Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Computational Study on *N*-Triflylphosphoramide Catalyzed Enantioselective Hydroamination of Alkenyl Thiourea

Ryukichi Takagi,* Duyen Thi Duong

Department of Chemistry, Graduate School of Science, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima 739-8526, Japan
rtakagi@hiroshima-u.ac.jp

Table of Contents

Computational study on the HBr-catalyzed hydroamination S2
Summary of the calculated energies S3
Cartesian coordinates of the structures S7

Computational study on the NPTA-catalyzed hydroamination S38
Summary of the calculated energies S39
Cartesian coordinates of the structures S47

Computational study

on

the HBr-catalyzed hydroamination

Summary of the calculated energies

Table S1. Calculated Gibbs free energies for the HBr-catalyzed hydroamination of alkenyl thiourea at 298.15 K

TS^{HBr}	M06-2x/ def2-TZVP //M06-2x/ 6-31g(d)[a]	ΔG_{298}[b]	M06-2x/ 6-311g(d,p) //M06-2x/ 6-31g(d)[a]	ΔG_{298}[b]	M06-2x/ 6-311+g(d,p) //M06-2x/ 6-31g(d)[a]	ΔG_{298}[b]
TS^{HBr}_{A}	-3858.608345	11.50	-3858.483053	12.18	-3858.493533	11.63
TS^{HBr}_{B}	-3858.594372	20.27	-3858.469971	20.39	-3858.479497	20.44
TS^{HBr}_{C}	-3858.626668	0	-3858.50247	0	-3858.512073	0
$TS^{HBr}_{D\_TS1}$	-3858.608846	11.18	-3858.484752	11.12	-3858.495133	10.63
$TS^{HBr}_{E\_TS1}$	-3858.640652	-8.77	-3858.516228	-8.63	-3858.525906	-8.68
TS^{HBr}_{D,E_int}	-3858.637992	-7.11	-3858.514792	-7.73	-3858.524704	-7.93
$TS^{HBr}_{E\_TS2}$	-3858.636426	-6.12	-3858.514163	-7.34	-3858.523724	-7.31

TS^{HBr}	M06-2x/ def2-TZVP// B3LYP +GB3BJ/ 6-31g(d)[a]	ΔG_{298}[b]	M06-2x/ 6-311g(d,p)// B3LYP +GB3BJ/ 6-31(d)[a]	ΔG_{298}[b]
TS^{HBr}_{A}	-3858.621325	12.44	-3858.496589	12.67
TS^{HBr}_{B}	-3858.607414	21.17	-3858.482919	21.25
TS^{HBr}_{C}	-3858.641156	0	-3858.516784	0
$TS^{HBr}_{D\_TS1}$	-3858.621184	12.53	-3858.497675	11.99
$TS^{HBr}_{E\_TS1}$	-3858.654513	-8.38	-3858.52962	-8.05
TS^{HBr}_{D,E_int}	-3858.650271	-5.72	-3858.527746	-6.88
$TS^{HBr}_{E\_TS2}$	-3858.648602	-4.67	-3858.526972	-6.39

TS^{HBr}	M06-2x/ def2-TZVP// B3LYP/ 6-31g(d,p)[a]	ΔG_{298}[b]	M06-2x/ 6-311g(d,p)// B3LYP/6- 31(d,p)[a]	ΔG_{298}[b]	M06-2x/ 6-311+g(d,p)// B3LYP/6- 31(d,p)[a]	ΔG_{298}[b]
TS^{HBr}_{A}	-3858.609425	14.02	-3858.484966	13.83	-3858.486708	18.88
TS^{HBr}_{B}	-3858.598611	20.80	-3858.47141	22.34	-3858.481298	22.28
TS^{HBr}_{C}	-3858.631762	0	-3858.507012	0	-3858.516798	0
$TS^{HBr}_{D\_TS1}$	-3858.61142	12.76	-3858.488162	11.83	-3858.488162	17.97
$TS^{HBr}_{E\_TS1}$	-3858.647834	-10.10	-3858.521298	-8.96	-3858.531315	-9.11
TS^{HBr}_{D,E_int}	-3858.638813	-4.42	-3858.515675	-5.44	-3858.525623	-5.54
$TS^{HBr}_{E\_TS2}$	-3858.636672	-3.08	-3858.514235	-4.53	-3858.523984	-4.51

[a] a.u. [b] kcal/mol.

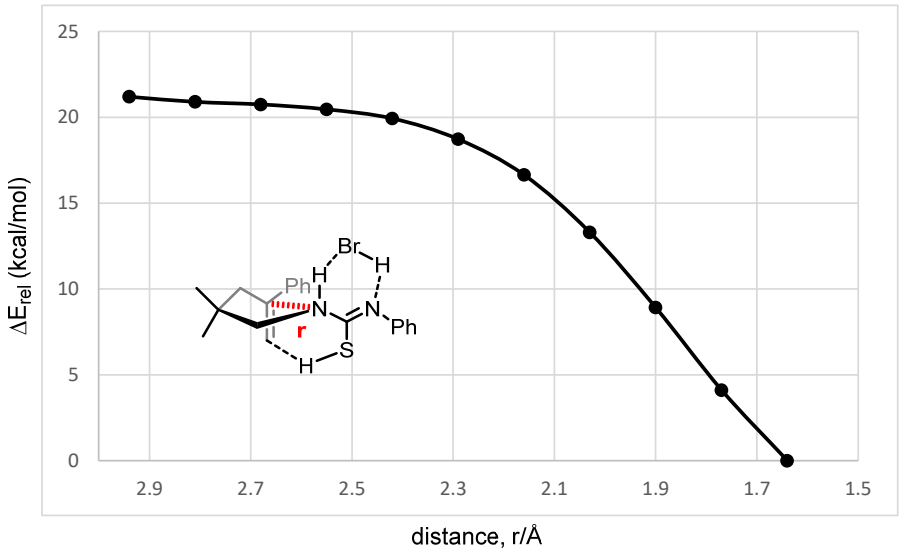


Fig. S1 Potential energy surface scanned by the bond length r (Å) of the forming C-N bond from the transition state C. The energies, ΔE_{rel} in kcal/mol, are relative to the product.

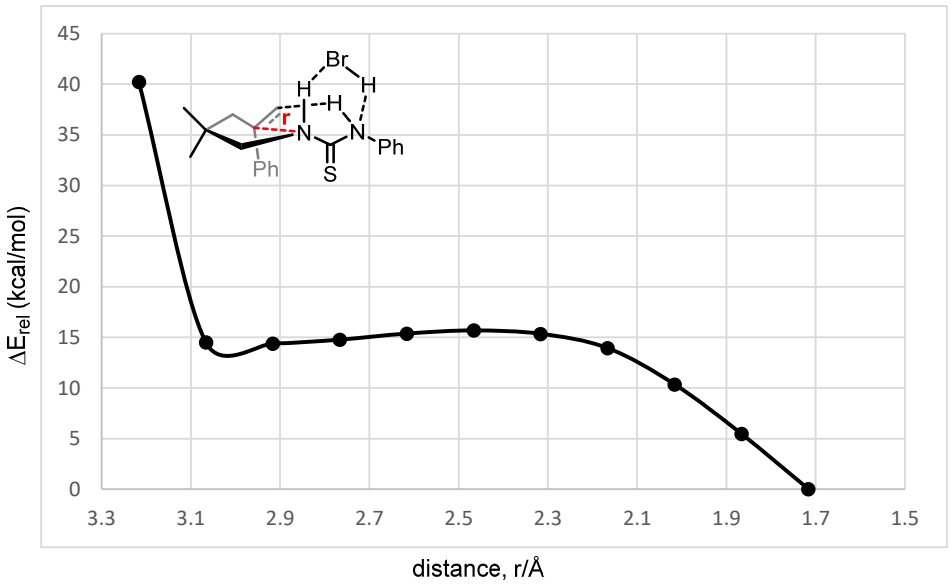


Fig. S2 Potential energy surface scanned by the bond length r (Å) of the forming C-N bond from the transition state $TS^{HBr}{}_{D\_TS1}$. The energies, ΔE_{rel} in kcal/mol, are relative to the product.

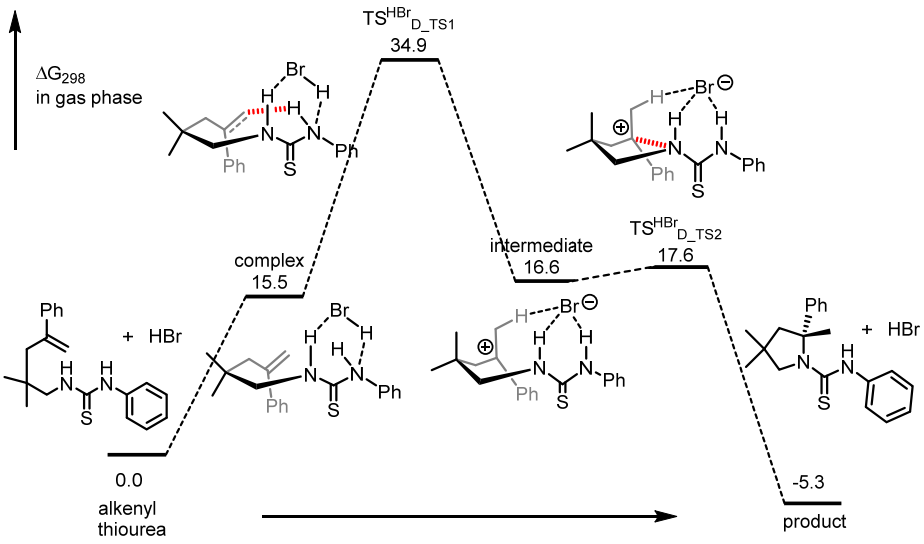


Fig. S3 Calculated Gibbs free-energy profile for the HBr-catalyzed hydroamination of alkenyl thiourea via transition state structure D at 298.15 K at the M06-2X/def2-TZVP//M06-2x/6-31G(d) level of theory.

Table S2. Calculated Gibbs free energies for the HBr-catalyzed hydroamination of alkenyl thiourea via transition state D at the M06-2X/def2-TZVP//M06-2X/ 6-31G(d) level of theory

	G_{298} (a.u.)	ΔG_{298} (kcal/mol)
thiourea + HBr	-3858.664407	0
complex	-3858.639644	15.5387825
$TS^{HBr}_{D\_TS1}$	-3858.608846	34.8645275
intermediate	-3858.637992	16.5754125
$TS^{HBr}_{D\_TS2}$	-3858.636426	17.5580775
product +HBr	-3858.668621	-5.29108

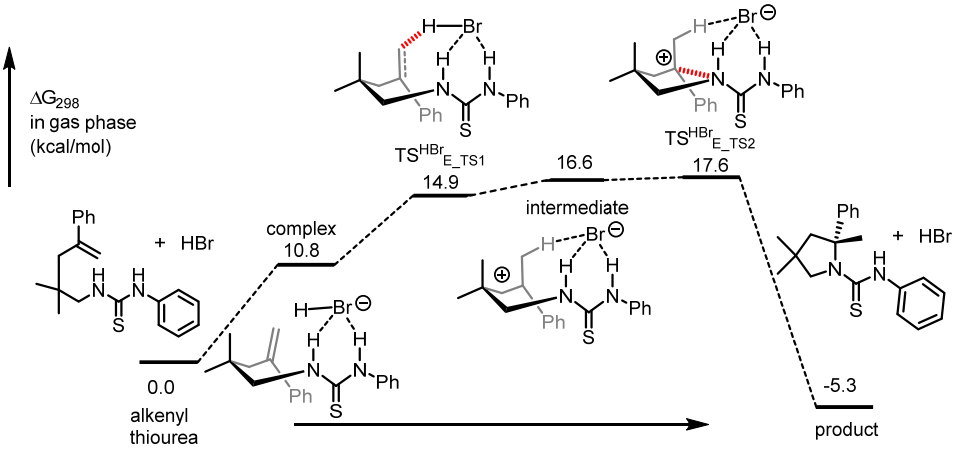


Fig. S4 Calculated Gibbs free-energy profile for the HBr-catalyzed hydroamination of alkenyl thiourea via transition state structure E at 298.15 K at the M06-2X/def2-TZVP//M06-2X/6-31G(d) level of theory.

Table S3. Calculated Gibbs free energies for the HBr-catalyzed hydroamination of alkenyl thiourea via transition state E at the M06-2X/def2-TZVP//M06-2X/6-31G(d) level of theory

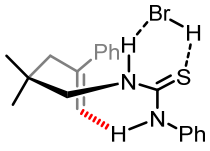
	G_{298} (a.u.)	ΔG_{298} (kcal/mol)
thiourea + HBr	-3858.664407	0
complex	-3858.647272	10.7522125
$TS^{HBr}_{E\_TS1}$	-3858.640652	14.9062625
intermediate	-3858.637992	16.5754125
$TS^{HBr}_{E\_TS2}$	-3858.636426	17.5580775
product +HBr	-3858.672839	-5.29108

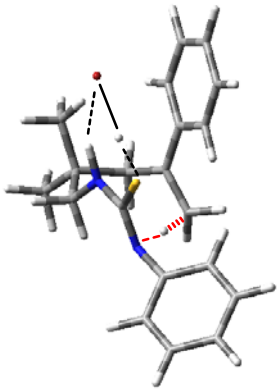
Cartesian coordinates of the structures

on

the HBr-catalyzed hydroamination

Transition state A (TS^{HBr}_{A})





E(RM06-2X/6-31G(d)) = -3856.188711 a.u.
Imaginary Freq = 1: -573.90 cm-1
Zero-point correction = 0.407583Thermal Correction to Energy = 0.430576
Thermal Correction to Enthalpy = 0.431520
Thermal Correction to Free Energy = 0.354905
EE + Zero-point Energy = -3855.781128
EE + Thermal Energy Correction = -3855.758135
EE + Thermal Enthalpy Correction = -3855.757191
EE + Thermal Free Energy Correction = -3855.833806
Truhlar's quasiharmonic corrected Gibbs energy = -3855.830030

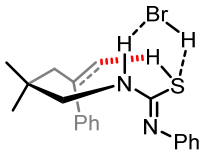
E_{sp}(RM06-2X/def2-TZVP) = -3858.967026
E_{sp}(RM06-2X/6-311G(d,p) = -3858.841734
E_{sp}(RM06-2X/6-311+G(d,p) = -3858.852214

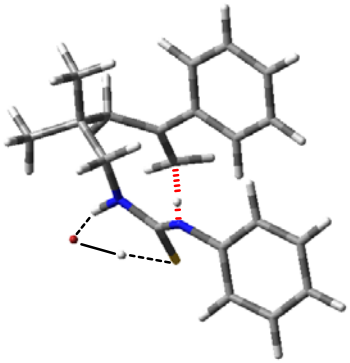
Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000024067	0.000010888	-0.000000526
2	6	-0.000001341	-0.000005763	-0.000001198
3	6	-0.000001931	0.000001492	0.000007460
4	6	-0.000003348	0.000001660	0.000000792
5	7	-0.000001644	0.000002432	0.000013347
6	1	0.000000124	0.000000372	-0.000000997
7	1	-0.000001726	0.000000781	-0.000001098

8	1	-0.000002685	0.000001810	-0.000001191
9	1	-0.000000605	0.000001539	0.000000006
10	6	0.000000334	0.000000043	-0.000002736
11	1	-0.000002642	0.000001942	-0.000004451
12	1	0.000001486	-0.000000564	0.000001809
13	1	-0.000002891	0.000001545	0.000003601
14	6	0.000001088	0.000003030	0.000000578
15	1	-0.000000067	0.000002739	0.000000171
16	1	-0.000001546	-0.000001089	-0.000000492
17	1	-0.000004249	0.000002293	-0.000000276
18	6	0.000008691	-0.000002767	-0.000002464
19	6	0.000000421	0.000000216	-0.000000482
20	6	-0.000003094	-0.000001417	0.000000716
21	6	-0.000000143	-0.000000532	-0.000000645
22	6	0.000004046	0.000000453	-0.000000000
23	6	-0.000001130	0.000003333	-0.000003487
24	1	0.000002503	0.000001818	-0.000000047
25	1	-0.000001677	0.000001534	-0.000002793
26	1	0.000000683	0.000000011	-0.000001696
27	1	0.000002360	-0.000001051	-0.000000690
28	1	0.000002350	-0.000000598	-0.000001504
29	6	0.000007166	0.000001156	0.000000555
30	1	0.000001600	-0.000000474	0.000000075
31	1	-0.000000409	-0.000000738	-0.000000615
32	6	0.000005694	-0.000002964	0.000001390
33	7	0.000000074	0.000001204	0.000000451
34	1	0.000000596	-0.000001916	-0.000003077
35	6	-0.000001370	-0.000000900	0.000001068
36	6	0.000000601	-0.000001021	0.000001650
37	6	0.000000770	-0.000000129	0.000001434
38	6	0.000000293	-0.000000616	0.000001438
39	6	0.000000428	-0.000001266	0.000000908
40	6	-0.000000235	-0.000000914	0.000001852
41	1	-0.000000936	-0.000000456	0.000001942
42	1	0.000001308	-0.000002418	-0.000000355
43	1	0.000001384	-0.000001170	0.000000761

44	1	-0.000000364	-0.000000758	0.000002314
45	1	0.000000686	-0.000001220	0.000001739
46	1	0.000007768	-0.000011512	-0.000023991
47	16	0.000000159	-0.000004563	0.000000998
48	1	0.000002375	0.000004425	0.000003919
49	35	0.000003111	0.000000101	0.000003835

Transition state B (TS^{HBr}_{B})





E(RM02-2X/6-31G(d)) = -3856.175143 a.u.
Imaginary Freq = 1: -668.52 cm-1
Zero-point Energy Correction = 0.405273
Thermal Correction to Energy = 0.428296
Thermal Correction to Enthalpy = 0.42924
Thermal Correction to Free Energy = 0.35245
EE + Zero-point Energy = -3855.769869
EE + Thermal Energy Correction = -3855.746846
EE + Thermal Enthalpy Correction = -3855.745902
EE + Thermal Free Energy Correction = -3855.822693
Truhlar's quasiharmonic corrected Gibbs energy = -3855.818689

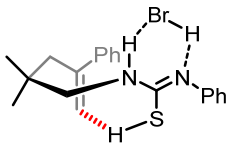
E_{sp}(RM06-2X/def2-TZVP) = -3858.950826
E_{sp}(RM06-2X/6-311G(d,p)) = -3858.826425
E_{sp}(RM06-2X/6-311+G(d,p)) = -3858.835951

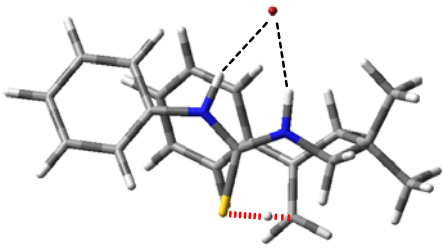
Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.043617	-0.041116	0.039059
2	6	0	-0.016696	0.013888	1.540984
3	6	0	1.362663	0.032178	2.299419
4	6	0	2.483870	-0.543368	1.416833
5	7	0	1.982846	-1.694454	0.708290
6	1	0	-0.593824	-0.846935	1.892301
7	1	0	-0.586963	0.906999	1.840299
8	1	0	3.358409	-0.779866	2.039730
9	1	0	2.813358	0.178681	0.662953
10	6	0	1.786869	1.430334	2.762504
11	1	0	1.001436	1.900612	3.364808
12	1	0	2.029221	2.088197	1.924023
13	1	0	2.682451	1.355377	3.388632
14	6	0	1.170607	-0.845056	3.548985
15	1	0	0.380288	-0.431194	4.185597
16	1	0	2.093523	-0.880811	4.136805
17	1	0	0.878536	-1.869597	3.292752
18	6	0	0.637501	0.978020	-0.762933
19	6	0	1.846935	2.938166	-2.350610
20	6	0	1.150052	0.651814	-2.030907
21	6	0	0.738567	2.302501	-0.307244
22	6	0	1.328380	3.276907	-1.101914
23	6	0	1.759915	1.625214	-2.810855
24	1	0	1.106263	-0.373648	-2.389390
25	1	0	0.312679	2.578041	0.651814
26	1	0	1.380556	4.301581	-0.748678
27	1	0	2.174848	1.350664	-3.775287
28	1	0	2.315761	3.699066	-2.966633
29	6	0	-0.794267	-1.027739	-0.627942
30	1	0	-1.455755	-1.640483	-0.016144
31	1	0	-1.181521	-0.757153	-1.609572
32	6	0	2.434313	-2.081411	-0.527491
33	7	0	3.461642	-1.520384	-1.035303
34	6	0	3.918946	-1.743809	-2.339447

35	6	0	4.945361	-2.031677	-4.938166
36	6	0	4.338274	-0.625393	-3.073103
37	6	0	4.063063	-3.015562	-2.911011
38	6	0	4.569395	-3.151110	-4.199669
39	6	0	4.832866	-0.766782	-4.364374
40	1	0	4.272977	0.348786	-2.598171
41	1	0	3.791984	-3.894248	-2.335374
42	1	0	4.674941	-4.143791	-4.627158
43	1	0	5.147422	0.112868	-4.919088
44	1	0	5.338731	-2.145416	-5.943321
45	16	0	1.266132	-3.205521	-1.318909
46	1	0	0.059313	-1.898028	-0.979840
47	1	0	1.430322	-2.363150	1.235443
48	1	0	0.366295	-3.714940	0.136803
49	35	0	-0.479129	-3.874780	1.512889

Transition state C (TS^{HBr}_{C})





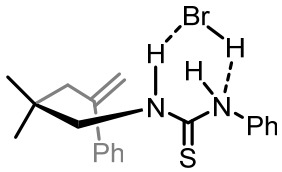
E(RM06-2X/6-31G(d)) = -3856.219755 a.u.
Imaginary Freq = 1: -153.06 cm-1
Zero-point Energy Correction = 0.413800
Thermal Correction to Energy = 0.436560
Thermal Correction to Enthalpy = 0.437504
Thermal Correction to Free Energy = 0.360684
EE + Zero-point Energy = -3855.805956
EE + Thermal Energy Correction = -3855.783196
EE + Thermal Enthalpy Correction = -3855.782251
EE + Thermal Free Energy Correction = -3855.859071
Truhlar's quasiharmonic corrected Gibbs energy = -3855.854462

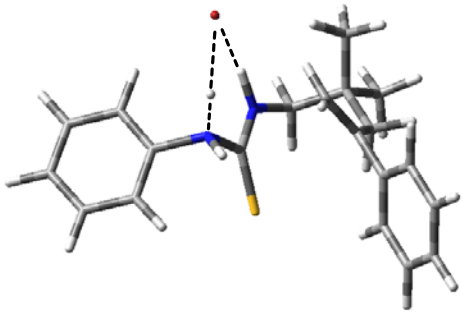
E_{sp}(RM06/def2-TZVP) = -3858.991961
E_{sp}(RM06/6-311G(d,p)) = -3858.867763
E_{sp}(RM06/6-311+G(d,p)) = -3858.877366

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.009090	0.065217	0.022731
2	6	0	-0.004582	0.135872	1.519762
3	6	0	1.327187	0.025197	2.326692
4	7	0	1.645500	-2.114655	1.132924
5	1	0	-0.453528	1.116530	1.750809
6	1	0	-0.707425	-0.606068	1.906484
7	6	0	0.933669	-0.515212	3.713164
8	1	0	0.222845	0.166228	4.194229
9	1	0	0.459322	-1.501947	3.653091
10	1	0	1.816835	-0.586899	4.356726
11	6	0	2.027806	1.374781	2.529894
12	1	0	1.376038	2.067598	3.071773
13	1	0	2.932617	1.234768	3.131297
14	1	0	2.330560	1.853758	1.594735
15	6	0	-1.015409	-0.686298	-0.683517
16	6	0	-2.850480	-2.251785	-2.109044
17	6	0	-1.387471	-0.341213	-2.002275
18	6	0	-1.599475	-1.824304	-0.093054
19	6	0	-2.494315	-2.605563	-0.811008
20	6	0	-2.304548	-1.108730	-2.698610
21	1	0	-0.994080	0.557633	-2.464443
22	1	0	-1.312981	-2.173292	0.896526
23	1	0	-2.899392	-3.496889	-0.342619
24	1	0	-2.595174	-0.821598	-3.703561
25	1	0	-3.553372	-2.863134	-2.666579
26	6	0	1.051051	0.664147	-0.724277
27	1	0	1.752158	-0.327757	-0.917801

28	1	0	1.674683	1.396629	-0.220610
29	6	0	1.777036	-2.697550	-0.073309
30	7	0	1.140511	-3.880796	-0.158974
31	6	0	0.707475	-4.639335	-1.271301
32	6	0	-0.329542	-6.245324	-3.304743
33	6	0	1.388402	-4.743678	-2.484533
34	6	0	-0.475118	-5.362643	-1.064552
35	6	0	-0.986895	-6.160023	-2.078408
36	6	0	0.854448	-5.540587	-3.494921
37	1	0	2.322123	-4.220662	-2.636300
38	1	0	-0.971352	-5.284833	-0.098289
39	1	0	-1.902151	-6.718233	-1.906767
40	1	0	1.385672	-5.616736	-4.438679
41	1	0	-0.729672	-6.867423	-4.098941
42	16	0	2.632883	-1.950333	-1.361368
43	1	0	0.844398	0.902228	-1.766830
44	6	0	2.323000	-0.946876	1.652718
45	1	0	2.876936	-0.470861	0.842618
46	1	0	3.059924	-1.256481	2.406112
47	1	0	1.034459	-2.617885	1.802247
48	1	0	0.645247	-4.145409	0.708039
49	35	0	-0.678193	-3.869743	2.606957

HBr-complex for Transition state D





E(RM06-2X/6-31G(d)) = -3856.230697 a.u.

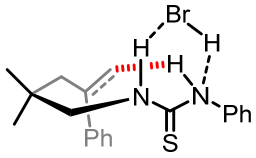
Imaginary Freq = 0
Zero-point Energy Correction = 0.417365
Thermal Correction to Energy = 0.440878
Thermal Correction to Enthalpy = 0.441822
Thermal Correction to Free Energy = 0.362611
EE + Zero-point Energy = -3855.813331
EE + Thermal Energy Correction = -3855.789818
EE + Thermal Enthalpy Correction = -3855.788874
EE + Thermal Free Energy Correction = -3855.868086
Truhlar's quasiharmonic corrected Gibbs energy = -3855.863075

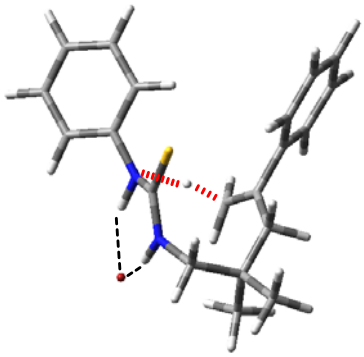
E_{sp}(RM06-2X/def2-TZVP) = -3859.007266
E_{sp}(RM06-2X/6-311G(d,p)) = -3858.883067
E_{sp}(RM06-2X/6-311+G(d,p)) = -3858.892614

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000001590	-0.000010576	0.000024258
2	6	-0.000035373	-0.000006897	0.000004136
3	6	0.000008874	0.000005411	0.000026362
4	7	0.000037509	0.000021271	0.000063398
5	1	0.000001945	-0.000009419	-0.000010614
6	1	0.000006176	0.000006740	-0.000006243
7	6	0.000000964	0.000005875	0.000004590
8	1	-0.000002590	-0.000004162	0.000003387
9	1	-0.000008276	0.000002605	0.000009389
10	1	-0.000007986	-0.000004130	0.000003338
11	6	0.000001318	0.000007372	-0.000018784
12	1	-0.000003805	0.000002666	0.000006900
13	1	0.000001410	0.000009691	-0.000002038
14	1	-0.000005179	0.000003424	0.000008522
15	6	0.000008433	-0.000011424	0.000000256
16	6	-0.000018161	-0.000006060	-0.000012765
17	6	0.000012323	0.000007707	-0.000010983

18	6	-0.000010632	-0.000017299	0.000002559
19	6	0.000003769	-0.000017978	0.000012358
20	6	-0.000009964	0.000006141	-0.000010130
21	1	-0.000012883	-0.000003074	0.000001746
22	1	-0.000003293	-0.000008393	0.000000422
23	1	-0.000003308	-0.000006480	-0.000002305
24	1	-0.000000117	-0.000005386	-0.000005522
25	1	-0.000002305	-0.000009485	-0.000001864
26	6	0.000001087	0.000018615	0.000006644
27	1	0.000005254	-0.000001504	-0.000019989
28	1	0.000005411	-0.000001616	0.000002194
29	6	0.000031517	-0.000060819	-0.000053270
30	7	0.000048003	0.000063159	0.000005717
31	1	0.000016204	-0.000013177	0.000003599
32	16	-0.000045478	-0.000001402	0.000012102
33	6	0.000037262	-0.000028273	0.000001094
34	6	0.000012148	-0.000009527	-0.000004263
35	6	-0.000015905	0.000029700	0.000028873
36	6	-0.000016445	0.000023826	-0.000006769
37	6	0.000005195	-0.000016712	-0.000006241
38	6	0.000019837	-0.000003815	-0.000000225
39	1	0.000010099	-0.000000848	-0.000014857
40	1	0.000003100	-0.000000510	-0.000001912
41	1	0.000007620	0.000002606	-0.000000403
42	1	0.000007000	0.000008890	0.000003893
43	1	0.000005450	0.000004190	0.000005118
44	6	-0.000031660	0.000011114	-0.000010691
45	1	0.000000741	-0.000004655	0.000006072
46	1	0.000010499	0.000004776	0.000000181
47	1	-0.000005147	0.000019999	-0.000003908
48	1	-0.000105838	-0.000012401	-0.000052016
49	35	0.000036785	0.000010244	0.000008683

Transition state D_TS1 ($TS^{HBr}_{D\_TS1}$)





E(RM06-2X/6-31G(d)) = -3856.195292 a.u
Imaginary Freq = 1: -667.52 cm-1Zero-point Energy Correction = 0.411933
Thermal Correction to Energy = 0.434798
Thermal Correction to Enthalpy = 0.435742
Thermal Correction to Free Energy = 0.358352
EE + Zero-point Energy = -3855.783359
EE + Thermal Energy Correction = -3855.760494
EE + Thermal Enthalpy Correction = -3855.759550
EE + Thermal Free Energy Correction = -3855.836940
Truhlar's quasiharmonic corrected Gibbs energy = -3855.832147

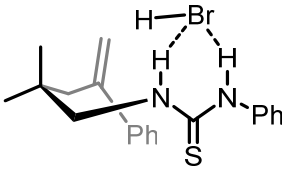
E_{sp}(RM06-2X/def2-TZVP) = -3858.971991
E_{sp}(RM06-2X/6-311G(d,p)) = -3858.847897
E_{sp}(RM06-2X/6-311+G(d,p)) = -3858.858278

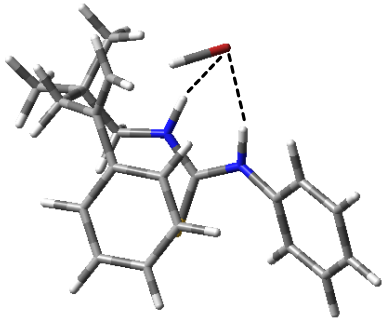
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.578524	-0.699400	-0.681668
2	6	0	1.920547	-1.883531	0.180908
3	6	0	0.966073	-3.014880	0.629913
4	7	0	-0.901525	-1.488133	1.208038
5	1	0	2.710631	-2.363676	-0.427236
6	1	0	2.457225	-1.510662	1.060553
7	6	0	1.867187	-4.059630	1.310511
8	1	0	2.549079	-4.517279	0.585920

9	1	0	2.465761	-3.615584	2.113687
10	1	0	1.257623	-4.858736	1.743882
11	6	0	0.233876	-3.699537	-0.534836
12	1	0	0.908476	-3.844146	-1.386896
13	1	0	-0.105178	-4.690681	-0.214522
14	1	0	-0.656337	-3.166471	-0.883288
15	6	0	2.630251	0.334745	-0.765294
16	6	0	4.648638	2.260295	-0.997722
17	6	0	2.989771	0.846215	-2.022916
18	6	0	3.302494	0.802810	0.375926
19	6	0	4.291987	1.769420	0.257384
20	6	0	4.001117	1.791916	-2.137787
21	1	0	2.505873	0.467325	-2.917412
22	1	0	2.998452	0.459016	1.359342
23	1	0	4.782253	2.145302	1.149216
24	1	0	4.281997	2.162378	-3.118052
25	1	0	5.429442	3.009098	-1.085867
26	6	0	0.429996	-0.533308	-1.464392
27	1	0	-0.248885	-1.364818	-1.650627
28	1	0	0.489678	0.204255	-2.265996
29	6	0	-0.690064	-0.179066	1.374842
30	7	0	-1.341999	0.548771	0.359461
31	1	0	-0.281886	0.132715	-0.667620
32	16	0	0.380977	0.509570	2.454987
33	6	0	-1.647383	1.945615	0.388139
34	6	0	-2.353981	4.628519	0.285516
35	6	0	-2.983780	2.301836	0.209426
36	6	0	-0.654489	2.919290	0.482858
37	6	0	-1.019373	4.261154	0.441515
38	6	0	-3.333511	3.646717	0.159876
39	1	0	-3.730587	1.520120	0.095081
40	1	0	0.383179	2.625541	0.590983
41	1	0	-0.251598	5.023914	0.523608
42	1	0	-4.373380	3.924553	0.022260
43	1	0	-2.628187	5.678073	0.251230
44	6	0	-0.035669	-2.532371	1.703992

45	1	0	-0.659161	-3.380928	2.005247
46	1	0	0.490067	-2.158994	2.585944
47	1	0	-1.638676	-1.767358	0.535085
48	1	0	-2.090985	-0.005967	-0.125643
49	35	0	-2.979689	-1.632155	-1.294523

HBr-complex for Transition state E





E(RM06-2X/6-31G(d)) = -3856.233502 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 0.412311
Thermal Correction to Energy = 0.436415
Thermal Correction to Enthalpy = 0.437359
Thermal Correction to Free Energy = 0.357953
EE + Zero-point Energy = -3855.82191
EE + Thermal Energy Correction = -3855.797087
EE + Thermal Enthalpy Correction = -3855.796143
EE + Thermal Free Energy Correction = -3855.875549
Truhlar's quasiharmonic corrected Gibbs energy = -3855.871049

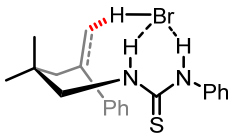
E_{sp}(RM06-2X/def2-TZVP) = -3859.009725
E_{sp}(RM06-2X/6-311G(d,p)) = -3858.883716
E_{sp}(RM06-2X/6-311+G(d,p)) = -3858.893585

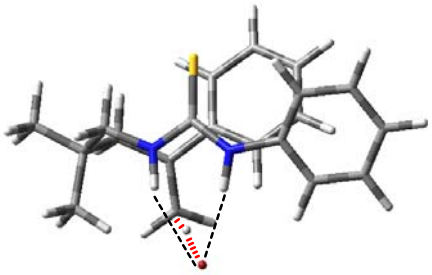
Center	Atomic	Forces (Hartrees/Bohr)

Number	Number	X	Y	Z
1	6	0.000004771	0.000002183	-0.000004683
2	6	-0.000001132	0.000006867	0.000003560
3	6	-0.000004097	0.000012861	-0.000000495
4	7	-0.000006314	0.000008866	0.000004903
5	1	0.000002080	0.000011136	0.000005205
6	1	-0.000002879	0.000008394	-0.000002032
7	6	-0.000000776	0.000017949	0.000001734
8	1	-0.000001975	0.000018056	0.000001301
9	1	-0.000006622	0.000015312	-0.000001596
10	1	-0.000003278	0.000017808	0.000000676
11	6	0.000002313	0.000012508	0.000004848
12	1	0.000004603	0.000014883	0.000004730
13	1	0.000003587	0.000015112	0.000003815
14	1	0.000004042	0.000007939	0.000002801
15	6	0.000000504	-0.000000823	0.000002578
16	6	-0.000005796	-0.000008195	-0.000003568
17	6	-0.000002977	-0.000003841	-0.000001472
18	6	-0.000006523	0.000002360	-0.000003096
19	6	-0.000008046	-0.000004770	-0.000005451
20	6	-0.000000705	-0.000008344	-0.000001620
21	1	0.000005698	-0.000005230	0.000002050
22	1	-0.000008125	0.000003420	-0.000003496
23	1	-0.000011464	-0.000003337	-0.000006852
24	1	-0.000000135	-0.000012016	-0.000001732
25	1	-0.000007364	-0.000011103	-0.000006501
26	6	0.000003634	0.000011528	0.000003473
27	1	0.000007269	0.000005236	0.000006642
28	1	0.000005818	-0.000000259	0.000004016
29	6	0.000004957	-0.000002777	-0.000000962
30	7	-0.000002419	-0.000002613	-0.000004073
31	16	-0.000004297	-0.000001094	-0.000005059
32	6	0.000004185	-0.000007185	0.000002537
33	6	0.000001634	-0.000018416	-0.000001228
34	6	-0.000004220	-0.000010314	-0.000003549

35	6	0.000005317	-0.000009227	0.000000317
36	6	0.000004546	-0.000015934	0.000000013
37	6	-0.000001111	-0.000015771	-0.000003370
38	1	-0.000005246	-0.000007750	-0.000003884
39	1	0.000006431	-0.000009506	0.000002052
40	1	0.000008106	-0.000018158	0.000001261
41	1	-0.000004804	-0.000016546	-0.000005254
42	1	0.000001443	-0.000021502	-0.000002483
43	6	-0.000004010	0.000006624	0.000000136
44	1	-0.000003323	0.000010330	-0.000000341
45	1	-0.000005995	0.000008418	-0.000002392
46	1	0.000004235	0.000003768	-0.000000192
47	1	0.000003185	-0.000001502	0.000003991
48	35	0.000016714	-0.000000152	0.000001403
49	1	0.000008562	-0.000005195	0.000011342

Transition state E_TS1 ($TS^{HBr}_{E\_TS1}$)





E(RM06-2X/6-31G(d)) = -3856.231004 a.u.
Imaginary Freq = 1: -434.51 cm-1
Zero-point Energy Correction = 0.411601
Thermal Correction to Energy = 0.434756
Thermal Correction to Enthalpy = 0.435700
Thermal Correction to Free Energy = 0.359000
EE + Zero-point Energy = -3855.819402
EE + Thermal Energy Correction = -3855.796248
EE + Thermal Enthalpy Correction = -3855.795304
EE + Thermal Free Energy Correction = -3855.872004

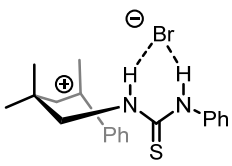
Truhlar's quasiharmonic corrected Gibbs energy = -3855.868277

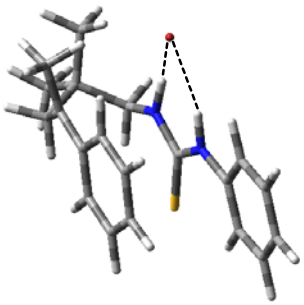
E_{sp}(RM06-2X/def2-TZVP) = -3859.003379
E_{sp}(RM06-2X/6-311G(d,p)) = -3858.878955
E_{sp}(RM06-2X/6-311+G(d,p)) = -3858.888633

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000001835	-0.000003627	0.000001384
2	6	-0.000002067	0.000009142	0.000002037
3	6	-0.000000945	-0.000005381	0.000001478
4	7	0.000005544	0.000004199	-0.000001151
5	1	-0.000005605	0.000004687	0.000001690
6	1	0.000001237	0.000004973	0.000000951
7	6	0.000001032	-0.000001337	-0.000000845
8	1	-0.000000917	-0.000001489	-0.000000447
9	1	0.000003959	-0.000000763	0.000000921
10	1	0.000001704	-0.000004152	-0.000002225
11	6	-0.000004592	-0.000003918	-0.000004269
12	1	-0.000009033	-0.000003684	-0.000004042
13	1	-0.000005486	-0.000009057	-0.000003619
14	1	-0.000007389	-0.000004759	-0.000005397
15	6	-0.000000582	0.000006596	0.000002586
16	6	0.000003898	0.000009127	0.000002971
17	6	-0.000002373	0.000006893	0.000002442
18	6	0.000001154	0.000007927	0.000003614
19	6	0.000004646	0.000011583	0.000007867
20	6	-0.000000147	0.000005766	0.000004844
21	1	-0.000005565	0.000000439	0.000000625
22	1	0.000003332	0.000009300	0.000006170
23	1	0.000006757	0.000013289	0.000007497
24	1	-0.000000787	0.000007069	0.000001953
25	1	0.000005036	0.000011169	0.000006759
26	6	-0.000021220	-0.000000050	-0.000000533

27	1	-0.000011394	0.000001774	-0.000002409
28	1	-0.000009444	0.000006158	-0.000001363
29	6	0.000000668	-0.000005676	0.000002790
30	7	0.000005806	0.000000047	-0.000001688
31	16	0.000009598	0.000000352	-0.000000852
32	6	0.000002424	-0.000006886	-0.000001950
33	6	0.000003762	-0.000000724	0.000001736
34	6	0.000008878	-0.000001782	-0.000000606
35	6	-0.000000519	-0.000003763	-0.000001181
36	6	-0.000000240	-0.000003231	-0.000001270
37	6	0.000008573	-0.000000948	0.000000517
38	1	0.000010027	-0.000003236	0.000002126
39	1	-0.000004695	-0.000004591	-0.000003085
40	1	-0.000003367	-0.000002236	-0.000002022
41	1	0.000012066	-0.000000725	0.000002262
42	1	0.000004624	0.000000271	0.000000464
43	6	0.000002196	-0.000012013	-0.000007626
44	1	0.000003655	-0.000007192	-0.000003895
45	1	0.000005352	-0.000003716	-0.000000793
46	1	-0.000002083	-0.000007749	-0.000001795
47	1	-0.000002419	-0.000007360	-0.000003894
48	35	-0.000008138	-0.000006831	-0.000006740
49	1	-0.000005085	-0.000003882	-0.000001989

Intermediate from transition states TS^{HBr}_{D,E_TS1}





E(RM06-2X/6-31G(d)) = -3856.236658 a.u.

