290
16	1	0	1.902504	2.083317	2.243667
17	1	0	3.365922	2.743717	1.424796
18	1	0	3.032679	0.965638	1.458149
19	1	0	-3.311746	2.076276	-1.374989
20	1	0	-3.252982	3.745526	-0.700210
21	1	0	-2.025453	3.200349	-1.899532
22	1	0	-2.118831	1.673923	2.604274
23	1	0	-3.237360	2.942861	1.980423
24	1	0	-3.420489	1.216286	1.479067
25	46	0	-0.248700	0.551735	-0.264154
26	6	0	-1.950261	-0.616276	-0.210668
27	6	0	-2.155970	-1.451039	0.904349
28	6	0	-2.873297	-0.651281	-1.270109
29	6	0	-3.261643	-2.316010	0.943112
30	1	0	-1.439260	-1.449437	1.728235
31	6	0	-3.978189	-1.522158	-1.223342
32	1	0	-2.728924	-0.015687	-2.148016
33	6	0	-4.188879	-2.365113	-0.117238
34	1	0	-3.401711	-2.971381	1.807799
35	1	0	-4.683423	-1.548922	-2.059682
36	6	0	-5.360465	-3.326986	-0.078793
37	1	0	-5.784898	-3.403080	0.935786
38	1	0	-6.161063	-3.010411	-0.766271
39	1	0	-5.048395	-4.343337	-0.378106
40	8	0	1.164944	-3.390438	0.349219
41	16	0	1.560602	-1.970077	0.330575
42	8	0	1.519992	-1.205596	1.608995
43	8	0	0.988395	-1.174783	-0.856091
44	6	0	3.396180	-1.982069	-0.138680
45	9	0	4.108897	-2.677328	0.767643
46	9	0	3.589042	-2.520405	-1.356585
47	9	0	3.890066	-0.703776	-0.162878

Complex : **Pd(C≡CSiMe$_3$)(dmpe)(OTf)** (optimized by B97D/BS1)
E (BS1) = -2494.2408142 au
Δ H (BS1) = 0.388099 au
Δ G(BS1) = 0.284513 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.028175	3.781279	0.629770
2	6	0	1.273517	3.679734	-0.278769
3	15	0	1.946300	1.925341	-0.236528
4	6	0	3.077132	1.789193	-1.687222
5	6	0	3.033466	1.850667	1.251229
6	15	0	-1.167767	2.374548	0.282874
7	6	0	-2.245014	2.927922	-1.104082
8	6	0	-2.257412	2.260515	1.759964
9	1	0	-0.480511	4.752665	0.511095
10	1	0	0.321095	3.684565	1.688193
11	1	0	2.039753	4.413040	0.022443
12	1	0	0.998705	3.890274	-1.325674
13	1	0	3.495705	0.774488	-1.692132
14	1	0	3.892756	2.528547	-1.635516
15	1	0	2.498216	1.935696	-2.611107
16	1	0	2.429712	2.055575	2.147221
17	1	0	3.861178	2.575274	1.178903
18	1	0	3.419158	0.826828	1.336042
19	1	0	-2.920977	2.093103	-1.338093
20	1	0	-2.820175	3.826928	-0.828726
21	1	0	-1.623791	3.136983	-1.987335
22	1	0	-1.645862	2.001266	2.636438
23	1	0	-2.786952	3.210958	1.936624
24	1	0	-2.967551	1.442975	1.574734
25	46	0	0.033782	0.566971	-0.203484
26	8	0	1.218806	-3.354904	0.532448
27	16	0	1.771302	-1.992549	0.440487
28	8	0	1.884833	-1.176780	1.679391
29	8	0	1.239401	-1.176501	-0.759334
30	6	0	3.565063	-2.225906	-0.123895
31	9	0	4.239813	-2.979946	0.762803
32	9	0	3.630001	-2.805277	-1.335804
33	9	0	4.196881	-1.012208	-0.203720
34	6	0	-1.740151	-0.355519	-0.196958
35	6	0	-2.902398	-0.791868	-0.176878
36	14	0	-4.558351	-1.584942	-0.137221
37	6	0	-4.385837	-3.471366	-0.304396
38	1	0	-3.760314	-3.881211	0.505474
39	1	0	-5.372275	-3.965800	-0.261637
40	1	0	-3.908052	-3.740719	-1.260702
41	6	0	-5.407686	-1.162184	1.520422
42	1	0	-4.809259	-1.522409	2.373842
43	1	0	-5.545933	-0.073569	1.639824
44	1	0	-6.403667	-1.634589	1.582613
45	6	0	-5.619689	-0.901508	-1.569378
46	1	0	-5.751589	0.191298	-1.488434
47	1	0	-5.151457	-1.112993	-2.545223
48	1	0	-6.623374	-1.361617	-1.568886

Complex : **Pd(dmpe)(Me)(OTf)** (optimized by B97D/BS1)
E (BS1) = -2048.8627323 au
Δ H (BS1) = 0.296278 au
Δ G(BS1) = 0.211996 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.864085	2.023540	-0.135759
2	6	0	-3.536548	0.902243	0.686624
3	15	0	-2.889180	-0.776951	0.156800
4	6	0	-3.414275	-1.935872	1.494195
5	6	0	-3.932100	-1.244085	-1.299075
6	15	0	-0.994100	1.802390	-0.123567
7	6	0	-0.471316	2.578774	1.473376
8	6	0	-0.379554	2.961416	-1.425372
9	1	0	-3.152062	3.014144	0.254054
10	1	0	-3.190753	1.970085	-1.187938
11	1	0	-4.635625	0.934599	0.596496
12	1	0	-3.282969	1.012442	1.753963
13	1	0	-3.119574	-2.956936	1.212626
14	1	0	-4.503706	-1.895953	1.656648
15	1	0	-2.889317	-1.668092	2.422825
16	1	0	-3.788795	-0.501227	-2.097535
17	1	0	-4.999848	-1.295111	-1.028592
18	1	0	-3.598674	-2.222005	-1.675733
19	1	0	0.625567	2.539618	1.520993
20	1	0	-0.818884	3.622997	1.543555
21	1	0	-0.875334	1.993048	2.312551
22	1	0	-0.737563	2.627092	-2.411014
23	1	0	-0.714854	3.995219	-1.239813
24	1	0	0.718282	2.911525	-1.406695
25	46	0	-0.725181	-0.585192	-0.264663
26	6	0	-0.590203	-2.691578	-0.313377
27	1	0	-1.458739	-3.204443	-0.755756
28	1	0	0.312905	-2.860803	-0.916894
29	1	0	-0.433647	-3.023972	0.725196
30	8	0	1.911745	-0.074135	1.676930
31	16	0	2.247461	0.252395	0.269811
32	8	0	2.392364	1.695628	-0.067992
33	8	0	1.413773	-0.530086	-0.760822
34	6	0	3.948106	-0.509741	-0.050047
35	9	0	4.851669	0.052236	0.778907
36	9	0	3.914405	-1.837562	0.179910
37	9	0	4.332653	-0.296087	-1.324175

Complex : **Na(OTf)** (optimized by B97D/BS1)
E (BS1) = -1689.1290095 au
Δ H (BS1) = 0.260892 au
Δ G(BS1) = 0.167837 au

Optimized coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	-0.043026	-0.974002	-0.361736
2	6	0	-1.786133	-2.282665	0.027409
3	6	0	-2.071889	-2.652111	1.347459
4	6	0	-2.547562	-2.734138	-1.057436
5	6	0	-3.167599	-3.499816	1.584241
6	1	0	-1.463980	-2.291170	2.177806
7	6	0	-3.639701	-3.581622	-0.803669
8	1	0	-2.306257	-2.436430	-2.078440
9	6	0	-3.947919	-3.961960	0.512294
10	1	0	-3.405860	-3.795940	2.607411
11	1	0	-4.245212	-3.941352	-1.637527
12	1	0	-4.795921	-4.621983	0.702516
13	6	0	-1.209646	0.693757	-0.152357
14	6	0	-1.713706	1.811939	-0.065255
15	14	0	-2.511667	3.492263	0.074505
16	6	0	-4.109749	3.467693	-0.951629
17	1	0	-4.820784	2.714830	-0.573703
18	1	0	-4.605776	4.452670	-0.908692
19	1	0	-3.902402	3.240019	-2.009961
20	6	0	-2.886101	3.811026	1.908532
21	1	0	-1.965793	3.785835	2.514457
22	1	0	-3.348723	4.804766	2.036859
23	1	0	-3.582560	3.059167	2.314653
24	6	0	-1.267892	4.751042	-0.608203
25	1	0	-1.041464	4.554833	-1.668600
26	1	0	-1.675939	5.773464	-0.528789
27	1	0	-0.318344	4.717143	-0.050263
28	8	0	1.827654	0.767779	-0.791636
29	16	0	3.145793	-0.017392	-0.798229
30	8	0	2.894761	-1.491456	-0.883186
31	6	0	3.746426	0.235511	0.975531
32	9	0	2.808361	-0.224798	1.844812
33	9	0	3.954050	1.542444	1.227798
34	9	0	4.892773	-0.438544	1.189506
35	8	0	4.190365	0.564801	-1.657389

Complex : **PhI** (optimized by B97D/BS1)
E (BS1) = -242.8682329 au
Δ H (BS1) = 0.094736 au
Δ G(BS1) = 0.055835 au