Imaginary Freq = 0

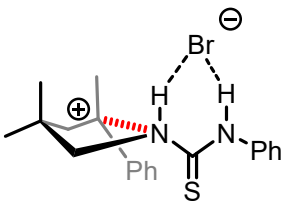
Zero-point Energy Correction 0.417827
Thermal Correction to Energy 0.440966
Thermal Correction to Enthalpy = 0.441910
Thermal Correction to Free Energy = 0.366174
EE + Zero-point Energy = -3855.818830
EE + Thermal Energy Correction = -3855.795692
EE + Thermal Enthalpy Correction = -3855.794747
EE + Thermal Free Energy Correction = -3855.870484
Truhlar's quasiharmonic corrected Gibbs energy = -3855.867609

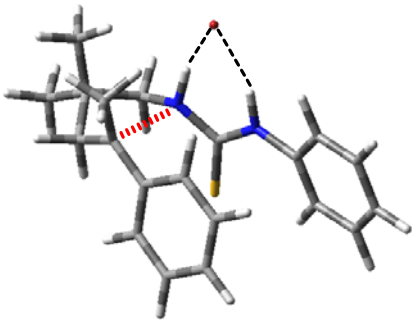
E_{sp}(RM06-2X/def2-TZVP) = -3859.007041
E_{sp}(RM06-2X/6-311G(d,p)) = -3858.883841
E_{sp}(RM06-2X/6-311+G(d,p)) = -3858.893753

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000001728	-0.000008341	0.000007540
2	6	0.000001458	0.000003892	0.000006588
3	6	-0.000000239	-0.000015836	-0.000001365
4	7	0.000000418	0.000000226	-0.000009250
5	1	0.000004318	-0.000002017	0.000001715
6	1	0.000004251	-0.000001665	0.000006384
7	6	0.000001800	-0.000012054	0.000007206
8	1	0.000003439	-0.000008928	0.000008831
9	1	0.000005732	-0.000007708	0.000010566
10	1	0.000002761	-0.000010453	0.000009156
11	6	-0.000005330	-0.000008830	0.000002899
12	1	-0.000002397	-0.000010149	-0.000001329
13	1	-0.000004071	-0.000010403	0.000003673
14	1	-0.000003612	-0.000006395	0.000001916
15	6	0.000010018	0.000004554	-0.000003361
16	6	-0.000002696	-0.000004956	-0.000002442
17	6	0.000006507	0.000004999	0.000001467
18	6	-0.000007040	0.000005197	0.000001265

19	6	0.000014867	0.000014906	0.000005836
20	6	-0.000009843	0.000012546	-0.000004538
21	1	-0.000004038	0.000004166	-0.000009729
22	1	0.000007605	0.000002168	0.000004114
23	1	0.000005587	0.000007082	0.000000823
24	1	0.000000435	0.000008091	-0.000007087
25	1	0.000003341	0.000011770	-0.000002395
26	6	-0.000006670	0.000002800	0.000007039
27	1	0.000001804	-0.000002815	0.000000012
28	1	-0.000001290	0.000000110	-0.000005342
29	6	0.000004072	0.000001682	0.000005125
30	7	-0.000007767	-0.000007547	-0.000006861
31	16	0.000010697	-0.000000625	0.000003623
32	6	0.000006844	0.000004016	-0.000004900
33	6	-0.000002625	0.000009129	-0.000007587
34	6	-0.000002713	0.000006080	-0.000001131
35	6	-0.000004523	0.000002903	-0.000006578
36	6	-0.000003151	0.000005622	-0.000006448
37	6	-0.000000467	0.000006725	-0.000002720
38	1	0.000000523	0.000000722	0.000000589
39	1	-0.000005233	0.000002863	-0.000006524
40	1	-0.000004850	0.000008054	-0.000010945
41	1	0.000002641	0.000009099	-0.000001529
42	1	-0.000001444	0.000011068	-0.000006904
43	6	-0.000005169	-0.000009621	0.000014616
44	1	-0.000002563	-0.000007427	0.000004871
45	1	0.000003535	-0.000004642	0.000004207
46	1	0.000000057	-0.000009156	0.000000930
47	1	-0.000004932	-0.000000133	0.000000089
48	35	-0.000005141	-0.000001555	-0.000006445
49	1	-0.000003173	0.000000784	-0.000005672

Transition state D,E_TS2 (TS^{HBr}_{D,E_TS2})





E(RM06-2X/6-31G(d)) = -3856.234322 a.u.
Imaginary Freq = 1: -133.34 cm-1
Zero-point Energy Correction = 0.416846
Thermal Correction to Energy = 0.439573
Thermal Correction to Enthalpy = 0.440517
Thermal Correction to Free Energy = 0.364465
EE + Zero-point Energy = -3855.817476
EE + Thermal Energy Correction = -3855.794749
EE + Thermal Enthalpy Correction = -3855.793805
EE + Thermal Free Energy Correction = -3855.869856
Truhlar's quasiharmonic corrected Gibbs energy = -3855.865973

E_{sp}(RM06-2X/def2-TZVP) = -3859.004775
E_{sp}(RM06-2X/6-311G(d,p)) = -3858.882512
E_{sp}(RM06-2X/6-311+G(d,p)) = -3858.892073

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.708037	-0.640556	1.280499
2	6	0	-2.857625	-1.346367	0.641424
3	6	0	-3.558120	-0.566507	-0.513950
4	7	0	-1.262703	0.123482	-1.025468
5	1	0	-3.602630	-1.528094	1.430104
6	1	0	-2.544966	-2.308604	0.227473
7	6	0	-4.697349	-1.435905	-1.050208
8	1	0	-5.493420	-1.541328	-0.305632

9	1	0	-4.342973	-2.436006	-1.321170
10	1	0	-5.134742	-0.977507	-1.943342
11	6	0	-4.117057	0.807443	-0.119796
12	1	0	-4.786536	0.737925	0.744804
13	1	0	-4.705830	1.196401	-0.957631
14	1	0	-3.338966	1.548369	0.096860
15	6	0	-0.406864	-1.241608	1.456123
16	6	0	2.145391	-2.315338	1.825280
17	6	0	0.688314	-0.400314	1.767553
18	6	0	-0.186559	-2.624698	1.313677
19	6	0	1.075916	-3.157790	1.536734
20	6	0	1.955505	-0.933983	1.923062
21	1	0	0.546015	0.679696	1.788964
22	1	0	-1.007453	-3.288471	1.068307
23	1	0	1.230804	-4.227868	1.449397
24	1	0	2.801272	-0.276234	2.097160
25	1	0	3.139352	-2.730864	1.960454
26	6	0	-2.000901	0.565478	2.091644
27	1	0	-3.069242	0.722818	2.225253
28	1	0	-1.517410	0.475820	3.068114
29	6	0	-0.010561	-0.391163	-1.362520
30	7	0	0.960641	0.513231	-1.123811
31	16	0	0.175843	-1.974911	-1.872126
32	6	0	2.352475	0.383705	-0.947437
33	6	0	5.086937	0.335199	-0.360189
34	6	0	3.124097	-0.716428	-1.328056
35	6	0	2.955604	1.463819	-0.282282
36	6	0	4.312155	1.435833	0.005631
37	6	0	4.485696	-0.726000	-1.027224
38	1	0	2.670180	-1.550014	-1.843760
39	1	0	2.337200	2.308244	0.018219
40	1	0	4.764481	2.278497	0.519771
41	1	0	5.079831	-1.584441	-1.326725
42	1	0	6.148394	0.312079	-0.134695
43	6	0	-2.490742	-0.395603	-1.602092
44	1	0	-2.855829	0.290275	-2.377739

45	1	0	-2.262154	-1.357723	-2.064154
46	1	0	-1.257167	1.138854	-0.837567
47	1	0	0.617141	1.436853	-0.813305
48	35	0	-0.555492	3.078642	0.260474
49	1	0	-1.561839	1.475126	1.625990

HBr

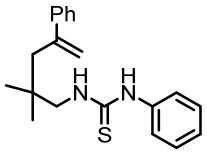
E(RM06-2X/6-31G(d)) = -2572.364093 a.u.
Imaginary Freq = 0Zero-point Energy Correction = 0.006154
Thermal Correction to Energy = 0.008514
Thermal Correction to Enthalpy = 0.009459
Thermal Correction to Free Energy = -0.013082
EE + Zero-point Energy = -2572.357940
EE + Thermal Energy Correction = -2572.355579
EE + Thermal Enthalpy Correction = -2572.354635
EE + Thermal Free Energy Correction = -2572.377175
Truhlar's quasiharmonic corrected Gibbs energy = -2572.377175

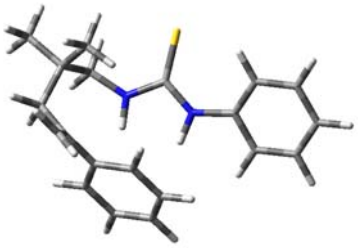
E_{sp}(RM06-2X/def2-TZVP) = -2574.790511
E_{sp}(RM06-2X/6-311G(d,p)) = -2574.766668
E_{sp}(RM06-2X/6-311+G(d,p)) = -2574.766971

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	0.039776
2	1	0	0.000000	0.000000	-1.392170

Alkenyl thiourea

NH,NH-isomer





E(RM06-2X/6-31G(d)) = -1283.849963 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 0.404113
Thermal Correction to Energy = 0.425859
Thermal Correction to Enthalpy = 0.426803
Thermal Correction to Free Energy = 0.351353
EE + Zero-point Energy = -1283.445849
EE + Thermal Energy Correction = -1283.424104
EE + Thermal Enthalpy Correction = -1283.423160
EE + Thermal Free Energy Correction = -1283.498610
Truhlar's quasiharmonic corrected Gibbs energy = -1283.492394

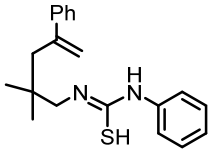
E_{sp}(RM06-2X/def2-TZVP) = -1284.212167
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -1284.212167
E_{sp}(RM06-2X/6-311G(d,p)) = -1284.109326
E_{sp}(RM06-2X/6-311+G(d,p)) = -1284.118127

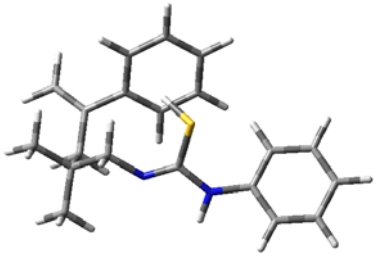
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.796889	1.108962	0.998117
2	6	0	3.597533	0.131047	0.160659
3	6	0	3.007665	-1.295317	-0.060463
4	7	0	0.747781	-0.666159	-1.029234
5	1	0	4.561153	-0.001319	0.665933
6	1	0	3.830454	0.563518	-0.822495
7	6	0	4.180389	-2.195422	-0.476720
8	1	0	4.925469	-2.254591	0.323320
9	1	0	4.678329	-1.809250	-1.374521

10	1	0	3.833351	-3.211586	-0.690952
11	6	0	2.381481	-1.833182	1.225616
12	1	0	3.097315	-1.771081	2.054069
13	1	0	2.079118	-2.876455	1.096452
14	1	0	1.491568	-1.261670	1.507085
15	6	0	1.683516	1.882458	0.383398
16	6	0	-0.450740	3.300230	-0.783070
17	6	0	1.815784	2.466023	-0.885876
18	6	0	0.462914	2.026679	1.055732
19	6	0	-0.591270	2.736149	0.485020
20	6	0	0.758486	3.163883	-1.464734
21	1	0	2.755596	2.377980	-1.423957
22	1	0	0.331990	1.543156	2.019442
23	1	0	-1.535657	2.816817	1.016200
24	1	0	0.881408	3.608069	-2.447774
25	1	0	-1.274887	3.843489	-1.235620
26	6	0	3.085474	1.292836	2.290439
27	1	0	3.891928	0.746929	2.771767
28	1	0	2.537302	2.003169	2.902481
29	6	0	-0.440745	-1.222061	-0.680601
30	7	0	-1.413972	-0.268639	-0.553412
31	16	0	-0.663100	-2.871194	-0.474331
32	6	0	-2.759697	-0.334483	-0.141166
33	6	0	-5.437658	-0.194390	0.672014
34	6	0	-3.575689	0.729953	-0.546406
35	6	0	-3.290901	-1.328162	0.685785
36	6	0	-4.624555	-1.248910	1.076060
37	6	0	-4.901414	0.801009	-0.140263
38	1	0	-3.160618	1.499965	-1.193687
39	1	0	-2.668783	-2.148961	1.012240
40	1	0	-5.027213	-2.028115	1.716215
41	1	0	-5.516499	1.633931	-0.466980
42	1	0	-6.475061	-0.147600	0.986895
43	6	0	1.998295	-1.366921	-1.226766
44	1	0	1.748535	-2.414083	-1.415746
45	1	0	2.469222	-0.963169	-2.133385

46	1	0	0.779016	0.338517	-1.149471
47	1	0	-1.134638	0.672755	-0.810343

SH,NH-isomer





E(RM06-2X/6-31G(d)) = -1283.825515 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 0.399947
Thermal Correction to Energy = 0.422017
Thermal Correction to Enthalpy = 0.422961
Thermal Correction to Free Energy = 0.347129
EE + Zero-point Energy = -1283.425568
EE + Thermal Energy Correction = -1283.403498
EE + Thermal Enthalpy Correction = -1283.402554
EE + Thermal Free Energy Correction = -1283.478386
Truhlar's quasiharmonic corrected Gibbs energy = -1283.472000

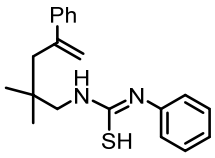
E_{sp}(RM06-2X/def2-TZVP) = -1284.190206

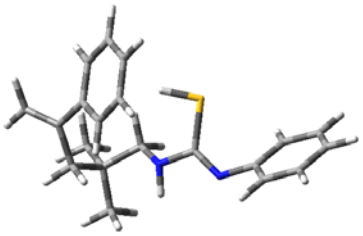
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.239686	0.685199	-0.920488
2	6	0	-3.030424	-0.780007	-1.238424
3	6	0	-2.906769	-1.711236	-0.007509
4	7	0	-0.457830	-1.452443	0.076384
5	1	0	-3.870223	-1.134121	-1.849364
6	1	0	-2.120789	-0.908634	-1.836181

7	6	0	-2.753272	-3.150303	-0.510654
8	1	0	-3.624833	-3.450030	-1.103494
9	1	0	-1.856446	-3.248284	-1.128562
10	1	0	-2.663673	-3.845295	0.332352
11	6	0	-4.153447	-1.608813	0.875788
12	1	0	-5.057034	-1.839094	0.299735
13	1	0	-4.094238	-2.321091	1.706369
14	1	0	-4.272720	-0.604097	1.294460
15	6	0	-2.055680	1.515362	-0.547686
16	6	0	0.134231	3.153330	0.105879
17	6	0	-2.135976	2.438791	0.504602
18	6	0	-0.850929	1.414209	-1.251975
19	6	0	0.227658	2.237113	-0.940607
20	6	0	-1.051177	3.248810	0.831831
21	1	0	-3.061202	2.507835	1.071432
22	1	0	-0.760637	0.700568	-2.064877
23	1	0	1.145350	2.160509	-1.516905
24	1	0	-1.131498	3.954097	1.653731
25	1	0	0.982177	3.784062	0.357174
26	6	0	-4.453925	1.243334	-0.964518
27	1	0	-0.212268	0.541485	1.995832
28	1	0	-5.331448	0.659838	-1.229965
29	6	0	0.658645	-1.035638	0.518726
30	7	0	1.810427	-1.423275	-0.141628
31	6	0	3.081493	-0.815128	-0.228419
32	6	0	5.659904	0.250369	-0.503375
33	6	0	3.301416	0.552951	-0.038312
34	6	0	4.161267	-1.640333	-0.564310
35	6	0	5.436870	-1.108615	-0.711176
36	6	0	4.587293	1.070302	-0.163159
37	1	0	2.470915	1.203181	0.206557
38	1	0	3.988462	-2.704708	-0.699633
39	1	0	6.261181	-1.763909	-0.975818
40	1	0	4.745325	2.133430	-0.006745
41	1	0	6.657169	0.665221	-0.608078
42	16	0	0.950716	-0.130367	2.045991

43	1	0	-4.604182	2.297904	-0.751022
44	6	0	-1.683420	-1.321643	0.834090
45	1	0	-1.842429	-0.299457	1.209544
46	1	0	-1.637489	-1.972764	1.721955
47	1	0	1.606466	-2.129066	-0.839440

NH,SH-isomer





E(RM06-2X/6-31G(d))= -1283.827957 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 0.400694
Thermal Correction to Energy = 0.422571
Thermal Correction to Enthalpy = 0.423515
Thermal Correction to Free Energy = 0.348487
EE + Zero-point Energy = -1283.427264
EE + Thermal Energy Correction = -1283.405386
EE + Thermal Enthalpy Correction = -1283.404442
EE + Thermal Free Energy Correction = -1283.479471
Truhlar's quasiharmonic corrected Gibbs energy = -1283.475016

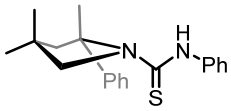
E_{sp}(RM06-2X/def2-TZVP) = -1284.192942

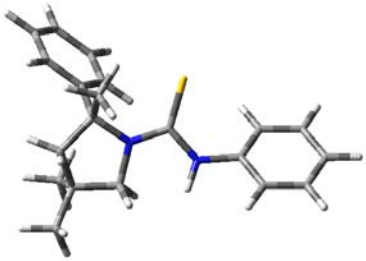
Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000085163	-0.000070921	-0.000015298
2	6	0.000014549	0.000050289	0.000028799
3	6	-0.000025474	0.000003771	-0.000012468

4	7	0.000032788	0.000005003	-0.000031478
5	1	-0.000008541	0.000010601	-0.000009778
6	1	-0.000018367	-0.000026424	0.000002317
7	6	0.000013692	-0.000019315	-0.000001086
8	1	0.000006864	0.000002254	-0.000007117
9	1	-0.000001110	0.000009614	-0.000011717
10	1	0.000002233	-0.000001838	0.000008268
11	6	0.000020293	-0.000005901	-0.000002046
12	1	-0.000010597	0.000006942	0.000001392
13	1	-0.000010630	-0.000000327	0.000004152
14	1	0.000002956	0.000003639	0.000005663
15	6	0.000000949	0.000067585	-0.000020420
16	6	-0.000006652	-0.000020814	-0.000000173
17	6	0.000032435	0.000019890	0.000034648
18	6	0.000037020	0.000007551	0.000006644
19	6	-0.000000633	0.000004519	-0.000007313
20	6	-0.000004388	-0.000014809	0.000020835
21	1	0.000008029	-0.000004591	0.000002911
22	1	0.000001133	0.000029510	-0.000005295
23	1	0.000002367	-0.000001202	-0.000000298
24	1	0.000006315	0.000002315	0.000000548
25	1	-0.000000044	-0.000005107	-0.000006017
26	6	0.000027796	-0.000032892	-0.000030596
27	1	-0.000008717	0.000007188	0.000013620
28	1	-0.000001210	0.000002636	0.000023375
29	6	-0.000063604	-0.000069211	0.000102928
30	7	0.000007403	0.000018163	-0.000114085
31	6	0.000005705	0.000001067	0.000087552
32	6	0.000002014	0.000010742	0.000006599
33	6	-0.000017904	0.000002652	-0.000039461
34	6	0.000033442	-0.000001667	-0.000015329
35	6	-0.000018187	-0.000007537	-0.000004367
36	6	0.000002203	-0.000020130	-0.000008778
37	1	0.000005204	0.000013852	-0.000000485
38	1	-0.000024945	0.000004854	0.000002656
39	1	-0.000004707	-0.000004912	0.000005314

40	1	-0.000004402	0.000003970	0.000000690
41	1	-0.000002528	-0.000005250	0.000003841
42	16	0.000039600	0.000032025	-0.000021531
43	1	0.000001323	-0.000007344	-0.000002201
44	6	-0.000000888	0.000011763	-0.000009124
45	1	0.000004333	-0.000005381	-0.000005436
46	1	0.000010672	0.000002867	0.000004025
47	1	-0.000002626	-0.000009688	0.000015126

Hydroamination product





E(RM06-2X/6-31G(d)) = -1283.866433 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 0.404707
Thermal Correction to Energy = 0.425804
Thermal Correction to Enthalpy = 0.426748
Thermal Correction to Free Energy = 0.354253
EE + Zero-point Energy = -1283.461726
EE + Thermal Energy Correction = -1283.440629
EE + Thermal Enthalpy Correction = -1283.439685
EE + Thermal Free Energy Correction = -1283.512181
Truhlar's quasiharmonic corrected Gibbs energy = -1283.762963

E_{sp}(RM06-2X/def2-TZVP) = -1284.223499
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -1284.258805
E_{sp}(RM06-2X/6-311G(d,p)) = -1284.121434
E_{sp}(RM06-2X/6-311+G(d,p)) = -1284.129962

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	0.317570	0.708320	0.296399
2	6	0	1.630014	0.392878	0.929543
3	6	0	2.386050	1.729890	0.729340
4	6	0	1.808791	2.400148	-0.522251
5	6	0	0.333460	1.995890	-0.409623
6	1	0	2.185278	2.370058	1.598478
7	1	0	3.467155	1.573574	0.669057
8	1	0	-0.143218	1.898787	-1.392684
9	1	0	-0.216394	2.758864	0.167311
10	6	0	1.970341	3.919323	-0.479420
11	1	0	1.549112	4.339670	0.440243
12	1	0	1.470348	4.391093	-1.332836
13	1	0	3.030029	4.191806	-0.523236
14	6	0	2.430618	1.863320	-1.815842
15	1	0	2.276506	0.789247	-1.935395
16	1	0	3.509746	2.049890	-1.822271
17	1	0	1.994629	2.372193	-2.683104
18	6	0	-0.824779	-0.024410	0.433148
19	16	0	-0.901208	-1.550936	1.116518
20	7	0	-1.934402	0.615594	-0.074590
21	6	0	-3.263293	0.128912	-0.145350
22	6	0	-5.928831	-0.663779	-0.399599
23	6	0	-4.293357	0.987482	0.239272
24	6	0	-3.568476	-1.128472	-0.670116
25	6	0	-4.897167	-1.518385	-0.784102
26	6	0	-5.621387	0.594257	0.106802
27	1	0	-4.050624	1.962964	0.654011
28	1	0	-2.767479	-1.788723	-0.977229
29	1	0	-5.126689	-2.499946	-1.187281
30	1	0	-6.413208	1.271990	0.410457
31	1	0	-6.963342	-0.977268	-0.496074
32	1	0	-1.873608	1.619890	-0.169745
33	6	0	1.516184	0.129988	2.441229
34	1	0	2.494829	0.295550	2.903378

35	1	0	1.184253	-0.882686	2.657656
36	1	0	0.809386	0.839207	2.883689
37	6	0	2.355941	-0.763281	0.231492
38	6	0	3.784850	-2.839797	-1.014562
39	6	0	3.614122	-1.152073	0.700317
40	6	0	1.825410	-1.435010	-0.870139
41	6	0	2.533031	-2.461188	-1.489386
42	6	0	4.323535	-2.180233	0.085643
43	1	0	4.053560	-0.647016	1.557157
44	1	0	0.847337	-1.156855	-1.247429
45	1	0	2.096102	-2.970577	-2.342912
46	1	0	5.299024	-2.463850	0.469344
47	1	0	4.334067	-3.643031	-1.495913

Computational study

on

the NPTA-catalyzed hydroamination

Summary of the calculated energies

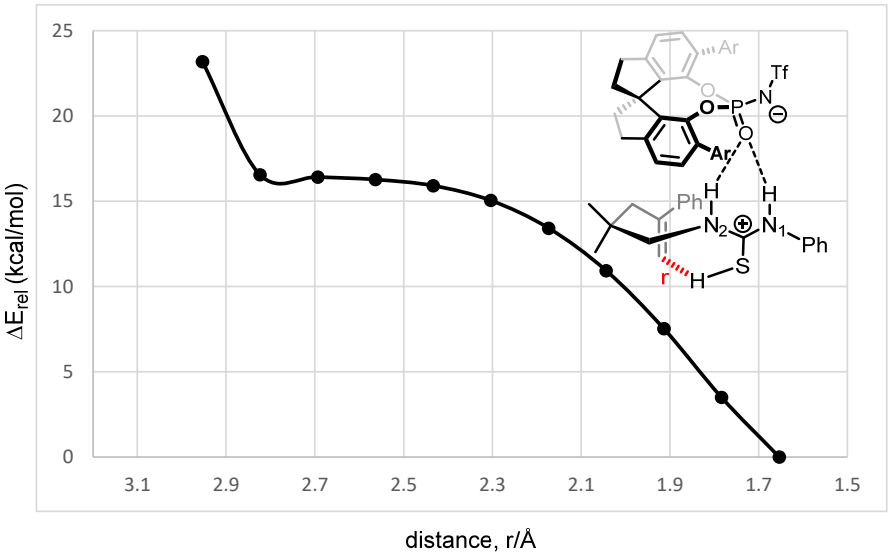


Fig. S5 Potential energy surface scanned by the bond length r (Å) of the forming C-N bond from the transition state $TS^{NPTA}_{C1\_S}$. The energies, ΔE_{rel} in kcal/mol, are relative to the product.

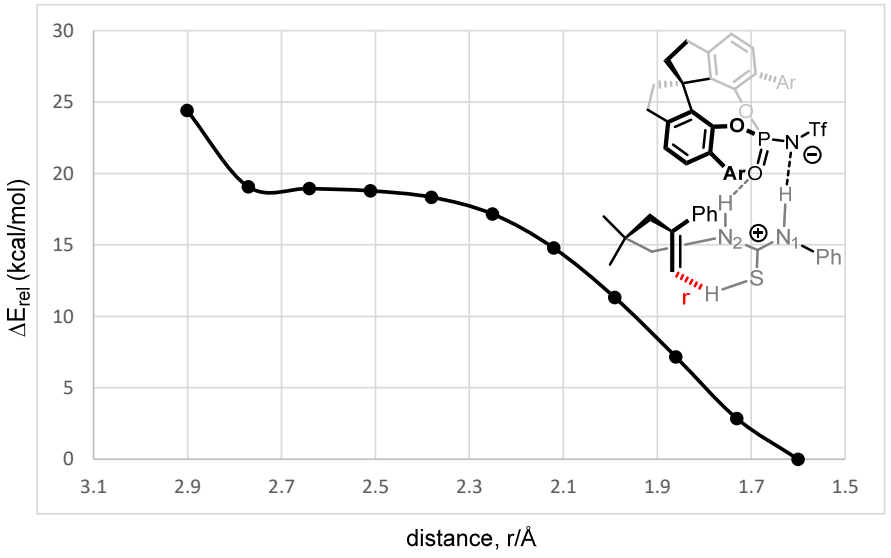


Fig. S6 Potential energy surface scanned by the bond length r (Å) of the forming C-N bond from the transition state $TS^{NPTA}_{C1\_R}$. The energies, ΔE_{rel} in kcal/mol, are relative to the product.

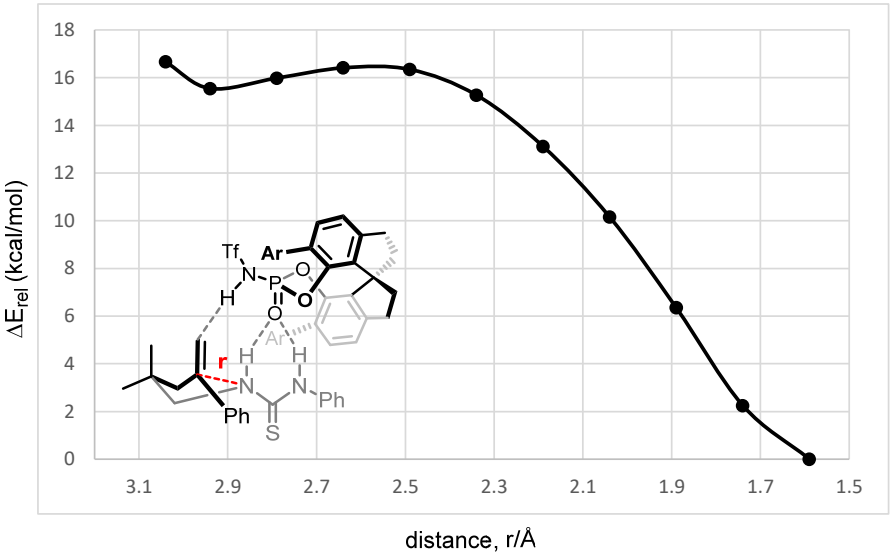


Fig. S7 Potential energy surface scanned by the bond length r (Å) of the forming C-N bond from the transition state $TS^{NPTA}{}_{E\_S\_TS1}$. The energies, ΔE_{rel} in kcal/mol, are relative to the product.

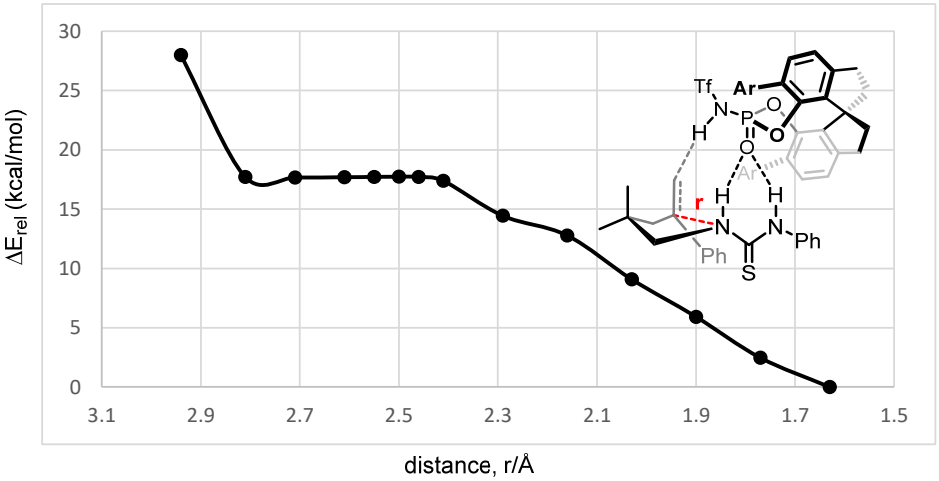


Fig. S8 Potential energy surface scanned by the bond length r (Å) of the forming C-N bond from the transition state $TS^{NPTA}{}_{E\_R\_TS1}$. The energies, ΔE_{rel} in kcal/mol, are relative to the product.

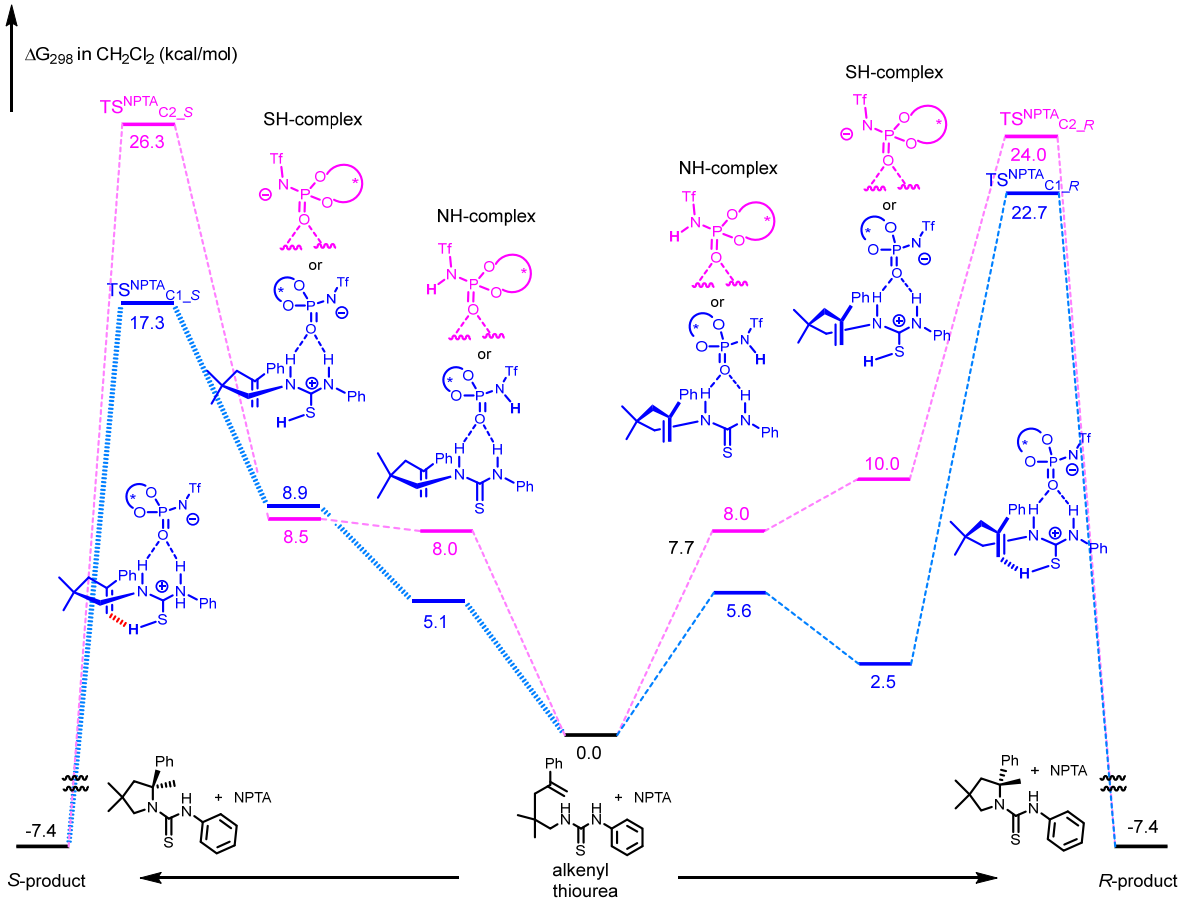


Fig. S9 Summary of the calculated Gibbs free-energy profile for the NPTA-catalyzed hydroamination of alkenyl thiourea vis $TS^{NPTA}_{C1,C2}$ at 298.15 K at the M06-2X/def2-TZVP/SMD(CH_2Cl_2)//M06-2X /6-31G(d) level of theory.

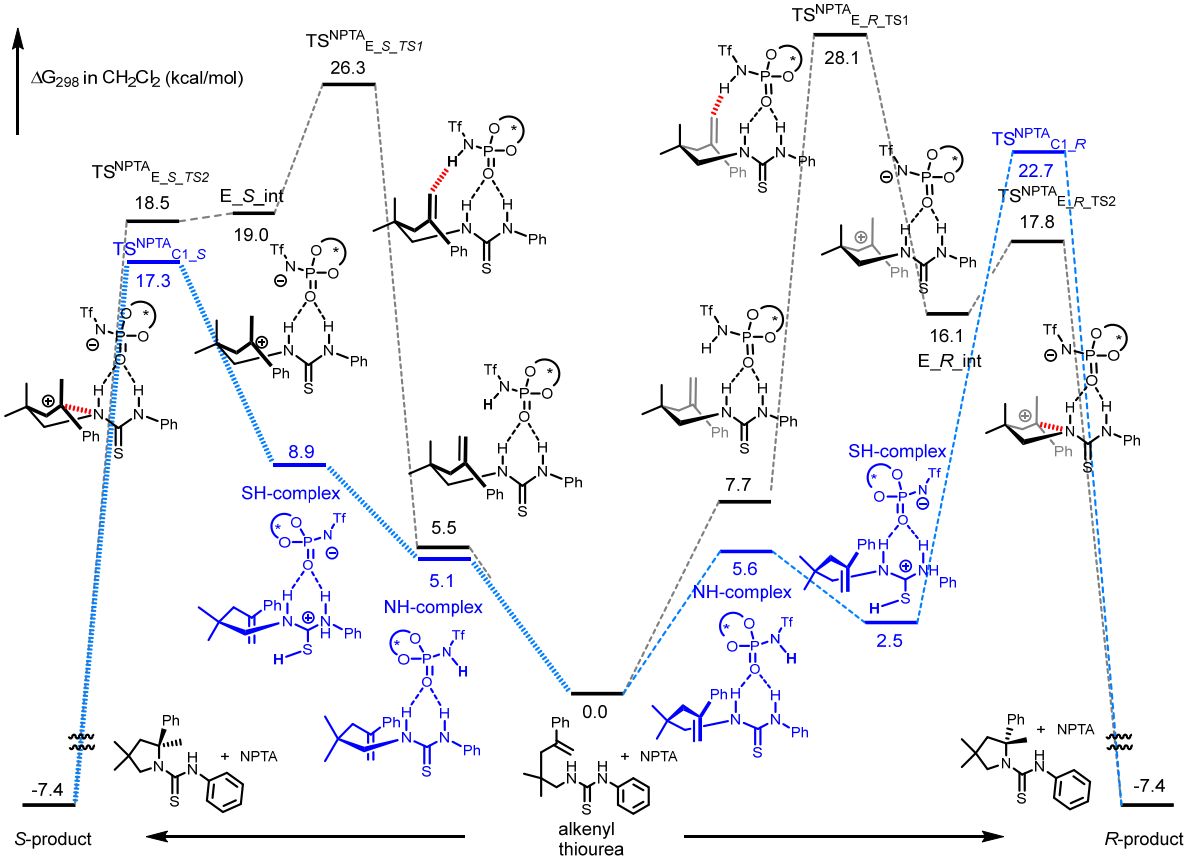


Fig. S10 Summary of the calculated Gibbs free-energy profile for the NPTA-catalyzed hydroamination of alkenyl thiourea via $TS^{NPTA}_{C1,E}$ at 298.15 K at the M06-2X/def2-TZVP/SMD(CH_2Cl_2)//M06-2X /6-31G(d) level of theory.

Table S4. Calculated Gibbs free energies for TS^{NPTA}_{C1} in gas and CH_2Cl_2 using differnent methodthe at M06-2X/6-31G(d) level of theory

	$TS^{NPTA}_{C1\_S}$	$TS^{NPTA}_{C1\_R}$	ΔG_{298} (kcal/mol)
M06-2X/6-311G(d,p)			
gas	-4524.366000	-4524.358036	4.99741
SMD	-4524.441578	-4524.432935	5.423483
IEPPCM	-4524.393277	-4524.382757	6.6013
M06-2X/6-311+G(d,p)			
gas	-4524.407375	-4524.40022	4.489763
SMD	-4524.481891	-4524.473988	4.959133
IEPPCM	-4524.430906	-4524.423901	4.395638
M06-2X/def2-TZVP			
gas	-4524.857823	-4524.849764	5.057023
SMD	-4524.930187	-4524.921531	5.43164
IEPPCM	-4524.892496	-4524.885063	4.664208

Table S5. Calculated Gibbs free energies for $TS^{NPTA}_{C1\_S}$ at the M06-2X/def2-TZVP/SMD(CH_2Cl_2)//M06-2X/ 6-31G(d) level of theory

	G_{298} (a.u.)	ΔG_{298} (kcal/mol)
thiourea + NPTA	-4524.957711	0
C1_S_NH-complex	-4524.949579	5.10283
C1_S_SH-complex	-4524.943529	8.899205
$TS^{NPTA}_{C1\_S}$	-4524.930187	14.77135
product +NPTA	-4524.969535	-7.41956

Table S6. Calculated Gibbs free energies for $TS^{NPTA}_{C1\_R}$ at the M06-2X/def2-TZVP/SMD(CH_2Cl_2)//M06-2X/ 6-31G(d) level of theory

	G_{298} (a.u.)	ΔG_{298} (kcal/mol)
thiourea + NPTA	-4524.957711	0
C1_R_NH-complex	-4524.948838	5.5678075
C1_R_SH-complex	-4524.953749	2.486155
$TS^{NPTA}_{C1\_R}$	-4524.921531	22.70295
product +NPTA	-4524.969535	-7.41956

Table S7. Calculated Gibbs free energies for $TS^{NPTA}_{C2\_S}$ at the M06-2X/def2-TZVP/SMD(CH_2Cl_2)//M06-2X/ 6-31G(d) level of theory

	G_{298} (a.u.)	ΔG_{298} (kcal/mol)
thiourea + NPTA	-4524.957711	0
C2_S_NH-complex	-4524.944915	8.02949
C2_S_SH-complex	-4524.944148	8.5107825
$TS^{NPTA}_{C2\_S}$	-4524.915827	26.28221
product +NPTA	-4524.969535	-7.41956

Table S8. Calculated Gibbs free energies for $TS^{NPTA}_{C2\_R}$ at the M06-2X/def2-TZVP/SMD(CH_2Cl_2)//M06-2X/ 6-31G(d) level of theory

	G_{298} (a.u.)	ΔG_{298} (kcal/mol)
thiourea + NPTA	-4524.957711	0
C2_R_NH-complex	-4524.944998	7.9774075
C2_R_SH-complex	-4524.941738	10.0230575
$TS^{NPTA}_{C2\_R}$	-4524.919515	23.96799
product +NPTA	-4524.969535	-7.41956

Table S9. Calculated Gibbs free energies for $TS^{NPTA}_{E\_S}$ at the M06-2X/def2-TZVP/SMD(CH_2Cl_2)//M06-2X/ 6-31G(d) level of theory

	G_{298} (a.u.)	ΔG_{298} (kcal/mol)
thiourea + NPTA	-4524.957711	0
E_S_NH-complex	-4524.948897	5.530785
$TS^{NPTA}_{E\_S\_TS1}$	-4524.915796	26.3016625
E_S_int	-4524.927461	18.981875
$TS^{NPTA}_{E\_S\_TS2}$	-4524.928232	18.4980725
product +NPTA	-4524.969535	-7.41956

Table S10. Calculated Gibbs free energies for $TS^{NPTA}_{E\_R}$ at the M06-2X/def2-TZVP/SMD(CH_2Cl_2)//M06-2X/ 6-31G(d) level of theory

	G_{298} (a.u.)	ΔG_{298} (kcal/mol)
thiourea + NPTA	-4524.957711	0
E_R_NH-complex	-4524.945484	7.6724425
$TS^{NPTA}_{E\_R\_TS1}$	-4524.912863	28.14212
E_R_int	-4524.932108	16.0658825
$TS^{NPTA}_{E\_R\_TS2}$	-4524.929353	17.794645
product +NPTA	-4524.969535	-7.41956

Distortion/interaction model

In this model, the activation energy $\Delta E^{\ddagger}$ of the reaction can be written as $\Delta E^{\ddagger} = \Delta E^{\ddagger}_{dist\_cat} + \Delta E^{\ddagger}_{dist\_sub} + \Delta E^{\ddagger}_{int}$. The distortion energy $\Delta E^{\ddagger}_{dist}$ can be obtained by calculating the energy difference between the distorted geometry in transition structure and the optimized geometry in reactants. In this work, $\Delta E^{\ddagger}_{dist\_cat}$ is the energy required to distort the anion form of NPTA from its ground-state geometry to its transition-state geometry, and $\Delta E^{\ddagger}_{dist\_sub}$ is the distortional energy for the *S*-protonated form of alkenyl thiourea. The interaction energy ($\Delta E^{\ddagger}_{int}$) refers to the energy difference between the catalyst plus the substrates and the transition state structure. For this distortion/interaction analysis, the calculated Gibbs free energy in CH_2Cl_2 was used for comparison with Fig. 3.

Table S11. Distortion/interaction analysis for $TS^{NPTA}_{C1\_S}$ and $TS^{NPTA}_{C1\_R}$[a]

	$\Delta G^{\ddagger}_{dist}$	$\Delta G^{\ddagger}_{dist\_cat}$	$\Delta G^{\ddagger}_{dist\_sub}$	$\Delta G^{\ddagger}_{int}$	$\Delta G^{\ddagger}$
$TS^{NPTA}_{C1\_S}$	20.1	0.3	19.8	-2.9	17.3
$TS^{NPTA}_{C1\_R}$	20.0	1.1	18.9	2.7	22.7
$\Delta\Delta G^{\ddagger}$	-0.1	0.8	-0.9	5.6	5.4

[a] Energies are shown in kcal/mol. $\Delta G^{\ddagger}_{dist} = \Delta G^{\ddagger}_{dist\_cat} + \Delta G^{\ddagger}_{dist\_sub}$.

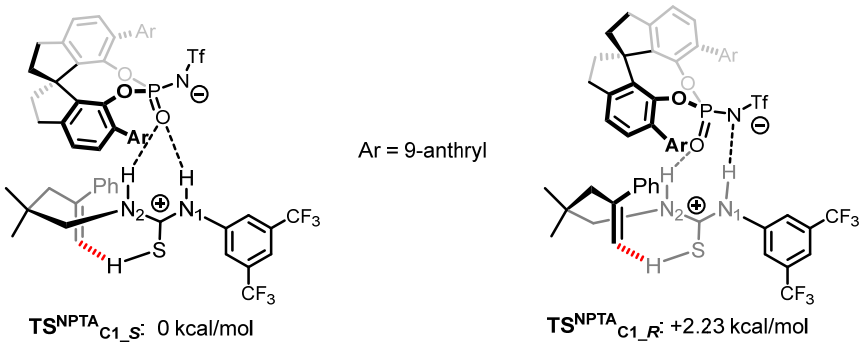


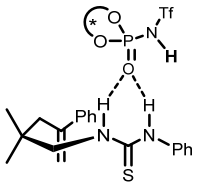
Fig. S11 Relative Gibbs free energies of $TS^{NPTA}_{C1\_S}$ and $TS^{NPTA}_{C1\_R}$ at 273.15 K in the NPTA-catalyzed hydroamination of real alkenyl thiourea at the M06-2X/def2-TZVP/SMD(CH_2Cl_2)//M06-2X/6-31G(d) level of theory

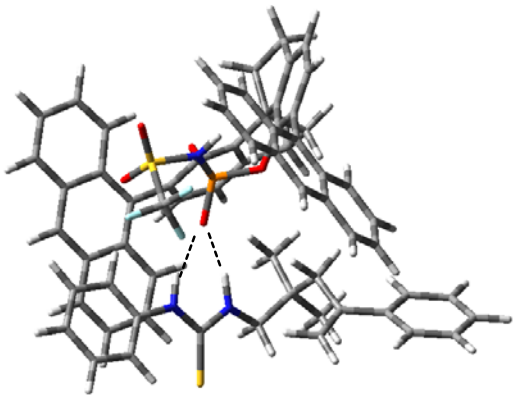
Cartesian coordinates of the structures

on

the NPTA-catalyzed hydroamination

NH-complex_c1_*s*





E (RM06-2X/6-31G(d)) = -4524.425531 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 1.080078
Thermal Correction to Energy = 1.146845
Thermal Correction to Enthalpy = 1.147789
Thermal Correction to Free Energy = 0.977312
EE + Zero-point Energy = -4523.345453
EE + Thermal Energy Correction = -4523.278686
EE + Thermal Enthalpy Correction = -4523.277742
EE + Thermal Free Energy Correction = -4523.448219
Truhlar's quasiharmonic corrected Gibbs energy = -4523.429999

E_{sp} (RM06-2X/def2-TZVP) = -4525.869943
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.945111

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.031058	2.645158	-0.299980
2	6	0	3.139350	1.865991	0.653313
3	6	0	2.428351	2.703022	1.751700
4	7	0	0.493369	3.123475	0.259158
5	1	0	3.708300	1.068384	1.146154
6	1	0	2.370308	1.352514	0.063013
7	6	0	1.667443	1.738087	2.672681

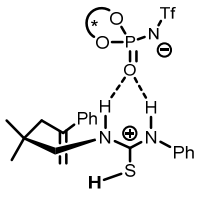
8	1	0	2.363726	1.032897	3.144432
9	1	0	0.915452	1.142761	2.139387
10	1	0	1.157859	2.285740	3.474805
11	6	0	3.429568	3.495775	2.599502
12	1	0	4.056744	2.827320	3.198742
13	1	0	2.898677	4.155563	3.295003
14	1	0	4.081663	4.115057	1.974647
15	6	0	5.513247	2.591179	-0.135033
16	6	0	8.326265	2.469994	0.141363
17	6	0	6.112899	2.174364	1.061538
18	6	0	6.369727	2.927645	-1.197097
19	6	0	7.751104	2.873800	-1.062070
20	6	0	7.497872	2.118173	1.200692
21	1	0	5.493809	1.893708	1.905569
22	1	0	5.946016	3.215497	-2.154040
23	1	0	8.381926	3.139076	-1.905213
24	1	0	7.927128	1.797332	2.145164
25	1	0	9.405483	2.422807	0.246661
26	6	0	3.470089	3.371068	-1.276300
27	1	0	2.393719	3.375429	-1.423142
28	1	0	4.049422	4.001955	-1.942276
29	6	0	-0.336379	3.824298	-0.554749
30	7	0	-1.297519	3.029082	-1.109062
31	6	0	-2.389809	3.318108	-1.947187
32	6	0	-4.652913	3.646368	-3.572777
33	6	0	-3.424320	2.370707	-1.936524
34	6	0	-2.487960	4.426701	-2.792737
35	6	0	-3.622245	4.580127	-3.588160
36	6	0	-4.541351	2.532174	-2.742154
37	1	0	-3.356866	1.515964	-1.266560
38	1	0	-1.692292	5.156435	-2.821737
39	1	0	-3.688849	5.448907	-4.236514
40	1	0	-5.326297	1.781344	-2.713345
41	1	0	-5.527525	3.780600	-4.201360
42	16	0	-0.153039	5.479974	-0.788386
43	6	0	1.465655	3.734797	1.140639

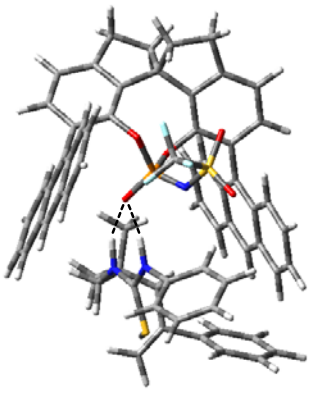
44	1	0	2.021713	4.487898	0.576733
45	1	0	0.955584	4.269692	1.958345
46	1	0	0.231869	2.162188	0.460325
47	6	0	0.963466	-2.697249	3.360527
48	6	0	2.261877	-2.178201	4.040948
49	6	0	1.758543	-1.325054	5.222422
50	1	0	2.798036	-1.542366	3.326237
51	1	0	2.928925	-2.992213	4.339971
52	1	0	1.614903	-1.933861	6.123586
53	1	0	2.451093	-0.519777	5.485521
54	6	0	0.412542	-3.922911	4.145044
55	1	0	-0.644515	-4.053590	3.887771
56	1	0	0.483571	-3.784418	5.227516
57	6	0	1.226627	-5.115900	3.618502
58	1	0	0.684859	-6.063755	3.682425
59	6	0	0.062615	-1.493461	3.551445
60	6	0	-1.494232	0.603961	4.480854
61	6	0	0.441959	-0.795381	4.700797
62	6	0	-1.039483	-1.062090	2.832357
63	6	0	-1.850133	-0.007485	3.270335
64	6	0	-0.344618	0.243682	5.180104
65	1	0	-0.064791	0.780663	6.081986
66	1	0	-2.120805	1.412138	4.846124
67	1	0	2.163080	-5.240062	4.176526
68	6	0	1.249525	-3.342179	2.013981
69	6	0	2.101754	-4.922265	-0.119020
70	6	0	1.350764	-2.808504	0.735936
71	6	0	1.504017	-4.707703	2.190937
72	6	0	1.933891	-5.499882	1.135138
73	6	0	1.799971	-3.574738	-0.349884
74	1	0	2.137111	-6.556283	1.283894
75	1	0	2.453703	-5.518446	-0.955903
76	8	0	-1.299591	-1.679518	1.597583
77	8	0	1.010402	-1.469630	0.508627
78	15	0	-0.522093	-1.021806	0.362770
79	8	0	-0.647174	0.436020	0.222198

80	7	0	-1.089440	-1.939501	-0.926108
81	1	0	-1.321322	2.078382	-0.745146
82	16	0	-2.547668	-1.677418	-1.675621
83	8	0	-3.007507	-2.929997	-2.223202
84	8	0	-3.339337	-0.834818	-0.811841
85	6	0	-2.006926	-0.647853	-3.109692
86	9	0	-3.076541	-0.236300	-3.764412
87	9	0	-1.307749	0.385872	-2.673298
88	9	0	-1.247979	-1.392768	-3.900597
89	6	0	-3.021431	0.471257	2.484684
90	6	0	-5.237398	1.396814	1.013658
91	6	0	-3.073073	1.822172	2.070599
92	6	0	-4.076352	-0.412584	2.176647
93	6	0	-5.193961	0.062613	1.410810
94	6	0	-4.216445	2.289627	1.336971
95	1	0	-6.085718	1.752932	0.432157
96	6	0	1.967571	-2.996241	-1.715343
97	6	0	2.326446	-1.956293	-4.308762
98	6	0	2.942699	-2.003207	-1.942285
99	6	0	1.175355	-3.479126	-2.780829
100	6	0	1.363482	-2.941971	-4.100475
101	6	0	3.116003	-1.473898	-3.266352
102	1	0	2.461530	-1.549666	-5.308720
103	6	0	-2.025162	2.767580	2.327980
104	1	0	-1.123567	2.435747	2.831433
105	6	0	-2.132020	4.068249	1.930489
106	1	0	-1.318905	4.763867	2.117894
107	6	0	-3.271148	4.525711	1.207344
108	1	0	-3.303082	5.552569	0.858721
109	6	0	-4.277174	3.656170	0.916065
110	1	0	-5.136459	3.972367	0.330482
111	6	0	-6.243698	-0.844067	1.062164
112	1	0	-7.070299	-0.464113	0.467532
113	6	0	-6.209037	-2.145040	1.460734
114	1	0	-7.007644	-2.827338	1.187472
115	6	0	-5.121662	-2.613236	2.255223

116	1	0	-5.113886	-3.645789	2.590875
117	6	0	-4.100178	-1.780282	2.603666
118	1	0	-3.293018	-2.153961	3.225198
119	6	0	0.132869	-4.452338	-2.603449
120	1	0	-0.039118	-4.875484	-1.617414
121	6	0	-0.655279	-4.843977	-3.647870
122	1	0	-1.456513	-5.555432	-3.476981
123	6	0	-0.441915	-4.328623	-4.958087
124	1	0	-1.072330	-4.662997	-5.775226
125	6	0	0.542941	-3.412178	-5.173063
126	1	0	0.712203	-2.999116	-6.163955
127	6	0	4.104252	-0.464909	-3.495310
128	1	0	4.208501	-0.069250	-4.501913
129	6	0	4.892004	-0.016117	-2.480488
130	1	0	5.641744	0.749412	-2.652118
131	6	0	4.742912	-0.558070	-1.169793
132	1	0	5.391731	-0.197735	-0.376394
133	6	0	3.802015	-1.509544	-0.907481
134	1	0	3.706761	-1.912987	0.095516
135	1	0	-0.533985	-2.698273	-1.326398

SH-complex_C1_*S*





E(RM06-2X/6-31G(d)) = -4524.413905

Imaginary Freq = 0

Zero-point Energy Correction = 1.077851

Thermal Correction to Energy = 1.144063
Thermal Correction to Enthalpy = 1.145007
Thermal Correction to Free Energy = 0.97782
EE + Zero-point Energy = -4523.3369054
EE + Thermal Energy Correction = -4523.269842
EE + Thermal Enthalpy Correction = -4523.268898
EE + Thermal Free Energy Correction = -4523.436085
Truhlar's quasiharmonic corrected Gibbs energy = -4523.420574

E_{sp} (RM06-2X/def2-TZVP) = -4525.861367
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.93686

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.543516	-0.841922	-1.566256
2	6	0	4.285475	-0.037787	-1.793887
3	6	0	3.283687	-0.380544	-2.897174
4	7	0	1.832143	-1.730092	-1.447299
5	1	0	4.591111	1.008100	-1.947348
6	1	0	3.748053	-0.007766	-0.830878
7	6	0	2.195133	0.699490	-2.854121
8	1	0	2.626490	1.680699	-3.082598
9	1	0	1.724182	0.775291	-1.864800
10	1	0	1.408973	0.486745	-3.589141
11	6	0	3.923985	-0.363920	-4.285021
12	1	0	4.390179	0.609869	-4.464342
13	1	0	3.159704	-0.514530	-5.055331
14	1	0	4.692370	-1.128889	-4.414249
15	6	0	6.383836	-0.295667	-0.463835
16	6	0	7.910156	0.757797	1.627042
17	6	0	6.938833	0.980979	-0.565152
18	6	0	6.608305	-1.040659	0.691415
19	6	0	7.364560	-0.515629	1.733904
20	6	0	7.701977	1.503107	0.470354

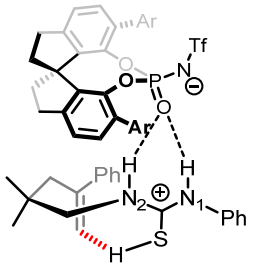
21	1	0	6.784665	1.561485	-1.471468
22	1	0	6.165879	-2.029660	0.782151
23	1	0	7.522150	-1.102401	2.633003
24	1	0	8.135840	2.492957	0.374525
25	1	0	8.498911	1.167996	2.440374
26	6	0	5.946253	-1.954632	-2.186282
27	1	0	5.407076	-2.412429	-3.007902
28	1	0	6.884760	-2.423704	-1.904245
29	6	0	1.856872	-2.565367	-0.424332
30	7	0	0.825149	-2.597400	0.395424
31	6	0	0.719944	-3.267846	1.648222
32	6	0	0.397901	-4.498147	4.096161
33	6	0	0.390283	-2.495497	2.756280
34	6	0	0.869727	-4.645445	1.736983
35	6	0	0.724502	-5.256569	2.976628
36	6	0	0.219339	-3.122880	3.982049
37	1	0	0.249298	-1.421324	2.654308
38	1	0	1.066680	-5.232552	0.843488
39	1	0	0.844558	-6.331335	3.060186
40	1	0	-0.063285	-2.521051	4.839529
41	1	0	0.268388	-4.984125	5.057341
42	16	0	3.234691	-3.594582	-0.063093
43	1	0	4.101427	-2.842993	-0.768048
44	6	0	2.610118	-1.737525	-2.672764
45	1	0	3.316389	-2.568805	-2.666959
46	1	0	1.900815	-1.927937	-3.488195
47	1	0	0.987555	-1.136979	-1.465305
48	6	0	-3.574067	3.236912	-0.530491
49	6	0	-3.521171	4.455528	-1.501263
50	6	0	-4.391370	4.059667	-2.708510
51	1	0	-2.479620	4.585022	-1.839642
52	1	0	-3.841693	5.386101	-1.007239
53	1	0	-5.453429	4.312542	-2.547802
54	1	0	-4.070782	4.554903	-3.637227
55	6	0	-4.798284	3.370142	0.408587
56	1	0	-4.961232	2.400846	0.906782

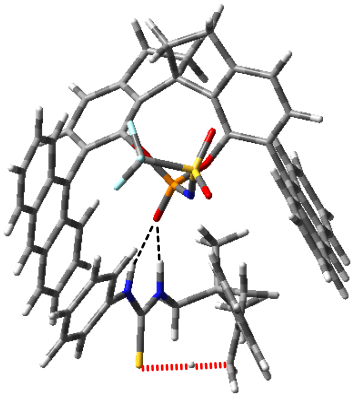
57	1	0	-5.712866	3.653046	-0.137476
58	6	0	-4.352035	4.412375	1.458621
59	1	0	-4.820009	4.239198	2.439065
60	6	0	-3.669842	2.120038	-1.540073
61	6	0	-4.110832	0.306219	-3.632069
62	6	0	-4.191587	2.564486	-2.760948
63	6	0	-3.353933	0.775228	-1.402840
64	6	0	-3.541535	-0.152787	-2.430920
65	6	0	-4.434647	1.661248	-3.803532
66	1	0	-4.848216	2.009331	-4.755875
67	1	0	-4.269702	-0.410984	-4.444821
68	1	0	-4.604888	5.439837	1.146044
69	6	0	-2.461342	3.336540	0.491616
70	6	0	-0.568647	4.316727	2.294106
71	6	0	-1.164216	2.831867	0.499812
72	6	0	-2.855244	4.197171	1.523599
73	6	0	-1.915231	4.687291	2.433297
74	6	0	-0.173043	3.359022	1.345738
75	1	0	-2.216490	5.368713	3.235611
76	1	0	0.193499	4.740465	2.956940
77	8	0	-2.867762	0.320382	-0.209619
78	8	0	-0.807861	1.806672	-0.352943
79	15	0	-1.285631	0.311815	0.034257
80	8	0	-0.571036	-0.602227	-0.899654
81	7	0	-1.121506	-0.120383	1.548502
82	1	0	0.060983	-1.955614	0.146732
83	16	0	-2.036549	-0.011896	2.826321
84	8	0	-1.330730	-0.653520	3.923839
85	8	0	-2.645475	1.286889	3.062851
86	6	0	-3.468168	-1.149972	2.563069
87	9	0	-4.473668	-0.566651	1.932837
88	9	0	-3.090296	-2.219724	1.882772
89	9	0	-3.912039	-1.527940	3.750621
90	6	0	-3.104524	-1.558034	-2.204408
91	6	0	-2.267444	-4.228081	-1.800836
92	6	0	-1.989543	-2.058135	-2.912378

93	6	0	-3.793097	-2.373659	-1.278480
94	6	0	-3.359086	-3.732704	-1.073983
95	6	0	-1.571567	-3.421635	-2.711239
96	1	0	-1.945305	-5.265402	-1.645676
97	6	0	1.256968	2.978037	1.124682
98	6	0	3.973013	2.336305	0.613223
99	6	0	1.864794	3.378982	-0.090508
100	6	0	2.009738	2.272646	2.096039
101	6	0	3.383327	1.926218	1.814891
102	6	0	3.247991	3.064214	-0.338822
103	1	0	5.024098	2.084345	0.416964
104	6	0	-1.233822	-1.243709	-3.821800
105	1	0	-1.519059	-0.193652	-3.944762
106	6	0	-0.172734	-1.763651	-4.521410
107	1	0	0.376223	-1.133507	-5.230628
108	6	0	0.227647	-3.125235	-4.336658
109	1	0	1.073846	-3.521535	-4.906930
110	6	0	-0.448613	-3.922981	-3.448978
111	1	0	-0.150838	-4.965263	-3.287911
112	6	0	-4.056640	-4.551803	-0.128318
113	1	0	-3.709197	-5.580679	0.016786
114	6	0	-5.121192	-4.058032	0.580885
115	1	0	-5.645670	-4.688295	1.305247
116	6	0	-5.549382	-2.708815	0.384716
117	1	0	-6.393197	-2.324823	0.965893
118	6	0	-4.908295	-1.893957	-0.513713
119	1	0	-5.235128	-0.857128	-0.647125
120	6	0	1.466249	1.882920	3.364489
121	1	0	0.442867	2.181812	3.608899
122	6	0	2.208698	1.154107	4.261025
123	1	0	1.750434	0.835851	5.202187
124	6	0	3.556856	0.785453	3.960811
125	1	0	4.130762	0.204209	4.689410
126	6	0	4.128927	1.170030	2.775777
127	1	0	5.165312	0.909325	2.529599
128	6	0	3.856123	3.500388	-1.560929

129	1	0	4.918545	3.272181	-1.711803
130	6	0	3.137122	4.189401	-2.505933
131	1	0	3.611239	4.522106	-3.434605
132	6	0	1.758700	4.486020	-2.272215
133	1	0	1.193608	5.037849	-3.029382
134	6	0	1.147288	4.097659	-1.105085
135	1	0	0.094115	4.341413	-0.928252

Transition state $TS^{NPTA}_{C1\_S}$





E (RM06-2X/6-31G(d)) = -4524.411469 a.u.
Imaginary Freq = 1: -618.99 cm-1
Zero-point Energy Correction = 1.076218
Thermal Correction to Energy = 1.14098
Thermal Correction to Enthalpy = 1.141924
Thermal Correction to Free Energy = 0.980645
EE + Zero-point Energy = -4523.335250
EE + Thermal Energy Correction = -4523.270489
EE + Thermal Enthalpy Correction = -4523.269545
EE + Thermal Free Energy Correction = -4523.430824
Truhlar's quasiharmonic corrected Gibbs energy = -4523.418451

E_{sp} (RM06-2X/6-311G(d,p)) = -4525.359018
E_{sp} (RM06-2X/6-311G(d,p)/SMD (CH_2Cl_2)) = -4525.434596
E_{sp} (RM06-2X/6-311G(d,p)/IEFPCM (CH_2Cl_2)) = -4525.386295

E_{sp} (RM06-2X/6-311+G(d,p)) = -4525.400393
E_{sp} (RM06-2X/6-311G+(d,p)/SMD (CH_2Cl_2)) = -4525.474909
E_{sp} (RM06-2X/6-311G+(d,p)/IEFPCM (CH_2Cl_2)) = -4525.423924

E_{sp} (RM06-2X/def2-TZVP) = -4525.850841
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.923205
E_{sp} (RM06-2X/def2-TZVP/IEFPCM (CH_2Cl_2)) = -4525.873141

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000059093	-0.000060179	0.000045056
2	6	0.000012788	0.000010345	-0.000022324
3	6	-0.000010239	0.000003494	-0.000002501
4	7	0.000045522	0.000029975	0.000043716
5	1	-0.000007568	0.000008683	0.000002754
6	1	0.000003649	0.000009664	-0.000002650
7	6	-0.000010212	-0.000007568	0.000001495
8	1	0.000003743	-0.000000317	-0.000002477
9	1	0.000002521	-0.000006004	-0.000000311
10	1	0.000002360	-0.000002764	-0.000000433
11	6	0.000003760	-0.000001235	-0.000000538
12	1	0.000000643	0.000001338	-0.000001050
13	1	0.000002191	0.000000864	-0.000004286
14	1	-0.000002264	-0.000001420	-0.000003728
15	6	-0.000012810	-0.000019005	-0.000009807
16	6	-0.000000254	0.000008071	0.000004418
17	6	-0.000013815	-0.000005560	0.000006236
18	6	0.000009239	0.000002432	0.000000449
19	6	-0.000005739	-0.000002384	0.000010684
20	6	-0.000002644	-0.000003134	0.000000093
21	1	-0.000000084	0.000005007	-0.000002739
22	1	-0.000000954	-0.000000517	0.000003880
23	1	-0.000006229	0.000012441	0.000014426
24	1	-0.000001451	0.000001545	0.000000468

25	1	-0.000000029	-0.000000554	-0.000000556
26	6	0.000085072	0.000122078	-0.000066195
27	1	-0.000000698	0.000005146	-0.000000944
28	1	-0.000007795	-0.000004916	0.000004842
29	6	-0.000023511	-0.000032891	-0.000048141
30	7	-0.000019446	-0.000012903	0.000001770
31	6	-0.000007301	-0.000004248	0.000002189
32	6	-0.000000735	0.000001537	0.000000750
33	6	-0.000001898	-0.000000575	-0.000005981
34	6	-0.000008473	-0.000003569	-0.000001671
35	6	-0.000001998	0.000000681	-0.000001128
36	6	-0.000000720	-0.000001202	-0.000000360
37	1	-0.000005392	-0.000000827	-0.000000692
38	1	-0.000005722	-0.000000678	0.000003769
39	1	-0.000001461	-0.000001111	-0.000002955
40	1	-0.000001772	0.000000766	-0.000000606
41	1	-0.000000758	0.000001776	0.000000909
42	16	0.000004521	0.000014410	0.000005090
43	1	-0.000003265	-0.000078435	0.000036067
44	6	-0.000008271	-0.000018281	0.000018240
45	1	-0.000010280	0.000001222	-0.000019375
46	1	-0.000002548	-0.000004550	-0.000001280
47	1	0.000025955	0.000005082	-0.000026208
48	6	0.000001775	0.000000180	0.000004445
49	6	0.000000435	-0.000003123	0.000001373
50	6	0.000002250	0.000000151	-0.000001699
51	1	0.000000421	-0.000001167	0.000000507
52	1	0.000000584	-0.000000581	-0.000000795
53	1	0.000000610	-0.000001510	0.000000438
54	1	0.000001672	-0.000000916	-0.000000078
55	6	-0.000001763	0.000003163	0.000000386
56	1	0.000001599	-0.000001363	-0.000009759
57	1	0.000001244	-0.000001269	0.000000915
58	6	0.000001270	-0.000000412	0.000001216
59	1	0.000000467	-0.000000394	0.000002731
60	6	0.000000839	0.000000569	0.000005489

61	6	0.000000982	-0.000001422	-0.000006514
62	6	0.000001620	-0.000000495	0.000001670
63	6	-0.000001330	-0.000002972	-0.000002620
64	6	0.000005756	0.000001576	0.000003373
65	6	-0.000001413	-0.000000212	0.000002218
66	1	0.000001227	-0.000000681	-0.000000229
67	1	0.000000396	-0.000001091	-0.000000530
68	1	0.000001223	-0.000001537	0.000001657
69	6	0.000003418	0.000005006	0.000001765
70	6	-0.000002965	0.000003446	0.000001036
71	6	-0.000001145	-0.000002695	-0.000003019
72	6	0.000004274	-0.000001991	0.000000721
73	6	0.000000185	-0.000000310	0.000000819
74	6	0.000000632	0.000001594	-0.000003832
75	1	0.000000731	-0.000000730	0.000001383
76	1	0.000000394	0.000000021	0.000000145
77	8	-0.000000792	-0.000006876	0.000010324
78	8	-0.000003124	-0.000009507	-0.000001262
79	15	0.000004671	-0.000009486	0.000018573
80	8	-0.000063575	0.000038767	-0.000018705
81	7	0.000008628	-0.000010851	-0.000018487
82	1	0.000053712	0.000022116	-0.000003578
83	16	-0.000005166	-0.000008670	-0.000011287
84	8	0.000002039	0.000005714	0.000001090
85	8	0.000002109	0.000000973	0.000003912
86	6	0.000003542	-0.000003770	-0.000001170
87	9	0.000000461	0.000000020	0.000001409
88	9	-0.000001398	0.000000794	0.000014019
89	9	0.000007135	0.000005295	0.000001664
90	6	-0.000003458	-0.000000451	-0.000003092
91	6	0.000000534	0.000000167	-0.000002445
92	6	0.000003991	0.000003362	0.000001454
93	6	-0.000002078	-0.000000413	-0.000001008
94	6	-0.000005163	-0.000001561	-0.000000705
95	6	-0.000000597	-0.000001142	0.000001189
96	1	0.000001807	0.000001504	-0.000000434

97	6	0.000002147	-0.000001224	0.000005078
98	6	-0.000001919	-0.000001534	-0.000000107
99	6	0.000000024	0.000000068	-0.000000347
100	6	-0.000003388	-0.000002295	-0.000000948
101	6	-0.000004894	-0.000000403	0.000001009
102	6	-0.000004726	-0.000002610	0.000004205
103	1	0.000000453	-0.000000042	0.000000253
104	6	0.000000509	0.000001272	0.000002069
105	1	0.000000466	-0.000001888	-0.000001102
106	6	0.000003601	0.000004418	0.000002244
107	1	-0.000000505	-0.000001275	-0.000001051
108	6	-0.000004709	-0.000001967	-0.000003156
109	1	0.000001638	0.000001217	-0.000000944
110	6	0.000010673	0.000006240	0.000007981
111	1	0.000001116	0.000000656	0.000001020
112	6	-0.000001819	-0.000001825	0.000000221
113	1	-0.000000251	0.000003157	0.000001707
114	6	0.000002753	0.000001723	0.000001538
115	1	-0.000000943	0.000000212	0.000000793
116	6	0.000000036	0.000000145	-0.000000642
117	1	0.000000004	-0.000000062	0.000001304
118	6	0.000001173	0.000000780	0.000000474
119	1	0.000000194	0.000000196	0.000001021
120	6	0.000001801	0.000001732	0.000001560
121	1	0.000000101	-0.000000306	0.000001847
122	6	0.000001895	-0.000001271	-0.000002294
123	1	-0.000000664	-0.000000095	0.000001676
124	6	0.000004877	0.000005400	-0.000002042
125	1	0.000000228	0.000000547	0.000000188
126	6	0.000003597	0.000000081	0.000002399
127	1	-0.000001151	0.000000116	0.000000682
128	6	-0.000000672	-0.000000005	0.000000576
129	1	0.000000617	-0.000000089	-0.000000046
130	6	0.000003574	0.000002021	-0.000000171
131	1	0.000000829	-0.000000909	-0.000000738
132	6	-0.000001834	0.000000156	0.000000971

133	1	0.000001331	-0.000000444	-0.000000317
134	6	-0.000002375	-0.000001594	0.000001438
135	1	0.000001013	0.000001154	-0.000001394

$TS^{NPTA}_{C1\_S\_conf\text{-}2}$

E(RM06-2X/6-31G(d)) = -4524.411101 a.u.
Imaginary Freq = 1: -614.85 cm-1
Zero-point Energy Correction = 1.076135
Thermal Correction to Energy = 1.140776
Thermal Correction to Enthalpy = 1.14172
Thermal Correction to Free Energy = 0.980685
EE + Zero-point Energy = -4523.334965
EE + Thermal Energy Correction = -4523.270325
EE + Thermal Enthalpy Correction = -4523.269381
EE + Thermal Free Energy Correction = -4523.430416