Optimized coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.275446	-1.224418	0.000000
2	6	0	-0.592688	0.000017	0.000000
3	6	0	-1.275456	1.224423	0.000002
4	6	0	-2.680908	1.213889	0.000000
5	6	0	-3.385328	-0.000006	-0.000002
6	6	0	-2.680878	-1.213905	0.000001
7	1	0	-0.730002	-2.167723	0.000006
8	1	0	-0.730059	2.167755	0.000006
9	1	0	-3.219516	2.163807	-0.000005
10	1	0	-4.476732	-0.000035	0.000004
11	1	0	-3.219505	-2.163813	0.000000
12	53	0	1.579623	0.000000	0.000000

Complex : **(*p*-Tol-C≡C-SiMe$_3$)** (optimized by B97D/BS1)
E (BS1) = -756.025566 au
Δ H (BS1) = 0.251490 au
Δ G(BS1) = 0.187430 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.154756	0.002214	-0.002450
2	6	0	-1.386743	0.002866	-0.000851
3	14	0	-3.229548	-0.000083	0.002018
4	6	0	-3.854464	1.797736	0.002759
5	1	0	-4.957899	1.823207	0.005697
6	1	0	-3.501459	2.344617	0.892570
7	1	0	-3.506185	2.343939	-0.889324
8	6	0	-3.854992	-0.900857	-1.554054
9	1	0	-3.494241	-1.942120	-1.586808
10	1	0	-4.958504	-0.924268	-1.571104
11	1	0	-3.512730	-0.396787	-2.472818
12	6	0	-3.850198	-0.899761	1.560679
13	1	0	-4.953652	-0.923944	1.580503
14	1	0	-3.488600	-1.940707	1.593849
15	1	0	-3.506043	-0.394244	2.477942
16	6	0	1.271782	0.001436	-0.003343
17	6	0	1.995844	-1.217100	-0.006288
18	6	0	1.997567	1.218916	-0.006602
19	6	0	3.393735	-1.209400	-0.010319
20	1	0	1.447780	-2.160316	-0.009876
21	6	0	3.395476	1.209158	-0.010627
22	1	0	1.450857	2.162920	-0.010431
23	6	0	4.118307	-0.000637	-0.009044
24	1	0	3.937165	-2.157655	-0.016604
25	1	0	3.940295	2.156611	-0.017157
26	6	0	5.632554	-0.001829	0.021151
27	1	0	6.007470	-0.003644	1.060298
28	1	0	6.041678	-0.894983	-0.476797
29	1	0	6.043076	0.892076	-0.474265

Complex : **(Me-C≡C-SiMe$_3$)** (optimized by B97D/BS1)
E (BS1) = -525.1450748 au
Δ H (BS1) = 0.166810 au
Δ G(BS1) = 0.167755 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.210382	0.000010	-0.000900
2	6	0	0.982448	0.000264	-0.001770
3	14	0	-0.860025	-0.000090	-0.000074
4	6	0	-1.487142	-0.298837	1.772522
5	1	0	-2.590671	-0.302170	1.798185

6	1	0	-1.137161	-1.268424	2.163577
7	1	0	-1.135698	0.488202	2.460011
8	6	0	-1.487684	1.684676	-0.626804
9	1	0	-1.137839	1.885900	-1.652825
10	1	0	-2.591193	1.710117	-0.634515
11	1	0	-1.135169	2.507627	0.016625
12	6	0	-1.489048	-1.385479	-1.144466
13	1	0	-2.592624	-1.404479	-1.160511
14	1	0	-1.138618	-1.240543	-2.179692
15	1	0	-1.139009	-2.374597	-0.805775
16	6	0	3.674164	-0.000420	0.000383
17	1	0	4.073207	-0.972301	-0.337653
18	1	0	4.074030	0.778357	-0.671659
19	1	0	4.072375	0.192292	1.011479

Complex : **(xylene)** (optimized by B97D/BS1)
E (BS1) = -310.6454613 au
Δ H (BS1) = 0.160778 au
Δ G(BS1) = 0.117364 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.426687	0.000067	-0.014712
2	6	0	0.700732	-1.206100	-0.008477
3	6	0	0.701064	1.206184	-0.008632
4	6	0	-0.700960	-1.206013	0.008587
5	1	0	1.241628	-2.156401	-0.014401
6	6	0	-0.700834	1.206271	0.008446
7	1	0	1.242050	2.156427	-0.014679
8	6	0	-1.426686	0.000299	0.014687
9	1	0	-1.241925	-2.156281	0.014616
10	1	0	-1.241750	2.156548	0.014347
11	6	0	-2.942156	-0.000081	-0.004542
12	1	0	-3.328721	-0.023951	-1.039222
13	1	0	-3.348561	-0.881519	0.516822
14	1	0	-3.348282	0.903991	0.476447
15	6	0	2.942156	-0.000242	0.004608
16	1	0	3.348570	0.894533	-0.493346
17	1	0	3.328649	-0.004222	1.039588
18	1	0	3.348333	-0.891437	-0.499964

Complex : **4a**$^{/}$ (optimized by B97D/BS1)
E (BS1) = -1843.4905743 au
Δ H (BS1) = 0.512988 au
Δ G(BS1) = 0.406959 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.049137	-3.240130	-0.828777
2	6	0	-0.741551	-3.821012	-0.242439

3	15	0	0.630828	-2.548735	-0.333612
4	6	0	1.967809	-3.099543	0.806672
5	6	0	1.349657	-2.669012	-2.029431
6	15	0	-2.475754	-1.586344	-0.052961
7	6	0	-3.307158	-2.015755	1.540416
8	6	0	-3.787020	-0.851725	-1.119396
9	1	0	-2.884766	-3.946721	-0.696106
10	1	0	-1.937371	-3.061941	-1.911111
11	1	0	-0.461397	-4.748492	-0.767436
12	1	0	-0.877273	-4.071865	0.822641
13	1	0	2.752490	-2.328758	0.791103
14	1	0	2.387375	-4.070041	0.498866
15	1	0	1.572362	-3.181265	1.830298
16	1	0	0.568547	-2.483456	-2.782023
17	1	0	1.798906	-3.659423	-2.204324
18	1	0	2.119239	-1.888778	-2.124745
19	1	0	-3.606961	-1.096192	2.064226
20	1	0	-4.203912	-2.627167	1.354188
21	1	0	-2.612044	-2.576092	2.183354
22	1	0	-3.382998	-0.694328	-2.130590
23	1	0	-4.670486	-1.507011	-1.172438
24	1	0	-4.066211	0.127428	-0.704309
25	46	0	-0.409607	-0.396576	0.119217
26	6	0	-0.337414	-0.136372	2.241708
27	1	0	-1.359717	-0.356584	2.561282
28	1	0	0.402319	-0.884052	2.544492
29	1	0	-0.024823	0.886526	2.455657
30	6	0	-1.360678	1.454701	0.161666
31	6	0	-0.877799	2.371841	-0.787568
32	6	0	-2.505168	1.757517	0.915514
33	6	0	-1.600978	3.553523	-1.032348
34	1	0	0.047488	2.176685	-1.329577
35	6	0	-3.205778	2.950181	0.671081
36	1	0	-2.868338	1.079034	1.690287
37	6	0	-2.768083	3.864470	-0.309111
38	1	0	-1.231392	4.254623	-1.784669
39	1	0	-4.104073	3.173538	1.252413
40	6	0	-3.505733	5.166593	-0.540687
41	1	0	-4.586748	5.050388	-0.367181
42	1	0	-3.143880	5.947965	0.149987
43	1	0	-3.353413	5.535339	-1.566185
44	6	0	1.430612	0.350112	0.124839
45	6	0	2.618836	0.707678	0.127102
46	14	0	4.385600	1.273912	0.053067
47	6	0	4.807644	2.148057	1.686052
48	1	0	4.171334	3.034440	1.842534
49	1	0	4.674758	1.477120	2.550828
50	1	0	5.858913	2.483267	1.678587
51	6	0	5.478225	-0.269591	-0.178049
52	1	0	5.362380	-0.975866	0.661683
53	1	0	5.230183	-0.802900	-1.111395
54	1	0	6.543881	0.011814	-0.229169
55	6	0	4.580753	2.454012	-1.422826
56	1	0	5.621492	2.813954	-1.491433
57	1	0	4.333860	1.954961	-2.374479
58	1	0	3.925463	3.334504	-1.320099