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.970887	4.032115	-0.603478
2	6	0	0.759814	3.750972	-1.439480
3	6	0	0.910250	3.248581	-2.906740
4	7	0	2.340527	1.489871	-1.973500
5	1	0	0.207574	4.704084	-1.470422
6	1	0	0.096464	3.075730	-0.891310
7	6	0	-0.329878	2.385250	-3.188616
8	1	0	-1.240718	2.965470	-3.008106
9	1	0	-0.375851	1.500460	-2.542094
10	1	0	-0.335963	2.054411	-4.233553
11	6	0	0.929468	4.399775	-3.917919
12	1	0	-0.014243	4.953893	-3.868949
13	1	0	1.036032	4.008616	-4.935844
14	1	0	1.749024	5.104759	-3.746781

15	6	0	1.984743	3.629095	0.798000
16	6	0	2.149949	2.795751	3.462888
17	6	0	2.705086	4.384415	1.745421
18	6	0	1.330536	2.455186	1.224634
19	6	0	1.424495	2.039147	2.544781
20	6	0	2.779432	3.974775	3.066975
21	1	0	3.168679	5.320828	1.452191
22	1	0	0.796618	1.826446	0.517508
23	1	0	0.906462	1.142246	2.866210
24	1	0	3.324423	4.575286	3.788257
25	1	0	2.207402	2.467574	4.496540
26	6	0	3.112370	4.640070	-1.149024
27	1	0	3.025109	5.120992	-2.119708
28	1	0	3.807963	5.122801	-0.463628
29	6	0	3.447962	1.197307	-1.271027
30	7	0	3.292766	0.177264	-0.419000
31	6	0	4.095761	-0.316166	0.636860
32	6	0	5.452470	-1.526721	2.749617
33	6	0	5.490330	-0.326724	0.640895
34	6	0	3.384297	-0.924950	1.673783
35	6	0	4.058693	-1.529051	2.724925
36	6	0	6.156543	-0.926486	1.708243
37	1	0	6.046111	0.106426	-0.180425
38	1	0	2.298182	-0.962663	1.638818
39	1	0	3.480108	-2.012175	3.506417
40	1	0	7.242437	-0.932529	1.713082
41	1	0	5.987289	-1.997392	3.568834
42	16	0	4.884373	2.134840	-1.428123
43	1	0	3.839792	3.597955	-1.342114
44	6	0	2.180608	2.393266	-3.091491
45	1	0	3.081910	2.997457	-3.196197
46	1	0	2.074917	1.810588	-4.017901
47	1	0	1.531143	0.891052	-1.775744
48	6	0	-3.810908	-2.216389	-1.449221
49	6	0	-4.577207	-1.874303	-2.762384
50	6	0	-4.064667	-2.896270	-3.795283

51	1	0	-4.291295	-0.863326	-3.075245
52	1	0	-5.662916	-1.894145	-2.627257
53	1	0	-4.646370	-3.826206	-3.756405
54	1	0	-4.119229	-2.524741	-4.822863
55	6	0	-4.541402	-3.355887	-0.687634
56	1	0	-3.843731	-3.786136	0.039168
57	1	0	-4.879748	-4.153015	-1.356990
58	6	0	-5.688544	-2.644245	0.055892
59	1	0	-5.972747	-3.156487	0.979898
60	6	0	-2.485407	-2.666983	-2.027299
61	6	0	-0.330405	-3.768157	-3.386639
62	6	0	-2.644540	-3.131463	-3.333959
63	6	0	-1.232283	-2.708895	-1.441434
64	6	0	-0.126904	-3.265417	-2.094825
65	6	0	-1.571193	-3.690195	-4.016771
66	1	0	-1.691514	-4.060351	-5.030996
67	1	0	0.516713	-4.209616	-3.904423
68	1	0	-6.590200	-2.577332	-0.566033
69	6	0	-3.943131	-1.089191	-0.437189
70	6	0	-4.836561	0.905271	1.284395
71	6	0	-3.180183	0.051286	-0.229290
72	6	0	-5.105033	-1.274164	0.321100
73	6	0	-5.553619	-0.286563	1.186460
74	6	0	-3.638576	1.091795	0.589882
75	1	0	-6.453695	-0.433980	1.776625
76	1	0	-5.191544	1.707540	1.925275
77	8	0	-1.090439	-2.168887	-0.175427
78	8	0	-1.928177	0.167141	-0.818950
79	15	0	-0.700756	-0.602759	-0.069093
80	8	0	0.515162	-0.252213	-0.863522
81	7	0	-0.776148	-0.246285	1.485626
82	1	0	2.363776	-0.258847	-0.450451
83	16	0	-0.480589	-1.226993	2.692524
84	8	0	0.547993	-2.229363	2.427356
85	8	0	-0.400407	-0.454386	3.927394
86	6	0	-2.040081	-2.203204	2.917097

87	9	0	-2.120552	-3.218697	2.062984
88	9	0	-2.068195	-2.690231	4.152913
89	9	0	-3.103670	-1.417649	2.741767
90	6	0	1.212560	-3.326886	-1.444702
91	6	0	3.772224	-3.520886	-0.275694
92	6	0	2.311487	-2.674136	-2.043606
93	6	0	1.382310	-4.044753	-0.241650
94	6	0	2.682412	-4.107458	0.364758
95	6	0	3.619864	-2.816868	-1.468636
96	1	0	4.755713	-3.571363	0.190004
97	6	0	-2.923468	2.402357	0.636960
98	6	0	-1.710638	4.949616	0.705226
99	6	0	-2.997619	3.248567	-0.492698
100	6	0	-2.265357	2.834012	1.804888
101	6	0	-1.650896	4.134741	1.834556
102	6	0	-2.376183	4.542496	-0.451221
103	1	0	-1.246500	5.934592	0.735500
104	6	0	2.180686	-1.815665	-3.186283
105	1	0	1.191675	-1.641490	-3.597742
106	6	0	3.268127	-1.199883	-3.736211
107	1	0	3.142247	-0.549400	-4.597846
108	6	0	4.574642	-1.394739	-3.196475
109	1	0	5.425699	-0.901855	-3.656200
110	6	0	4.738515	-2.180413	-2.095627
111	1	0	5.719875	-2.321041	-1.649595
112	6	0	2.839825	-4.766248	1.624305
113	1	0	3.827813	-4.768023	2.078245
114	6	0	1.780809	-5.361934	2.237660
115	1	0	1.904638	-5.848746	3.200022
116	6	0	0.499999	-5.352233	1.613066
117	1	0	-0.336177	-5.840096	2.104620
118	6	0	0.308319	-4.725660	0.418652
119	1	0	-0.676140	-4.727434	-0.036663
120	6	0	-2.185240	2.024881	2.984396
121	1	0	-2.599457	1.023761	2.961503
122	6	0	-1.566524	2.483896	4.108965

123	1	0	-1.493241	1.836095	4.976054
124	6	0	-0.978769	3.783051	4.139766
125	1	0	-0.487729	4.126512	5.045979
126	6	0	-1.007033	4.576716	3.033518
127	1	0	-0.544385	5.560671	3.036894
128	6	0	-2.456500	5.393565	-1.599725
129	1	0	-1.974668	6.368115	-1.550240
130	6	0	-3.138752	5.008902	-2.716356
131	1	0	-3.202230	5.669121	-3.576237
132	6	0	-3.788606	3.740068	-2.749424
133	1	0	-4.345021	3.448760	-3.634917
134	6	0	-3.714943	2.891622	-1.682605
135	1	0	-4.217552	1.930719	-1.722148

$TS^{NPTA}_{C1\_S\_conf\text{-}3}$

E(RM06-2X/6-31G(d)) = -4524.410126 a.u.
Imaginary Freq = 1: -649.25 cm-1
Zero-point Energy Correction = 1.075906
Thermal Correction to Energy = 1.140866
Thermal Correction to Enthalpy = 1.14181
Thermal Correction to Free Energy = 0.979043
EE + Zero-point Energy = -4523.334221
EE + Thermal Energy Correction = -4523.269260
EE + Thermal Enthalpy Correction = -4523.268316
EE + Thermal Free Energy Correction = -4523.431083

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000195	0.000008834	0.000000522
2	6	0.000000946	-0.000002410	0.000003220
3	6	-0.000005588	-0.000002005	0.000000669
4	7	0.000000210	-0.000000332	0.000003127

5	1	0.000002344	0.000000776	0.000004235
6	1	0.000003417	0.000002002	-0.000003696
7	6	-0.000001941	-0.000000828	0.000001835
8	1	-0.000002988	0.000000134	0.000001185
9	1	-0.000000621	-0.000000971	0.000001645
10	1	-0.000000454	0.000000215	0.000000678
11	6	-0.000000439	-0.000000010	0.000001778
12	1	-0.000001597	-0.000000093	0.000002198
13	1	-0.000001179	0.000000186	0.000002014
14	1	-0.000000978	-0.000000357	0.000002430
15	6	0.000000101	-0.000000293	0.000003226
16	6	-0.000000169	-0.000004125	-0.000001385
17	6	0.000001987	-0.000003535	0.000002514
18	6	-0.000001722	0.000000132	0.000003959
19	6	-0.000000233	0.000003664	0.000000093
20	6	0.000000424	-0.000002519	-0.000000391
21	1	0.000002696	-0.000000099	0.000000946
22	1	-0.000001709	-0.000008308	-0.000001397
23	1	0.000000539	0.000001577	0.000002021
24	1	0.000001599	-0.000001046	-0.000000176
25	1	0.000001336	-0.000001184	-0.000000735
26	6	0.000001484	-0.000002677	0.000003799
27	1	0.000000345	-0.000000955	0.000002146
28	1	-0.000000673	-0.000002327	0.000001249
29	6	0.000000216	-0.000005708	-0.000008728
30	7	0.000005055	-0.000000505	0.000000604
31	6	0.000004134	0.000003613	-0.000001506
32	6	0.000000562	-0.000000966	-0.000002122
33	6	0.000002143	-0.000002562	-0.000000470
34	6	0.000006152	0.000000337	0.000004761
35	6	0.000001011	-0.000005396	0.000001699
36	6	0.000000145	-0.000001505	-0.000003303
37	1	0.000002729	-0.000000897	0.000002675
38	1	0.000002131	-0.000001939	-0.000006262
39	1	0.000002235	0.000000262	-0.000001110
40	1	0.000002133	-0.000002730	0.000000621

41	1	0.000002283	-0.000002639	0.000000083
42	16	0.000011839	0.000019090	0.000002269
43	1	-0.000014966	-0.000026249	0.000001889
44	6	0.000000402	-0.000000478	0.000001168
45	1	0.000003912	0.000001161	0.000001301
46	1	0.000000040	-0.000000885	0.000001566
47	1	0.000006358	0.000003641	0.000000793
48	6	0.000002866	0.000005226	-0.000003516
49	6	-0.000000196	0.000004222	-0.000002099
50	6	-0.000001437	0.000002720	0.000000670
51	1	-0.000002992	0.000001715	0.000000352
52	1	-0.000002562	0.000001179	-0.000002687
53	1	-0.000001405	0.000001616	-0.000000992
54	1	-0.000001992	0.000001253	0.000000185
55	6	-0.000005425	-0.000001627	-0.000000536
56	1	-0.000000890	0.000000668	-0.000004615
57	1	-0.000001296	0.000002212	-0.000000673
58	6	0.000002506	0.000003621	-0.000000296
59	1	-0.000000614	0.000002416	-0.000001943
60	6	-0.000006034	0.000000623	0.000004948
61	6	0.000001105	0.000000364	-0.000003169
62	6	-0.000004236	0.000001408	0.000000115
63	6	0.000007342	-0.000003864	-0.000010455
64	6	0.000000231	0.000004339	0.000004240
65	6	-0.000001046	0.000000610	0.000005774
66	1	-0.000000975	0.000001667	0.000000655
67	1	-0.000000297	0.000001221	0.000000129
68	1	-0.000002208	0.000000768	-0.000001400
69	6	0.000000718	-0.000002798	-0.000004903
70	6	-0.000000221	-0.000000092	-0.000003409
71	6	0.000000113	0.000004234	0.000001858
72	6	0.000005919	0.000003533	-0.000001975
73	6	-0.000002350	0.000003663	-0.000001817
74	6	-0.000007732	0.000002061	-0.000007424
75	1	0.000000054	0.000002217	-0.000001693
76	1	-0.000001879	0.000001313	-0.000000063

77	8	0.000000394	0.000010872	0.000002831
78	8	-0.000001477	-0.000001699	0.000004048
79	15	-0.000008026	0.000000042	-0.000000103
80	8	0.000004251	-0.000011548	-0.000002269
81	7	0.000001335	0.000008445	-0.000013189
82	1	-0.000003460	-0.000002530	-0.000002302
83	16	-0.000002167	0.000004525	0.000004832
84	8	0.000004382	0.000001495	-0.000006248
85	8	0.000000452	-0.000001530	-0.000002570
86	6	-0.000003604	-0.000004721	0.000001857
87	9	-0.000000514	0.000004118	-0.000003115
88	9	0.000004809	-0.000001103	-0.000004974
89	9	-0.000007312	-0.000007685	0.000008846
90	6	-0.000003973	0.000001060	-0.000002688
91	6	0.000003905	-0.000004149	-0.000003830
92	6	0.000005841	0.000004025	-0.000015203
93	6	-0.000000314	0.000005434	-0.000009731
94	6	-0.000008341	0.000001843	0.000005013
95	6	0.000002671	-0.000005985	0.000011610
96	1	0.000000957	-0.000003181	-0.000001560
97	6	0.000000167	0.000001954	-0.000002081
98	6	0.000001159	-0.000002445	0.000004415
99	6	-0.000000418	0.000007235	-0.000004413
100	6	0.000003572	0.000004729	-0.000000145
101	6	-0.000005793	-0.000003515	0.000001156
102	6	-0.000003594	-0.000003781	0.000000321
103	1	0.000000135	0.000001671	0.000001212
104	6	-0.000006975	0.000000574	0.000000265
105	1	0.000000343	-0.000000330	0.000000692
106	6	0.000000752	-0.000002326	0.000000408
107	1	0.000000472	0.000000144	0.000002278
108	6	0.000000396	-0.000008610	0.000008916
109	1	-0.000000109	-0.000001696	0.000001485
110	6	-0.000000680	0.000005672	0.000001529
111	1	0.000000911	-0.000002155	0.000003065
112	6	0.000007158	-0.000005223	-0.000000113

113	1	0.000003790	0.000004208	0.000003217
114	6	0.000000126	0.000002559	-0.000003602
115	1	0.000001691	-0.000000798	-0.000002015
116	6	-0.000002634	0.000000595	0.000000432
117	1	-0.000000109	0.000000274	-0.000001563
118	6	0.000003445	-0.000011863	0.000000414
119	1	0.000005841	0.000005307	-0.000002862
120	6	0.000003391	0.000000119	-0.000001992
121	1	0.000000233	-0.000003937	0.000003915
122	6	-0.000000914	-0.000000328	-0.000002302
123	1	0.000000232	-0.000000583	-0.000000033
124	6	0.000000475	0.000000623	0.000002575
125	1	0.000001592	-0.000000123	-0.000001359
126	6	-0.000001940	0.000000216	0.000002237
127	1	-0.000000011	-0.000000433	0.000000300
128	6	-0.000002201	0.000001894	0.000002579
129	1	-0.000001417	0.000001948	0.000001140
130	6	-0.000001356	0.000001143	0.000001970
131	1	-0.000001879	0.000000472	0.000001240
132	6	-0.000002379	0.000000450	0.000000342
133	1	-0.000002438	0.000002231	0.000000719
134	6	-0.000000313	0.000000432	0.000004346
135	1	-0.000001061	0.000000387	0.000001156

$TS^{NPTA}_{C1\_S\_conf\text{-}4}$

E(RM06-2X/6-31G(d)) = -4524.403602 a.u.

Imaginary Freq = 1: -389.68 cm-1

Zero-point Energy Correction = 1.076044

Thermal Correction to Energy = 1.141097

Thermal Correction to Enthalpy = 1.142041

Thermal Correction to Free Energy = 0.979798

EE + Zero-point Energy = -4523.327558

EE + Thermal Energy Correction = -4523.262506

EE + Thermal Enthalpy Correction = -4523.261561

EE + Thermal Free Energy Correction = -4523.423804

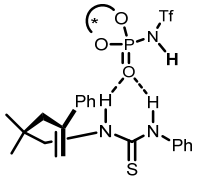
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.840419	4.006537	0.552304
2	6	0	-0.006556	3.156790	1.455965
3	6	0	-0.441629	2.846113	2.912681
4	7	0	-2.332719	1.595903	1.949393
5	1	0	0.963462	3.683203	1.498963
6	1	0	0.227965	2.218133	0.940827
7	6	0	0.379724	1.619518	3.352111
8	1	0	1.450945	1.842511	3.303794
9	1	0	0.199669	0.748139	2.713381
10	1	0	0.135991	1.354539	4.387305
11	6	0	-0.115998	3.983772	3.889073
12	1	0	0.964861	4.163558	3.899782
13	1	0	-0.414589	3.701942	4.904932
14	1	0	-0.614687	4.926888	3.650193
15	6	0	-0.773367	3.796210	-0.889984
16	6	0	-0.867825	3.386211	-3.652404
17	6	0	-0.868197	4.892051	-1.772892
18	6	0	-0.712281	2.496107	-1.420335
19	6	0	-0.787152	2.294754	-2.794796
20	6	0	-0.890952	4.687347	-3.141288
21	1	0	-0.865667	5.903716	-1.378487
22	1	0	-0.669045	1.633503	-0.764218
23	1	0	-0.779117	1.281686	-3.183561
24	1	0	-0.933736	5.537996	-3.814188
25	1	0	-0.909768	3.226112	-4.725665
26	6	0	-1.771297	4.948077	1.026875
27	1	0	-1.695125	5.294235	2.052610
28	1	0	-2.131067	5.691885	0.316540
29	6	0	-3.250385	1.749549	0.982645
30	7	0	-3.261854	0.745910	0.092115

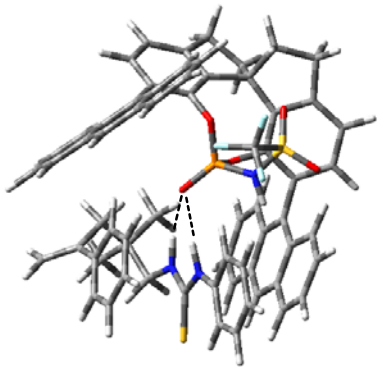
31	6	0	-3.937212	0.582418	-1.140081
32	6	0	-5.116338	0.018860	-3.597122
33	6	0	-5.273775	0.918161	-1.350693
34	6	0	-3.200615	-0.053910	-2.141931
35	6	0	-3.787167	-0.332729	-3.368012
36	6	0	-5.850219	0.639482	-2.588273
37	1	0	-5.852094	1.380722	-0.560187
38	1	0	-2.166462	-0.341916	-1.963623
39	1	0	-3.190283	-0.830671	-4.125799
40	1	0	-6.889634	0.904353	-2.757592
41	1	0	-5.582397	-0.196030	-4.553785
42	16	0	-4.285765	3.124986	0.892255
43	1	0	-2.786799	4.196511	1.017817
44	6	0	-1.949397	2.506573	3.005122
45	1	0	-2.588642	3.388421	2.959571
46	1	0	-2.135876	2.021775	3.972742
47	1	0	-1.731691	0.774397	1.855454
48	6	0	2.776807	-3.668747	0.444112
49	6	0	3.742576	-4.080587	1.601858
50	6	0	2.982002	-5.152522	2.398181
51	1	0	3.910712	-3.207188	2.242656
52	1	0	4.713759	-4.415316	1.226069
53	1	0	3.118985	-6.147737	1.956150
54	1	0	3.298369	-5.214324	3.443487
55	6	0	2.993711	-4.596391	-0.778727
56	1	0	2.150435	-4.472257	-1.463867
57	1	0	3.069124	-5.649365	-0.488575
58	6	0	4.281596	-4.053301	-1.440971
59	1	0	4.270768	-4.187116	-2.526531
60	6	0	1.440910	-3.833299	1.149123
61	6	0	-0.773165	-4.383543	2.741741
62	6	0	1.552200	-4.694258	2.242987
63	6	0	0.209722	-3.256693	0.872527
64	6	0	-0.915357	-3.491610	1.669910
65	6	0	0.446066	-4.989416	3.030850
66	1	0	0.533931	-5.663859	3.877717

67	1	0	-1.640590	-4.578041	3.366178
68	1	0	5.180065	-4.553659	-1.058573
69	6	0	3.255170	-2.344551	-0.132819
70	6	0	4.828493	-0.249353	-1.060420
71	6	0	2.936335	-1.033141	0.179560
72	6	0	4.266521	-2.585868	-1.067899
73	6	0	5.053860	-1.542683	-1.536375
74	6	0	3.753429	0.035195	-0.213076
75	1	0	5.840857	-1.725075	-2.262406
76	1	0	5.467147	0.569248	-1.380535
77	8	0	0.109763	-2.439253	-0.233279
78	8	0	1.737625	-0.742714	0.817890
79	15	0	0.414273	-0.859750	-0.130552
80	8	0	-0.648720	-0.122324	0.615637
81	7	0	0.736876	-0.407811	-1.631531
82	1	0	-2.498025	0.073472	0.213408
83	16	0	0.641813	-1.339929	-2.915337
84	8	0	1.227871	-2.669700	-2.790217
85	8	0	-0.649884	-1.216470	-3.592618
86	6	0	1.797199	-0.475313	-4.051177
87	9	0	3.044973	-0.529699	-3.592429
88	9	0	1.753334	-1.077841	-5.232968
89	9	0	1.459230	0.805446	-4.217051
90	6	0	-2.220696	-2.798339	1.457052
91	6	0	-4.804098	-1.678611	1.248665
92	6	0	-2.701312	-1.936450	2.468619
93	6	0	-2.995253	-3.031659	0.301668
94	6	0	-4.310163	-2.456686	0.202980
95	6	0	-4.025862	-1.388940	2.368891
96	1	0	-5.802125	-1.251919	1.167288
97	6	0	3.535696	1.415530	0.321896
98	6	0	3.414698	4.061365	1.320713
99	6	0	3.747540	1.663020	1.697552
100	6	0	3.200126	2.483285	-0.536787
101	6	0	3.153393	3.827956	-0.029101
102	6	0	3.682802	3.010123	2.197780

103	1	0	3.389276	5.080919	1.702589
104	6	0	-1.900129	-1.537950	3.590891
105	1	0	-0.877690	-1.895317	3.656844
106	6	0	-2.398023	-0.711055	4.557459
107	1	0	-1.770111	-0.425912	5.397128
108	6	0	-3.731821	-0.211835	4.477904
109	1	0	-4.112045	0.437211	5.261085
110	6	0	-4.512143	-0.532294	3.407631
111	1	0	-5.519964	-0.135879	3.314023
112	6	0	-5.086289	-2.677033	-0.979005
113	1	0	-6.065164	-2.209254	-1.044676
114	6	0	-4.590800	-3.414184	-2.010037
115	1	0	-5.174119	-3.551405	-2.915147
116	6	0	-3.292124	-3.996270	-1.913374
117	1	0	-2.904732	-4.577098	-2.744200
118	6	0	-2.528852	-3.826498	-0.796413
119	1	0	-1.544766	-4.278126	-0.742348
120	6	0	2.878479	2.274485	-1.914744
121	1	0	2.877495	1.260421	-2.289077
122	6	0	2.546466	3.318575	-2.727242
123	1	0	2.283350	3.129203	-3.762599
124	6	0	2.524434	4.652399	-2.225878
125	1	0	2.259102	5.469112	-2.890601
126	6	0	2.816193	4.897337	-0.917274
127	1	0	2.794870	5.908901	-0.518931
128	6	0	3.891484	3.252267	3.593549
129	1	0	3.842786	4.279211	3.948007
130	6	0	4.142321	2.226674	4.454598
131	1	0	4.292753	2.420572	5.512006
132	6	0	4.222153	0.890926	3.963071
133	1	0	4.435785	0.081197	4.653651
134	6	0	4.043367	0.621785	2.637733
135	1	0	4.123872	-0.398750	2.280582

NH-complex_C1_*R*





E(RM06-2X/6-31G(d)) = -4524.438678 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 1.081026
Thermal Correction to Energy = 1.146952
Thermal Correction to Enthalpy = 1.147896
Thermal Correction to Free Energy = 0.98366
EE + Zero-point Energy = -4523.357652
EE + Thermal Energy Correction = -4523.291726
EE + Thermal Enthalpy Correction = -4523.290782
EE + Thermal Free Energy Correction = -4523.455018
Truhlar's quasiharmonic corrected Gibbs energy = -4523.441834

E_{sp} (RM06-2X/def2-TZVP) = -4525.877954
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.945682

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.981521	2.352592	-3.057275
2	6	0	-2.042718	1.208413	-3.380544
3	6	0	-2.697032	-0.199219	-3.465278
4	7	0	-3.037502	-0.274201	-1.025200
5	1	0	-1.557597	1.391120	-4.348130
6	1	0	-1.236239	1.179934	-2.637899
7	6	0	-1.574748	-1.242951	-3.458496
8	1	0	-0.871029	-1.050142	-4.277327

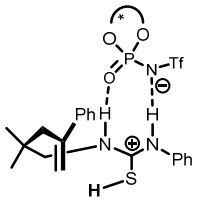
9	1	0	-1.002908	-1.232260	-2.523351
10	1	0	-1.983351	-2.249241	-3.588471
11	6	0	-3.500303	-0.333654	-4.761978
12	1	0	-2.850185	-0.199318	-5.633907
13	1	0	-3.953324	-1.329425	-4.828768
14	1	0	-4.302150	0.409942	-4.811035
15	6	0	-3.120338	2.768201	-1.631161
16	6	0	-3.353142	3.627363	1.035177
17	6	0	-4.376949	2.976554	-1.054835
18	6	0	-1.981169	2.979718	-0.842618
19	6	0	-2.094305	3.421876	0.470866
20	6	0	-4.492106	3.391239	0.271057
21	1	0	-5.270024	2.770629	-1.638780
22	1	0	-0.995778	2.804030	-1.261152
23	1	0	-1.192462	3.588574	1.056034
24	1	0	-5.477529	3.506577	0.711665
25	1	0	-3.444659	3.933830	2.073276
26	6	0	-3.663947	2.992087	-4.014090
27	1	0	-3.563977	2.716261	-5.061046
28	1	0	-4.329398	3.818093	-3.779550
29	6	0	-3.718908	-0.081352	0.121769
30	7	0	-2.896981	0.350042	1.128921
31	6	0	-3.126570	0.710343	2.463959
32	6	0	-3.303131	1.445756	5.171268
33	6	0	-4.366139	0.708009	3.113274
34	6	0	-1.985798	1.105959	3.180566
35	6	0	-2.072624	1.465736	4.517706
36	6	0	-4.436546	1.072942	4.455888
37	1	0	-5.255965	0.424702	2.570825
38	1	0	-1.025474	1.143646	2.668097
39	1	0	-1.175402	1.767039	5.048073
40	1	0	-5.406418	1.064889	4.945065
41	1	0	-3.375850	1.725791	6.217084
42	16	0	-5.375464	-0.376736	0.217035
43	6	0	-3.675913	-0.454269	-2.312674
44	1	0	-4.529170	0.232593	-2.380982

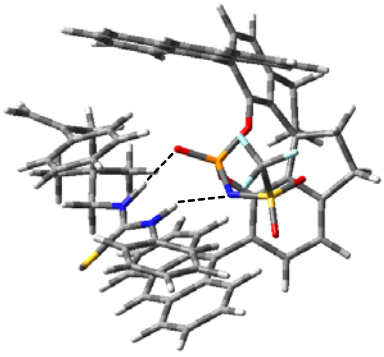
45	1	0	-4.077210	-1.474402	-2.390421
46	1	0	-2.044740	-0.052781	-1.028634
47	6	0	3.927086	-2.159931	-1.244880
48	6	0	4.897299	-1.957152	-3.487407
49	1	0	5.982206	-1.999611	-3.328835
50	1	0	4.718079	-2.146032	-4.549644
51	6	0	5.188529	-2.258607	-0.343320
52	1	0	5.131237	-1.477580	0.421589
53	1	0	6.113519	-2.124852	-0.912522
54	6	0	5.073153	-3.645629	0.324270
55	1	0	5.532904	-3.669101	1.316258
56	6	0	3.707958	-0.761261	-1.794769
57	6	0	3.817022	1.712617	-3.076932
58	6	0	4.344201	-0.626719	-3.034529
59	6	0	3.072203	0.346967	-1.257399
60	6	0	3.133812	1.608734	-1.860243
61	6	0	4.401139	0.601490	-3.679000
62	1	0	4.902086	0.698941	-4.637710
63	1	0	3.874829	2.687879	-3.551381
64	1	0	5.556741	-4.425225	-0.277282
65	6	0	2.922001	-2.897698	-0.384288
66	6	0	1.455565	-4.777194	1.050526
67	6	0	1.544226	-2.820020	-0.320913
68	6	0	3.577106	-3.858531	0.393905
69	6	0	2.850693	-4.796345	1.114186
70	6	0	0.773373	-3.777657	0.351635
71	1	0	3.357278	-5.540748	1.721298
72	1	0	0.872807	-5.525003	1.580553
73	8	0	2.380460	0.221733	-0.047942
74	8	0	0.890745	-1.706693	-0.865348
75	15	0	0.899231	-0.352740	-0.003159
76	8	0	-0.214139	0.520589	-0.419744
77	7	0	0.851998	-0.761895	1.634858
78	1	0	-1.973376	0.630876	0.803405
79	16	0	2.061288	-0.766219	2.781341
80	8	0	1.576492	-1.547786	3.895530

81	8	0	3.357208	-0.985961	2.188546
82	6	0	2.011630	1.005884	3.331205
83	9	0	1.775868	1.796684	2.298020
84	9	0	1.037606	1.148108	4.218959
85	9	0	3.168958	1.306556	3.891607
86	6	0	2.547471	2.808727	-1.202307
87	6	0	1.478008	5.089441	0.055893
88	6	0	1.519069	3.537083	-1.834720
89	6	0	3.067076	3.231027	0.039166
90	6	0	2.497118	4.377685	0.687952
91	6	0	0.993086	4.712820	-1.196059
92	1	0	1.058215	5.966108	0.545041
93	6	0	-0.716165	-3.707350	0.285153
94	6	0	-3.518260	-3.440091	0.081857
95	6	0	-1.467528	-3.311968	1.408345
96	6	0	-1.365139	-4.027645	-0.926688
97	6	0	-2.792626	-3.905324	-1.016384
98	6	0	-2.889613	-3.144365	1.290335
99	1	0	-4.591835	-3.292281	-0.006321
100	6	0	4.157915	-2.945324	-2.570972
101	1	0	4.699071	-3.881138	-2.404592
102	1	0	3.181688	-3.189550	-3.004913
103	6	0	2.999236	4.779847	1.966713
104	1	0	2.541758	5.639722	2.449072
105	6	0	4.027959	4.111666	2.558027
106	1	0	4.403633	4.425538	3.526910
107	6	0	4.629923	3.001376	1.894752
108	1	0	5.461567	2.486380	2.365493
109	6	0	4.166401	2.574966	0.686078
110	1	0	4.640628	1.729410	0.198826
111	6	0	0.949581	3.152282	-3.093918
112	1	0	1.293978	2.240972	-3.571622
113	6	0	-0.025546	3.903436	-3.684283
114	1	0	-0.450188	3.590296	-4.633215
115	6	0	-0.523808	5.083065	-3.058863
116	1	0	-1.315305	5.648401	-3.539721

117	6	0	-0.033204	5.467136	-1.848179
118	1	0	-0.423723	6.345072	-1.340887
119	6	0	-3.452287	-4.281474	-2.229365
120	1	0	-4.533774	-4.180194	-2.273841
121	6	0	-2.748235	-4.771807	-3.289209
122	1	0	-3.259426	-5.069204	-4.199502
123	6	0	-1.329839	-4.889572	-3.205652
124	1	0	-0.777194	-5.278518	-4.055459
125	6	0	-0.661903	-4.519629	-2.074121
126	1	0	0.417227	-4.625814	-2.023104
127	6	0	-0.867826	-3.042003	2.684021
128	1	0	0.193763	-3.219721	2.818590
129	6	0	-1.609428	-2.563258	3.727257
130	1	0	-1.119018	-2.339665	4.670082
131	6	0	-3.014681	-2.362689	3.592237
132	1	0	-3.580627	-1.954147	4.423282
133	6	0	-3.633136	-2.661807	2.415472
134	1	0	-4.699441	-2.499223	2.286828
135	1	0	-0.040958	-1.101745	2.017337

SH-complex_C1_*R*





E(RM06-2X/6-31G(d)) = -4524.433013 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 1.078199
Thermal Correction to Energy = 1.143923
Thermal Correction to Enthalpy = 1.144868

Thermal Correction to Free Energy = 0.981158
EE + Zero-point Energy = -4523.354814
EE + Thermal Energy Correction = -4523.289089
EE + Thermal Enthalpy Correction = -4523.288145
EE + Thermal Free Energy Correction = -4523.451855
Truhlar's quasiharmonic corrected Gibbs energy = -4523.438796

E_{sp} (RM06-2X/def2-TZVP) = -4525.878783
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.947966

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000836853	0.002045790	0.000487913
2	6	0.001280499	0.001029721	0.001073865
3	6	0.000651556	0.000820340	-0.000084846
4	7	0.004913660	-0.003090024	0.001226529
5	1	0.000675968	0.000769923	-0.000560708
6	1	-0.001282356	0.000226339	0.000611415
7	6	0.000787918	-0.001311936	-0.002340134
8	1	-0.000055701	-0.000130993	-0.000493501
9	1	-0.000334191	-0.000509409	-0.000024031
10	1	0.000427858	-0.000122963	-0.000541077
11	6	-0.002476769	-0.000908488	-0.000347037
12	1	-0.000527189	-0.000229201	-0.000225959
13	1	-0.001166948	-0.000597098	-0.000489293
14	1	-0.000123414	-0.000589569	-0.000069056
15	6	0.000655960	-0.002332565	-0.002157894
16	6	-0.000390855	0.003464322	-0.000199864
17	6	-0.001185262	-0.001105667	0.001407921
18	6	0.001250141	-0.000001450	-0.001876952
19	6	-0.000005932	0.002948675	-0.000667806
20	6	-0.001215128	-0.000350709	0.000769591
21	1	-0.000076529	0.000351132	0.000193742
22	1	-0.000474397	0.000136912	0.000595941

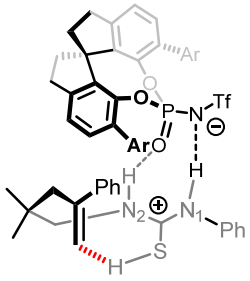
23	1	0.000008686	0.000051809	0.000065824
24	1	-0.000279109	-0.000074663	0.000335253
25	1	0.000076871	-0.000006525	-0.000164522
26	6	0.000649819	-0.003002044	0.001383838
27	1	0.000005540	-0.000370224	0.000776200
28	1	0.000160669	-0.000654762	-0.000025045
29	6	0.001290457	-0.000012027	-0.000143905
30	7	0.001212832	0.002789646	-0.000124465
31	6	0.000681015	-0.002027632	0.000188964
32	6	-0.000119122	0.001552089	0.000050362
33	6	0.000815312	-0.001655009	0.001257253
34	6	0.000161163	0.000094077	-0.002056708
35	6	-0.000230776	0.000960081	-0.001154249
36	6	0.000320245	0.000085991	0.002229461
37	1	0.002400731	-0.001077018	0.001978125
38	1	-0.000119489	0.000796040	0.001091236
39	1	0.000075359	0.000025380	-0.000117244
40	1	0.000015158	0.000086483	0.000312564
41	1	-0.000048966	0.000385947	0.000107594
42	16	-0.005383271	0.002407453	0.000578915
43	1	-0.000973998	-0.000886594	0.000590001
44	6	-0.001490613	0.000700136	0.000019815
45	1	-0.000064028	0.000589104	-0.001158307
46	1	-0.002634346	-0.000777111	-0.001023077
47	1	-0.000668120	0.000350136	0.000652352
48	6	-0.000223823	-0.000117464	0.000659249
49	6	0.004748688	-0.007536658	-0.007570020
50	1	-0.001790280	-0.000030139	0.004524756
51	1	-0.000669274	0.004850660	0.000779086
52	6	0.012752087	0.003316220	-0.002366655
53	1	-0.003804941	-0.004442366	-0.001063992
54	1	-0.003765629	0.001688819	0.003661714
55	6	-0.004901314	0.001297043	-0.011334956
56	1	0.000780580	-0.003670249	0.003242987
57	6	0.008326762	-0.000761099	0.005944262
58	6	0.002564638	0.001424872	0.002187749

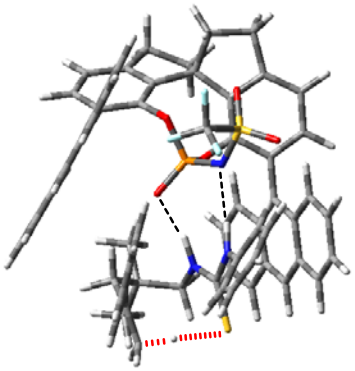
59	6	0.002945288	0.004030958	0.005345048
60	6	0.007224722	-0.010055230	-0.005963063
61	6	-0.005131164	-0.005171193	-0.006436784
62	6	-0.000868306	-0.000971556	-0.001942653
63	1	-0.002945104	0.004945491	0.001959463
64	1	-0.005725013	0.001274967	-0.002831356
65	1	0.001381170	0.002678280	0.004013542
66	6	-0.008620809	0.003181463	0.004379186
67	6	-0.003080416	-0.000261979	0.003134643
68	6	-0.008013940	0.002255518	-0.012351668
69	6	-0.003514577	-0.001059140	0.006561240
70	6	0.001009518	0.000101902	-0.003018860
71	6	0.005853033	0.000021282	-0.008290754
72	1	0.003302360	-0.002214852	0.004553443
73	1	0.006239021	-0.001460728	-0.000950554
74	8	0.002515928	0.003883672	-0.001617332
75	8	-0.000717522	-0.006389900	0.006480936
76	15	-0.002240837	0.006170137	0.000476371
77	8	-0.004196000	-0.000559187	0.003201410
78	7	0.001025518	-0.001668408	0.004051333
79	1	-0.000207327	-0.000729750	-0.000276479
80	16	0.002024292	-0.003128299	0.000325444
81	8	-0.011263813	0.004890106	-0.000328334
82	8	0.004902687	-0.002238972	-0.008624713
83	6	0.000831040	-0.000318278	0.000537372
84	9	0.004736998	-0.001379041	0.002422298
85	9	-0.002890957	0.004413756	0.004548835
86	9	0.001517491	0.003788255	-0.004658265
87	6	0.002232378	0.004274872	0.003892612
88	6	0.000585404	0.000333358	0.000443745
89	6	0.001613132	0.005424375	-0.001933338
90	6	0.001469051	-0.003073613	0.004677532
91	6	-0.001455458	-0.005034051	0.001969692
92	6	-0.000600394	0.002749102	-0.005315600
93	1	-0.003072243	-0.003420885	-0.004281972
94	6	-0.001596306	-0.002105963	0.006820888

95	6	-0.001288333	-0.000560361	0.001176057
96	6	-0.001438723	-0.005261994	0.000581764
97	6	-0.002427329	0.005184867	0.001906417
98	6	0.003694881	0.005733086	0.000655510
99	6	0.001392621	-0.005256510	-0.002951953
100	1	0.003808632	0.001188962	-0.005822963
101	6	-0.011972175	-0.003278565	-0.001360642
102	1	0.003791530	0.000810718	0.004376165
103	1	0.003455128	0.002346287	-0.003309273
104	6	0.001931504	0.007212362	-0.005120264
105	1	-0.002840253	-0.003193869	-0.004303114
106	6	0.003440170	0.001841357	0.007647241
107	1	-0.002062262	-0.005514662	0.001174745
108	6	-0.003697295	-0.006941923	-0.003444780
109	1	0.000913697	-0.002046170	0.005615187
110	6	0.000351681	0.005939299	-0.008134255
111	1	0.003402153	0.003833389	0.005582432
112	6	-0.001385967	-0.008038513	0.005192713
113	1	0.003557386	0.004208975	0.004445779
114	6	-0.003117314	-0.002509763	-0.007431600
115	1	0.002184049	0.005554641	-0.001337646
116	6	0.004281156	0.006840899	0.002864187
117	1	-0.000891181	0.001963169	-0.005568679
118	6	0.000198711	-0.005706354	0.006795912
119	1	-0.002957508	-0.003471227	-0.004039244
120	6	-0.000193018	-0.009694808	0.000613228
121	1	0.002781868	0.000730167	-0.005730952
122	6	-0.003287587	0.001940157	0.008267884
123	1	0.001292146	0.005590522	-0.002127871
124	6	0.003860030	0.004748929	-0.006222349
125	1	-0.001603714	0.004503818	0.003414004
126	6	0.001808412	-0.009321764	-0.002946767
127	1	-0.003412179	-0.000725806	0.006528946
128	6	0.000953414	0.009172720	-0.000836046
129	1	-0.002538716	-0.000650573	0.006910887
130	6	0.003495095	-0.001312281	-0.007342384

131	1	-0.001457247	-0.005945722	0.002006564
132	6	-0.003918542	-0.004394267	0.005911401
133	1	0.001652382	-0.004493929	-0.003621627
134	6	-0.000520769	0.007993280	0.003727630
135	1	0.003123073	0.000941510	-0.005318726

Transition state $TS^{NPTA}_{C1\_R}$





E (RM06-2X/6-31G(d)) = -4524.406906 a.u.
Imaginary Freq = 1: -189.39 cm-1
Zero-point Energy Correction = 1.077314
Thermal Correction to Energy = 1.141887
Thermal Correction to Enthalpy = 1.142831
Thermal Correction to Free Energy = 0.981692
EE + Zero-point Energy = -4523.329592
EE + Thermal Energy Correction = -4523.265020
EE + Thermal Enthalpy Correction = -4523.264076
EE + Thermal Free Energy Correction = -4523.425215
Truhlar's quasiharmonic corrected Gibbs energy = -4523.412455

E_{sp} (RM06-2X/6-311G(d,p)) = -4525.352487
E_{sp} (RM06-2X/6-311G(d,p)/SMD (CH_2Cl_2)) = -4525.427386
E_{sp} (RM06-2X/6-311G(d,p)/IEFPCM (CH_2Cl_2)) = -4525.377208

E_{sp} (RM06-2X/6-311+G(d,p)) = -4525.394671
E_{sp} (RM06-2X/6-311G+(d,p)/SMD (CH_2Cl_2)) = -4525.468439

E_{sp} (RM06-2X/6-311G+(d,p)/IEFPCM (CH_2Cl_2)) = -4525.418352

E_{sp} (RM06-2X/def2-TZVP) = -4525.844215
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.915982
E_{sp} (RM06-2X/def2-TZVP/IEFPCM (CH_2Cl_2)) = -4525.866755

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001532630	0.001246048	-0.000244582
2	6	0.000669363	0.000053730	-0.000967928
3	6	0.000122356	0.001975694	0.000251208
4	7	-0.001930746	-0.001941668	-0.000655715
5	1	0.001245789	-0.000002419	-0.001084185
6	1	-0.000387367	0.000549649	0.000653473
7	6	-0.000066275	-0.000798062	-0.000661457
8	1	-0.000650348	-0.000706828	-0.000445127
9	1	0.001085010	-0.000531528	-0.000192501
10	1	0.000127688	0.001178660	0.000159867
11	6	0.000284992	-0.000364429	0.001328069
12	1	0.000093399	-0.000166416	0.000982633
13	1	0.000909113	-0.000198147	-0.000553117
14	1	-0.000781160	0.000310562	-0.000898163
15	6	-0.000459029	-0.000841230	-0.000331057
16	6	0.000357442	0.000066775	-0.000221684
17	6	-0.000502867	0.000383594	0.000609848
18	6	0.000814503	-0.000168469	-0.000674535
19	6	0.000524623	-0.000167458	-0.000550883
20	6	-0.000023640	-0.000313496	0.000078234
21	1	0.000481894	-0.000053136	-0.000208489
22	1	-0.000586283	-0.000042087	-0.000138268
23	1	0.000180646	0.000503658	-0.001057932
24	1	0.000108582	-0.000042630	-0.000061662
25	1	-0.000248384	0.000163698	0.000041727
26	6	-0.003910139	0.001855912	0.001027377

27	1	0.001003280	-0.000640014	0.000238088
28	1	0.000697213	-0.000773902	-0.000432967
29	6	-0.001143438	-0.000180120	0.001129450
30	7	-0.000530652	-0.001181271	0.002286351
31	6	0.000071218	-0.000000252	-0.001895079
32	6	-0.000099414	-0.000168802	0.000277588
33	6	-0.000083279	0.001970744	-0.001111107
34	6	-0.000203947	0.000190706	-0.000244672
35	6	0.000028625	0.000011291	-0.000135805
36	6	0.000407076	0.000569353	-0.000415886
37	1	0.001119400	0.002779346	-0.002759708
38	1	-0.000965055	-0.000519379	0.000041482
39	1	-0.000106942	-0.000013245	0.000024879
40	1	-0.000452704	-0.000046654	0.000178335
41	1	0.000126553	0.000028515	-0.000105759
42	16	0.001320922	0.000369911	-0.000121548
43	1	0.001178102	-0.000517314	-0.000574812
44	6	0.001098310	-0.000938130	0.000168891
45	1	-0.000318926	-0.000413071	-0.000503327
46	1	-0.000513665	0.000438241	-0.000168272
47	1	0.001409630	0.001471777	0.000371711
48	6	0.000187063	0.000836617	0.001275197
49	6	-0.000241285	-0.000337074	-0.000215679
50	1	0.000104095	-0.000131523	0.000048334
51	1	-0.000169032	0.000198839	-0.000125678
52	6	0.001018284	0.000170729	-0.000564697
53	1	-0.000847653	-0.000021889	0.000258980
54	1	0.000406122	-0.000125808	0.000253635
55	6	0.000603059	-0.000027913	0.000553396
56	1	-0.000028557	-0.000090333	0.000106775
57	6	-0.000504382	0.000301890	-0.000362529
58	6	-0.000520704	0.000304983	-0.000212701
59	6	0.000701706	0.000284431	-0.000357886
60	6	-0.001925140	-0.001294796	0.001602594
61	6	0.003311569	-0.003088497	-0.003676098
62	6	-0.000229684	0.000005706	0.000337271

63	1	0.000123117	0.000153979	-0.000005119
64	1	0.000060330	0.000082278	-0.000152375
65	1	0.000037725	0.000033822	-0.000095329
66	6	-0.001124716	-0.000563574	-0.000635667
67	6	-0.000679897	-0.000230553	-0.000534459
68	6	0.002223637	0.003132126	0.003265139
69	6	-0.000462797	-0.001044332	-0.001551291
70	6	0.000868584	0.000428070	0.000659458
71	6	-0.001378896	0.000388119	-0.000664468
72	1	-0.000167604	-0.000132176	-0.000324103
73	1	0.000025376	-0.000011525	-0.000036155
74	8	-0.006004866	-0.004347674	-0.004622297
75	8	-0.002059006	-0.002330853	-0.000924045
76	15	0.005341909	0.003837301	0.000665094
77	8	0.001301671	0.000481545	0.002137327
78	7	-0.012116554	-0.002483495	-0.008010699
79	1	0.000149110	0.000639411	-0.000403496
80	16	0.017107681	-0.001964580	0.010218735
81	8	0.001209849	-0.006883586	0.002775600
82	8	-0.002102920	0.001235869	-0.002395378
83	6	0.002081327	0.001756295	-0.012599888
84	9	-0.012536409	0.006726837	0.014147570
85	9	-0.000124051	-0.002171253	0.005997624
86	9	0.000979895	0.003121657	-0.004265799
87	6	-0.000916859	0.000176022	-0.001085748
88	6	-0.000803176	-0.001421603	0.000050485
89	6	0.000365964	0.001004525	0.000434918
90	6	0.001216077	0.003584661	0.000593209
91	6	0.000680013	0.002153847	0.000781697
92	6	0.000202510	0.000793137	0.000955552
93	1	-0.000006081	-0.000062523	0.000002285
94	6	0.000150456	0.000042856	0.000384357
95	6	-0.000139979	0.000016295	-0.000192715
96	6	0.000368603	0.000320833	0.000468847
97	6	-0.000812112	0.000581762	-0.000179879
98	6	0.001159159	-0.000508922	0.000399771

99	6	0.000600287	0.000061452	-0.000038675
100	1	-0.000153438	0.000064624	-0.000012910
101	6	-0.000273889	0.000776545	-0.000107061
102	1	-0.000501170	-0.000258585	0.000218981
103	1	0.000770674	-0.000490017	0.000150373
104	6	0.000654759	-0.001414682	-0.000355052
105	1	-0.000206760	-0.000019858	0.000044116
106	6	0.000024876	0.001366639	-0.002153810
107	1	-0.000238226	0.000102404	0.000228891
108	6	0.001447449	-0.000180338	0.003313651
109	1	-0.000264017	0.000386438	0.000047731
110	6	0.003440156	-0.006167628	-0.000208490
111	1	0.000635017	-0.001070980	0.000493244
112	6	-0.000868703	-0.000230150	-0.000185772
113	1	0.000018338	0.000210960	-0.000003725
114	6	-0.001980905	0.000583054	0.000790466
115	1	-0.000222361	-0.000014034	-0.000016269
116	6	-0.001424873	0.000191680	0.001603452
117	1	0.000017865	0.000083875	0.000088940
118	6	0.000310505	-0.000486380	-0.000381558
119	1	-0.000058349	-0.000080511	0.000002452
120	6	-0.000201284	0.000078971	-0.000159047
121	1	0.000129088	-0.000080875	0.000028257
122	6	-0.000356602	0.000113237	0.000054576
123	1	0.000051939	-0.000002680	0.000000542
124	6	0.000326522	-0.000084449	0.000083065
125	1	-0.000043468	0.000022212	-0.000002273
126	6	-0.000171882	0.000084738	-0.000057084
127	1	0.000048310	-0.000055852	0.000028453
128	6	0.000316355	-0.000343001	-0.000092235
129	1	0.000585087	-0.001300452	0.000841952
130	6	-0.002329453	0.000651064	-0.000931893
131	1	0.000130704	-0.000157587	0.000110518
132	6	-0.000364186	0.000368885	-0.000030478
133	1	-0.000100840	0.000170706	-0.000024237
134	6	0.001202524	-0.000815970	0.000017787

135	1	-0.000066672	0.000028879	0.000000468

$TS^{NPTA}_{C1\_R\_conf\text{-}2}$

E(RM06-2X/6-31G(d)) = -4524.406906 a.u.
Imaginary Freq = 1: -188.66 cm-1
Zero-point Energy Correction = 1.077317
Thermal Correction to Energy = 1.141889
Thermal Correction to Enthalpy = 1.142834
Thermal Correction to Free Energy = 0.981696
EE + Zero-point Energy = -4523.329590
EE + Thermal Energy Correction = -4523.265017
EE + Thermal Enthalpy Correction = -4523.264073
EE + Thermal Free Energy Correction = -4523.425210

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.529444	1.185199	2.477799
2	6	0	2.255507	0.923518	3.220652
3	6	0	1.902849	-0.525182	3.677553
4	7	0	2.176834	-1.072396	1.258734
5	1	0	2.322798	1.554172	4.123296
6	1	0	1.411336	1.331649	2.657519
7	6	0	0.379029	-0.563412	3.891333
8	1	0	0.084023	0.171147	4.648826
9	1	0	-0.164980	-0.337518	2.970339
10	1	0	0.079996	-1.558428	4.239397
11	6	0	2.546503	-0.937779	5.009479
12	1	0	2.241247	-0.257563	5.811632
13	1	0	2.201934	-1.943365	5.276711
14	1	0	3.638285	-0.970678	4.983696
15	6	0	3.558103	2.106925	1.347759
16	6	0	3.700864	3.688630	-0.963275

17	6	0	4.739881	2.812468	1.025337
18	6	0	2.438310	2.250443	0.503805
19	6	0	2.524205	3.011490	-0.656305
20	6	0	4.801231	3.608141	-0.106171
21	1	0	5.596518	2.773445	1.689696
22	1	0	1.511610	1.722286	0.707290
23	1	0	1.667244	3.059975	-1.320773
24	1	0	5.709645	4.157671	-0.330515
25	1	0	3.765933	4.278024	-1.872772
26	6	0	4.720900	0.500503	2.819462
27	1	0	4.765125	0.031487	3.797078
28	1	0	5.661283	0.951814	2.505896
29	6	0	3.085357	-1.128853	0.273272
30	7	0	2.633110	-0.730151	-0.933766
31	6	0	3.358052	-0.184935	-2.024252
32	6	0	4.557390	1.024723	-4.239663
33	6	0	2.731007	-0.223915	-3.270626
34	6	0	4.574037	0.487150	-1.878387
35	6	0	5.169033	1.075680	-2.989058
36	6	0	3.330089	0.381231	-4.369697
37	1	0	1.768575	-0.715193	-3.374610
38	1	0	5.041694	0.568116	-0.905766
39	1	0	6.115675	1.593991	-2.865169
40	1	0	2.819544	0.350991	-5.327369
41	1	0	5.027607	1.491613	-5.099483
42	16	0	4.700869	-1.649471	0.558466
43	1	0	4.697149	-0.422502	2.004430
44	6	0	2.297494	-1.578384	2.613814
45	1	0	3.318516	-1.938964	2.752176
46	1	0	1.629478	-2.436074	2.736958
47	1	0	1.285552	-0.598868	1.049343
48	6	0	-4.652897	-1.138601	0.140389
49	6	0	-6.187182	-0.767660	2.023863
50	1	0	-7.141347	-0.502418	1.550788
51	1	0	-6.405186	-1.044045	3.059629
52	6	0	-5.542364	-0.888460	-1.106729

53	1	0	-5.044871	-0.145337	-1.738734
54	1	0	-6.538377	-0.520146	-0.840323
55	6	0	-5.561442	-2.248841	-1.835577
56	1	0	-5.678083	-2.138387	-2.917315
57	6	0	-4.295018	0.134377	0.885771
58	6	0	-4.104639	2.444697	2.430437
59	6	0	-5.206266	0.376018	1.918514
60	6	0	-3.273125	1.045040	0.667363
61	6	0	-3.153180	2.214448	1.430883
62	6	0	-5.123690	1.530146	2.686889
63	1	0	-5.839103	1.717185	3.482562
64	1	0	-4.024788	3.354175	3.019472
65	1	0	-6.381140	-2.886752	-1.481374
66	6	0	-3.622589	-2.081908	-0.455603
67	6	0	-2.254387	-4.213777	-1.592975
68	6	0	-2.300433	-2.323790	-0.121940
69	6	0	-4.211918	-2.831161	-1.477860
70	6	0	-3.535318	-3.900513	-2.046679
71	6	0	-1.599619	-3.419019	-0.645700
72	1	0	-3.989780	-4.485198	-2.841089
73	1	0	-1.721429	-5.063867	-2.009320
74	8	0	-2.369117	0.803098	-0.351230
75	8	0	-1.620752	-1.419977	0.686940
76	15	0	-1.055412	-0.087981	-0.065949
77	8	0	-0.104806	0.532571	0.904040
78	7	0	-0.427577	-0.467001	-1.500638
79	1	0	1.614175	-0.721462	-1.074510
80	16	0	-1.120680	-0.209773	-2.915125
81	8	0	-0.399045	-0.923934	-3.960874
82	8	0	-2.575416	-0.265535	-2.915367
83	6	0	-0.701309	1.575981	-3.228656
84	9	0	-0.628959	2.247598	-2.076958
85	9	0	0.478085	1.676091	-3.834098
86	9	0	-1.626854	2.134954	-3.996830
87	6	0	-2.044772	3.175542	1.171958
88	6	0	0.095298	4.930402	0.633134

89	6	0	-1.060175	3.403581	2.156184
90	6	0	-1.984268	3.850041	-0.063554
91	6	0	-0.879954	4.725042	-0.340947
92	6	0	0.020112	4.308266	1.878790
93	1	0	0.930993	5.594560	0.420397
94	6	0	-0.212025	-3.747403	-0.200515
95	6	0	2.380413	-4.538511	0.609658
96	6	0	0.850650	-3.751315	-1.129614
97	6	0	0.024861	-4.127769	1.140357
98	6	0	1.337410	-4.561468	1.534568
99	6	0	2.170504	-4.133003	-0.706507
100	1	0	3.380374	-4.831771	0.922590
101	6	0	-5.468400	-1.880529	1.243283
102	1	0	-6.144514	-2.629901	0.821832
103	1	0	-4.764411	-2.395179	1.907266
104	6	0	-0.804331	5.372871	-1.615290
105	1	0	0.046354	6.020990	-1.811460
106	6	0	-1.774166	5.186948	-2.552777
107	1	0	-1.707551	5.679655	-3.517795
108	6	0	-2.892426	4.348269	-2.267237
109	1	0	-3.662582	4.214069	-3.019940
110	6	0	-2.993946	3.704917	-1.070636
111	1	0	-3.847863	3.066507	-0.870843
112	6	0	-1.080500	2.765083	3.440066
113	1	0	-1.857340	2.038090	3.651210
114	6	0	-0.148455	3.062675	4.391880
115	1	0	-0.200518	2.584596	5.366378
116	6	0	0.911271	3.977163	4.117224
117	1	0	1.646338	4.196416	4.886494
118	6	0	1.004149	4.557803	2.887806
119	1	0	1.816963	5.240255	2.651487
120	6	0	1.565861	-4.973693	2.886877
121	1	0	2.566457	-5.302260	3.157306
122	6	0	0.566262	-4.936852	3.812409
123	1	0	0.751043	-5.246843	4.836497
124	6	0	-0.736965	-4.500611	3.429549

125	1	0	-1.531704	-4.482452	4.169121
126	6	0	-0.998463	-4.121355	2.144759
127	1	0	-2.001119	-3.812489	1.870004
128	6	0	0.677829	-3.361427	-2.496650
129	1	0	-0.298544	-3.048471	-2.841374
130	6	0	1.731580	-3.336080	-3.361057
131	1	0	1.568403	-3.005643	-4.382478
132	6	0	3.043670	-3.691093	-2.930192
133	1	0	3.871966	-3.636537	-3.629657
134	6	0	3.253286	-4.078851	-1.641625
135	1	0	4.246307	-4.343252	-1.289028

$TS^{NPTA}_{C1\_R\_conf\text{-}3}$

E(RM06-2X/6-31G(d)) = -4524.405842 a.u.
Imaginary Freq = 1: -861.63 cm-1
Zero-point Energy Correction = 1.076104
Thermal Correction to Energy = 1.140925
Thermal Correction to Enthalpy = 1.141869
Thermal Correction to Free Energy = 0.980583
EE + Zero-point Energy = -4523.329738
EE + Thermal Energy Correction = -4523.264917
EE + Thermal Enthalpy Correction = -4523.263972
EE + Thermal Free Energy Correction = -4523.425259

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000008986	0.000010106	-0.000001618
2	6	0.000000974	0.000000046	-0.000001626
3	6	0.000001553	-0.000004399	0.000002185
4	7	0.000001994	-0.000006753	-0.000003300
5	1	0.000000123	0.000000824	-0.000000479
6	1	-0.000001867	-0.000001430	-0.000000785

7	6	0.000001799	0.000000230	-0.000003257
8	1	0.000000702	-0.000000030	-0.000001348
9	1	-0.000000601	-0.000000133	0.000000385
10	1	0.000000790	0.000000204	-0.000000764
11	6	0.000001347	-0.000000818	-0.000001979
12	1	0.000000213	0.000000020	-0.000001128
13	1	0.000001103	0.000000333	-0.000000746
14	1	-0.000000790	0.000000384	-0.000002581
15	6	-0.000006074	-0.000003846	-0.000002846
16	6	-0.000000504	0.000000633	-0.000001765
17	6	0.000002458	-0.000002695	0.000000388
18	6	0.000002148	0.000002248	-0.000001713
19	6	0.000000889	-0.000000509	-0.000000643
20	6	-0.000002458	-0.000003972	-0.000000784
21	1	-0.000002531	-0.000004229	-0.000000772
22	1	0.000002007	0.000000722	0.000001072
23	1	-0.000000127	-0.000000303	-0.000000393
24	1	-0.000000241	-0.000001051	-0.000000070
25	1	-0.000000255	0.000000053	0.000000351
26	6	-0.000995225	0.000727392	0.000268341
27	1	0.000003859	-0.000000121	-0.000000067
28	1	0.000002480	0.000000565	0.000001902
29	6	-0.000005855	-0.000007334	0.000000646
30	7	0.000012048	-0.000000825	0.000005197
31	6	-0.000013027	-0.000002082	-0.000005778
32	6	-0.000000713	-0.000001876	0.000001879
33	6	0.000002070	-0.000003826	-0.000001936
34	6	-0.000000750	0.000003087	0.000000568
35	6	-0.000000054	-0.000002628	-0.000002300
36	6	0.000001472	0.000001932	0.000001458
37	1	0.000001069	-0.000001988	0.000000237
38	1	0.000001205	0.000000427	-0.000000585
39	1	0.000000125	-0.000000805	0.000000596
40	1	-0.000000376	-0.000001810	-0.000000839
41	1	-0.000000597	-0.000001060	0.000000366
42	16	0.000004455	-0.000005274	-0.000003184

43	1	0.000985038	-0.000719051	-0.000264632
44	6	-0.000001217	0.000005002	0.000000251
45	1	-0.000000886	0.000001064	-0.000000693
46	1	0.000001185	-0.000000386	-0.000001764
47	1	-0.000001937	0.000014081	0.000005111
48	6	-0.000000956	0.000001179	-0.000000729
49	6	0.000000347	0.000002171	0.000000157
50	1	0.000000046	0.000001016	0.000000603
51	1	-0.000000121	0.000001002	0.000000012
52	6	-0.000000106	0.000001050	0.000001936
53	1	-0.000000249	0.000000885	0.000000682
54	1	-0.000000315	0.000000764	0.000000470
55	6	-0.000000538	-0.000000093	0.000000757
56	1	-0.000000427	0.000000764	0.000000973
57	6	0.000000225	0.000000193	0.000000288
58	6	0.000000119	0.000001984	0.000000764
59	6	0.000000570	-0.000000433	-0.000001781
60	6	-0.000000040	-0.000000053	0.000002519
61	6	0.000000733	-0.000000698	-0.000001262
62	6	-0.000000657	0.000002334	0.000000686
63	1	0.000000473	0.000001004	-0.000000143
64	1	0.000000275	0.000001307	-0.000000430
65	1	-0.000000792	0.000000587	0.000000418
66	6	0.000001104	0.000000286	0.000001552
67	6	0.000000253	-0.000000850	-0.000000963
68	6	0.000001397	0.000003632	-0.000001534
69	6	0.000000287	-0.000000178	0.000001016
70	6	-0.000000935	-0.000000471	0.000000310
71	6	-0.000001899	0.000001770	0.000001194
72	1	-0.000000456	0.000000524	0.000000772
73	1	-0.000000848	-0.000000436	0.000000507
74	8	0.000000050	0.000002944	-0.000002340
75	8	-0.000002763	-0.000004730	0.000002571
76	15	-0.000003445	0.000004222	0.000008158
77	8	0.000005956	-0.000010302	-0.000006814
78	7	-0.000001226	0.000002968	-0.000006682

79	1	0.000001265	-0.000001704	0.000000713
80	16	-0.000001959	-0.000003161	0.000005335
81	8	0.000000180	0.000001059	-0.000000549
82	8	0.000000303	0.000001208	-0.000000245
83	6	0.000000668	0.000002053	0.000000626
84	9	-0.000000772	-0.000002372	0.000001630
85	9	-0.000000739	-0.000001194	-0.000000301
86	9	-0.000000882	-0.000000802	0.000002400
87	6	0.000000122	0.000001506	0.000000164
88	6	0.000001459	0.000001093	0.000000584
89	6	0.000000363	-0.000000555	-0.000000881
90	6	-0.000000626	0.000000110	0.000000624
91	6	-0.000000568	0.000000209	0.000000175
92	6	-0.000001131	0.000000263	0.000000154
93	1	-0.000000344	0.000000651	-0.000000167
94	6	0.000000319	-0.000000008	0.000000355
95	6	-0.000000632	-0.000001327	-0.000000072
96	6	-0.000000159	-0.000000665	-0.000000176
97	6	0.000000073	-0.000001195	-0.000000742
98	6	0.000000229	0.000000160	-0.000000665
99	6	-0.000000010	-0.000000459	0.000000514
100	1	0.000000790	-0.000001885	0.000000024
101	6	0.000000454	0.000000402	0.000001473
102	1	-0.000000233	0.000001207	0.000000164
103	1	-0.000000081	0.000000442	0.000000063
104	6	0.000000147	0.000000424	0.000000285
105	1	-0.000000300	0.000000747	0.000000664
106	6	0.000000135	0.000000528	0.000001684
107	1	-0.000000345	0.000000704	0.000000622
108	6	-0.000001414	0.000001666	0.000000387
109	1	-0.000000246	0.000000575	0.000000969
110	6	-0.000000519	0.000002127	0.000000565
111	1	0.000000604	0.000001086	0.000001114
112	6	0.000000387	0.000001841	-0.000000416
113	1	0.000000738	0.000000249	0.000000307
114	6	0.000000427	0.000000484	0.000000299

115	1	0.000000712	0.000000674	-0.000001043
116	6	0.000000718	-0.000000548	-0.000000544
117	1	0.000000413	0.000001048	-0.000000717
118	6	0.000000428	0.000001323	-0.000000566
119	1	0.000000396	0.000000585	-0.000000279
120	6	-0.000000009	-0.000001551	-0.000001615
121	1	0.000000333	-0.000000792	-0.000000359
122	6	0.000000691	-0.000000696	0.000000578
123	1	0.000000279	-0.000000497	-0.000000756
124	6	-0.000000311	0.000000032	-0.000001142
125	1	0.000000292	-0.000000003	-0.000000003
126	6	-0.000000315	-0.000000175	-0.000000748
127	1	-0.000000538	-0.000000651	0.000000337
128	6	0.000000876	-0.000000903	0.000001484
129	1	0.000000144	-0.000001269	0.000000952
130	6	-0.000000711	-0.000000581	0.000000601
131	1	-0.000001246	-0.000000476	0.000000803
132	6	-0.000000931	-0.000000613	0.000000340
133	1	-0.000000648	-0.000001411	0.000000178
134	6	-0.000000470	-0.000001896	0.000000582
135	1	0.000000125	-0.000001528	0.000000012

$TS^{NPTA}_{C1\_R\_conf\text{-}4}$

E(RM06-2X/6-31G(d)) = -4524.399936 a.u.

Imaginary Freq = 1: -922.04 cm-1

Zero-point Energy Correction = 1.076694

Thermal Correction to Energy = 1.141306

Thermal Correction to Enthalpy = 1.14225

Thermal Correction to Free Energy = 0.982

EE + Zero-point Energy = -4523.323242

EE + Thermal Energy Correction = -4523.258631

EE + Thermal Enthalpy Correction = -4523.257686

EE + Thermal Free Energy Correction = -4523.417936

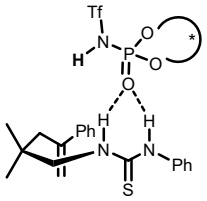
Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000007109	0.000018269	-0.000011703
2	6	-0.000006494	-0.000003156	0.000001495
3	6	0.000004766	-0.000004000	0.000003615
4	7	-0.000006884	-0.000000723	-0.000025078
5	1	0.000001012	-0.000000028	0.000001189
6	1	0.000000433	-0.000000904	-0.000001826
7	6	0.000002742	0.000003918	-0.000003129
8	1	0.000001004	-0.000000706	-0.000000180
9	1	0.000000905	-0.000001433	0.000000868
10	1	0.000002211	-0.000001663	0.000001885
11	6	0.000004153	0.000001491	-0.000001203
12	1	-0.000000297	-0.000002263	-0.000000072
13	1	0.000001358	0.000000392	0.000000170
14	1	-0.000001439	-0.000001766	0.000000110
15	6	-0.000005379	-0.000004115	0.000001425
16	6	-0.000001156	0.000001313	0.000001772
17	6	-0.000001557	-0.000001107	0.000001181
18	6	0.000004386	0.000008018	0.000000716
19	6	0.000000870	-0.000001036	-0.000004502
20	6	-0.000001593	0.000000001	0.000002389
21	1	0.000000825	-0.000001046	0.000000019
22	1	-0.000001034	-0.000000147	0.000001879
23	1	0.000000113	0.000001308	0.000001881
24	1	-0.000002200	0.000000640	-0.000001168
25	1	-0.000001462	0.000000320	0.000000430
26	6	-0.000468725	0.000386966	0.000175535
27	1	-0.000003032	0.000000995	0.000000274
28	1	0.000004434	-0.000003983	-0.000001473
29	6	0.000007793	-0.000003587	0.000010852
30	7	-0.000005688	0.000005570	-0.000006686
31	6	-0.000011781	0.000000934	0.000003800
32	6	-0.000000366	0.000004313	-0.000003607

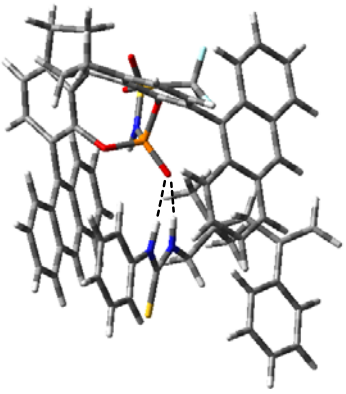
33	6	-0.000007781	0.000013910	-0.000007074
34	6	-0.000002381	-0.000000908	0.000000213
35	6	-0.000003286	0.000001121	-0.000004245
36	6	-0.000006988	-0.000003873	-0.000004113
37	1	-0.000000687	0.000000217	-0.000000543
38	1	-0.000001644	0.000002722	-0.000001172
39	1	-0.000001390	-0.000000405	0.000000429
40	1	-0.000002170	0.000001324	-0.000001330
41	1	-0.000002013	0.000000702	-0.000000829
42	16	-0.000005230	0.000005259	-0.000000925
43	1	0.000461684	-0.000398090	-0.000166150
44	6	-0.000005860	0.000005138	0.000009119
45	1	0.000000630	0.000001956	0.000000653
46	1	0.000000734	-0.000001044	-0.000000965
47	1	-0.000009520	-0.000005026	-0.000003240
48	6	0.000006232	0.000002357	0.000001324
49	6	0.000001821	0.000000829	0.000000851
50	1	0.000001990	-0.000000572	0.000000899
51	1	0.000001897	-0.000000239	0.000000140
52	6	-0.000001341	-0.000000876	0.000000932
53	1	0.000000192	0.000000247	0.000000700
54	1	0.000000917	-0.000000454	-0.000000497
55	6	0.000001819	-0.000000284	0.000001043
56	1	0.000000375	0.000000399	-0.000000432
57	6	0.000000320	-0.000000304	-0.000004661
58	6	0.000003324	0.000001295	-0.000002153
59	6	-0.000000111	0.000001798	0.000000300
60	6	0.000000534	-0.000008872	0.000003072
61	6	-0.000001966	0.000000216	0.000002664
62	6	0.000001969	-0.000002572	0.000001923
63	1	0.000002075	-0.000000710	0.000001799
64	1	0.000001007	0.000000159	0.000001096
65	1	0.000000907	-0.000000978	0.000000175
66	6	0.000000877	-0.000001820	0.000001594
67	6	-0.000000237	-0.000000668	0.000000316
68	6	0.000005643	-0.000005467	-0.000000482

69	6	0.000000496	0.000000104	-0.000002997
70	6	0.000000525	0.000001331	-0.000002236
71	6	-0.000000373	0.000003142	-0.000000619
72	1	0.000000279	-0.000000851	-0.000000521
73	1	0.000000422	-0.000000032	-0.000002245
74	8	-0.000000527	0.000017344	-0.000001513
75	8	-0.000007305	0.000003204	0.000001336
76	15	0.000002378	-0.000013878	0.000014193
77	8	0.000013627	-0.000001714	-0.000006678
78	7	0.000003909	0.000015574	-0.000006852
79	1	0.000003068	-0.000002382	0.000002172
80	16	-0.000010497	-0.000016889	-0.000004705
81	8	-0.000000149	0.000003149	0.000002451
82	8	0.000004120	0.000000232	0.000004107
83	6	-0.000000110	0.000002860	0.000000636
84	9	-0.000005396	-0.000000319	-0.000000077
85	9	0.000000128	-0.000001582	-0.000000099
86	9	-0.000001813	-0.000000043	0.000000117
87	6	0.000000834	0.000000107	-0.000001174
88	6	0.000001555	-0.000000470	0.000001836
89	6	0.000000537	-0.000001527	0.000002202
90	6	0.000000012	0.000002342	0.000002746
91	6	-0.000000958	-0.000000110	0.000002848
92	6	0.000001262	-0.000000548	0.000001538
93	1	-0.000000877	0.000000839	0.000001897
94	6	0.000001061	-0.000000986	-0.000003570
95	6	0.000000769	-0.000000763	-0.000001202
96	6	-0.000001250	0.000000548	-0.000001254
97	6	-0.000000156	-0.000003235	-0.000001221
98	6	0.000000412	-0.000001357	-0.000000653
99	6	0.000001751	-0.000000535	-0.000001060
100	1	0.000000803	0.000000281	-0.000002172
101	6	0.000000171	-0.000002290	-0.000001041
102	1	0.000001980	-0.000001565	-0.000000622
103	1	0.000001440	-0.000000483	-0.000000767
104	6	0.000000028	0.000001211	0.000002463

105	1	-0.000000905	0.000000831	0.000002136
106	6	-0.000001640	-0.000000172	0.000001037
107	1	-0.000000935	0.000000324	0.000001777
108	6	-0.000000134	0.000000447	0.000002037
109	1	-0.000000284	-0.000000231	0.000001414
110	6	0.000000159	0.000000390	0.000003246
111	1	0.000000793	-0.000000211	0.000001692
112	6	-0.000001272	-0.000000202	0.000000099
113	1	0.000000629	-0.000001457	0.000001997
114	6	0.000002027	-0.000002085	0.000000190
115	1	0.000001648	-0.000000319	0.000001333
116	6	0.000001058	0.000001032	0.000001438
117	1	0.000000804	-0.000000308	0.000001478
118	6	0.000000816	-0.000000413	0.000001442
119	1	0.000000118	0.000000076	0.000001783
120	6	0.000000378	0.000000525	-0.000002270
121	1	0.000000846	-0.000000537	-0.000001991
122	6	0.000002230	0.000000033	-0.000000586
123	1	0.000001403	-0.000000461	-0.000001231
124	6	0.000000200	-0.000001295	-0.000002370
125	1	0.000001590	-0.000001211	-0.000000948
126	6	0.000000810	-0.000000576	-0.000002738
127	1	0.000000100	-0.000001211	-0.000000841
128	6	0.000000860	0.000001527	0.000006429
129	1	-0.000000692	-0.000000983	-0.000000549
130	6	-0.000000072	0.000002454	0.000001249
131	1	0.000001882	-0.000002194	0.000000688
132	6	0.000005203	-0.000004338	0.000007527
133	1	0.000002572	-0.000000761	-0.000002669
134	6	0.000000485	0.000000718	0.000000397
135	1	-0.000000199	0.000000628	-0.000001749

NH-complex_C2_*S*





E(RM06-2X/6-31G(d)) = -4524.434530 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 1.080888
Thermal Correction to Energy = 1.147145
Thermal Correction to Enthalpy = 1.14809
Thermal Correction to Free Energy = 0.980718
EE + Zero-point Energy = -4523.353642
EE + Thermal Energy Correction = -4523.287385
EE + Thermal Enthalpy Correction = -4523.286441
EE + Thermal Free Energy Correction = -4523.453812
Truhlar's quasiharmonic corrected Gibbs energy = -4523.437887

E_{sp} (RM06-2X/def2-TZVP) = -4525.874382
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.941558

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000000009	-0.000001454	0.000002378
2	6	-0.000004653	0.000000959	-0.000002797
3	6	0.000005915	-0.000002877	-0.000002907
4	7	0.000008867	-0.000011762	0.000001614
5	1	-0.000000025	0.000001329	-0.000001957
6	1	-0.000000060	-0.000000140	-0.000001868
7	6	-0.000003367	0.000001413	0.000003343
8	1	0.000000114	0.000000024	-0.000001975