Complex : **4b**$^{/}$ (optimized by B97D/BS1)
E (BS1) = -1843.4807074 au

Δ H (BS1) = 0.512447 au
Δ G(BS1) = 0.406803 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.891349	-2.792033	1.842005
2	6	0	2.065597	-2.438422	0.900609
3	15	0	1.497156	-2.294021	-0.874015
4	15	0	-0.509719	-1.561042	1.670201
5	1	0	1.236152	-2.829323	2.888166
6	1	0	0.486937	-3.787695	1.594655
7	1	0	2.869234	-3.188105	0.985730
8	1	0	2.485416	-1.453860	1.161425
9	46	0	-0.415422	-0.738044	-0.658918
10	6	0	-0.256230	-0.006937	-2.651844
11	1	0	0.774673	-0.075216	-3.009968
12	1	0	-0.928056	-0.741557	-3.130706
13	1	0	-0.653511	1.010209	-2.696992
14	6	0	-2.063408	0.466499	-0.334065
15	6	0	-3.230183	-0.291034	-0.147377
16	6	0	-2.120180	1.862679	-0.449521
17	6	0	-4.480401	0.358494	-0.141761
18	1	0	-3.190763	-1.377427	-0.021274
19	6	0	-3.372897	2.493876	-0.412289
20	1	0	-1.209061	2.445764	-0.578548
21	6	0	-4.568554	1.756949	-0.264780
22	1	0	-5.390706	-0.233311	-0.020065
23	1	0	-3.423738	3.581235	-0.510782
24	6	0	0.819515	0.724263	-0.359321
25	6	0	1.678256	1.578358	-0.115625
26	6	0	-5.908282	2.462427	-0.238561
27	1	0	-5.923339	3.256482	0.525663
28	1	0	-6.116188	2.942237	-1.209803
29	1	0	-6.727730	1.760739	-0.024245
30	6	0	2.953794	-1.638570	-1.792897
31	1	0	3.856785	-2.236068	-1.592361
32	1	0	2.745099	-1.656100	-2.873281
33	1	0	3.110773	-0.597014	-1.477035
34	6	0	1.272840	-4.039678	-1.455098
35	1	0	0.965403	-4.037976	-2.511763
36	1	0	2.210349	-4.609999	-1.354268
37	1	0	0.484491	-4.532434	-0.866228
38	6	0	-0.072466	-0.155606	2.778534
39	1	0	-0.918616	0.547507	2.795291
40	1	0	0.144504	-0.502485	3.801136
41	1	0	0.793556	0.371948	2.354465
42	6	0	-1.978797	-2.361646	2.457614
43	1	0	-2.829497	-1.666177	2.406609
44	1	0	-2.241550	-3.283107	1.916252
45	1	0	-1.773671	-2.606160	3.511805
46	6	0	4.668874	2.094550	-0.081686
47	1	0	4.755651	1.877240	-1.159428
48	1	0	5.474669	2.800781	0.181391
49	1	0	4.853583	1.158729	0.472577
50	6	0	2.831722	3.147204	2.217230
51	1	0	3.573740	3.897402	2.539462
52	1	0	1.832447	3.525351	2.489368

53	1	0	3.017413	2.226437	2.795808
54	6	0	2.643238	4.420058	-0.641440
55	1	0	2.682897	4.233015	-1.727050
56	1	0	1.653558	4.844478	-0.405246
57	1	0	3.402743	5.184059	-0.402889
58	14	0	2.969391	2.834126	0.347227

Complex : **4c**/ (optimized by B97D/BS1)
E (BS1) = -1843.4899173 au
Δ H (BS1) = 0.512889 au
Δ G(BS1) = 0.408066 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.220488	-2.400052	1.708015
2	6	0	3.308268	-1.457177	1.140479
3	15	0	2.918878	-0.930171	-0.618933
4	15	0	0.490105	-1.727656	1.419548
5	1	0	2.398606	-2.588305	2.779043
6	1	0	2.262056	-3.374423	1.194112
7	1	0	4.296403	-1.945375	1.171731
8	1	0	3.380754	-0.542267	1.750071
9	46	0	0.564125	-0.524331	-0.707051
10	6	0	0.664957	0.168978	-2.718223
11	1	0	1.416685	0.958363	-2.826800
12	1	0	0.940753	-0.748685	-3.263963
13	1	0	-0.337802	0.514482	-2.986695
14	6	0	0.633980	1.508410	-0.214514
15	6	0	-0.191445	2.451235	-0.828828
16	6	0	1.494601	1.846978	0.830097
17	6	0	-0.129142	3.781408	-0.378111
18	1	0	-0.884902	2.169209	-1.615666
19	6	0	1.537494	3.189105	1.261076
20	1	0	2.123067	1.110744	1.326896
21	6	0	0.733259	4.174724	0.664585
22	1	0	-0.780723	4.520856	-0.849775
23	1	0	2.212864	3.456929	2.077124
24	6	0	-1.412284	-0.437810	-0.625136
25	6	0	-2.640601	-0.392524	-0.448677
26	14	0	-4.481327	-0.342684	-0.214087
27	6	0	-5.250055	0.760721	-1.554340
28	1	0	-6.344590	0.818446	-1.426978
29	1	0	-4.851499	1.787663	-1.505895
30	1	0	-5.049170	0.365518	-2.563702
31	6	0	-4.805019	0.379892	1.518319
32	1	0	-5.889629	0.447571	1.709755
33	1	0	-4.364765	-0.251360	2.308625
34	1	0	-4.382071	1.393354	1.616105
35	6	0	-5.152842	-2.117628	-0.329821
36	1	0	-4.712243	-2.769756	0.443009
37	1	0	-6.246985	-2.122498	-0.188066
38	1	0	-4.939115	-2.564807	-1.314471
39	6	0	-0.652964	-3.169459	1.531618
40	1	0	-0.642979	-3.616182	2.538156
41	1	0	-1.663206	-2.808387	1.288312

42	1	0	-0.366419	-3.929172	0.789077
43	6	0	4.101022	0.418550	-1.037869
44	1	0	5.138830	0.124167	-0.817344
45	1	0	4.009900	0.644922	-2.110928
46	1	0	3.834813	1.320604	-0.469044
47	6	0	3.413110	-2.373262	-1.664176
48	1	0	3.223778	-2.136513	-2.721737
49	1	0	4.481097	-2.608647	-1.532185
50	1	0	2.810801	-3.253053	-1.392215
51	6	0	0.053972	-0.661402	2.858537
52	1	0	-0.969346	-0.291039	2.695808
53	1	0	0.100348	-1.227493	3.802220
54	1	0	0.725909	0.205918	2.907309
55	6	0	0.791154	5.617877	1.120576
56	1	0	-0.220722	6.021666	1.282966
57	1	0	1.358980	5.719712	2.057133
58	1	0	1.276855	6.250652	0.358679

Complex : **4a'_TS2** (optimized by B97D/BS1)
E (BS1) = -1843.4836891 au
Δ H (BS1) = 0.511442 au
Δ G(BS1) = 0.405978 au
Imaginary frequency = -252.5i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.107519	-3.154189	-0.954432
2	6	0	-0.933860	-3.835433	-0.210852
3	15	0	0.543730	-2.684347	-0.111577
4	6	0	1.693499	-3.400441	1.140793
5	6	0	1.424479	-2.854344	-1.726456
6	15	0	-2.469339	-1.455050	-0.248674
7	6	0	-3.506256	-1.746445	1.250561
8	6	0	-3.567837	-0.600384	-1.452677
9	1	0	-3.010308	-3.785431	-0.919767
10	1	0	-1.849791	-3.004035	-2.015933
11	1	0	-0.662833	-4.781316	-0.707480
12	1	0	-1.225202	-4.079126	0.824438
13	1	0	2.572522	-2.741644	1.210237
14	1	0	2.017719	-4.414745	0.859994
15	1	0	1.200150	-3.434161	2.123907
16	1	0	0.746310	-2.575004	-2.546916
17	1	0	1.786037	-3.882948	-1.883648
18	1	0	2.274892	-2.156459	-1.728143
19	1	0	-3.766721	-0.773325	1.691151
20	1	0	-4.430958	-2.286169	0.991675
21	1	0	-2.936176	-2.329271	1.989041
22	1	0	-3.028217	-0.460218	-2.400697
23	1	0	-4.490435	-1.174616	-1.630199
24	1	0	-3.811938	0.391392	-1.045563
25	46	0	-0.357911	-0.461211	0.204703
26	6	0	0.302513	0.145106	2.261353
27	1	0	-0.671893	-0.231232	2.601579
28	1	0	1.144879	-0.433840	2.638214
29	1	0	0.398363	1.224590	2.368273

30	6	0	-1.345863	1.378683	0.174411
31	6	0	-1.121707	2.163373	-0.967462
32	6	0	-2.267394	1.793402	1.144151
33	6	0	-1.844578	3.357479	-1.139189
34	1	0	-0.387355	1.861588	-1.717044
35	6	0	-2.982126	2.992372	0.961652
36	1	0	-2.441974	1.199186	2.044975
37	6	0	-2.783824	3.789768	-0.181523
38	1	0	-1.666109	3.966297	-2.029340
39	1	0	-3.703314	3.309439	1.719483
40	6	0	-3.531048	5.095600	-0.361125
41	1	0	-3.733949	5.297385	-1.424287
42	1	0	-4.488878	5.086523	0.181370
43	1	0	-2.938693	5.942304	0.027051
44	6	0	1.461465	0.289236	0.360973
45	6	0	2.624407	0.705885	0.228846
46	14	0	4.335371	1.344966	-0.127118
47	6	0	5.091295	1.922578	1.518013
48	1	0	4.500857	2.737918	1.966691
49	1	0	5.154789	1.101532	2.250853
50	1	0	6.113792	2.300832	1.347763
51	6	0	5.348200	-0.081577	-0.874186
52	1	0	5.423059	-0.933303	-0.177381
53	1	0	4.897963	-0.444697	-1.813531
54	1	0	6.374419	0.251490	-1.104921
55	6	0	4.183226	2.784693	-1.355046
56	1	0	5.179989	3.191651	-1.596460
57	1	0	3.714071	2.461128	-2.298830
58	1	0	3.575338	3.603279	-0.936306

Complex : **4a'_TS3** (optimized by B97D/BS1)
E (BS1) = -1843.4886584 au
Δ H (BS1) = 0.512104 au
Δ G(BS1) = 0.408799 au
Imaginary frequency = -160.6i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.983898	-3.297553	-0.786102
2	6	0	-0.605919	-3.797582	-0.309840
3	15	0	0.661083	-2.424534	-0.426722
4	6	0	2.110297	-2.962336	0.569678
5	6	0	1.235193	-2.369344	-2.176085
6	15	0	-2.460861	-1.673423	0.027671
7	6	0	-3.223184	-2.153420	1.642661
8	6	0	-3.853318	-1.069224	-1.025125
9	1	0	-2.762997	-4.054101	-0.597806
10	1	0	-1.966124	-3.108470	-1.872062
11	1	0	-0.282615	-4.673648	-0.895534
12	1	0	-0.648574	-4.103882	0.748261
13	1	0	2.864341	-2.165016	0.519825
14	1	0	2.521417	-3.907263	0.180424
15	1	0	1.805621	-3.097733	1.618058
16	1	0	0.383909	-2.166638	-2.842713
17	1	0	1.715801	-3.316858	-2.466987

18	1	0	1.953031	-1.540827	-2.261733
19	1	0	-3.562487	-1.252445	2.175108
20	1	0	-4.082758	-2.825087	1.490748
21	1	0	-2.468729	-2.657382	2.264971
22	1	0	-3.474128	-0.885204	-2.041378
23	1	0	-4.660640	-1.817550	-1.063802
24	1	0	-4.239606	-0.121652	-0.628191
25	46	0	-0.439917	-0.415411	0.208299
26	6	0	-0.540307	0.461551	2.244271
27	1	0	-1.562683	0.448799	2.623732
28	1	0	0.073729	-0.369450	2.616311
29	1	0	-0.034707	1.420236	2.357395
30	6	0	-1.406252	1.470047	0.301945
31	6	0	-0.693972	2.504905	-0.332318
32	6	0	-2.756084	1.661480	0.650739
33	6	0	-1.378286	3.668199	-0.723190
34	1	0	0.371014	2.401748	-0.531592
35	6	0	-3.419633	2.833960	0.266415
36	1	0	-3.293771	0.914794	1.237200
37	6	0	-2.745261	3.852744	-0.439562
38	1	0	-0.826779	4.456675	-1.240632
39	1	0	-4.470937	2.967870	0.532957
40	6	0	-3.470280	5.108694	-0.870526
41	1	0	-2.777378	5.958490	-0.962268
42	1	0	-3.947519	4.962941	-1.855591
43	1	0	-4.263995	5.377922	-0.156914
44	6	0	1.436021	0.273543	0.166686
45	6	0	2.623627	0.625376	0.121581
46	14	0	4.394805	1.173782	0.055043
47	6	0	4.704301	2.415851	1.458292
48	1	0	4.060373	3.304998	1.356483
49	1	0	4.506224	1.965226	2.444854
50	1	0	5.753623	2.756960	1.448269
51	6	0	5.484957	-0.372674	0.282854
52	1	0	5.288886	-0.866490	1.249609
53	1	0	5.315890	-1.110312	-0.520104
54	1	0	6.553631	-0.099196	0.261323
55	6	0	4.725668	1.968828	-1.639115
56	1	0	5.778013	2.292533	-1.711723
57	1	0	4.534629	1.261827	-2.463592
58	1	0	4.089847	2.855243	-1.799042

Complex : **4b'_TS1** (optimized by B97D/BS1)
E (BS1) = -1843.4770799 au
Δ H (BS1) = 0.511728 au
Δ G(BS1) = 0.407396 au
Imaginary frequency = -105.6i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.090522	-0.685149	1.973012
2	6	0	3.576767	0.512747	1.128013
3	15	0	3.055238	0.340285	-0.662848
4	15	0	1.240884	-0.907287	1.776479
5	1	0	3.351645	-0.538189	3.033815

6	1	0	3.575591	-1.617230	1.638288
7	1	0	4.671985	0.619401	1.191385
8	1	0	3.131017	1.449678	1.499750
9	46	0	0.774707	-0.487429	-0.596659
10	6	0	0.610641	-0.008115	-2.681132
11	1	0	0.997505	0.997431	-2.873767
12	1	0	1.224031	-0.790168	-3.158912
13	1	0	-0.447263	-0.081569	-2.948525
14	6	0	-1.120238	-1.394415	-0.485344
15	6	0	-1.334794	-2.264051	-1.564225
16	6	0	-1.967009	-1.417142	0.635279
17	6	0	-2.350994	-3.235337	-1.463174
18	1	0	-0.720206	-2.228761	-2.462443
19	6	0	-2.983942	-2.377705	0.705487
20	1	0	-1.852854	-0.684478	1.431205
21	6	0	-3.190318	-3.306525	-0.338553
22	1	0	-2.495416	-3.933984	-2.290311
23	1	0	-3.637095	-2.397990	1.581553
24	6	0	-0.540937	0.944295	-0.436362
25	6	0	-1.267088	1.927763	-0.253872
26	6	0	0.526928	0.426344	2.839017
27	1	0	-0.569741	0.369385	2.825349
28	1	0	0.886561	0.335947	3.876262
29	1	0	0.811595	1.403029	2.423451
30	6	0	0.826184	-2.499161	2.614532
31	1	0	-0.254817	-2.675214	2.514582
32	1	0	1.358788	-3.323617	2.116995
33	1	0	1.102314	-2.474540	3.680423
34	6	0	3.211495	2.031534	-1.380402
35	1	0	4.177858	2.489288	-1.117141
36	1	0	3.129925	1.969716	-2.475271
37	1	0	2.384106	2.650242	-1.002446
38	6	0	4.383774	-0.669226	-1.463786
39	1	0	4.141843	-0.811760	-2.527752
40	1	0	5.361734	-0.169016	-1.380082
41	1	0	4.439203	-1.658315	-0.984601
42	6	0	-4.309863	-4.321707	-0.255136
43	1	0	-5.293054	-3.825884	-0.322455
44	1	0	-4.245405	-5.058435	-1.069113
45	1	0	-4.283800	-4.861840	0.705220
46	14	0	-2.303283	3.418836	0.134396
47	6	0	-2.921388	3.233484	1.924809
48	1	0	-3.550579	4.094172	2.208745
49	1	0	-3.529122	2.321115	2.045635
50	1	0	-2.082671	3.183979	2.639743
51	6	0	-3.759547	3.462891	-1.082062
52	1	0	-4.407551	4.331671	-0.874722
53	1	0	-3.410442	3.542906	-2.124472
54	1	0	-4.376505	2.553175	-0.999534
55	6	0	-1.218659	4.970727	-0.037178
56	1	0	-1.803987	5.878032	0.189934
57	1	0	-0.362414	4.943262	0.657635
58	1	0	-0.824367	5.074095	-1.061643

Complex : **4c'_TS1** (optimized by B97D/BS1)
E (BS1) = -1843.4849162 au
Δ H (BS1) = 0.511744 au
Δ G(BS1) = 0.408686 au
Imaginary frequency = -184.6i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.840931	-2.099512	1.484367
2	6	0	3.571239	-0.775644	1.157167
3	15	0	3.107810	-0.139957	-0.546554
4	6	0	3.605288	1.633729	-0.567367
5	6	0	4.241788	-1.005608	-1.720700
6	15	0	0.988585	-1.909538	1.231478
7	6	0	0.280248	-1.488280	2.888880
8	6	0	0.334915	-3.600086	0.879615
9	1	0	3.069070	-2.422622	2.512879
10	1	0	3.179410	-2.900740	0.806468
11	1	0	4.663973	-0.901446	1.231691
12	1	0	3.278652	0.010810	1.872428
13	1	0	3.463683	2.032014	-1.583188
14	1	0	4.657216	1.762853	-0.268158
15	1	0	2.945148	2.186451	0.117051
16	1	0	4.088580	-2.092943	-1.648022
17	1	0	5.294485	-0.770519	-1.498275
18	1	0	4.010611	-0.690245	-2.748949
19	1	0	-0.762602	-1.165579	2.751954
20	1	0	0.311264	-2.362997	3.557371
21	1	0	0.847594	-0.667081	3.351385
22	1	0	0.780629	-3.981064	-0.051391
23	1	0	0.550597	-4.297766	1.704214
24	1	0	-0.752966	-3.519640	0.734883
25	46	0	0.762460	-0.432083	-0.717272
26	6	0	0.807394	0.329475	-2.702765
27	1	0	1.276645	1.319636	-2.731431
28	1	0	1.385491	-0.418863	-3.266762
29	1	0	-0.238029	0.362605	-3.028636
30	6	0	-0.123795	1.421499	-0.097804
31	6	0	-0.670727	2.377095	-0.955805
32	6	0	0.190497	1.708054	1.230626
33	6	0	-0.835992	3.683935	-0.470544
34	1	0	-0.971941	2.126850	-1.969262
35	6	0	0.026987	3.031384	1.687394
36	1	0	0.561350	0.940981	1.904915
37	6	0	-0.484747	4.036877	0.849213
38	1	0	-1.258586	4.438943	-1.137727
39	1	0	0.289131	3.267305	2.721411
40	6	0	-0.666117	5.456756	1.343456
41	1	0	-0.501758	5.527700	2.428724
42	1	0	0.043748	6.139748	0.846691
43	1	0	-1.680531	5.825509	1.122535
44	6	0	-1.210564	-0.540788	-0.577266
45	6	0	-2.438049	-0.695296	-0.452348
46	14	0	-4.272374	-0.929207	-0.267591
47	6	0	-5.082330	-0.808390	-1.979483
48	1	0	-4.897472	0.175739	-2.440468
49	1	0	-4.696336	-1.581920	-2.663482
50	1	0	-6.174471	-0.943837	-1.899639
51	6	0	-4.581217	-2.634198	0.515570
52	1	0	-4.192081	-3.446570	-0.120571
53	1	0	-4.103494	-2.714935	1.506467
54	1	0	-5.662758	-2.805050	0.650915
55	6	0	-4.882992	0.460950	0.879610