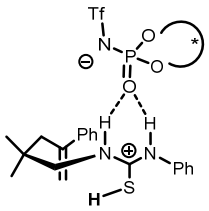
9	1	0.000000469	-0.000001151	-0.000004111
10	1	0.000002156	-0.000000393	-0.000001583
11	6	-0.000001249	0.000001306	-0.000001592
12	1	-0.000000086	0.000001319	-0.000001620
13	1	0.000000014	0.000001350	-0.000001161
14	1	-0.000000468	0.000001717	-0.000000993
15	6	0.000000178	0.000004713	-0.000002019
16	6	0.000000151	0.000000740	-0.000001735
17	6	-0.000000815	0.000000940	0.000001022
18	6	0.000000280	0.000003980	0.000000000
19	6	0.000000491	0.000002518	0.000004582
20	6	0.000000827	0.000005634	-0.000002309
21	1	-0.000000399	0.000003202	-0.000000956
22	1	0.000000689	0.000001562	0.000000815
23	1	-0.000000012	0.000002513	0.000000001
24	1	-0.000000069	0.000003615	-0.000000366
25	1	0.000000280	0.000003743	0.000000787
26	6	-0.000001465	0.000001497	-0.000002517
27	1	-0.000000448	0.000002516	-0.000001019
28	6	0.000004846	0.000007705	0.000006494
29	7	-0.000002542	-0.000005085	-0.000000585
30	6	0.000001209	-0.000002514	-0.000000703
31	6	0.000001053	0.000002083	0.000002079
32	6	-0.000000893	0.000000588	0.000000692
33	6	0.000000869	0.000001965	0.000001811
34	6	-0.000000815	0.000000738	0.000003292
35	6	0.000000433	-0.000000244	0.000002950
36	1	0.000000365	-0.000000179	0.000001819
37	1	-0.000000460	0.000002633	0.000002152
38	1	0.000001053	0.000000795	0.000002111
39	1	0.000000526	-0.000000775	0.000002345
40	1	0.000000572	0.000000202	0.000002948
41	16	-0.000002935	-0.000003280	-0.000006372
42	1	-0.000000612	0.000003179	-0.000001090
43	6	-0.000001908	0.000002885	-0.000000833
44	1	-0.000000788	0.000000913	-0.000001099

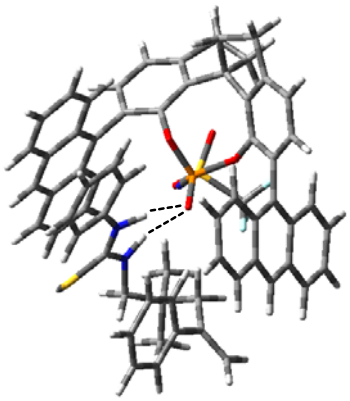
45	1	-0.000000165	0.000001958	0.000000189
46	1	-0.000001742	0.000011843	0.000002555
47	6	-0.000003195	-0.000005438	0.000000392
48	6	-0.000000636	-0.000001067	0.000000452
49	6	0.000001672	-0.000001493	0.000000734
50	1	0.000000510	-0.000001915	0.000001610
51	1	0.000000050	-0.000002212	0.000000319
52	1	-0.000000254	-0.000002482	0.000000888
53	1	0.000000665	-0.000002131	0.000002322
54	6	-0.000001032	-0.000000825	-0.000000358
55	1	0.000000242	-0.000001462	-0.000000018
56	1	0.000000013	-0.000002702	0.000000158
57	6	0.000001573	-0.000002197	0.000001778
58	1	-0.000000204	-0.000003076	-0.000001122
59	6	0.000003248	0.000001694	0.000003996
60	6	0.000001029	0.000003534	0.000006143
61	6	0.000000321	-0.000001835	0.000000035
62	6	-0.000008204	0.000000575	-0.000005136
63	6	-0.000000724	-0.000003065	-0.000003349
64	6	-0.000000716	-0.000003311	-0.000003000
65	1	0.000001048	-0.000000879	0.000001264
66	1	0.000000580	0.000000002	0.000000736
67	1	-0.000000340	-0.000004051	-0.000000226
68	6	0.000003817	-0.000000441	0.000002922
69	6	-0.000000301	-0.000003340	0.000003495
70	6	-0.000000425	-0.000000717	-0.000002105
71	6	-0.000001532	-0.000001804	-0.000003692
72	6	0.000002954	-0.000002931	-0.000001409
73	6	-0.000003220	0.000001755	-0.000000626
74	1	-0.000000695	-0.000002432	-0.000000421
75	1	-0.000000465	-0.000002382	-0.000000913
76	8	0.000013020	0.000001813	0.000003368
77	8	0.000007657	-0.000002103	0.000003041
78	15	-0.000009658	0.000008691	0.000006152
79	8	0.000001431	-0.000025956	-0.000002598
80	7	-0.000000585	-0.000014250	0.000000627

81	16	0.000006962	0.000001008	-0.000004649
82	8	-0.000002806	0.000000486	-0.000000615
83	8	-0.000001927	0.000000486	-0.000001931
84	6	0.000000825	0.000003109	0.000000135
85	9	-0.000000631	-0.000001915	-0.000004083
86	9	-0.000002188	-0.000001938	-0.000002393
87	9	0.000001054	-0.000000633	-0.000001439
88	6	0.000001347	0.000006352	-0.000000999
89	6	0.000000074	-0.000001182	0.000000359
90	6	-0.000002022	-0.000000716	-0.000002070
91	6	-0.000001187	-0.000002337	0.000002044
92	6	-0.000000275	0.000003065	-0.000001557
93	6	0.000000124	0.000001978	-0.000000983
94	1	0.000000172	0.000002521	-0.000001277
95	6	0.000000358	-0.000004200	0.000001802
96	6	0.000000506	-0.000001482	0.000000614
97	6	0.000000285	-0.000000771	0.000000298
98	6	-0.000001381	-0.000002895	-0.000000200
99	6	0.000000632	-0.000000633	-0.000000803
100	6	0.000000548	0.000000475	0.000000883
101	1	-0.000000551	0.000000210	0.000001889
102	6	-0.000000700	0.000000418	-0.000000869
103	1	-0.000001249	0.000001494	-0.000001299
104	6	-0.000000686	0.000001023	-0.000003029
105	1	-0.000000208	0.000000841	-0.000001919
106	6	0.000000534	0.000000610	-0.000001176
107	1	-0.000000439	-0.000000314	-0.000002333
108	6	0.000000265	-0.000001738	-0.000001774
109	1	-0.000000634	-0.000001062	-0.000001605
110	6	0.000001327	0.000000531	0.000000518
111	1	-0.000000462	-0.000000180	0.000000557
112	6	-0.000000117	0.000001477	0.000000706
113	1	0.000001801	0.000000908	0.000001997
114	6	0.000000220	0.000002112	0.000002958
115	1	-0.000000519	0.000001332	0.000000685
116	6	-0.000001370	0.000002125	0.000001111

117	1	-0.000000155	0.000003211	-0.000000370
118	6	-0.000001775	-0.000000857	-0.000001894
119	1	0.000000042	-0.000001640	-0.000001557
120	6	-0.000000814	-0.000000419	-0.000002007
121	1	-0.000000124	-0.000000647	-0.000001769
122	6	-0.000001920	-0.000001304	-0.000000699
123	1	-0.000000349	-0.000000035	-0.000001003
124	6	-0.000000508	-0.000000231	-0.000000249
125	1	-0.000000544	-0.000000342	-0.000000242
126	6	0.000001031	-0.000000373	0.000002333
127	1	0.000000115	-0.000000152	0.000002731
128	6	0.000000449	-0.000000739	0.000003225
129	1	0.000001228	-0.000001057	0.000003142
130	6	0.000000455	-0.000001299	0.000001435
131	1	0.000000439	-0.000001413	0.000001530
132	6	-0.000000104	-0.000002506	0.000000366
133	1	0.000000410	-0.000001853	0.000001084
134	1	-0.000000990	0.000002438	-0.000001741
135	1	-0.000007606	0.000022863	-0.000001139

SH-complex_C2_*S*





E(RM06-2X/6-31G(d)) = -4524.428403
Imaginary Freq = 0
Zero-point Energy Correction = 1.078258
Thermal Correction to Energy = 1.14385

Thermal Correction to Enthalpy = 1.144794
Thermal Correction to Free Energy = 0.981322
EE + Zero-point Energy = -4523.350145
EE + Thermal Energy Correction = -4523.284553
EE + Thermal Enthalpy Correction = -4523.283609
EE + Thermal Free Energy Correction = -4523.447081
Truhlar's quasiharmonic corrected Gibbs energy = -4523.433660

E_{sp} (RM06-2X/def2-TZVP) = -4525.871551
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.938891

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.821487	-2.681485	-1.308006
2	6	0	-2.534633	-2.079539	-1.825825
3	6	0	-2.698726	-0.966934	-2.899852
4	7	0	-2.356629	0.783925	-1.182764
5	1	0	-1.937329	-2.878194	-2.282013
6	1	0	-1.924712	-1.718166	-0.984514
7	6	0	-1.348627	-0.750078	-3.588369
8	1	0	-1.027965	-1.663099	-4.097150
9	1	0	-0.548840	-0.472436	-2.892508
10	1	0	-1.433260	0.044561	-4.335364
11	6	0	-3.729601	-1.388511	-3.951677
12	1	0	-3.452928	-2.358043	-4.378409
13	1	0	-3.764851	-0.658885	-4.768623
14	1	0	-4.734638	-1.481079	-3.526366
15	6	0	-4.790795	-1.772151	-0.639396
16	6	0	-6.613599	-0.024280	0.586123
17	6	0	-6.138217	-1.762008	-1.018345
18	6	0	-4.370883	-0.897686	0.369107
19	6	0	-5.277751	-0.038878	0.982457
20	6	0	-7.042005	-0.892721	-0.414194
21	1	0	-6.467059	-2.433629	-1.807322

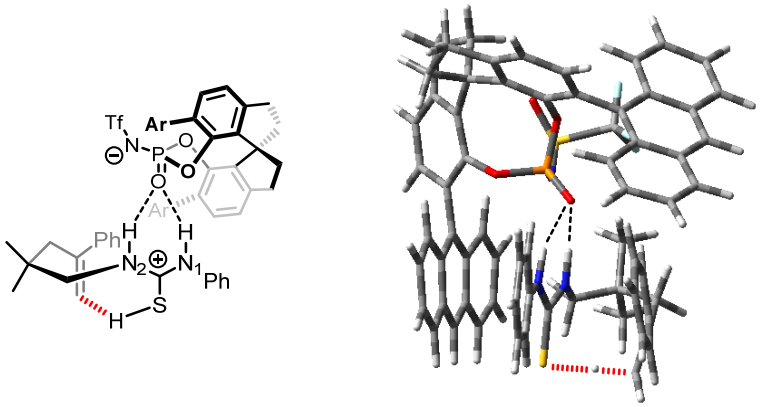
22	1	0	-3.331605	-0.904907	0.691082
23	1	0	-4.934888	0.595407	1.795939
24	1	0	-8.081709	-0.892940	-0.727328
25	1	0	-7.317130	0.653743	1.059381
26	6	0	-4.102493	-3.979015	-1.454611
27	1	0	-3.906687	2.707775	-1.894473
28	1	0	-3.414157	-4.652221	-1.957748
29	6	0	-2.643026	1.701021	-0.280985
30	7	0	-2.004874	1.692288	0.884637
31	6	0	-2.050743	2.666903	1.917369
32	6	0	-2.022421	4.422470	4.066559
33	6	0	-0.835210	3.136244	2.404288
34	6	0	-3.254443	3.052191	2.505485
35	6	0	-3.234281	3.942423	3.574412
36	6	0	-0.826054	4.016428	3.479798
37	1	0	0.088503	2.821941	1.923561
38	1	0	-4.193120	2.635709	2.151648
39	1	0	-4.168723	4.246018	4.035060
40	1	0	0.123041	4.390487	3.851809
41	1	0	-2.011683	5.107542	4.908203
42	16	0	-3.833606	2.958338	-0.580094
43	1	0	-5.019940	-4.407763	-1.059726
44	6	0	-3.171852	0.387634	-2.328980
45	1	0	-4.218450	0.341506	-2.006377
46	1	0	-3.077230	1.133875	-3.131954
47	1	0	-1.557200	0.183100	-0.927462
48	1	0	-1.259146	0.975873	0.965316
49	6	0	4.588512	-0.116960	1.367403
50	6	0	5.291871	0.856193	2.363333
51	6	0	5.278580	0.119969	3.710331
52	1	0	4.691630	1.771164	2.440817
53	1	0	6.293381	1.135891	2.020825
54	1	0	6.131490	-0.566944	3.794726
55	1	0	5.317233	0.794024	4.571948
56	6	0	5.631048	-1.105073	0.781022
57	1	0	5.099632	-1.939924	0.315768

58	1	0	6.308120	-1.493470	1.550248
59	6	0	6.355465	-0.285625	-0.308929
60	1	0	6.687870	-0.913437	-1.141333
61	6	0	3.567902	-0.755389	2.295152
62	6	0	1.991974	-1.761736	4.367104
63	6	0	3.981975	-0.648265	3.627906
64	6	0	2.353619	-1.371888	2.022547
65	6	0	1.529302	-1.849855	3.049690
66	6	0	3.216805	-1.168934	4.664323
67	1	0	3.552416	-1.086937	5.695054
68	1	0	1.354261	-2.137485	5.163721
69	1	0	7.239143	0.231163	0.089701
70	6	0	4.202479	0.650621	0.115395
71	6	0	4.115037	2.238677	-2.171755
72	6	0	3.029580	1.291507	-0.250000
73	6	0	5.294920	0.694175	-0.757852
74	6	0	5.260908	1.490956	-1.893504
75	6	0	2.969016	2.126289	-1.380172
76	1	0	6.105955	1.517376	-2.576384
77	1	0	4.081718	2.880056	-3.048930
78	8	0	1.952224	-1.534790	0.711476
79	8	0	1.839467	0.990594	0.411821
80	15	0	1.144098	-0.402150	-0.098267
81	8	0	-0.303172	-0.309854	0.288139
82	7	0	1.409209	-0.648465	-1.648607
83	16	0	2.468297	-1.611425	-2.328655
84	8	0	2.649627	-1.252537	-3.727562
85	8	0	3.651628	-1.916217	-1.532748
86	6	0	1.534080	-3.203654	-2.374068
87	9	0	0.678351	-3.222656	-3.395021
88	9	0	2.373563	-4.222770	-2.510088
89	9	0	0.840433	-3.360556	-1.248910
90	6	0	0.151817	-2.332348	2.753605
91	6	0	-2.482695	-3.155096	2.179519
92	6	0	-0.936512	-1.554647	3.195953
93	6	0	-0.067079	-3.519995	2.029781

94	6	0	-1.410270	-3.912095	1.703832
95	6	0	-2.275619	-2.006462	2.944760
96	1	0	-3.501071	-3.467531	1.948097
97	6	0	1.701294	2.846147	-1.698446
98	6	0	-0.732184	4.188272	-2.216347
99	6	0	1.230212	3.827987	-0.798631
100	6	0	0.985555	2.575376	-2.884439
101	6	0	-0.245164	3.273613	-3.149782
102	6	0	-0.016893	4.492053	-1.054800
103	1	0	-1.662844	4.717127	-2.420271
104	6	0	-1.620793	-5.089116	0.918551
105	1	0	-2.642816	-5.353123	0.655581
106	6	0	-0.568493	-5.858707	0.518525
107	1	0	-0.738128	-6.752858	-0.075201
108	6	0	0.762777	-5.499439	0.883498
109	1	0	1.591138	-6.125757	0.564505
110	6	0	1.005941	-4.368187	1.606097
111	1	0	2.024511	-4.092231	1.863833
112	6	0	-0.769261	-0.293840	3.862258
113	1	0	0.234732	0.095932	4.002847
114	6	0	-1.844207	0.421478	4.306502
115	1	0	-1.694646	1.383046	4.792393
116	6	0	-3.170524	-0.070132	4.121006
117	1	0	-4.012427	0.502245	4.503602
118	6	0	-3.374835	-1.246095	3.460296
119	1	0	-4.380792	-1.625977	3.294806
120	6	0	1.438924	1.626222	-3.857769
121	1	0	2.311927	1.021443	-3.648455
122	6	0	0.768793	1.444078	-5.031407
123	1	0	1.136045	0.707612	-5.740362
124	6	0	-0.422909	2.175966	-5.313861
125	1	0	-0.935998	2.023378	-6.260191
126	6	0	-0.928021	3.041574	-4.388423
127	1	0	-1.842550	3.599424	-4.583582
128	6	0	-0.472878	5.499793	-0.147564
129	1	0	-1.432526	5.972183	-0.346508

130	6	0	0.284907	5.878333	0.921323
131	1	0	-0.065841	6.655161	1.595227
132	6	0	1.540135	5.246481	1.161834
133	1	0	2.147538	5.564807	2.005624
134	6	0	1.986102	4.245059	0.345370
135	1	0	2.946750	3.775292	0.538352

Transition state $TS^{NPTA}_{C2\_S}$



E (RM06-2X/6-31G(d)) = -4524.396822 a.u.
Imaginary Freq = 1: -627.33 cm-1
Zero-point Energy Correction = 1.076722
Thermal Correction to Energy = 1.141544
Thermal Correction to Enthalpy = 1.142488
Thermal Correction to Free Energy = 0.979411
EE + Zero-point Energy = -4523.320101
EE + Thermal Energy Correction = -4523.255279
EE + Thermal Enthalpy Correction = -4523.254335
EE + Thermal Free Energy Correction = -4523.417411
Truhlar's quasiharmonic corrected Gibbs energy = -4523.402718

E_{sp} (RM06-2X/def2-TZVP) = -4525.83653
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.909931

Center Atomic Forces (Hartrees/Bohr)

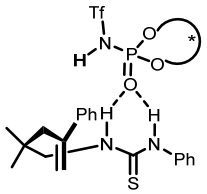
Number	Number	X	Y	Z
1	6	0.000009667	-0.000039367	0.000020144
2	6	-0.000048813	0.000001705	0.000000694
3	6	0.000022847	0.000006705	-0.000008815
4	7	0.000057650	0.000011346	0.000002017
5	1	-0.000000937	0.000001915	-0.000000918
6	1	0.000000180	0.000009708	0.000007116
7	6	0.000004354	0.000004985	0.000005946
8	1	-0.000005814	0.000001579	-0.000000701
9	1	0.000004775	-0.000003575	0.000001986
10	1	-0.000000278	0.000006021	-0.000004801
11	6	0.000004809	-0.000019336	-0.000000509
12	1	-0.000000354	0.000000408	0.000000631
13	1	0.000004520	0.000004671	-0.000000322
14	1	0.000000530	0.000001325	0.000004976
15	6	0.000006473	-0.000023472	0.000019298
16	6	-0.000013836	0.000005538	0.000007340
17	6	0.000001123	0.000013291	-0.000020414
18	6	0.000002674	0.000004497	-0.000000722
19	6	-0.000005405	0.000008523	-0.000012516
20	6	-0.000000423	-0.000009082	0.000005615
21	1	-0.000012690	0.000009714	-0.000005032
22	1	-0.000007352	-0.000000786	0.000007382
23	1	0.000004280	0.000004225	-0.000008199
24	1	0.000003572	0.000005791	-0.000003071
25	1	-0.000003138	0.000001692	-0.000006873
26	6	-0.003125243	-0.001508008	0.000935734
27	1	0.003110790	0.001515950	-0.000942632
28	1	0.000015396	-0.000003815	-0.000015013
29	6	-0.000007161	0.000026478	0.000080676
30	7	-0.000009494	0.000006913	-0.000032849
31	6	0.000002401	0.000055906	0.000002742
32	6	-0.000002557	0.000002666	-0.000000611
33	6	-0.000001897	0.000007515	0.000015342
34	6	0.000002603	-0.000027435	0.000000361

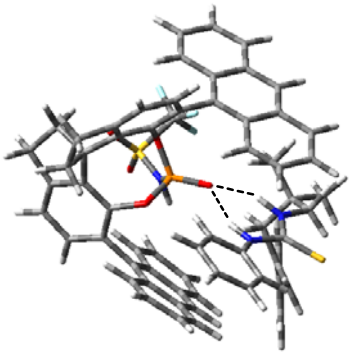
35	6	-0.000008142	0.000003061	-0.000006801
36	6	-0.000001606	0.000003616	-0.000006954
37	1	-0.000005602	0.000005970	-0.000009171
38	1	-0.000008318	-0.000015268	-0.000010884
39	1	0.000000579	-0.000002982	0.000006482
40	1	0.000000572	-0.000002843	-0.000000148
41	1	0.000001567	-0.000003812	-0.000001467
42	16	-0.000002192	-0.000026802	-0.000042805
43	1	-0.000000010	-0.000005419	-0.000001161
44	6	-0.000024089	0.000004064	-0.000022243
45	1	0.000003175	0.000006996	0.000007612
46	1	0.000013418	-0.000015834	0.000008951
47	1	-0.000042247	-0.000039790	-0.000038236
48	1	0.000076461	-0.000012707	0.000011270
49	6	-0.000012464	-0.000003515	0.000003947
50	6	0.000002741	0.000000581	-0.000002960
51	6	0.000000362	-0.000006135	-0.000004160
52	1	0.000002928	0.000001771	0.000002686
53	1	-0.000000660	-0.000003204	-0.000000862
54	1	-0.000002276	0.000001753	0.000000577
55	1	0.000001611	-0.000000192	0.000006263
56	6	-0.000016544	-0.000001831	0.000001633
57	1	0.000006488	0.000005717	0.000000443
58	1	-0.000000865	-0.000005013	-0.000001445
59	6	0.000022727	0.000014625	-0.000015300
60	1	-0.000006601	-0.000005474	0.000000739
61	6	0.000001866	-0.000004273	-0.000008038
62	6	0.000010175	-0.000003235	0.000004934
63	6	-0.000003020	0.000009488	-0.000010319
64	6	-0.000015847	0.000018262	0.000001481
65	6	-0.000000112	-0.000004564	0.000008164
66	6	0.000001241	0.000001525	0.000007848
67	1	-0.000000472	-0.000005779	-0.000000773
68	1	0.000003213	0.000001377	0.000004096
69	1	-0.000003618	-0.000008352	0.000008982
70	6	0.000030338	-0.000002717	0.000010519

71	6	0.000009629	-0.000003455	0.000012817
72	6	-0.000013276	-0.000023448	0.000008363
73	6	-0.000014025	0.000005057	-0.000003426
74	6	0.000001072	-0.000008395	-0.000002964
75	6	-0.000025043	0.000022696	-0.000010837
76	1	0.000001545	0.000001212	-0.000006431
77	1	-0.000005087	-0.000000143	0.000000054
78	8	0.000005392	-0.000010144	0.000013065
79	8	0.000029388	0.000008948	-0.000005782
80	15	-0.000018435	0.000016577	0.000021362
81	8	-0.000025349	0.000031778	0.000014556
82	7	-0.000062768	-0.000025138	-0.000004558
83	16	0.000019822	-0.000004990	0.000008883
84	8	-0.000008734	0.000003927	0.000009797
85	8	0.000000273	0.000005795	0.000002652
86	6	0.000056212	0.000003145	0.000033990
87	9	-0.000007682	0.000012359	-0.000030930
88	9	0.000000524	-0.000011764	-0.000018435
89	9	-0.000012469	0.000002890	-0.000010901
90	6	0.000011342	0.000009644	-0.000007707
91	6	-0.000006676	-0.000000833	0.000006075
92	6	-0.000013699	-0.000009332	0.000005672
93	6	0.000006871	-0.000007679	0.000008433
94	6	0.000006885	0.000004644	-0.000004268
95	6	-0.000001454	0.000002960	-0.000004874
96	1	0.000006850	0.000001991	-0.000000073
97	6	-0.000005794	0.000000584	-0.000002765
98	6	0.000009402	0.000004473	-0.000000538
99	6	-0.000003561	-0.000014895	-0.000000054
100	6	-0.000007246	-0.000006691	0.000008530
101	6	-0.000001387	0.000006548	0.000000561
102	6	0.000001317	-0.000004236	-0.000004321
103	1	-0.000002372	0.000003784	0.000008226
104	6	-0.000004150	0.000000776	0.000007027
105	1	0.000005663	0.000002134	-0.000000608
106	6	-0.000006342	-0.000006166	-0.000000856

107	1	0.000005197	0.000003257	-0.000002456
108	6	0.000006559	0.000002161	-0.000022020
109	1	0.000003493	-0.000005930	0.000005657
110	6	-0.000010872	0.000006360	0.000007562
111	1	0.000004755	-0.000010525	-0.000004856
112	6	0.000005591	0.000008007	-0.000006266
113	1	-0.000009520	-0.000005203	-0.000001805
114	6	0.000010173	-0.000007712	0.000003134
115	1	-0.000011112	0.000005500	0.000005406
116	6	-0.000007686	0.000008495	0.000001616
117	1	0.000006480	-0.000007424	0.000001679
118	6	0.000004799	-0.000012295	-0.000001537
119	1	0.000005723	0.000006507	-0.000000188
120	6	0.000001730	0.000011841	-0.000004447
121	1	0.000000958	-0.000002902	-0.000003679
122	6	-0.000005005	-0.000001774	-0.000000429
123	1	0.000003569	0.000000142	-0.000004196
124	6	-0.000002241	-0.000005380	-0.000000344
125	1	-0.000000207	0.000004720	-0.000000219
126	6	0.000009708	-0.000002132	-0.000001241
127	1	-0.000005195	0.000003307	0.000002650
128	6	-0.000001967	0.000006523	0.000000327
129	1	-0.000002387	0.000006275	0.000002383
130	6	-0.000008135	-0.000004720	0.000001077
131	1	0.000003256	-0.000001110	0.000005091
132	6	0.000019097	-0.000007899	0.000011846
133	1	-0.000000318	-0.000001781	-0.000001446
134	6	0.000012511	0.000012922	-0.000002701
135	1	-0.000003625	-0.000007099	-0.000007232

NH-complex_C2_*R*





E(RM06-2X/6-31G(d)) = -4524.430078
Imaginary Freq = 0
Zero-point Energy Correction = 1.08072
Thermal Correction to Energy = 1.147142
Thermal Correction to Enthalpy = 1.148087
Thermal Correction to Free Energy = 0.978568
EE + Zero-point Energy = -4523.349357
EE + Thermal Energy Correction = -4523.282935
EE + Thermal Enthalpy Correction = -4523.281991
EE + Thermal Free Energy Correction = -4523.451509
Truhlar's quasiharmonic corrected Gibbs energy = -4523.433455

E_{sp} (RM06-2X/def2-TZVP) = -4525.870574
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.941621

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000266	-0.000014171	0.000004909
2	6	-0.000004244	0.000004868	0.000004628
3	6	-0.000000877	0.000005437	-0.000005062
4	7	-0.000028652	-0.000006029	-0.000023374
5	1	0.000001723	-0.000001104	-0.000003820
6	1	-0.000000696	0.000002418	0.000000315
7	6	-0.000002525	-0.000001446	0.000001080
8	1	0.000000634	0.000000320	0.000000119
9	1	0.000000434	0.000000675	-0.000000003

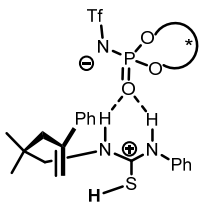
10	1	-0.000000975	0.000001154	0.000000378
11	6	-0.000004007	0.000001481	-0.000001296
12	1	0.000000080	0.000001506	-0.000000259
13	1	0.000000360	0.000000350	0.000000137
14	1	-0.000001254	0.000000179	0.000000913
15	6	-0.000005607	0.000003135	-0.000005724
16	6	-0.000002293	-0.000003702	-0.000002470
17	6	0.000001841	0.000006390	-0.000001276
18	6	-0.000000595	-0.000003421	0.000004484
19	6	-0.000001259	0.000004307	-0.000001574
20	6	0.000000203	0.000000280	0.000003319
21	1	0.000000419	-0.000001089	0.000001018
22	1	0.000000293	-0.000000891	0.000000367
23	1	-0.000001885	0.000000032	0.000000565
24	1	-0.000000418	0.000000162	-0.000001251
25	1	-0.000001489	0.000000399	0.000000225
26	6	0.000000090	-0.000001675	0.000003201
27	1	-0.000000423	-0.000000577	-0.000004822
28	6	-0.000018760	0.000001774	0.000021974
29	7	0.000035965	0.000029694	-0.000023833
30	6	-0.000009205	0.000000486	-0.000004272
31	6	-0.000002798	-0.000003245	0.000012385
32	6	0.000000777	-0.000015557	-0.000001668
33	6	0.000002630	0.000011395	-0.000004264
34	6	-0.000001319	-0.000008668	-0.000005578
35	6	0.000007376	0.000007243	-0.000003099
36	1	0.000002970	0.000005094	0.000000068
37	1	0.000000275	-0.000003456	0.000003805
38	1	0.000000519	0.000002163	0.000002473
39	1	-0.000000237	-0.000000933	-0.000000607
40	1	0.000000041	0.000000196	-0.000001126
41	16	0.000001924	-0.000011122	-0.000005146
42	1	-0.000002363	0.000004691	-0.000001308
43	6	0.000001399	0.000001559	-0.000006358
44	1	0.000002007	-0.000002643	0.000005196
45	1	-0.000002984	0.000002832	0.000002665

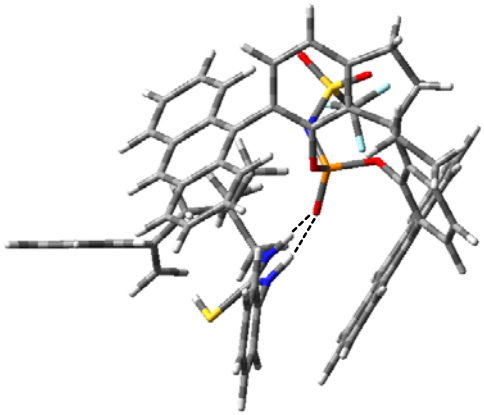
46	1	0.000026352	-0.000014356	0.000023330
47	1	-0.000022946	-0.000026146	0.000012912
48	6	0.000000041	-0.000000646	0.000004957
49	6	0.000004785	0.000000980	0.000003246
50	6	-0.000001163	-0.000001052	-0.000005319
51	1	-0.000000979	-0.000000319	0.000001345
52	1	-0.000000922	0.000000615	-0.000001716
53	1	0.000001022	-0.000001137	0.000000767
54	1	0.000000707	-0.000000912	0.000002796
55	6	-0.000003789	0.000003000	-0.000007326
56	1	0.000000648	-0.000001193	0.000003477
57	1	0.000001442	0.000000816	-0.000000338
58	6	0.000008020	-0.000006227	-0.000001152
59	1	0.000001321	-0.000000527	0.000001011
60	6	0.000002263	0.000004347	-0.000000169
61	6	0.000001310	0.000003857	0.000000536
62	6	0.000008582	0.000003720	0.000002392
63	6	-0.000009883	-0.000005688	-0.000004630
64	6	-0.000002736	-0.000007925	0.000001526
65	6	-0.000003197	-0.000003463	-0.000001515
66	1	-0.000000824	0.000001660	0.000000569
67	1	-0.000000686	0.000001329	-0.000000494
68	1	-0.000002589	0.000001138	0.000002227
69	6	-0.000002360	-0.000006175	-0.000004984
70	6	0.000004388	0.000001820	-0.000002065
71	6	0.000004118	0.000001641	-0.000006824
72	6	-0.000010351	0.000002904	-0.000002097
73	6	0.000001948	-0.000002250	0.000009085
74	6	0.000008363	0.000000152	-0.000001677
75	1	0.000001197	-0.000000710	-0.000000055
76	1	-0.000000699	-0.000001515	0.000002148
77	8	0.000011390	0.000001523	0.000009803
78	8	-0.000010068	-0.000020713	0.000015963
79	15	0.000008221	0.000001973	-0.000011906
80	8	0.000010596	0.000040410	-0.000011406
81	7	-0.000011974	-0.000002995	0.000000605

82	16	0.000009174	0.000002668	0.000003330
83	8	-0.000001302	-0.000000820	-0.000000881
84	8	-0.000001237	-0.000003272	-0.000000067
85	6	-0.000005158	-0.000003998	-0.000006178
86	9	0.000004324	0.000001016	0.000003172
87	9	-0.000002647	0.000002512	0.000003766
88	9	0.000008870	0.000005286	-0.000001712
89	6	0.000001977	0.000003148	0.000004867
90	6	0.000000256	-0.000003133	0.000000019
91	6	0.000003047	-0.000002020	-0.000001579
92	6	-0.000002633	0.000003421	0.000000846
93	6	0.000000527	0.000004956	0.000002017
94	6	0.000000875	0.000008472	-0.000003882
95	1	-0.000002090	0.000000266	-0.000001882
96	6	-0.000013923	0.000004126	-0.000000735
97	6	-0.000000874	0.000007256	-0.000001709
98	6	0.000003243	-0.000007208	0.000001386
99	6	-0.000005523	-0.000003476	0.000010333
100	6	0.000004545	-0.000002384	-0.000005288
101	6	0.000000331	-0.000009358	0.000003989
102	1	-0.000000566	-0.000000888	0.000000372
103	6	-0.000000903	-0.000003790	0.000003810
104	1	0.000002073	0.000002763	-0.000005320
105	6	-0.000001923	0.000002838	-0.000003418
106	1	0.000003478	0.000002073	0.000005960
107	6	0.000002613	-0.000000790	0.000005034
108	1	-0.000000586	0.000001862	-0.000000582
109	6	0.000002972	-0.000004273	0.000002921
110	1	-0.000001355	-0.000000465	-0.000002401
111	6	0.000005297	-0.000004407	-0.000005116
112	1	-0.000001306	0.000000463	0.000000209
113	6	-0.000008094	0.000000418	0.000004641
114	1	0.000001469	-0.000001002	0.000000180
115	6	0.000003950	0.000004893	-0.000001948
116	1	0.000001299	-0.000000436	-0.000000825
117	6	0.000004750	-0.000007431	-0.000004148

118	1	-0.000001933	0.000001422	-0.000001200
119	6	0.000001337	0.000008048	-0.000004784
120	1	-0.000001203	-0.000000001	0.000001945
121	6	-0.000002560	-0.000006480	0.000012212
122	1	-0.000004986	0.000004557	-0.000002694
123	6	0.000006285	-0.000003300	-0.000008597
124	1	-0.000000266	0.000002133	0.000002706
125	6	-0.000001187	0.000009833	-0.000002982
126	1	-0.000000149	-0.000001181	0.000000558
127	6	-0.000001533	0.000000439	-0.000003991
128	1	0.000002564	0.000000320	-0.000001390
129	6	0.000000790	-0.000001289	-0.000000651
130	1	-0.000001242	-0.000001954	-0.000000587
131	6	0.000001452	0.000001952	0.000000933
132	1	0.000000567	0.000000140	-0.000002693
133	6	-0.000001553	-0.000001224	-0.000001478
134	1	-0.000001212	-0.000001394	0.000002395
135	1	0.000001507	0.000000261	0.000000065

SH-complex_C2_*R*





E(RM06-2x/6-31G(d)) = -4524.409575
Imaginary Freq = 0
Zero-point Energy Correction = 1.077669
Thermal Correction to Energy = 1.143939
Thermal Correction to Enthalpy = 1.144884

Thermal Correction to Free Energy = 0.97517
EE + Zero-point Energy = -4523.331906
EE + Thermal Energy Correction = -4523.265636
EE + Thermal Enthalpy Correction = -4523.264692
EE + Thermal Free Energy Correction = -4523.434405
Truhlar's quasiharmonic corrected Gibbs energy = -4523.416110

E_{sp} (RM06-2X/def2-TZVP) = -4525.858121
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.935203

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.421917	-1.934611	-0.861190
2	6	0	-4.003510	-1.948753	-1.389379
3	6	0	-2.982203	-3.019091	-0.966177
4	7	0	-2.156909	-1.690388	0.954259
5	1	0	-4.068899	-1.969297	-2.486350
6	1	0	-3.554352	-0.970519	-1.167306
7	6	0	-1.678147	-2.704670	-1.720972
8	1	0	-1.825226	-2.824789	-2.798332
9	1	0	-1.329244	-1.678060	-1.555069
10	1	0	-0.873269	-3.384862	-1.418839
11	6	0	-3.412012	-4.442351	-1.347414
12	1	0	-3.640491	-4.484968	-2.417029
13	1	0	-2.594364	-5.145735	-1.154801
14	1	0	-4.293318	-4.794493	-0.806341
15	6	0	-6.272085	-0.824261	-1.381654
16	6	0	-7.921741	1.234405	-2.350002
17	6	0	-7.604218	-1.075027	-1.735669
18	6	0	-5.775855	0.476285	-1.539148
19	6	0	-6.597110	1.495124	-2.011753
20	6	0	-8.422032	-0.057831	-2.213475
21	1	0	-7.990217	-2.087276	-1.658553
22	1	0	-4.747774	0.714250	-1.282259

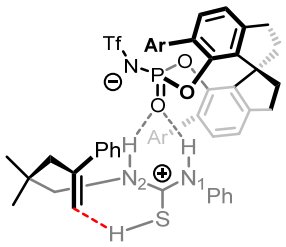
23	1	0	-6.195653	2.498679	-2.113527
24	1	0	-9.448422	-0.278442	-2.489978
25	1	0	-8.557281	2.030394	-2.725048
26	6	0	-5.954210	-2.817504	-0.003219
27	1	0	-4.745229	-1.545187	1.518367
28	1	0	-5.418648	-3.685184	0.363308
29	6	0	-2.571103	-0.875632	1.911655
30	7	0	-1.737413	0.065236	2.341290
31	6	0	-1.965936	1.074601	3.315283
32	6	0	-2.281952	3.092566	5.195555
33	6	0	-2.477294	0.768134	4.575803
34	6	0	-1.583085	2.377623	2.997837
35	6	0	-1.739921	3.383143	3.945059
36	6	0	-2.649200	1.786548	5.508101
37	1	0	-2.707676	-0.260937	4.835719
38	1	0	-1.166820	2.598031	2.017834
39	1	0	-1.438984	4.394403	3.691464
40	1	0	-3.053452	1.550455	6.487115
41	1	0	-2.407516	3.881607	5.929930
42	16	0	-4.195401	-0.941920	2.597076
43	1	0	-6.978487	-2.705791	0.340805
44	6	0	-2.686046	-2.984902	0.542026
45	1	0	-3.552599	-3.236207	1.155492
46	1	0	-1.910472	-3.729606	0.760293
47	1	0	-1.206195	-1.476359	0.619594
48	1	0	-0.818710	0.068645	1.859649
49	6	0	4.739801	1.404748	-0.131222
50	6	0	5.434265	2.460203	0.788164
51	6	0	6.197327	1.632609	1.845931
52	1	0	4.656919	3.045755	1.288303
53	1	0	6.072545	3.138342	0.218303
54	1	0	7.198303	1.360311	1.494322
55	1	0	6.303296	2.163771	2.794656
56	6	0	5.701313	0.965304	-1.267012
57	1	0	5.281455	0.073312	-1.738272
58	1	0	6.708909	0.757326	-0.898135