56	1	0	-5.975901	0.390302	1.013896
57	1	0	-4.414853	0.397007	1.875661
58	1	0	-4.655917	1.454805	0.460483

Complex : **(OTf)** (optimized by B97D/BS1)
E (BS1) = -961.1989929 au
Δ H (BS1) = 0.034239 au
Δ G(BS1) = -0.006864 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.262010	1.384850	-0.460872
2	16	0	-0.945741	-0.000125	-0.000071
3	8	0	-1.262360	-0.292855	1.429729
4	6	0	0.958741	0.000029	-0.000219
5	9	0	1.469682	0.946517	0.839866
6	9	0	1.469610	0.253962	-1.239638
7	9	0	1.469602	-1.200956	0.399670
8	8	0	-1.263208	-1.091228	-0.968435

Complex : **4a**$^{//}$ (optimized by B97D/BS1)
E (BS1) = -2036.5527623 au
Δ H (BS1) = 0.604494 au
Δ G(BS1) = 0.485497 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.053358	-3.272312	0.398770
2	6	0	0.793062	-3.851100	-0.283791
3	15	0	-0.592863	-2.590495	-0.239648
4	15	0	2.515597	-1.601190	-0.305380
5	1	0	2.903730	-3.967930	0.306795
6	1	0	1.867610	-3.103481	1.471094
7	1	0	0.489447	-4.794358	0.198257
8	1	0	0.999116	-4.074125	-1.343684
9	46	0	0.448763	-0.387906	-0.393923
10	6	0	0.424073	-0.174737	-2.497181
11	1	0	1.469200	-0.089712	-2.808237
12	1	0	-0.063142	-1.085594	-2.863894
13	1	0	-0.150313	0.723725	-2.732382
14	6	0	1.298444	1.532013	-0.485106
15	6	0	0.554866	2.637644	-0.033532
16	6	0	2.602652	1.748552	-0.962067
17	6	0	1.145307	3.911735	0.023561
18	1	0	-0.488405	2.515599	0.250637
19	6	0	3.183808	3.027382	-0.908504
20	1	0	3.183297	0.936931	-1.403516
21	6	0	2.471225	4.128440	-0.398809
22	1	0	0.552339	4.757405	0.382641
23	1	0	4.201905	3.170402	-1.280355

24	6	0	-1.444221	0.265340	-0.413158
25	6	0	-2.649182	0.553333	-0.404565
26	6	0	0.301718	0.078753	2.974169
27	8	0	0.742103	-0.581916	2.019678
28	6	0	0.758965	-0.245118	4.379624
29	1	0	-0.109844	-0.574788	4.975537
30	1	0	1.531019	-1.025781	4.380560
31	1	0	1.138562	0.669677	4.865452
32	6	0	-0.668793	1.214448	2.798452
33	1	0	-1.361536	0.999713	1.972897
34	1	0	-1.206002	1.439712	3.730707
35	1	0	-0.086883	2.105876	2.505952
36	14	0	-4.435334	1.036453	-0.335725
37	6	0	3.105543	5.500781	-0.310839
38	1	0	2.362455	6.295325	-0.480431
39	1	0	3.543400	5.668515	0.688923
40	1	0	3.913772	5.616631	-1.049021
41	6	0	-4.701560	2.588555	-1.397039
42	1	0	-5.759626	2.900639	-1.372083
43	1	0	-4.091869	3.431997	-1.032972
44	1	0	-4.428684	2.405297	-2.449371
45	6	0	-4.884522	1.381295	1.482745
46	1	0	-5.944805	1.673223	1.571594
47	1	0	-4.729810	0.490146	2.114549
48	1	0	-4.276510	2.202374	1.898464
49	6	0	-5.469864	-0.417215	-1.000771
50	1	0	-5.208746	-0.650375	-2.046756
51	1	0	-5.318301	-1.329846	-0.399404
52	1	0	-6.545888	-0.174852	-0.972316
53	6	0	-1.783961	-3.048145	-1.567946
54	1	0	-2.229475	-4.039110	-1.389449
55	1	0	-2.569808	-2.278609	-1.584443
56	1	0	-1.273124	-3.051708	-2.542349
57	6	0	-1.497371	-2.862660	1.343594
58	1	0	-2.281448	-2.094204	1.411794
59	1	0	-1.950426	-3.865704	1.381832
60	1	0	-0.801101	-2.734951	2.183808
61	6	0	3.832287	-0.971799	0.820242
62	1	0	4.684738	-1.667931	0.862810
63	1	0	4.168780	0.014429	0.472215
64	1	0	3.390705	-0.857113	1.819758
65	6	0	3.344353	-1.980219	-1.911887
66	1	0	3.680253	-1.049757	-2.392688
67	1	0	4.215976	-2.634591	-1.754280
68	1	0	2.632066	-2.478955	-2.585822

Complex : **4b**$^{//}$ (optimized by B97D/BS1)
E (BS1) = -2036.5469993 au
Δ H (BS1) = 0.604664 au
Δ G(BS1) = 0.488755 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.604351	-2.523238	2.188804
2	6	0	1.659245	-2.748170	1.084577

3	15	0	0.881018	-2.589362	-0.600395
4	15	0	-0.218884	-0.844820	2.029057
5	1	0	1.065513	-2.612668	3.185953
6	1	0	-0.187314	-3.288772	2.125556
7	1	0	2.142501	-3.732072	1.200890
8	1	0	2.439264	-1.971826	1.131783
9	46	0	-0.373371	-0.457593	-0.482944
10	6	0	-0.227813	-0.236425	-2.601615
11	1	0	0.749161	-0.599125	-2.933651
12	1	0	-1.057271	-0.865806	-2.954439
13	1	0	-0.362256	0.823548	-2.830701
14	6	0	-1.334087	1.400207	-0.377447
15	6	0	-2.377126	1.655232	-1.280147
16	6	0	-1.031130	2.343529	0.616321
17	6	0	-3.153471	2.820621	-1.144550
18	1	0	-2.608922	0.950404	-2.080100
19	6	0	-1.813363	3.504294	0.742160
20	1	0	-0.179443	2.192606	1.277329
21	6	0	-2.888749	3.760820	-0.130906
22	1	0	-3.971182	3.004557	-1.846872
23	1	0	-1.573123	4.228975	1.524881
24	6	0	1.334166	0.457502	-0.447849
25	6	0	2.474108	0.928700	-0.376191
26	6	0	-3.456163	-1.451938	-0.385400
27	8	0	-2.292810	-1.600084	-0.799400
28	6	0	-4.546880	-2.340947	-0.937861
29	1	0	-5.379478	-1.719769	-1.308485
30	1	0	-4.165272	-2.982872	-1.741822
31	1	0	-4.959855	-2.962918	-0.125067
32	6	0	-3.854838	-0.423499	0.638275
33	1	0	-4.398767	0.386655	0.124019
34	1	0	-4.545458	-0.866462	1.373809
35	1	0	-2.979084	0.020603	1.118011
36	14	0	4.175065	1.643610	-0.219113
37	6	0	0.962131	0.290958	2.889151
38	1	0	0.447837	1.229248	3.142430
39	1	0	1.334296	-0.172312	3.816518
40	1	0	1.794898	0.521385	2.210704
41	6	0	-1.635890	-0.966467	3.224078
42	1	0	-2.136885	0.010200	3.297397
43	1	0	-2.364719	-1.711873	2.873833
44	1	0	-1.274185	-1.257171	4.223196
45	6	0	-0.068326	-4.158399	-0.849114
46	1	0	-0.852895	-4.234302	-0.082189
47	1	0	-0.555720	-4.133137	-1.834856
48	1	0	0.589829	-5.039946	-0.789950
49	6	0	2.289311	-2.645832	-1.785657
50	1	0	1.904161	-2.708398	-2.814293
51	1	0	2.858581	-1.711417	-1.673135
52	1	0	2.941616	-3.511969	-1.593028
53	6	0	4.264322	3.254409	-1.217816
54	1	0	3.536115	3.994309	-0.847017
55	1	0	5.270121	3.702481	-1.145575
56	1	0	4.049506	3.075471	-2.284147
57	6	0	4.506907	1.975645	1.626655
58	1	0	4.468923	1.048084	2.223068
59	1	0	5.508482	2.417139	1.765401
60	1	0	3.770812	2.681236	2.046820
61	6	0	5.414561	0.361468	-0.885717
62	1	0	6.447712	0.739690	-0.802915
63	1	0	5.361436	-0.585912	-0.322410

64	1	0	5.226318	0.136882	-1.949045
65	6	0	-3.702969	5.032449	-0.009002
66	1	0	-3.170514	5.883726	-0.467251
67	1	0	-4.674680	4.936478	-0.516815
68	1	0	-3.885207	5.291671	1.045947

Complex : **4c**$^{//}$ (optimized by B97D/BS1)
E (BS1) = -2036.5540507 au
Δ H (BS1) = 0.604359 au
Δ G(BS1) = 0.487669 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.045572	-1.856340	2.280749
2	6	0	3.246497	-1.368443	1.436159
3	15	0	2.784352	-1.175244	-0.374379
4	15	0	0.506966	-0.821483	1.988983
5	1	0	2.314724	-1.886480	3.349155
6	1	0	1.767402	-2.878367	1.976770
7	1	0	4.089181	-2.073891	1.524722
8	1	0	3.604746	-0.392139	1.798552
9	46	0	0.517725	-0.399822	-0.424800
10	6	0	0.577937	-0.231968	-2.551842
11	1	0	1.370213	0.467909	-2.840470
12	1	0	0.778435	-1.248630	-2.921158
13	1	0	-0.406027	0.131404	-2.866312
14	6	0	1.025968	1.610393	-0.378091
15	6	0	0.352396	2.538082	-1.184177
16	6	0	2.046021	2.032947	0.480795
17	6	0	0.720128	3.891787	-1.125569
18	1	0	-0.456803	2.220986	-1.836868
19	6	0	2.403568	3.394936	0.524195
20	1	0	2.579321	1.332694	1.120815
21	6	0	1.749190	4.345604	-0.276176
22	1	0	0.184905	4.607721	-1.754406
23	1	0	3.205782	3.711095	1.195697
24	6	0	-1.392965	0.175730	-0.279458
25	6	0	-2.571172	0.513427	-0.099302
26	6	0	-1.082557	-3.255204	-1.001054
27	8	0	-0.093154	-2.713713	-0.476292
28	6	0	-1.455828	-4.664623	-0.602174
29	1	0	-1.439793	-5.315354	-1.493098
30	1	0	-0.777524	-5.060199	0.165086
31	1	0	-2.496276	-4.672435	-0.233001
32	6	0	-1.955898	-2.556490	-2.005569
33	1	0	-1.337819	-2.047247	-2.756248
34	1	0	-2.663743	-3.244705	-2.486899
35	1	0	-2.503913	-1.758295	-1.474067
36	14	0	-4.337745	1.010559	0.135144
37	6	0	-4.461677	2.053264	1.721838
38	1	0	-3.830884	2.955217	1.655455
39	1	0	-5.501372	2.381179	1.892377
40	1	0	-4.141539	1.479816	2.608133
41	6	0	-4.906807	2.017188	-1.372664
42	1	0	-4.832159	1.427179	-2.301289
43	1	0	-5.958245	2.331350	-1.256970

44	1	0	-4.295846	2.926260	-1.499836
45	6	0	-5.381403	-0.574921	0.305592
46	1	0	-6.445076	-0.326592	0.461174
47	1	0	-5.315389	-1.200299	-0.600965
48	1	0	-5.052013	-1.184201	1.164394
49	6	0	-0.903107	-1.857279	2.571723
50	1	0	-0.857747	-2.033770	3.657651
51	1	0	-1.832063	-1.327100	2.313759
52	1	0	-0.884079	-2.815982	2.036176
53	6	0	0.539680	0.600706	3.162136
54	1	0	-0.359714	1.206181	2.972915
55	1	0	0.535605	0.248551	4.205752
56	1	0	1.417500	1.235318	2.986809
57	6	0	4.111120	-0.159579	-1.148925
58	1	0	4.041718	0.873821	-0.783388
59	1	0	5.106758	-0.574870	-0.927537
60	1	0	3.956316	-0.154804	-2.238315
61	6	0	2.992784	-2.864060	-1.089238
62	1	0	2.766240	-2.829112	-2.164979
63	1	0	4.023696	-3.224412	-0.947102
64	1	0	2.283035	-3.548235	-0.606387
65	6	0	2.129820	5.810942	-0.232223
66	1	0	2.474539	6.159334	-1.219962
67	1	0	1.265707	6.435189	0.048969
68	1	0	2.935110	5.993920	0.494646

Complex : **4a$^{//}$_TS2** (optimized by B97D/BS1)
E (BS1) = -2036.5379584 au
Δ H (BS1) = 0.604359 au
Δ G(BS1) = 0.487669 au
Imaginary frequency = -327.8i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.089482	-3.170607	0.764796
2	6	0	0.908563	-3.893435	0.078611
3	15	0	-0.543120	-2.728235	-0.136171
4	15	0	2.478162	-1.560346	-0.102261
5	1	0	2.981859	-3.817361	0.787810
6	1	0	1.829064	-2.901587	1.798480
7	1	0	0.610392	-4.783250	0.656381
8	1	0	1.199106	-4.235923	-0.928457
9	46	0	0.374056	-0.529607	-0.518901
10	6	0	-0.402850	-0.033004	-2.593235
11	1	0	0.587513	-0.379111	-2.918306
12	1	0	-1.208823	-0.676204	-2.945765
13	1	0	-0.543045	1.030211	-2.783545
14	6	0	1.282692	1.353994	-0.645927
15	6	0	0.735159	2.382501	0.139112
16	6	0	2.398675	1.630122	-1.451407
17	6	0	1.337585	3.653811	0.156835
18	1	0	-0.174326	2.210343	0.713794
19	6	0	2.990368	2.906012	-1.434005
20	1	0	2.817837	0.864673	-2.108979
21	6	0	2.477951	3.934752	-0.620121
22	1	0	0.897160	4.446711	0.767941

23	1	0	3.859715	3.104138	-2.066652
24	6	0	-1.467114	0.170398	-0.758896
25	6	0	-2.639341	0.548070	-0.592202
26	6	0	0.464259	0.420945	2.926427
27	8	0	0.824099	-0.680757	2.500601
28	6	0	1.452134	1.412949	3.504099
29	1	0	1.051322	1.884262	4.415938
30	1	0	2.418754	0.935504	3.712173
31	1	0	1.595441	2.214748	2.757394
32	6	0	-0.997727	0.835343	2.883170
33	1	0	-1.449327	0.523321	1.930411
34	1	0	-1.530201	0.315928	3.699197
35	1	0	-1.127130	1.917740	3.028678
36	6	0	-1.622722	-3.480695	-1.430722
37	1	0	-1.959710	-4.488507	-1.141588
38	1	0	-2.499634	-2.829384	-1.565710
39	1	0	-1.076583	-3.539311	-2.384399
40	6	0	-1.522134	-2.823661	1.422811
41	1	0	-2.415044	-2.192388	1.301513
42	1	0	-1.824627	-3.859342	1.644887
43	1	0	-0.913528	-2.411494	2.238964
44	6	0	3.732238	-0.701244	0.930635
45	1	0	4.653118	-1.298706	1.019156
46	1	0	3.956556	0.272537	0.472266
47	1	0	3.286122	-0.538641	1.920463
48	6	0	3.359042	-2.070803	-1.648099
49	1	0	3.647323	-1.179257	-2.223186
50	1	0	4.265356	-2.648995	-1.407331
51	1	0	2.688995	-2.685344	-2.267865
52	6	0	3.135461	5.299079	-0.580229
53	1	0	3.593995	5.550045	-1.549113
54	1	0	2.408277	6.085375	-0.325800
55	1	0	3.935351	5.329663	0.180413
56	14	0	-4.362573	1.136006	-0.219865
57	6	0	-5.568392	0.138235	-1.298096
58	1	0	-5.493082	-0.943393	-1.096467
59	1	0	-6.607790	0.445897	-1.092279
60	1	0	-5.378744	0.299453	-2.372094
61	6	0	-4.684813	0.805574	1.627569
62	1	0	-3.981768	1.364971	2.266220
63	1	0	-5.706930	1.120673	1.898109
64	1	0	-4.589698	-0.265834	1.871425
65	6	0	-4.469271	2.990809	-0.603724
66	1	0	-3.752199	3.568730	0.002395
67	1	0	-4.254415	3.193669	-1.665702
68	1	0	-5.481091	3.373172	-0.385967

Complex : **4a$^{//}$_TS3** (optimized by B97D/BS1)
E (BS1) = -2036.5462887 au
Δ H (BS1) = 0.603676 au
Δ G(BS1) = 0.487846 au
Imaginary frequency = -216.6i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.887025	-3.303400	0.758741