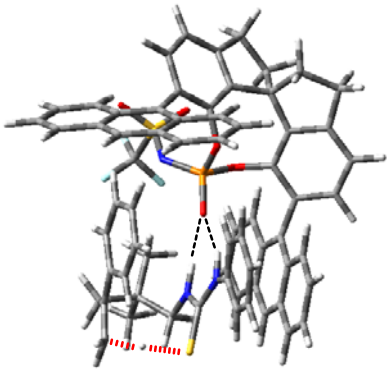
59	6	0	5.639211	2.133930	-2.285050
60	1	0	5.778732	1.781723	-3.309254
61	6	0	4.456238	0.315556	0.884680
62	6	0	4.370336	-1.590843	2.917328
63	6	0	5.323054	0.404827	1.975159
64	6	0	3.537046	-0.718178	0.845882
65	6	0	3.465309	-1.681411	1.854120
66	6	0	5.297484	-0.549674	2.985812
67	1	0	5.978478	-0.480234	3.828101
68	1	0	4.326358	-2.338801	3.702475
69	1	0	6.394397	2.899243	-2.077493
70	6	0	3.657513	2.087745	-0.950689
71	6	0	2.189977	3.857267	-2.517137
72	6	0	2.310451	2.283487	-0.713731
73	6	0	4.233728	2.667803	-2.086165
74	6	0	3.506418	3.547084	-2.876022
75	6	0	1.568092	3.216087	-1.444761
76	1	0	3.947318	3.990714	-3.762660
77	1	0	1.619541	4.578260	-3.093336
78	8	0	2.688867	-0.821515	-0.235113
79	8	0	1.633298	1.492144	0.210436
80	15	0	1.288639	-0.015228	-0.333941
81	8	0	0.255015	-0.521007	0.624995
82	7	0	0.887677	-0.061443	-1.866945
83	16	0	1.815296	-0.278763	-3.136293
84	8	0	1.313491	0.481960	-4.278413
85	8	0	3.256223	-0.299922	-2.892550
86	6	0	1.395580	-2.031644	-3.534920
87	9	0	0.145230	-2.120782	-3.987832
88	9	0	2.220989	-2.486911	-4.471704
89	9	0	1.508646	-2.797333	-2.450153
90	6	0	2.437987	-2.765206	1.804403
91	6	0	0.532993	-4.841471	1.788294
92	6	0	1.355504	-2.729350	2.701476
93	6	0	2.561146	-3.819244	0.879728
94	6	0	1.587695	-4.873162	0.875273

95	6	0	0.392907	-3.792506	2.697200
96	1	0	-0.192552	-5.651857	1.792209
97	6	0	0.185024	3.589134	-1.004660
98	6	0	-2.383230	4.430427	-0.191130
99	6	0	0.046962	4.472704	0.087124
100	6	0	-0.952273	3.140912	-1.699131
101	6	0	-2.257670	3.562714	-1.274275
102	6	0	-1.261551	4.901927	0.491615
103	1	0	-3.372652	4.755394	0.121462
104	6	0	1.158689	-1.644309	3.622897
105	1	0	1.861486	-0.819248	3.605838
106	6	0	0.112158	-1.639778	4.493086
107	1	0	-0.017661	-0.810794	5.180314
108	6	0	-0.830795	-2.716715	4.506226
109	1	0	-1.649735	-2.700386	5.218200
110	6	0	-0.695414	-3.751592	3.633034
111	1	0	-1.403184	-4.575948	3.628842
112	6	0	1.723588	-5.944988	-0.068546
113	1	0	0.978462	-6.735050	-0.055259
114	6	0	2.753866	-5.967509	-0.955863
115	1	0	2.848639	-6.778044	-1.670400
116	6	0	3.723072	-4.915568	-0.958354
117	1	0	4.532098	-4.943830	-1.679794
118	6	0	3.632285	-3.883905	-0.075470
119	1	0	4.365341	-3.085865	-0.088565
120	6	0	-1.389393	5.825949	1.582363
121	1	0	-2.388712	6.145459	1.864391
122	6	0	-0.291855	6.298739	2.234744
123	1	0	-0.396184	7.008302	3.049155
124	6	0	1.014014	5.868132	1.841055
125	1	0	1.879469	6.253553	2.369277
126	6	0	1.176328	4.992131	0.810919
127	1	0	2.169942	4.678320	0.512548
128	6	0	-0.855224	2.266640	-2.832701
129	1	0	0.118946	1.927570	-3.158482
130	6	0	-1.972143	1.839839	-3.484072

131	1	0	-1.869146	1.171587	-4.332062
132	6	0	-3.273317	2.255657	-3.057212
133	1	0	-4.148484	1.904676	-3.595740
134	6	0	-3.408710	3.088412	-1.988206
135	1	0	-4.386602	3.424894	-1.655042

Transition state $TS^{NPTA}_{C2\_R}$





E (RM06-2X/6-31G(d)) = -4524.399229 a.u.
Imaginary Freq = 1: -866.91 cm-1
Zero-point Energy Correction = 1.077017
Thermal Correction to Energy = 1.141822
Thermal Correction to Enthalpy = 1.142766
Thermal Correction to Free Energy = 0.979676
EE + Zero-point Energy = -4523.322212
EE + Thermal Energy Correction = -4523.257407
EE + Thermal Enthalpy Correction = -4523.256462
EE + Thermal Free Energy Correction = -4523.419553
Truhlar's quasiharmonic corrected Gibbs energy = -4523.405059

E_{sp} (RM06-2X/def2-TZVP) = -4525.842825
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.913685

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z

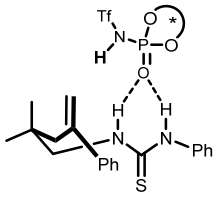
1	6	0.000090318	-0.000046073	0.000025972
2	6	-0.000146363	-0.000024440	0.000055006
3	6	0.000007876	0.000047341	0.000011950
4	7	-0.000032281	0.000023572	-0.000028656
5	1	-0.000030622	-0.000016962	-0.000001287
6	1	0.000013478	-0.000014375	-0.000001342
7	6	0.000005742	-0.000017409	0.000021010
8	1	-0.000003446	0.000004086	-0.000006788
9	1	-0.000055166	-0.000016723	-0.000049597
10	1	0.000013288	-0.000021684	0.000003980
11	6	0.000020457	-0.000006198	-0.000018634
12	1	0.000005698	-0.000003022	0.000001360
13	1	0.000009981	-0.000006856	0.000006916
14	1	0.000001290	0.000000406	0.000001962
15	6	-0.000029956	-0.000026577	0.000010427
16	6	0.000002956	-0.000044039	0.000047608
17	6	-0.000017155	-0.000013549	-0.000017447
18	6	0.000018884	0.000045458	0.000045384
19	6	0.000044392	-0.000000208	-0.000019593
20	6	-0.000021358	0.000014995	-0.000001333
21	1	-0.000009783	-0.000000687	-0.000001210
22	1	0.000036954	-0.000003583	0.000028149
23	1	0.000000247	-0.000035874	0.000032426
24	1	-0.000000394	0.000006717	0.000003092
25	1	-0.000017110	-0.000034644	0.000012286
26	6	-0.000748161	-0.000030413	0.000115968
27	1	0.000833491	0.000165908	-0.000101500
28	1	-0.000021089	-0.000004176	-0.000007885
29	6	0.000210287	-0.000020342	0.000027553
30	7	-0.000097905	-0.000072393	-0.000077379
31	6	-0.000042122	-0.000017064	-0.000012026
32	6	0.000002533	0.000010667	0.000000847
33	6	-0.000022158	0.000002965	-0.000015678
34	6	-0.000002335	0.000000474	-0.000000238
35	6	0.000002319	-0.000002123	0.000001222

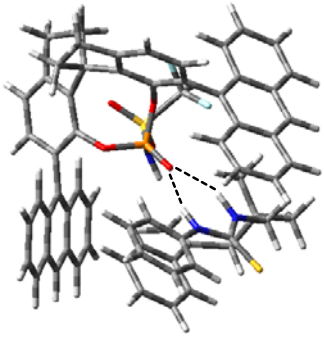
36	6	-0.000000700	0.000000679	-0.000007184
37	1	-0.000004198	-0.000014469	-0.000015272
38	1	-0.000004590	-0.000001105	0.000002550
39	1	-0.000004278	0.000015414	0.000004124
40	1	-0.000002144	0.000000399	-0.000001378
41	1	-0.000002714	0.000001303	-0.000001085
42	16	-0.000106220	-0.000071661	0.000075703
43	1	-0.000004571	0.000010832	-0.000040662
44	6	-0.000042352	-0.000014949	-0.000006817
45	1	-0.000018223	0.000009889	-0.000025638
46	1	-0.000010940	0.000003250	-0.000006338
47	1	-0.000008874	-0.000020459	-0.000003030
48	1	-0.000038130	0.000099060	0.000011939
49	6	0.000003603	-0.000010528	-0.000013660
50	6	0.000002497	-0.000004153	0.000001869
51	6	0.000003973	0.000004817	-0.000016113
52	1	0.000001090	0.000000389	0.000000322
53	1	-0.000000658	-0.000005531	0.000001037
54	1	-0.000001960	-0.000000986	-0.000000188
55	1	0.000002532	0.000001123	0.000001313
56	6	-0.000035911	0.000008268	-0.000018389
57	1	-0.000018353	0.000014008	0.000017451
58	1	-0.000004288	0.000006049	0.000001664
59	6	0.000006640	-0.000012394	-0.000020106
60	1	-0.000000628	0.000004399	-0.000003206
61	6	-0.000005500	0.000005121	0.000006590
62	6	-0.000007314	0.000019620	-0.000004167
63	6	0.000008956	0.000007187	0.000009195
64	6	0.000005158	-0.000005961	-0.000044433
65	6	0.000013404	-0.000014562	-0.000010997
66	6	-0.000002772	-0.000001891	-0.000008168
67	1	0.000000573	0.000001074	-0.000002950
68	1	-0.000000760	0.000005378	-0.000006988
69	1	0.000002331	-0.000001779	-0.000001313
70	6	-0.000001706	0.000001379	0.000014716
71	6	0.000016630	-0.000012730	0.000017403

72	6	0.000000148	-0.000011952	0.000010280
73	6	0.000012075	0.000010052	-0.000003827
74	6	0.000005716	-0.000009427	-0.000007045
75	6	-0.000017121	0.000012266	-0.000009014
76	1	0.000000349	-0.000001489	-0.000000083
77	1	0.000009338	-0.000002936	-0.000002469
78	8	-0.000000239	-0.000021446	0.000090600
79	8	0.000027912	-0.000010053	0.000012194
80	15	-0.000173182	-0.000006108	-0.000064488
81	8	0.000110179	-0.000031260	0.000027008
82	7	0.000049385	0.000039091	0.000060574
83	16	0.000011276	0.000046579	-0.000093717
84	8	0.000008069	-0.000014613	0.000096276
85	8	0.000040091	0.000026629	-0.000007534
86	6	0.000023768	-0.000009970	0.000004463
87	9	-0.000024421	0.000021964	0.000007944
88	9	-0.000002036	0.000004772	-0.000000551
89	9	-0.000013057	0.000002307	-0.000017966
90	6	-0.000002459	0.000019044	-0.000043915
91	6	0.000039464	-0.000012321	0.000004602
92	6	-0.000010549	0.000000877	0.000007716
93	6	0.000017179	0.000004384	0.000011745
94	6	-0.000000992	0.000009061	0.000005514
95	6	0.000007292	0.000001659	0.000009667
96	1	0.000007165	0.000002413	0.000002308
97	6	0.000019857	0.000036078	0.000000516
98	6	-0.000008718	-0.000041762	-0.000016569
99	6	-0.000000265	0.000042989	-0.000005832
100	6	-0.000013791	0.000030700	-0.000013227
101	6	0.000014523	0.000016947	0.000001655
102	6	0.000011858	-0.000031983	-0.000018731
103	1	-0.000004439	0.000005535	-0.000000339
104	6	0.000035024	0.000003784	0.000017931
105	1	0.000004527	-0.000017186	0.000009144
106	6	0.000069259	0.000003484	0.000023260
107	1	-0.000002659	0.000001667	-0.000004350

108	6	0.000034512	0.000007877	0.000012190
109	1	0.000002955	0.000000912	-0.000002084
110	6	0.000021533	0.000008521	0.000006886
111	1	0.000002308	0.000004055	0.000001307
112	6	-0.000014448	-0.000003146	-0.000006001
113	1	0.000003160	0.000001267	0.000003034
114	6	-0.000001414	0.000002066	-0.000004913
115	1	0.000001272	-0.000001758	-0.000001032
116	6	-0.000001319	-0.000003229	-0.000003786
117	1	0.000002749	0.000002782	0.000003391
118	6	-0.000018770	-0.000004348	0.000008400
119	1	0.000001730	-0.000003231	-0.000005496
120	6	0.000000146	0.000003083	0.000004375
121	1	-0.000002580	-0.000000159	-0.000001900
122	6	-0.000004890	-0.000009268	0.000004862
123	1	-0.000000616	0.000001081	-0.000003787
124	6	-0.000002991	-0.000004462	-0.000003389
125	1	0.000000806	0.000000676	-0.000001644
126	6	0.000001809	-0.000006095	-0.000013579
127	1	-0.000001036	-0.000002260	-0.000021843
128	6	0.000006078	-0.000011112	-0.000005329
129	1	-0.000044433	0.000016230	-0.000060273
130	6	0.000008438	0.000010624	-0.000011769
131	1	0.000000076	0.000002039	0.000004105
132	6	-0.000000251	-0.000002386	0.000005182
133	1	-0.000002082	0.000001014	0.000001369
134	6	-0.000004318	0.000000148	-0.000001809
135	1	-0.000001342	-0.000000351	-0.000000524

NH-complex_E_*S*





Electronic Energy (EE) = -4524.440151
Imaginary Freq = 0
Zero-point Energy Correction = 1.081359
Thermal Correction to Energy = 1.147003
Thermal Correction to Enthalpy = 1.147947
Thermal Correction to Free Energy = 0.983666
EE + Zero-point Energy = -4523.358792
EE + Thermal Energy Correction = -4523.293149
EE + Thermal Enthalpy Correction = -4523.292204
EE + Thermal Free Energy Correction = -4523.456486
Truhlar's quasiharmonic corrected Gibbs energy = -4523.442400

E_{sp} (RM06-2X/def2-TZVP) = -4525.877901
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.946648

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.053356	-0.778765	-3.007193
2	6	0	2.696430	0.380655	-3.747890
3	6	0	2.495551	1.848318	-3.272606
4	7	0	3.126558	1.433003	-0.906640
5	1	0	2.317485	0.341237	-4.775894
6	1	0	3.776859	0.207590	-3.820696
7	6	0	2.917311	2.753471	-4.439480
8	1	0	2.251962	2.613986	-5.297890
9	1	0	3.940751	2.530457	-4.761879

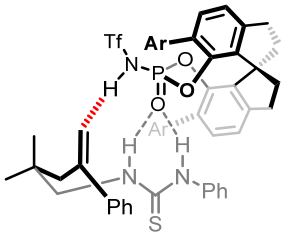
10	1	0	2.876379	3.808681	-4.148170
11	6	0	1.034158	2.132658	-2.933097
12	1	0	0.360557	1.791432	-3.731218
13	1	0	0.872918	3.207416	-2.789000
14	1	0	0.734242	1.630865	-2.009607
15	6	0	2.775218	-1.488886	-1.914841
16	6	0	4.076430	-2.898497	0.148600
17	6	0	4.172557	-1.539941	-1.849653
18	6	0	2.048685	-2.162134	-0.924412
19	6	0	2.686816	-2.843660	0.104251
20	6	0	4.815849	-2.244165	-0.833238
21	1	0	4.776540	-1.017438	-2.586332
22	1	0	0.962563	-2.135680	-0.942677
23	1	0	2.096259	-3.309010	0.887449
24	1	0	5.900280	-2.246050	-0.795681
25	1	0	4.574885	-3.413225	0.964503
26	6	0	0.859911	-1.241439	-3.428091
27	1	0	0.315582	-0.770764	-4.243914
28	1	0	0.412534	-2.140124	-3.012115
29	6	0	4.061781	0.908922	-0.076468
30	7	0	3.496306	0.138640	0.896071
31	16	0	5.710017	1.166902	-0.301849
32	6	0	3.987719	-0.452838	2.064760
33	6	0	4.706697	-1.699078	4.479843
34	6	0	3.004826	-0.935084	2.947999
35	6	0	5.338000	-0.611709	2.400915
36	6	0	5.677133	-1.226396	3.603850
37	6	0	3.363342	-1.551011	4.137971
38	1	0	1.955584	-0.830195	2.676587
39	1	0	6.105823	-0.263442	1.727992
40	1	0	6.728842	-1.338741	3.850752
41	1	0	2.585743	-1.918957	4.800394
42	1	0	4.990022	-2.179491	5.410938
43	6	0	3.408735	2.209455	-2.088777
44	1	0	3.296597	3.280808	-1.860630
45	1	0	4.456595	2.042085	-2.353934

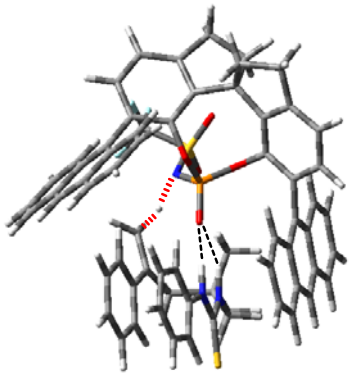
46	1	0	2.161298	1.387772	-0.592316
47	1	0	2.484104	0.059961	0.824839
48	1	0	-0.472113	-0.319030	-2.053709
49	6	0	-3.689344	-0.131719	2.631203
50	6	0	-3.677242	-0.773003	4.051709
51	6	0	-3.449546	0.405943	5.014247
52	1	0	-2.831151	-1.466443	4.114217
53	1	0	-4.591946	-1.337037	4.256412
54	1	0	-4.397293	0.882443	5.294221
55	1	0	-2.951286	0.107458	5.941159
56	6	0	-5.102604	0.426883	2.309509
57	1	0	-5.016303	1.117900	1.463042
58	1	0	-5.535574	0.967831	3.156857
59	6	0	-5.911634	-0.813746	1.887714
60	1	0	-6.715198	-0.577355	1.184436
61	6	0	-2.676625	0.978545	2.832108
62	6	0	-1.088927	3.115837	3.630880
63	6	0	-2.605921	1.340336	4.180162
64	6	0	-1.911766	1.672382	1.911808
65	6	0	-1.105258	2.756012	2.276891
66	6	0	-1.817480	2.410205	4.584868
67	1	0	-1.760710	2.691878	5.632192
68	1	0	-0.467023	3.955254	3.927438
69	1	0	-6.372565	-1.303677	2.754491
70	6	0	-3.577273	-1.208169	1.562673
71	6	0	-3.888752	-3.467503	-0.023510
72	6	0	-2.479315	-1.792844	0.948138
73	6	0	-4.853769	-1.693074	1.261358
74	6	0	-5.017632	-2.816631	0.464467
75	6	0	-2.599255	-2.964235	0.188110
76	1	0	-6.009775	-3.192501	0.232348
77	1	0	-3.992295	-4.375548	-0.610237
78	8	0	-1.937741	1.233654	0.575546
79	8	0	-1.217094	-1.190903	1.066646
80	15	0	-0.862113	0.109501	0.194194
81	8	0	0.563887	0.439447	0.354319

82	7	0	-1.273116	-0.142620	-1.423399
83	16	0	-2.682561	0.125824	-2.274382
84	8	0	-2.359578	-0.209004	-3.643813
85	8	0	-3.811098	-0.443684	-1.576066
86	6	0	-2.986073	1.971926	-2.276885
87	9	0	-3.817714	2.273978	-1.298074
88	9	0	-1.841132	2.621784	-2.154161
89	9	0	-3.552269	2.285364	-3.432966
90	6	0	-0.291075	3.525665	1.293634
91	6	0	1.230157	5.024471	-0.538539
92	6	0	1.115533	3.520137	1.386936
93	6	0	-0.941692	4.312667	0.325282
94	6	0	-0.161773	5.035797	-0.636988
95	6	0	1.885302	4.314429	0.469228
96	1	0	1.818738	5.601634	-1.250021
97	6	0	-1.429858	-3.724752	-0.344804
98	6	0	0.661375	-5.341062	-1.342389
99	6	0	-0.553322	-4.373083	0.550399
100	6	0	-1.271363	-3.896037	-1.737161
101	6	0	-0.190446	-4.700030	-2.239490
102	6	0	0.492460	-5.213505	0.034397
103	1	0	1.471001	-5.959101	-1.723983
104	6	0	-2.366245	4.442918	0.268792
105	1	0	-2.971212	3.938306	1.015500
106	6	0	-2.970346	5.177563	-0.708641
107	1	0	-4.053228	5.254774	-0.734523
108	6	0	-2.194855	5.838750	-1.705528
109	1	0	-2.694197	6.405955	-2.484531
110	6	0	-0.833318	5.773390	-1.662811
111	1	0	-0.227195	6.290642	-2.402019
112	6	0	3.308673	4.360539	0.606170
113	1	0	3.872923	4.970032	-0.094964
114	6	0	3.944170	3.650173	1.579409
115	1	0	5.025003	3.669265	1.661636
116	6	0	3.187139	2.828844	2.466660
117	1	0	3.709145	2.217885	3.198421

118	6	0	1.828760	2.753986	2.367732
119	1	0	1.275615	2.089627	3.024856
120	6	0	-0.015457	-4.837209	-3.653792
121	1	0	0.811813	-5.445367	-4.009429
122	6	0	-0.855907	-4.216252	-4.528540
123	1	0	-0.708623	-4.319159	-5.598787
124	6	0	-1.933285	-3.423055	-4.035867
125	1	0	-2.592860	-2.915732	-4.732361
126	6	0	-2.138255	-3.278770	-2.694457
127	1	0	-2.973648	-2.689359	-2.337390
128	6	0	-0.676235	-4.261646	1.973325
129	1	0	-1.470464	-3.649095	2.387482
130	6	0	0.170089	-4.930654	2.808572
131	1	0	0.052779	-4.833859	3.883455
132	6	0	1.206973	-5.762817	2.291414
133	1	0	1.873256	-6.277686	2.975821
134	6	0	1.358920	-5.896925	0.944925
135	1	0	2.147952	-6.517946	0.530202

Transition state $TS^{NPTA}_{E\_S\_TS1}$





E (RM06-2X /6-31G(d)) = -1151.35 a.u.
Imaginary Freq = 1: -1313.35 cm-1
Zero-point Energy Correction = 1.07575
Thermal Correction to Energy = 1.140816
Thermal Correction to Enthalpy = 1.14176
Thermal Correction to Free Energy = 0.979515

EE + Zero-point Energy = -4523.325768
EE + Thermal Energy Correction = -4523.260702
EE + Thermal Enthalpy Correction = -4523.259758
EE + Thermal Free Energy Correction = -4523.422003
Truhlar's quasiharmonic corrected Gibbs energy = -4523.409377

E_{sp} (RM06-2X/def2-TZVP) = -4525.839933
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.907937

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000041028	0.000005960	-0.000040200
2	6	-0.000081315	-0.000019570	-0.000021471
3	6	0.000022992	0.000007118	-0.000038719
4	7	0.000038900	0.000022839	0.000016262
5	1	-0.000014350	0.000011689	0.000017007
6	1	0.000016040	0.000020729	-0.000011389
7	6	0.000025548	0.000000653	0.000017266
8	1	-0.000001415	-0.000001234	-0.000002969
9	1	0.000004418	0.000002424	-0.000011296
10	1	-0.000010858	0.000002379	0.000003356
11	6	-0.000011767	0.000000702	0.000035083
12	1	0.000000815	0.000001202	0.000001905
13	1	-0.000019036	0.000004569	-0.000014267
14	1	0.000014318	0.000000579	-0.000013499
15	6	-0.000026615	-0.000024213	0.000044707
16	6	-0.000040403	-0.000005341	-0.000001186
17	6	-0.000009680	0.000000459	-0.000042830
18	6	0.000024577	0.000032500	-0.000039254
19	6	0.000032492	0.000012102	-0.000003418
20	6	-0.000010117	-0.000018875	-0.000005421
21	1	-0.000010434	-0.000012019	0.000019164
22	1	-0.000017550	0.000023954	0.000002673
23	1	-0.000001050	0.000006114	0.000023944

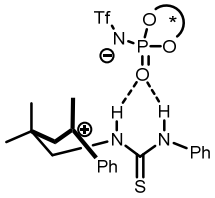
24	1	0.000010872	0.000012883	-0.000005466
25	1	0.000011387	0.000009891	0.000004099
26	6	-0.015442996	0.005087439	0.005389105
27	1	0.000020661	-0.000009988	-0.000029019
28	1	-0.000061836	-0.000001483	0.000052138
29	6	-0.000015653	-0.000004102	0.000029886
30	7	-0.000024362	0.000023877	-0.000019214
31	16	-0.000022754	-0.000006888	0.000001233
32	6	-0.000012142	-0.000021433	0.000007024
33	6	0.000005693	-0.000010434	-0.000014364
34	6	-0.000025357	-0.000005527	-0.000010858
35	6	-0.000028743	0.000017345	-0.000019979
36	6	-0.000002608	-0.000003731	0.000009360
37	6	-0.000002343	0.000008391	-0.000006397
38	1	-0.000003268	0.000001868	-0.000000146
39	1	-0.000006766	0.000000041	-0.000008830
40	1	0.000001055	-0.000002389	-0.000004605
41	1	0.000002301	-0.000004121	-0.000002943
42	1	0.000001440	-0.000002262	-0.000003815
43	6	-0.000010198	0.000004305	0.000006252
44	1	0.000018291	0.000017783	0.000008873
45	1	-0.000004250	0.000002300	-0.000002545
46	1	-0.000013228	0.000019376	0.000000765
47	1	0.000002233	0.000013204	-0.000003529
48	1	0.015584492	-0.005073709	-0.005336647
49	6	0.000014215	0.000004890	-0.000009688
50	6	0.000003908	0.000003964	0.000003934
51	6	-0.000000695	-0.000005726	0.000001566
52	1	0.000002137	-0.000004001	0.000002314
53	1	-0.000001751	-0.000004706	0.000004439
54	1	-0.000001190	-0.000002243	0.000004065
55	1	-0.000001205	-0.000001358	0.000001164
56	6	-0.000000282	0.000012043	-0.000001942
57	1	-0.000013858	0.000001180	0.000008272
58	1	-0.000002909	-0.000002333	0.000006811
59	6	-0.000006968	-0.000004636	0.000011057

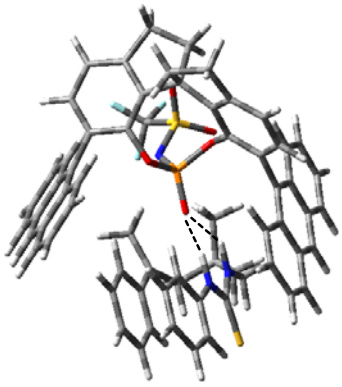
60	1	-0.000000953	-0.000004821	0.000002191
61	6	-0.000033625	-0.000000108	-0.000019263
62	6	0.000010661	-0.000014146	0.000000347
63	6	0.000005585	0.000001373	0.000016837
64	6	0.000024997	-0.000012640	0.000014390
65	6	0.000006332	0.000028436	0.000010161
66	6	-0.000010283	0.000002465	0.000013492
67	1	0.000000230	0.000001482	-0.000004565
68	1	0.000002309	0.000000028	-0.000001580
69	1	-0.000004537	0.000006418	0.000003136
70	6	-0.000011006	-0.000030201	0.000012910
71	6	0.000031749	0.000004586	0.000007773
72	6	0.000008886	0.000022316	0.000011311
73	6	0.000009678	-0.000001388	-0.000006534
74	6	-0.000007748	0.000015726	0.000000709
75	6	-0.000056739	-0.000016947	-0.000023487
76	1	-0.000005659	-0.000000709	0.000003755
77	1	-0.000004250	-0.000008738	0.000001015
78	8	-0.000016906	-0.000017728	-0.000019006
79	8	0.000024458	-0.000024283	0.000020714
80	15	-0.000074148	-0.000120389	0.000004837
81	8	-0.000000761	0.000020479	0.000011161
82	7	-0.000008798	-0.000019198	-0.000035926
83	16	-0.000004558	0.000067270	-0.000044919
84	8	0.000020738	0.000045221	0.000000507
85	8	-0.000013046	-0.000011830	0.000001076
86	6	0.000013574	-0.000012378	-0.000003639
87	9	0.000007053	0.000005755	0.000025617
88	9	-0.000012756	-0.000007857	0.000000177
89	9	-0.000019280	-0.000003429	0.000030571
90	6	-0.000001509	-0.000028244	0.000007116
91	6	-0.000010940	0.000004459	-0.000011126
92	6	0.000010221	0.000003649	-0.000001426
93	6	0.000017630	-0.000014433	-0.000008404
94	6	-0.000001677	-0.000003263	0.000003259
95	6	0.000003952	0.000000597	-0.000005264

96	1	0.000006071	0.000001880	0.000003808
97	6	0.000006775	-0.000023009	0.000003981
98	6	-0.000020308	-0.000018476	-0.000021340
99	6	0.000003730	0.000014569	-0.000002845
100	6	-0.000001695	-0.000007486	-0.000025482
101	6	0.000008369	-0.000009943	-0.000005509
102	6	0.000016308	-0.000009093	-0.000015074
103	1	0.000004006	0.000002151	0.000004704
104	6	-0.000004567	0.000018914	-0.000012698
105	1	-0.000002130	-0.000004833	0.000003028
106	6	0.000011897	0.000003308	0.000000234
107	1	-0.000004230	0.000001473	0.000002379
108	6	-0.000003183	0.000006822	0.000006049
109	1	-0.000003533	-0.000000643	-0.000000089
110	6	-0.000009431	0.000008699	-0.000000100
111	1	0.000002214	0.000004846	-0.000003248
112	6	0.000028602	0.000014629	-0.000009028
113	1	-0.000006264	-0.000002633	-0.000006088
114	6	0.000032299	-0.000007959	0.000028752
115	1	0.000006991	0.000000038	-0.000000163
116	6	0.000039721	-0.000021513	0.000009572
117	1	0.000010224	0.000002264	0.000005233
118	6	0.000035688	0.000012843	0.000000012
119	1	-0.000006511	0.000000463	0.000003046
120	6	-0.000010055	-0.000005778	0.000005337
121	1	0.000004717	-0.000000646	-0.000000944
122	6	0.000002781	0.000004027	0.000000434
123	1	-0.000000424	-0.000004461	-0.000001382
124	6	0.000005350	-0.000001558	0.000007161
125	1	-0.000003372	0.000000617	0.000001280
126	6	0.000007340	0.000019167	-0.000002627
127	1	-0.000007909	-0.000002316	-0.000003217
128	6	0.000007373	0.000003149	0.000007904
129	1	-0.000002222	0.000003128	-0.000002004
130	6	0.000001716	0.000000063	-0.000000741
131	1	-0.000000074	-0.000005126	-0.000004523

132	6	0.000000870	-0.000005696	-0.000001764
133	1	0.000001470	-0.000004282	-0.000001056
134	6	-0.000002517	-0.000006885	0.000000842
135	1	0.000005185	-0.000002674	0.000000423

Intermediate E_S_int





Electronic Energy (EE) = -4524.414450 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 1.080824
Thermal Correction to Energy = 1.14643
Thermal Correction to Enthalpy = 1.147374
Thermal Correction to Free Energy = 0.984535
EE + Zero-point Energy = -4523.333626
EE + Thermal Energy Correction = -4523.268019
EE + Thermal Enthalpy Correction = -4523.267075
EE + Thermal Free Energy Correction = -4523.429914
Truhlar's quasiharmonic corrected Gibbs energy = -4523.417614

E_{sp} (RM06-2X/def2-TZVP) = -4525.853292
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.924297

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

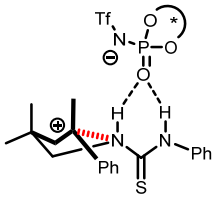
1	6	0	1.282848	2.244393	2.845282
2	6	0	2.159511	1.595711	3.859106
3	6	0	2.156971	0.015004	3.917921
4	7	0	2.919291	-0.185095	1.562024
5	1	0	1.779545	1.935116	4.831953
6	1	0	3.203957	1.902202	3.773402
7	6	0	2.619441	-0.367598	5.327154
8	1	0	1.876004	-0.074373	6.075163
9	1	0	3.574599	0.105730	5.580655
10	1	0	2.748243	-1.453232	5.391505
11	6	0	0.798423	-0.634886	3.644455
12	1	0	0.027313	-0.306118	4.348571
13	1	0	0.889671	-1.722408	3.743036
14	1	0	0.423654	-0.443009	2.635261
15	6	0	1.758159	2.987155	1.729209
16	6	0	2.638451	4.447246	-0.490660
17	6	0	3.118257	3.369999	1.603546
18	6	0	0.847432	3.368087	0.700534
19	6	0	1.290273	4.079787	-0.393409
20	6	0	3.543444	4.107809	0.511341
21	1	0	3.839064	3.102380	2.365001
22	1	0	-0.190232	3.050483	0.745876
23	1	0	0.604547	4.321208	-1.197799
24	1	0	4.590405	4.373952	0.420100
25	1	0	2.984828	4.977214	-1.373717
26	6	0	-0.173291	2.219565	3.122040
27	1	0	-0.388268	1.867943	4.129318
28	1	0	-0.607465	3.215283	2.979581
29	6	0	3.824732	0.304984	0.675214
30	7	0	3.259963	0.504906	-0.545275
31	16	0	5.415136	0.670000	1.115048
32	6	0	3.709692	1.100536	-1.732360
33	6	0	4.310541	2.316490	-4.190247
34	6	0	2.708455	1.305550	-2.697539
35	6	0	5.020758	1.496977	-2.013795
36	6	0	5.302771	2.100154	-3.239823

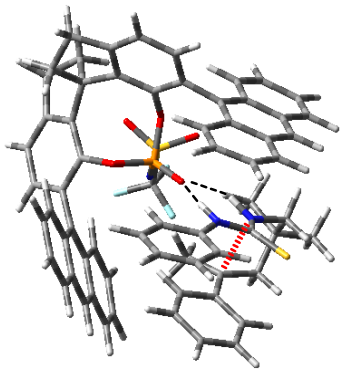
37	6	0	3.005270	1.909636	-3.909022
38	1	0	1.687915	0.997561	-2.474099
39	1	0	5.803541	1.329148	-1.288643
40	1	0	6.325621	2.400590	-3.448040
41	1	0	2.210401	2.065427	-4.632500
42	1	0	4.548884	2.788144	-5.138190
43	6	0	3.204491	-0.531132	2.932874
44	1	0	3.221570	-1.623297	3.037356
45	1	0	4.199512	-0.152189	3.174255
46	1	0	2.022640	-0.495318	1.179319
47	1	0	2.273597	0.236636	-0.594711
48	1	0	-0.706971	1.544760	2.432552
49	6	0	-3.253116	-2.388856	-2.305709
50	6	0	-3.559651	-2.363818	-3.835385
51	6	0	-2.833516	-3.592410	-4.403010
52	1	0	-3.124678	-1.452925	-4.262824
53	1	0	-4.634380	-2.352526	-4.038351
54	1	0	-3.453727	-4.494259	-4.322942
55	1	0	-2.559866	-3.479790	-5.456202
56	6	0	-4.276441	-3.303863	-1.582866
57	1	0	-3.900058	-3.524510	-0.579769
58	1	0	-4.438205	-4.244450	-2.118982
59	6	0	-5.548125	-2.434871	-1.471845
60	1	0	-6.124441	-2.665458	-0.571377
61	6	0	-1.841242	-2.950572	-2.327699
62	6	0	0.570043	-4.269669	-2.752654
63	6	0	-1.630654	-3.688447	-3.495980
64	6	0	-0.813880	-2.859014	-1.397046
65	6	0	0.418245	-3.493840	-1.594577
66	6	0	-0.438551	-4.369740	-3.704114
67	1	0	-0.285948	-4.957041	-4.605009
68	1	0	1.518906	-4.774553	-2.908813
69	1	0	-6.213300	-2.570724	-2.333868
70	6	0	-3.623563	-1.042636	-1.707461
71	6	0	-4.883432	1.327117	-0.980886
72	6	0	-2.881454	0.101985	-1.472768

73	6	0	-4.991509	-1.029881	-1.414186
74	6	0	-5.628009	0.150344	-1.060732
75	6	0	-3.495666	1.319294	-1.149259
76	1	0	-6.690492	0.161311	-0.836083
77	1	0	-5.370198	2.265167	-0.728707
78	8	0	-1.040629	-2.169155	-0.222594
79	8	0	-1.492077	0.040891	-1.434955
80	15	0	-0.878512	-0.572184	-0.052850
81	8	0	0.534808	-0.091052	0.015607
82	7	0	-1.825582	-0.219522	1.195741
83	16	0	-2.589839	-1.348295	2.024218
84	8	0	-3.739790	-1.934507	1.340651
85	8	0	-1.697517	-2.241254	2.757559
86	6	0	-3.338292	-0.310169	3.350553
87	9	0	-4.409557	0.352502	2.916889
88	9	0	-3.718713	-1.110788	4.338112
89	9	0	-2.463759	0.574261	3.836513
90	6	0	1.580178	-3.334520	-0.671906
91	6	0	3.899909	-3.230116	0.933787
92	6	0	2.777410	-2.794907	-1.194078
93	6	0	1.526286	-3.778668	0.668330
94	6	0	2.711316	-3.716978	1.479856
95	6	0	3.960739	-2.769036	-0.378853
96	1	0	4.797297	-3.194429	1.549528
97	6	0	-2.699507	2.570618	-0.983995
98	6	0	-1.377547	5.060692	-0.727934
99	6	0	-1.994868	3.113553	-2.082344
100	6	0	-2.704522	3.255040	0.251333
101	6	0	-2.038070	4.522524	0.375193
102	6	0	-1.336546	4.383766	-1.946909
103	1	0	-0.877152	6.022689	-0.635307
104	6	0	0.338704	-4.312143	1.264816
105	1	0	-0.567546	-4.378962	0.675066
106	6	0	0.316768	-4.704614	2.570555
107	1	0	-0.610764	-5.059938	3.005970
108	6	0	1.490746	-4.631211	3.374444