2	6	0	0.576796	-3.880640	0.194332
3	15	0	-0.724808	-2.541224	0.067842
4	15	0	2.420012	-1.769128	-0.168407
5	1	0	2.693013	-4.055057	0.733272
6	1	0	1.748919	-2.981611	1.801757
7	1	0	0.208156	-4.708086	0.822079
8	1	0	0.730176	-4.278175	-0.822590
9	46	0	0.398762	-0.537907	-0.548196
10	6	0	0.685293	0.111972	-2.659604
11	1	0	1.723415	0.202615	-2.981304
12	1	0	0.240679	-0.852131	-2.945665
13	1	0	0.054528	0.947038	-2.963807
14	6	0	1.268562	1.378830	-0.875362
15	6	0	0.436417	2.497748	-0.672010
16	6	0	2.663579	1.564544	-0.933451
17	6	0	1.007970	3.752451	-0.409175
18	1	0	-0.646355	2.388726	-0.705963
19	6	0	3.223001	2.821105	-0.668527
20	1	0	3.320527	0.740315	-1.210361
21	6	0	2.405608	3.936008	-0.388982
22	1	0	0.352161	4.608598	-0.233042
23	1	0	4.308180	2.944580	-0.701810
24	6	0	-1.496167	0.099722	-0.615689
25	6	0	-2.682363	0.445771	-0.511833
26	6	0	0.667864	0.577294	2.657547
27	8	0	0.977067	-0.611912	2.522661
28	6	0	1.702583	1.682777	2.641038
29	1	0	1.673169	2.227806	3.600200
30	1	0	2.710312	1.286429	2.467732
31	1	0	1.446262	2.407655	1.851412
32	6	0	-0.781731	1.003055	2.804185
33	1	0	-1.216101	1.066095	1.789712
34	1	0	-1.348778	0.244924	3.362583
35	1	0	-0.879267	1.986487	3.286832
36	6	0	3.011781	5.288498	-0.087303
37	1	0	3.220734	5.389132	0.992464
38	1	0	3.964634	5.428048	-0.620265
39	1	0	2.328969	6.104228	-0.368648
40	6	0	3.227091	-2.393618	-1.712546
41	1	0	3.602848	-1.546160	-2.305356
42	1	0	4.067789	-3.065045	-1.477148
43	1	0	2.486383	-2.934706	-2.319684
44	6	0	3.797474	-1.134797	0.886643
45	1	0	4.272147	-0.254357	0.435297
46	1	0	3.358420	-0.854474	1.853380
47	1	0	4.551582	-1.925329	1.028219
48	6	0	-1.961056	-3.154333	-1.151465
49	1	0	-2.390709	-4.113801	-0.822241
50	1	0	-2.748686	-2.393998	-1.240373
51	1	0	-1.480241	-3.285265	-2.132314
52	6	0	-1.593500	-2.478866	1.685570
53	1	0	-2.420425	-1.760808	1.592523
54	1	0	-1.984187	-3.472992	1.954819
55	1	0	-0.888134	-2.115878	2.444445
56	14	0	-4.412531	1.039780	-0.210833
57	6	0	-5.125398	0.004611	1.221261
58	1	0	-6.152537	0.326570	1.463244
59	1	0	-5.165807	-1.067665	0.964566
60	1	0	-4.518262	0.114031	2.136018
61	6	0	-4.327079	2.874230	0.282189
62	1	0	-3.708511	3.015308	1.184632

63	1	0	-3.894076	3.486760	-0.526169
64	1	0	-5.333912	3.269204	0.500143
65	6	0	-5.444584	0.800527	-1.787081
66	1	0	-6.479139	1.149609	-1.627928
67	1	0	-5.023917	1.368735	-2.632958
68	1	0	-5.491151	-0.260891	-2.082703

Complex : **4b$^{//}$_TS1** (optimized by B97D/BS1)
E (BS1) = -2036.5386066 au
Δ H (BS1) = 0.603009 au
Δ G(BS1) = 0.485754 au
Imaginary frequency = -245.2i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.510264	-2.925367	2.000541
2	6	0	0.371533	-3.439503	0.844727
3	15	0	-0.254186	-2.784979	-0.787071
4	15	0	-0.592337	-1.054961	1.978413
5	1	0	-0.122997	-3.272128	2.972503
6	1	0	-1.540596	-3.304892	1.900436
7	1	0	0.411992	-4.541016	0.835755
8	1	0	1.401797	-3.062802	0.950561
9	46	0	-0.604707	-0.417557	-0.425961
10	6	0	-0.650717	-0.242819	-2.556583
11	1	0	-1.098314	-1.152604	-2.976507
12	1	0	-1.283876	0.627171	-2.760814
13	1	0	0.375946	-0.093004	-2.907525
14	6	0	-0.284013	1.702724	-0.191674
15	6	0	-0.113770	2.553911	-1.301288
16	6	0	-0.614225	2.272429	1.052242
17	6	0	-0.350918	3.928442	-1.181772
18	1	0	0.215238	2.152815	-2.257498
19	6	0	-0.856262	3.652381	1.160533
20	1	0	-0.704794	1.660275	1.946845
21	6	0	-0.738611	4.504134	0.046836
22	1	0	-0.221651	4.569340	-2.057608
23	1	0	-1.133346	4.072478	2.130860
24	6	0	1.252395	0.198473	-0.327252
25	6	0	2.488952	0.246473	-0.263028
26	8	0	-2.930110	-0.719236	-0.372831
27	6	0	-3.828168	0.130906	-0.491664
28	6	0	-5.273928	-0.283366	-0.342178
29	1	0	-5.774725	0.368548	0.393801
30	1	0	-5.794712	-0.122764	-1.302380
31	1	0	-5.359687	-1.336587	-0.045044
32	6	0	-3.538706	1.586080	-0.761656
33	1	0	-2.708900	1.690616	-1.471081
34	1	0	-4.430777	2.122326	-1.113745
35	1	0	-3.188047	2.054025	0.174643
36	6	0	1.109487	-3.114773	-1.979529
37	1	0	1.430969	-4.167461	-1.949334
38	1	0	0.774716	-2.866579	-2.997348
39	1	0	1.949219	-2.453698	-1.716464
40	6	0	-1.654042	-3.893460	-1.266030
41	1	0	-2.045134	-3.578226	-2.245134

42	1	0	-1.334539	-4.946149	-1.325676
43	1	0	-2.462493	-3.791635	-0.527523
44	6	0	0.912018	-0.533123	2.914791
45	1	0	0.931193	0.562364	3.003938
46	1	0	0.932943	-0.987354	3.917976
47	1	0	1.800234	-0.828213	2.339418
48	6	0	-2.027432	-0.663269	3.084204
49	1	0	-2.113673	0.426018	3.212412
50	1	0	-2.951149	-1.036348	2.617198
51	1	0	-1.904936	-1.131031	4.074028
52	6	0	-0.975752	5.994155	0.164115
53	1	0	-1.435900	6.253241	1.129327
54	1	0	-0.025553	6.549310	0.083156
55	1	0	-1.631909	6.357400	-0.643437
56	14	0	4.326107	0.364106	-0.100374
57	6	0	4.838569	2.190677	-0.193752
58	1	0	5.932218	2.295341	-0.090605
59	1	0	4.546104	2.637408	-1.158300
60	1	0	4.364727	2.780581	0.608089
61	6	0	5.128216	-0.634905	-1.506734
62	1	0	6.228413	-0.575504	-1.447241
63	1	0	4.849107	-1.701154	-1.456061
64	1	0	4.824619	-0.251190	-2.494843
65	6	0	4.806891	-0.381279	1.586715
66	1	0	5.898172	-0.326719	1.739910
67	1	0	4.326522	0.160938	2.418401
68	1	0	4.515824	-1.443523	1.657485

Complex : **4b$^{//}$_TS2** (optimized by B97D/BS1)
E (BS1) = -2036.5308384 au
Δ H (BS1) = 0.602477 au
Δ G(BS1) = 0.482355 au
Imaginary frequency = -377.1i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.307756	-2.629415	2.295814
2	6	0	0.750940	-3.214077	1.334771
3	15	0	0.343228	-2.770530	-0.435892
4	15	0	-0.478851	-0.785486	2.023221
5	1	0	-0.036928	-2.836259	3.344368
6	1	0	-1.293766	-3.086440	2.107708
7	1	0	0.821029	-4.308016	1.450312
8	1	0	1.743456	-2.789604	1.556277
9	46	0	-0.394176	-0.434642	-0.357877
10	6	0	0.255102	0.007690	-2.470747
11	1	0	1.019293	-0.613316	-2.939733
12	1	0	-0.754334	-0.372961	-2.708198
13	1	0	0.337486	1.069480	-2.705463
14	6	0	-1.003124	1.554124	-0.184584
15	6	0	-2.043393	1.965266	-1.032569
16	6	0	-0.414007	2.480381	0.687983
17	6	0	-2.527217	3.283993	-0.961138
18	1	0	-2.483272	1.273594	-1.752478
19	6	0	-0.908798	3.794798	0.753539
20	1	0	0.450953	2.200893	1.287799

21	6	0	-1.978253	4.215924	-0.060183
22	1	0	-3.336882	3.593148	-1.627917
23	1	0	-0.441853	4.508370	1.437676
24	6	0	1.416957	0.206883	-0.781170
25	6	0	2.607962	0.520166	-0.632915
26	6	0	-3.756827	-0.977289	-0.762883
27	8	0	-2.601974	-1.292003	-1.076695
28	6	0	-4.929222	-1.425888	-1.609696
29	1	0	-5.348221	-0.543889	-2.125858
30	1	0	-4.614764	-2.166535	-2.356223
31	1	0	-5.735348	-1.831059	-0.976583
32	6	0	-4.066803	-0.139709	0.457098
33	1	0	-4.781798	0.659276	0.205210
34	1	0	-4.560847	-0.780532	1.209439
35	1	0	-3.151058	0.298223	0.865547
36	6	0	1.868797	-3.139826	-1.404190
37	1	0	2.279394	-4.130556	-1.153889
38	1	0	1.628470	-3.112257	-2.478095
39	1	0	2.607434	-2.352722	-1.193220
40	6	0	-0.900997	-4.037677	-0.954732
41	1	0	-1.222823	-3.830679	-1.985547
42	1	0	-0.480380	-5.054180	-0.895674
43	1	0	-1.783936	-3.964675	-0.303772
44	6	0	1.088773	-0.097832	2.723828
45	1	0	0.930821	0.954390	2.999334
46	1	0	1.395295	-0.656985	3.622043
47	1	0	1.875521	-0.137197	1.956047
48	6	0	-1.787620	-0.230209	3.206581
49	1	0	-2.732325	-0.753559	3.002567
50	1	0	-1.480826	-0.425104	4.246303
51	1	0	-1.944079	0.850434	3.069907
52	6	0	-2.522674	5.626633	0.033962
53	1	0	-3.309449	5.695817	0.805732
54	1	0	-1.731724	6.342122	0.306777
55	1	0	-2.967465	5.947934	-0.920336
56	14	0	4.355324	1.041047	-0.320997
57	6	0	4.503276	2.900559	-0.674808
58	1	0	3.813789	3.484434	-0.042815
59	1	0	5.528996	3.254859	-0.475111
60	1	0	4.266868	3.125774	-1.727628
61	6	0	5.503805	0.037517	-1.456929
62	1	0	5.408903	-1.046856	-1.277207
63	1	0	5.280367	0.225743	-2.520053
64	1	0	6.557710	0.313393	-1.281757
65	6	0	4.764858	0.677575	1.505361
66	1	0	4.111643	1.248284	2.186516
67	1	0	4.652031	-0.394099	1.742673
68	1	0	5.807658	0.958901	1.730874

Complex : **4c$^{//}$_TS1** (optimized by B97D/BS1)
E (BS1) = -2036.5414148 au
Δ H (BS1) = 0.602814 au
Δ G(BS1) = 0.484638 au
Imaginary frequency = -254.6i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.963228	-0.597902	2.105638
2	6	0	3.542129	0.676647	1.449511
3	15	0	2.894431	0.891835	-0.300775
4	6	0	2.942692	2.703722	-0.635052
5	6	0	4.163508	0.121201	-1.395201
6	15	0	1.092432	-0.554011	2.034030
7	6	0	0.607698	0.449159	3.517341
8	6	0	0.514056	-2.255128	2.456027
9	1	0	3.319146	-0.696028	3.144435
10	1	0	3.276360	-1.492779	1.546199
11	1	0	4.643959	0.650115	1.443341
12	1	0	3.238398	1.572520	2.016236
13	1	0	2.709047	2.877062	-1.696522
14	1	0	3.926666	3.140228	-0.402414
15	1	0	2.159296	3.184966	-0.030338
16	1	0	4.202943	-0.955477	-1.177097
17	1	0	5.155772	0.573821	-1.242550
18	1	0	3.861992	0.254045	-2.444833
19	1	0	-0.486733	0.558899	3.546734
20	1	0	0.944279	-0.048319	4.440979
21	1	0	1.061026	1.450579	3.464309
22	1	0	0.935085	-2.960580	1.727751
23	1	0	0.815222	-2.545265	3.474761
24	1	0	-0.582653	-2.272201	2.370487
25	46	0	0.688361	0.020562	-0.335661
26	6	0	0.753724	0.087810	-2.457674
27	1	0	0.976634	1.103622	-2.803952
28	1	0	1.543219	-0.622826	-2.737265
29	1	0	-0.234164	-0.244126	-2.796988
30	6	0	-0.672831	1.677588	-0.348379
31	6	0	-1.225006	2.208212	-1.523465
32	6	0	-0.654494	2.431062	0.832450
33	6	0	-1.706432	3.525019	-1.516540
34	1	0	-1.304804	1.611753	-2.428043
35	6	0	-1.133965	3.753395	0.813319
36	1	0	-0.285865	2.007452	1.760231
37	6	0	-1.661281	4.325985	-0.357414
38	1	0	-2.136908	3.930186	-2.435578
39	1	0	-1.107445	4.337497	1.736502
40	6	0	-2.169569	5.752101	-0.379289
41	1	0	-1.462343	6.415350	-0.906951
42	1	0	-3.134329	5.821111	-0.906526
43	1	0	-2.302678	6.145781	0.639432
44	6	0	-1.267259	-0.377483	-0.181864
45	6	0	-2.399584	-0.867142	-0.033966
46	14	0	-4.080790	-1.621277	0.158357
47	6	0	-4.357868	-2.006570	2.000818
48	1	0	-3.603806	-2.715770	2.382736
49	1	0	-4.306622	-1.091403	2.613927
50	1	0	-5.351369	-2.459874	2.158352
51	6	0	-5.369895	-0.377883	-0.474939
52	1	0	-5.314415	0.573812	0.078571
53	1	0	-5.218514	-0.156859	-1.544286
54	1	0	-6.389393	-0.782108	-0.353283
55	6	0	-4.123980	-3.223153	-0.868984
56	1	0	-5.116948	-3.699396	-0.801240
57	1	0	-3.920570	-3.020967	-1.933694
58	1	0	-3.378068	-3.952761	-0.511340
59	8	0	1.930212	-2.272030	-0.580604
60	6	0	1.490406	-3.234427	-1.224775

61	6	0	0.119669	-3.224043	-1.859545
62	1	0	0.234452	-2.905029	-2.910850
63	1	0	-0.320713	-4.232732	-1.875354
64	1	0	-0.541648	-2.508429	-1.354525
65	6	0	2.335410	-4.477826	-1.415264
66	1	0	1.859205	-5.321573	-0.885829
67	1	0	2.364068	-4.757075	-2.481805
68	1	0	3.352862	-4.328396	-1.030866

Complex : **4c$^{//}$_TS3** (optimized by B97D/BS1)
E (BS1) = -2036.5399436 au
Δ H (BS1) = 0.602997 au
Δ G(BS1) = 0.486395 au
Imaginary frequency = -168.3i

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.926858	-2.953869	1.910560
2	6	0	2.336197	-2.869401	1.293262
3	15	0	2.314195	-2.012366	-0.373614
4	6	0	4.114725	-1.838020	-0.770265
5	6	0	1.717228	-3.284346	-1.573802
6	15	0	0.092701	-1.290710	1.840219
7	6	0	0.942001	-0.224445	3.085309
8	6	0	-1.619923	-1.526016	2.452544
9	1	0	0.978042	-3.318715	2.949531
10	1	0	0.285629	-3.636128	1.333083
11	1	0	2.776848	-3.873582	1.183125
12	1	0	3.007097	-2.282658	1.942169
13	1	0	4.240956	-1.474168	-1.800904
14	1	0	4.605390	-2.820315	-0.681571
15	1	0	4.591954	-1.128554	-0.079139
16	1	0	0.655490	-3.486062	-1.376089
17	1	0	2.309996	-4.209752	-1.494361
18	1	0	1.814990	-2.879716	-2.593223
19	1	0	0.473955	0.770630	3.064760
20	1	0	0.859749	-0.652108	4.097536
21	1	0	2.001025	-0.109352	2.813011
22	1	0	-2.084741	-2.317852	1.852976
23	1	0	-1.612101	-1.805962	3.517615
24	1	0	-2.174622	-0.589635	2.304631
25	46	0	0.593104	-0.326615	-0.278454
26	6	0	0.774239	0.371204	-2.347750
27	1	0	1.778226	0.339668	-2.777350
28	1	0	0.165274	-0.494613	-2.655096
29	1	0	0.250460	1.307029	-2.550080
30	6	0	1.698620	1.482260	-0.533842
31	6	0	1.065203	2.668934	-0.130963
32	6	0	3.081609	1.441184	-0.747943
33	6	0	1.864445	3.783469	0.173295
34	1	0	-0.015111	2.724800	-0.033032
35	6	0	3.857526	2.570924	-0.435760
36	1	0	3.559575	0.567670	-1.178189
37	6	0	3.266694	3.755651	0.039971
38	1	0	1.373147	4.699079	0.511730
39	1	0	4.938018	2.529386	-0.593513

40	6	0	4.106011	4.966536	0.387529
41	1	0	5.082588	4.935560	-0.118532
42	1	0	3.595347	5.899638	0.103536
43	1	0	4.294327	5.013286	1.474308
44	6	0	-1.175814	0.583841	-0.112850
45	6	0	-2.304069	1.089748	-0.031032
46	14	0	-3.972448	1.889051	0.045632
47	6	0	-4.897464	1.200514	1.562036
48	1	0	-5.030768	0.106962	1.503653
49	1	0	-4.358555	1.426686	2.497618
50	1	0	-5.901174	1.651995	1.639837
51	6	0	-3.738199	3.767378	0.209545
52	1	0	-3.166765	4.021904	1.117681
53	1	0	-3.198362	4.180113	-0.658807
54	1	0	-4.714479	4.277457	0.273006
55	6	0	-4.917375	1.465391	-1.551004
56	1	0	-5.912346	1.942276	-1.549849
57	1	0	-4.375626	1.823709	-2.442111
58	1	0	-5.069865	0.378805	-1.661092
59	8	0	-1.419546	-2.921502	-0.494411
60	6	0	-2.378511	-2.416194	-1.084015
61	6	0	-2.249373	-1.837026	-2.478285
62	1	0	-2.238453	-0.737992	-2.369582
63	1	0	-1.316081	-2.168128	-2.952593
64	1	0	-3.111787	-2.101485	-3.109319
65	6	0	-3.733782	-2.266320	-0.419018
66	1	0	-4.554577	-2.473879	-1.122315
67	1	0	-3.816226	-2.916011	0.462453
68	1	0	-3.823090	-1.212604	-0.104379

Complex: **acetone** (optimized by B97D/BS1)
E (BS1) = -193.0253403 au
Δ H (BS1) = 0.088077 au
Δ G(BS1) = 0.052477 au

Optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.193450	0.000041
2	8	0	0.000000	1.415431	-0.000041
3	6	0	1.294004	-0.621908	0.000002
4	1	0	1.328603	-1.279638	0.885662
5	1	0	1.328416	-1.279907	-0.885465
6	1	0	2.163187	0.048918	-0.000181
7	6	0	-1.294004	-0.621908	0.000010
8	1	0	-1.328516	-1.279724	-0.885590
9	1	0	-1.328504	-1.279821	0.885537
10	1	0	-2.163187	0.048918	0.000048

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