109	1	0	1.454436	-4.958799	4.409083
110	6	0	2.653561	-4.161583	2.839299
111	1	0	3.565049	-4.116322	3.431725
112	6	0	5.181925	-2.256577	-0.923539
113	1	0	6.059250	-2.239587	-0.283318
114	6	0	5.234797	-1.779022	-2.196979
115	1	0	6.160912	-1.379049	-2.597489
116	6	0	4.055101	-1.758540	-2.997062
117	1	0	4.093983	-1.316922	-3.988797
118	6	0	2.873527	-2.239727	-2.515723
119	1	0	1.981568	-2.184844	-3.129754
120	6	0	-2.066747	5.205202	1.634450
121	1	0	-1.568919	6.168848	1.706684
122	6	0	-2.706742	4.664283	2.710496
123	1	0	-2.725817	5.193458	3.658515
124	6	0	-3.345838	3.393615	2.598568
125	1	0	-3.826588	2.952063	3.465479
126	6	0	-3.343627	2.717056	1.414130
127	1	0	-3.809691	1.745132	1.336148
128	6	0	-1.921172	2.458478	-3.355388
129	1	0	-2.432271	1.511415	-3.487263
130	6	0	-1.225908	3.004171	-4.394110
131	1	0	-1.181733	2.484436	-5.346181
132	6	0	-0.566848	4.261070	-4.251555
133	1	0	-0.025917	4.682942	-5.093056
134	6	0	-0.633810	4.932328	-3.067975
135	1	0	-0.147334	5.897031	-2.944645

Transition state $TS^{NPTA}_{E\_S\_TS2}$





E(RM06-2X/6-31G(d)) = -4524.412756 a.u.
Imaginary Freq = 1: -44.26 cm-1
Zero-point Energy Correction = 1.080378
Thermal Correction to Energy = 1.145577
Thermal Correction to Enthalpy = 1.146522
Thermal Correction to Free Energy = 0.983322
EE + Zero-point Energy = -4523.332377
EE + Thermal Energy Correction = -4523.267178
EE + Thermal Enthalpy Correction = -4523.266178
EE + Thermal Free Energy Correction = -4523.429433
Truhlar's quasiharmonic corrected Gibbs energy = -4523.416045

E_{sp} (RM06-2X/def2-TZVP) = -4525.851872
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.924943

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000100764	-0.000045999	-0.000006770
2	6	0.000019760	0.000019473	-0.000013712
3	6	-0.000018121	-0.000013306	-0.000008928
4	7	0.000063000	0.000062429	-0.000012633
5	1	-0.000010412	-0.000006524	-0.000000729
6	1	-0.000005269	-0.000003946	0.000002372
7	6	0.000002844	-0.000003598	-0.000007814
8	1	0.000000385	-0.000001482	-0.000002162

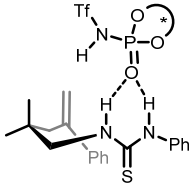
9	1	0.000000296	-0.000001822	0.000000720
10	1	-0.000001864	-0.000000177	0.000003286
11	6	0.000002880	-0.000001892	0.000002077
12	1	0.000001369	-0.000003423	0.000000863
13	1	-0.000001851	-0.000003514	0.000001728
14	1	-0.000004215	-0.000001062	-0.000005784
15	6	0.000035564	0.000005091	0.000019878
16	6	0.000001951	0.000010916	-0.000007456
17	6	-0.000007201	-0.000000957	-0.000004583
18	6	-0.000002634	0.000007788	-0.000005584
19	6	0.000007820	-0.000022344	-0.000000951
20	6	0.000015154	-0.000003703	0.000017233
21	1	-0.000002106	0.000006682	-0.000000144
22	1	-0.000000261	0.000006110	-0.000000426
23	1	-0.000010553	0.000015919	0.000023970
24	1	0.000004285	0.000000872	0.000005182
25	1	-0.000003076	-0.000000970	-0.000001387
26	6	0.000058130	0.000028439	0.000016261
27	1	-0.000012798	-0.000007529	0.000003244
28	1	-0.000024916	-0.000011639	-0.000003233
29	6	0.000006068	-0.000031784	0.000007237
30	7	0.000009671	0.000030819	-0.000028187
31	16	-0.000007345	0.000005648	-0.000011299
32	6	-0.000003160	-0.000003436	0.000007079
33	6	-0.000005451	0.000005722	0.000002669
34	6	0.000016200	0.000013677	-0.000012466
35	6	-0.000000946	-0.000006803	0.000003823
36	6	-0.000000313	0.000000090	-0.000002992
37	6	0.000012907	0.000001509	0.000005577
38	1	-0.000001688	0.000001519	0.000001425
39	1	0.000000950	0.000002014	0.000008886
40	1	0.000002435	0.000002734	0.000001515
41	1	0.000003372	0.000004166	0.000005147
42	1	0.000002230	0.000002060	0.000000926
43	6	-0.000004244	-0.000018739	0.000009629
44	1	0.000002232	0.000004959	0.000000727

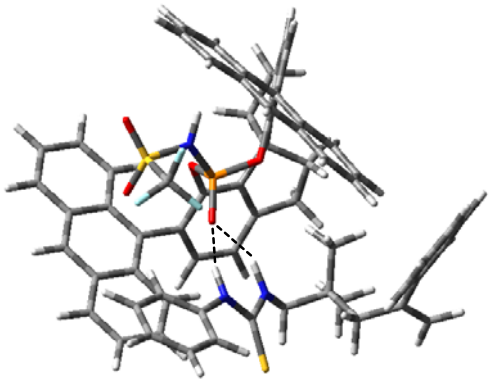
45	1	0.000002199	0.000002051	-0.000000500
46	1	0.000008545	0.000021605	-0.000018759
47	1	-0.000004591	-0.000014501	0.000041369
48	1	0.000000365	-0.000011790	-0.000014155
49	6	-0.000000716	0.000000087	-0.000005755
50	6	-0.000000714	0.000001858	-0.000001422
51	6	-0.000001385	-0.000004440	0.000005719
52	1	-0.000000108	0.000000711	-0.000001079
53	1	0.000001278	0.000001288	0.000000640
54	1	0.000000194	-0.000000447	-0.000000423
55	1	-0.000000459	0.000000538	0.000000504
56	6	-0.000001547	-0.000003810	-0.000002713
57	1	-0.000002278	-0.000000393	0.000000517
58	1	-0.000000328	-0.000001257	0.000000500
59	6	-0.000002378	0.000001148	-0.000002218
60	1	0.000000754	-0.000000742	-0.000001582
61	6	0.000005579	0.000016269	0.000007941
62	6	-0.000001873	-0.000007749	0.000011362
63	6	0.000004449	0.000000368	-0.000005269
64	6	-0.000020390	-0.000033480	-0.000001884
65	6	0.000004659	0.000011046	-0.000001579
66	6	0.000002107	-0.000000939	-0.000001612
67	1	0.000000481	-0.000000323	0.000002238
68	1	0.000003445	-0.000002652	0.000000954
69	1	-0.000002216	0.000000336	-0.000001465
70	6	0.000005758	-0.000009655	0.000007294
71	6	0.000008419	-0.000008644	-0.000010004
72	6	-0.000013454	-0.000015144	-0.000011965
73	6	0.000009066	0.000013312	0.000008976
74	6	-0.000012295	0.000007104	-0.000006609
75	6	0.000005030	-0.000000659	0.000006632
76	1	-0.000002269	0.000000366	-0.000000190
77	1	-0.000002443	0.000001417	0.000000435
78	8	0.000014496	0.000003696	-0.000010061
79	8	-0.000013972	0.000004407	0.000012538
80	15	0.000026665	0.000064718	-0.000041320

81	8	-0.000034927	-0.000061716	0.000065576
82	7	-0.000006166	-0.000016082	-0.000027565
83	16	-0.000003626	0.000005560	0.000010899
84	8	0.000003640	0.000002498	-0.000002036
85	8	0.000002622	0.000002932	0.000005049
86	6	-0.000001018	0.000000490	-0.000006168
87	9	-0.000001681	0.000003000	-0.000004154
88	9	-0.000005026	-0.000006279	0.000004055
89	9	-0.000004967	0.000016015	-0.000002952
90	6	0.000011636	-0.000012427	0.000013698
91	6	0.000000818	-0.000004064	0.000007676
92	6	0.000001249	0.000004992	-0.000005036
93	6	-0.000002763	0.000001058	-0.000005121
94	6	-0.000005842	-0.000000072	-0.000003059
95	6	-0.000000356	0.000006025	-0.000002688
96	1	-0.000001919	-0.000001358	0.000001629
97	6	-0.000001168	0.000015053	-0.000008644
98	6	-0.000000722	-0.000007105	-0.000009397
99	6	-0.000001556	-0.000001154	-0.000003037
100	6	-0.000003453	0.000007232	0.000004494
101	6	-0.000001126	0.000003226	0.000006515
102	6	-0.000000246	-0.000009418	-0.000006504
103	1	0.000001363	0.000000041	0.000000141
104	6	-0.000002499	-0.000002389	-0.000002463
105	1	-0.000002552	-0.000001702	-0.000003091
106	6	-0.000001047	-0.000001994	-0.000003186
107	1	-0.000000310	-0.000002336	0.000000717
108	6	0.000000422	0.000001637	0.000001966
109	1	-0.000001002	-0.000002840	0.000000616
110	6	-0.000000215	-0.000004423	0.000004210
111	1	-0.000000340	-0.000001702	0.000000081
112	6	0.000000631	-0.000006357	0.000005529
113	1	0.000001168	-0.000001017	0.000000891
114	6	0.000002522	-0.000000828	-0.000005960
115	1	-0.000000415	0.000000059	0.000004315
116	6	-0.000006261	0.000003893	0.000005792

117	1	0.000002567	-0.000002174	0.000000719
118	6	-0.000005733	-0.000004476	0.000000724
119	1	-0.000004882	0.000007268	0.000000851
120	6	-0.000001778	0.000004231	-0.000004994
121	1	0.000001856	0.000004151	0.000001513
122	6	-0.000002628	-0.000006971	-0.000002348
123	1	0.000000452	0.000001602	0.000000097
124	6	0.000002085	0.000003733	-0.000005218
125	1	0.000000500	-0.000003714	-0.000000557
126	6	0.000003583	-0.000005457	-0.000000290
127	1	0.000001512	0.000003289	0.000003890
128	6	0.000005450	0.000004300	-0.000000586
129	1	0.000000615	0.000000599	0.000001508
130	6	0.000003571	-0.000003979	-0.000000673
131	1	0.000000631	0.000001690	0.000000417
132	6	-0.000007498	-0.000000762	0.000000296
133	1	0.000001082	-0.000000356	-0.000001058
134	6	0.000000029	-0.000011117	-0.000017089
135	1	0.000003327	0.000000003	-0.000001260

NH-complex_E_*R*





E(RM06-2X/6-31G(d)) = -4524.420253
Zero-point Energy Correction = 1.07997
Thermal Correction to Energy = 1.14685
Thermal Correction to Enthalpy = 1.147794

Thermal Correction to Free Energy = 0.976352
EE + Zero-point Energy = -4523.340282
EE + Thermal Energy Correction = -4523.273403
EE + Thermal Enthalpy Correction = -4523.272458
EE + Thermal Free Energy Correction = -4523.443901
Truhlar's quasiharmonic corrected Gibbs energy = -4523.425005

E_{sp} (RM06-2X/def2-TZVP) = -4525.86474
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.940732

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000009217	-0.000134864	-0.000047794
2	6	0.000006458	0.000097058	0.000000321
3	6	0.000032024	0.000042826	-0.000002643
4	7	0.000127849	0.000202339	0.000034215
5	1	-0.000039638	-0.000034220	-0.000018339
6	1	0.000028890	-0.000040189	0.000031666
7	6	0.000042124	-0.000020330	0.000022956
8	1	0.000007131	0.000012926	0.000008127
9	1	-0.000002406	-0.000010703	-0.000005030
10	1	-0.000050261	-0.000036253	-0.000024498
11	6	0.000007336	0.000016841	-0.000055826
12	1	-0.000017626	-0.000014116	0.000001110
13	1	-0.000039127	0.000009426	-0.000029401
14	1	0.000005481	0.000006217	0.000007084
15	6	-0.000074150	0.000061521	0.000009939
16	6	-0.000019831	-0.000026906	0.000048867
17	6	-0.000027902	0.000016515	-0.000045503
18	6	0.000055103	-0.000000637	0.000013626
19	6	0.000008799	0.000011108	-0.000023651
20	6	0.000036788	0.000009125	0.000000859
21	1	0.000019391	-0.000021925	0.000004983
22	1	-0.000003396	-0.000007639	-0.000014689

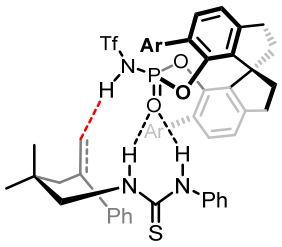
23	1	0.000009390	-0.000008097	0.000014278
24	1	-0.000006761	-0.000000234	0.000007772
25	1	-0.000018418	0.000008875	-0.000018878
26	6	0.000041455	0.000002751	0.000042331
27	1	-0.000004582	-0.000002054	-0.000019915
28	1	-0.000008735	0.000019262	0.000003550
29	6	0.000086560	0.000150827	-0.000017902
30	7	-0.000067029	-0.000047049	0.000050263
31	16	-0.000115493	-0.000010234	0.000027472
32	6	-0.000051529	0.000004016	0.000120755
33	6	-0.000016606	0.000018433	-0.000043276
34	6	0.000006353	-0.000051152	-0.000028039
35	6	0.000116685	-0.000000932	-0.000019176
36	6	-0.000059566	-0.000040568	0.000047191
37	6	0.000018915	-0.000003253	-0.000027088
38	1	0.000039619	-0.000025050	-0.000022434
39	1	0.000000369	0.000024372	-0.000017238
40	1	0.000000967	0.000008256	-0.000001508
41	1	-0.000000496	-0.000003551	0.000010588
42	1	0.000010009	0.000002642	0.000005862
43	6	-0.000108101	-0.000129357	0.000079569
44	1	-0.000046299	-0.000040219	0.000037664
45	1	0.000021810	0.000025463	-0.000023147
46	1	0.000030645	-0.000066633	0.000079288
47	1	0.000154916	-0.000069678	-0.000590277
48	1	0.000020754	-0.000004421	0.000020089
49	6	-0.000005830	-0.000043328	0.000016427
50	6	0.000034210	-0.000002536	-0.000010516
51	6	0.000066063	0.000041831	-0.000021670
52	1	-0.000037730	-0.000016730	0.000002500
53	1	0.000008203	0.000052631	0.000010313
54	1	0.000066590	0.000023698	0.000022541
55	1	-0.000023499	-0.000058525	-0.000002636
56	6	-0.000017674	0.000075808	-0.000048079
57	1	-0.000019173	-0.000072971	0.000040500
58	1	0.000026158	0.000041283	-0.000025682

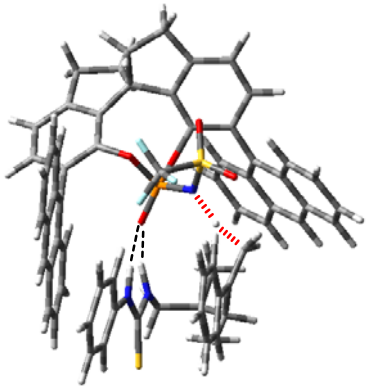
59	6	0.000079823	-0.000092831	0.000051072
60	1	0.000004275	-0.000010202	0.000019149
61	6	0.000054320	-0.000108364	-0.000080734
62	6	0.000029855	0.000062140	-0.000076231
63	6	-0.000091886	0.000042472	-0.000056357
64	6	0.000024221	0.000013786	-0.000020787
65	6	0.000079532	-0.000007277	0.000009835
66	6	0.000038229	-0.000080727	0.000052981
67	1	-0.000007121	0.000081321	-0.000007364
68	1	-0.000027907	0.000054607	0.000034424
69	1	-0.000045433	0.000053542	-0.000035679
70	6	-0.000160378	0.000151142	0.000054068
71	6	-0.000072685	-0.000009756	-0.000008591
72	6	0.000002520	0.000094203	0.000109885
73	6	0.000063669	-0.000032658	-0.000058050
74	6	-0.000034540	0.000057558	0.000033560
75	6	0.000074558	-0.000061310	-0.000056945
76	1	0.000070520	-0.000014450	-0.000018693
77	1	0.000023575	-0.000071814	-0.000013775
78	8	-0.000141085	-0.000096312	-0.000150795
79	8	-0.000161376	-0.000111803	-0.000010833
80	15	0.000345424	0.000187365	-0.000236298
81	8	-0.000247711	-0.000243469	0.000490466
82	7	-0.000026914	0.000089637	0.000115049
83	16	-0.000008291	-0.000074757	-0.000069084
84	8	-0.000027331	0.000080188	-0.000035522
85	8	-0.000036002	0.000063867	0.000021273
86	6	-0.000061033	-0.000053222	-0.000039046
87	9	0.000065254	-0.000100200	0.000108402
88	9	-0.000018027	0.000179145	0.000076067
89	9	0.000052672	0.000036707	-0.000080848
90	6	-0.000000209	-0.000008979	0.000004939
91	6	0.000069000	0.000023791	-0.000045931
92	6	-0.000138233	-0.000000752	0.000018914
93	6	-0.000009284	-0.000048544	0.000069308
94	6	-0.000090896	0.000011455	-0.000030076

95	6	-0.000028456	-0.000040031	0.000005259
96	1	-0.000023894	-0.000033731	0.000066120
97	6	0.000012445	-0.000069307	0.000026471
98	6	0.000025558	-0.000037252	-0.000012425
99	6	0.000000529	0.000002524	-0.000062290
100	6	-0.000039929	-0.000031719	-0.000044459
101	6	0.000006019	0.000014419	0.000036483
102	6	0.000032277	0.000059437	-0.000020882
103	1	-0.000065734	-0.000039386	0.000009640
104	6	0.000083160	-0.000053077	0.000095227
105	1	-0.000017836	0.000039598	-0.000071720
106	6	-0.000037463	0.000018411	-0.000034227
107	1	0.000076484	-0.000013052	0.000019120
108	6	-0.000105441	0.000020986	-0.000025089
109	1	0.000053884	-0.000031459	0.000042272
110	6	0.000056512	0.000037654	-0.000052747
111	1	-0.000027899	-0.000031778	0.000067357
112	6	0.000086377	0.000066583	-0.000054848
113	1	-0.000041431	-0.000032195	0.000077718
114	6	0.000145619	0.000088208	0.000020855
115	1	-0.000078207	-0.000022313	0.000008050
116	6	-0.000017265	-0.000019451	0.000087601
117	1	-0.000053461	0.000025975	0.000016353
118	6	-0.000056376	-0.000058823	0.000005335
119	1	0.000043045	0.000066429	-0.000062980
120	6	0.000049833	0.000050567	-0.000005505
121	1	-0.000063273	-0.000047100	-0.000003031
122	6	-0.000047437	0.000058951	-0.000033637
123	1	0.000024665	-0.000071669	0.000030989
124	6	0.000011490	0.000033091	-0.000031469
125	1	0.000036209	-0.000010262	0.000058664
126	6	-0.000047159	-0.000070967	0.000006683
127	1	0.000071014	0.000080516	-0.000015296
128	6	-0.000022054	-0.000041892	0.000042717
129	1	0.000080985	0.000088395	0.000062844
130	6	-0.000029484	-0.000050975	0.000046298

131	1	-0.000050709	0.000103765	-0.000080555
132	6	0.000043338	-0.000035997	0.000006391
133	1	-0.000025361	0.000024916	-0.000029503
134	6	0.000081082	0.000032290	0.000026560
135	1	-0.000058735	-0.000067472	0.000020033

Transition state $TS^{NPTA}_{E\_R\_TS1}$





E (RM06-2X /6-31G(d)) = -4524.402003 a.u.
Imaginary Freq = 1: -1242.06 cm-1
Zero-point Energy Correction = 1.076263
Thermal Correction to Energy = 1.141221
Thermal Correction to Enthalpy = 1.142165
Thermal Correction to Free Energy = 0.979417
EE + Zero-point Energy = -4523.325740
EE + Thermal Energy Correction = -4523.260782
EE + Thermal Enthalpy Correction = -4523.259838
EE + Thermal Free Energy Correction = -4523.422586
Truhlar's quasiharmonic corrected Gibbs energy = -4523.408843

E_{sp} (RM06-2X/def2-TZVP) = -4525.837786
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.906023

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z

1	6	0.000029688	0.000063491	0.000014001
2	6	-0.000000434	-0.000001503	-0.000015540
3	6	-0.000044078	-0.000059893	0.000019080
4	7	0.000028436	0.000047527	-0.000013729
5	1	0.000007435	0.000011639	0.000003413
6	1	-0.000045790	-0.000015384	-0.000029486
7	6	-0.000003295	0.000016062	-0.000017183
8	1	-0.000002827	-0.000000325	0.000002986
9	1	0.000004157	-0.000000505	-0.000015807
10	1	0.000002955	0.000001043	-0.000004508
11	6	0.000000009	0.000008937	0.000009824
12	1	-0.000006152	0.000028320	0.000003299
13	1	-0.000002559	-0.000004234	-0.000010508
14	1	-0.000006632	0.000004675	0.000013146
15	6	-0.000153845	-0.000014536	0.000033804
16	6	-0.000029456	0.000005316	0.000000883
17	6	0.000028342	0.000010156	0.000016330
18	6	0.000099609	0.000033637	-0.000031692
19	6	0.000008034	-0.000001066	-0.000023287
20	6	0.000000072	0.000006178	-0.000016587
21	1	-0.000027927	-0.000022931	-0.000024624
22	1	-0.000005810	0.000003115	0.000033716
23	1	-0.000000042	0.000007732	0.000012760
24	1	0.000000738	0.000008255	-0.000001883
25	1	0.000017485	-0.000017147	0.000000763
26	6	0.001570747	-0.000769657	-0.000572602
27	1	-0.000011608	0.000049364	-0.000049044
28	1	-0.000012262	0.000080707	0.000017459
29	6	-0.000006842	-0.000059643	0.000029844
30	7	-0.000036097	-0.000018852	-0.000038954
31	16	0.000062583	0.000098851	0.000028092
32	6	0.000014017	0.000017845	0.000012867
33	6	-0.000027266	-0.000000147	0.000018966
34	6	0.000033912	-0.000041071	-0.000031162
35	6	-0.000014132	-0.000016403	0.000003611

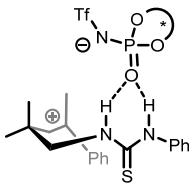
36	6	-0.000001726	-0.000004115	-0.000023428
37	6	0.000029036	0.000018693	0.000006133
38	1	-0.000000614	-0.000006299	0.000016699
39	1	0.000013221	-0.000007856	-0.000022961
40	1	0.000000020	-0.000005334	-0.000005164
41	1	-0.000001757	-0.000005800	-0.000001316
42	1	0.000001317	-0.000000148	-0.000002826
43	6	0.000041853	-0.000024646	0.000029746
44	1	-0.000034001	0.000021088	0.000005038
45	1	-0.000004926	-0.000020341	-0.000010751
46	1	0.000023750	-0.000023762	0.000027331
47	1	-0.000011093	0.000015366	-0.000013379
48	1	-0.001464204	0.000571641	0.000548709
49	6	-0.000003613	-0.000001678	0.000001178
50	6	-0.000005525	-0.000002862	0.000002132
51	6	0.000003008	-0.000004109	-0.000005038
52	1	0.000000270	-0.000000572	0.000004663
53	1	-0.000000487	-0.000000710	0.000000206
54	1	0.000001888	0.000000731	0.000000306
55	1	-0.000000997	-0.000000424	0.000001746
56	6	0.000001498	0.000002001	-0.000009173
57	1	-0.000001451	-0.000000415	0.000001374
58	1	0.000003368	-0.000000149	0.000000229
59	6	0.000007085	-0.000002178	0.000001998
60	1	0.000002260	-0.000001296	0.000001160
61	6	-0.000004114	-0.000009977	0.000001897
62	6	-0.000013020	0.000006502	-0.000009224
63	6	0.000008906	0.000007055	-0.000002301
64	6	-0.000030180	-0.000012194	0.000014951
65	6	0.000021231	-0.000015682	0.000018298
66	6	0.000003930	0.000009256	-0.000000532
67	1	-0.000001676	-0.000002149	0.000003149
68	1	0.000001108	-0.000000515	0.000003005
69	1	0.000003300	-0.000001438	-0.000000998
70	6	0.000005058	-0.000001742	-0.000014994
71	6	-0.000011087	-0.000003270	-0.000007961

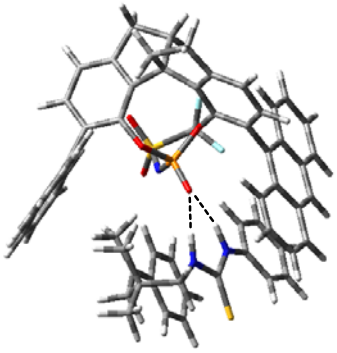
72	6	0.000030564	-0.000049953	0.000031160
73	6	-0.000025263	-0.000010644	0.000004286
74	6	-0.000004360	0.000004793	0.000011124
75	6	0.000007534	0.000052852	-0.000028746
76	1	0.000002471	-0.000002865	-0.000000109
77	1	-0.000007076	-0.000000221	-0.000002176
78	8	0.000027463	-0.000009353	-0.000074274
79	8	-0.000068380	0.000015525	-0.000050690
80	15	0.000037753	-0.000041633	0.000064397
81	8	-0.000000527	-0.000025142	-0.000058192
82	7	-0.000105762	0.000135878	0.000204941
83	16	0.000095579	-0.000023065	-0.000056009
84	8	-0.000025357	0.000035170	-0.000006480
85	8	-0.000015213	-0.000012121	0.000021933
86	6	0.000042920	0.000044449	-0.000030646
87	9	-0.000008516	-0.000023666	0.000010875
88	9	0.000006783	-0.000050305	0.000021208
89	9	-0.000016806	-0.000025324	-0.000000854
90	6	-0.000011322	0.000014975	-0.000013489
91	6	-0.000010060	0.000007411	-0.000007648
92	6	-0.000004606	-0.000009571	0.000005766
93	6	0.000000610	0.000020020	0.000002560
94	6	-0.000004752	-0.000011650	0.000004497
95	6	0.000011549	-0.000006101	0.000004986
96	1	-0.000001305	0.000002751	0.000003139
97	6	-0.000036920	-0.000044751	0.000015248
98	6	0.000013336	0.000002557	-0.000001245
99	6	0.000000820	0.000002971	-0.000018407
100	6	0.000016614	-0.000002252	0.000004485
101	6	0.000001753	-0.000002053	0.000018810
102	6	-0.000009957	-0.000009848	0.000002669
103	1	-0.000004413	0.000000300	-0.000002411
104	6	-0.000009249	0.000014344	-0.000012597
105	1	0.000000976	-0.000000977	-0.000000706
106	6	-0.000003724	0.000011398	0.000000956
107	1	0.000004674	-0.000006079	0.000000416

108	6	0.000003038	-0.000003523	0.000008440
109	1	-0.000003989	0.000003692	-0.000001660
110	6	-0.000011190	0.000002675	-0.000011304
111	1	-0.000002350	0.000004102	0.000002284
112	6	-0.000005177	0.000007231	-0.000017427
113	1	0.000001236	-0.000002542	0.000003543
114	6	0.000020026	0.000004500	0.000014099
115	1	-0.000008782	0.000004655	-0.000003700
116	6	-0.000009212	-0.000014619	0.000002626
117	1	0.000001024	0.000000881	0.000001135
118	6	-0.000014584	0.000026010	-0.000007490
119	1	0.000009044	-0.000005933	-0.000002318
120	6	-0.000000599	-0.000000856	0.000001287
121	1	-0.000000665	-0.000000381	-0.000000836
122	6	0.000002207	0.000000331	-0.000004503
123	1	-0.000001094	-0.000002921	0.000001592
124	6	-0.000004048	0.000000334	0.000004311
125	1	0.000003391	0.000002742	-0.000003449
126	6	0.000014857	0.000014613	-0.000002392
127	1	0.000013338	0.000000669	-0.000000047
128	6	0.000014420	0.000007520	0.000017475
129	1	-0.000000552	0.000001552	-0.000003006
130	6	0.000000721	0.000003125	-0.000013581
131	1	-0.000001390	-0.000003740	0.000001936
132	6	-0.000007584	0.000000885	-0.000000075
133	1	0.000000221	0.000000809	0.000001305
134	6	0.000006595	-0.000004987	0.000004350
135	1	0.000000471	0.000003133	0.000000481

---

intermediate E_R_int





E(RM06-2X/6-31G(d)) = -4524.418451
Imaginary Freq = 0
Zero-point Energy Correction = 1.08093
Thermal Correction to Energy = 1.146844
Thermal Correction to Enthalpy = 1.147788
Thermal Correction to Free Energy = 0.981985
EE + Zero-point Energy = -4523.337521
EE + Thermal Energy Correction = -4523.271607
EE + Thermal Enthalpy Correction = -4523.270663
EE + Thermal Free Energy Correction = -4523.436466
Truhlar's quasiharmonic corrected Gibbs energy = -4523.421472

E_{sp} (RM06-2X/def2-TZVP) = -4525.856736
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.929086

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.357113	-3.676862	-0.104664
2	6	0	-0.505518	-4.707402	0.967581
3	6	0	-0.646534	-4.234678	2.451195
4	7	0	1.206550	-2.694195	1.907572
5	1	0	-1.436092	-5.241278	0.713412
6	1	0	0.310120	-5.432819	0.943553
7	6	0	-0.906083	-5.488398	3.295788
8	1	0	-1.899292	-5.901209	3.090327
9	1	0	-0.159055	-6.265037	3.100338

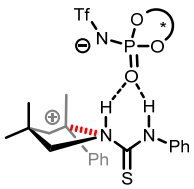
10	1	0	-0.862930	-5.239078	4.361243
11	6	0	-1.774132	-3.228847	2.725615
12	1	0	-2.741143	-3.576664	2.346728
13	1	0	-1.875956	-3.112797	3.810345
14	1	0	-1.582646	-2.233393	2.313415
15	6	0	0.661836	-3.693431	-1.099229
16	6	0	2.681450	-3.618025	-3.043328
17	6	0	0.695301	-2.661805	-2.085923
18	6	0	1.674745	-4.690286	-1.136261
19	6	0	2.666716	-4.646227	-2.101864
20	6	0	1.689015	-2.631131	-3.040744
21	1	0	-0.028564	-1.853479	-2.085742
22	1	0	1.683121	-5.497472	-0.416852
23	1	0	3.445609	-5.400459	-2.102883
24	1	0	1.696911	-1.821394	-3.762658
25	1	0	3.479151	-3.576072	-3.779383
26	6	0	-1.456532	-2.687457	-0.229933
27	1	0	-2.361295	-3.022948	0.273415
28	1	0	-1.686704	-2.463278	-1.270590
29	6	0	2.429394	-2.803736	1.299299
30	7	0	2.666650	-1.751591	0.488125
31	16	0	3.418833	-4.153675	1.501340
32	6	0	3.660133	-1.508535	-0.480725
33	6	0	5.454680	-0.781566	-2.502112
34	6	0	3.325838	-0.517872	-1.410394
35	6	0	4.908497	-2.132305	-0.554983
36	6	0	5.788517	-1.763367	-1.572533
37	6	0	4.213312	-0.152959	-2.411116
38	1	0	2.351568	-0.041264	-1.340371
39	1	0	5.187182	-2.884053	0.168733
40	1	0	6.756806	-2.252694	-1.626444
41	1	0	3.930543	0.630260	-3.107787
42	1	0	6.155696	-0.504845	-3.283579
43	6	0	0.703472	-3.630468	2.883751
44	1	0	0.573078	-3.125278	3.850086
45	1	0	1.451511	-4.415625	3.006095

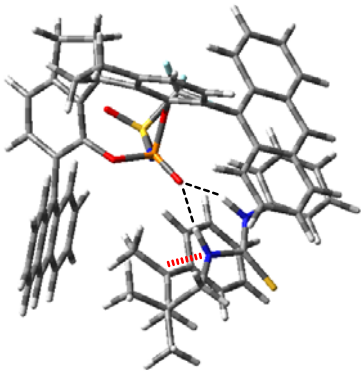
46	1	0	0.769771	-1.768678	1.871526
47	1	0	1.941628	-1.025968	0.509790
48	1	0	-1.135402	-1.746970	0.235275
49	6	0	-2.282350	3.904794	1.111167
50	6	0	-3.224219	4.169229	2.325126
51	6	0	-2.327868	4.828429	3.389840
52	1	0	-3.584400	3.203892	2.699160
53	1	0	-4.095377	4.770887	2.049747
54	1	0	-2.287717	5.917144	3.256876
55	1	0	-2.672600	4.640824	4.410955
56	6	0	-2.191160	5.169197	0.215400
57	1	0	-1.317712	5.063606	-0.438086
58	1	0	-2.078540	6.086754	0.801571
59	6	0	-3.478422	5.128088	-0.631111
60	1	0	-3.352073	5.596399	-1.611412
61	6	0	-0.986836	3.619719	1.836474
62	6	0	1.298906	3.520607	3.406492
63	6	0	-0.980083	4.207576	3.103202
64	6	0	0.136833	2.945356	1.395319
65	6	0	1.312887	2.901923	2.150656
66	6	0	0.158739	4.155428	3.896767
67	1	0	0.168058	4.608250	4.884087
68	1	0	2.206673	3.490850	4.002491
69	1	0	-4.306291	5.644777	-0.129293
70	6	0	-2.936193	2.933554	0.142184
71	6	0	-4.741860	1.596857	-1.479259
72	6	0	-2.928778	1.545044	0.092264
73	6	0	-3.749483	3.644484	-0.744039
74	6	0	-4.644577	2.981071	-1.570411
75	6	0	-3.887657	0.850619	-0.658078
76	1	0	-5.275604	3.530408	-2.262704
77	1	0	-5.477598	1.062026	-2.073065
78	8	0	0.075432	2.301210	0.167616
79	8	0	-1.958600	0.834339	0.792110
80	15	0	-0.449412	0.769189	0.166077
81	8	0	0.306663	-0.125805	1.092592

82	7	0	-0.415132	0.318632	-1.363346
83	16	0	-0.575300	1.097700	-2.729857
84	8	0	-0.243148	0.170258	-3.808470
85	8	0	-1.783389	1.908563	-2.847932
86	6	0	0.778651	2.373818	-2.794412
87	9	0	0.382691	3.518682	-2.255270
88	9	0	1.871260	1.950519	-2.160309
89	9	0	1.088553	2.590490	-4.068495
90	6	0	2.563066	2.290640	1.618155
91	6	0	5.027171	1.270005	0.706338
92	6	0	3.126142	1.159175	2.239360
93	6	0	3.212252	2.900426	0.523256
94	6	0	4.454191	2.358674	0.049730
95	6	0	4.397146	0.663459	1.791196
96	1	0	5.963478	0.856208	0.335188
97	6	0	-4.108753	-0.623140	-0.562702
98	6	0	-4.898582	-3.338417	-0.484978
99	6	0	-4.565541	-1.190783	0.649110
100	6	0	-3.992410	-1.428238	-1.715374
101	6	0	-4.387757	-2.809485	-1.669543
102	6	0	-4.980288	-2.568113	0.676077
103	1	0	-5.216799	-4.379082	-0.457641
104	6	0	2.687577	4.053732	-0.146904
105	1	0	1.765527	4.499408	0.211096
106	6	0	3.318557	4.587047	-1.231496
107	1	0	2.892758	5.451787	-1.731291
108	6	0	4.526822	4.015358	-1.727498
109	1	0	5.005546	4.447094	-2.601025
110	6	0	5.077893	2.939429	-1.099107
111	1	0	6.000814	2.491296	-1.458755
112	6	0	4.968305	-0.480434	2.435112
113	1	0	5.928587	-0.842223	2.076865
114	6	0	4.312617	-1.118636	3.443611
115	1	0	4.742434	-2.000169	3.907986
116	6	0	3.032047	-0.650120	3.867572
117	1	0	2.507257	-1.182749	4.656033

118	6	0	2.460182	0.446474	3.291440
119	1	0	1.475647	0.780890	3.601270
120	6	0	-4.194383	-3.628158	-2.827099
121	1	0	-4.510102	-4.667359	-2.779769
122	6	0	-3.601803	-3.126325	-3.947437
123	1	0	-3.436750	-3.763284	-4.811064
124	6	0	-3.192070	-1.760683	-3.991108
125	1	0	-2.696369	-1.370981	-4.874216
126	6	0	-3.405017	-0.934305	-2.925867
127	1	0	-3.099209	0.104965	-2.976270
128	6	0	-4.664736	-0.444824	1.869190
129	1	0	-4.376987	0.600383	1.869625
130	6	0	-5.114825	-1.023078	3.019820
131	1	0	-5.173869	-0.435832	3.930834
132	6	0	-5.525512	-2.388233	3.039861
133	1	0	-5.891714	-2.825877	3.963392
134	6	0	-5.466769	-3.131043	1.899568
135	1	0	-5.785012	-4.170761	1.893737

Transition state $TS^{NPTA}_{E\_R\_TS2}$





E(RM06-2X/6-31G(d)) = -4524.418350
Imaginary Freq = 1: -75.30 cm-1
Zero-point Energy Correction = 1.081178
Thermal Correction to Energy = 1.146206
Thermal Correction to Enthalpy = 1.14715

Thermal Correction to Free Energy = 0.983863
EE + Zero-point Energy = -4523.337172
EE + Thermal Energy Correction = -4523.272144
EE + Thermal Enthalpy Correction = -4523.271199
EE + Thermal Free Energy Correction = -4523.434487
Truhlar's quasiharmonic corrected Gibbs energy = -4523.420374

E_{sp} (RM06-2X/def2-TZVP) = -4525.855494
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -4525.927329

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.202149	3.657369	-0.051454
2	6	0	0.299372	4.785101	0.929249
3	6	0	0.494762	4.423903	2.427708
4	7	0	-1.163739	2.685033	1.796532
5	1	0	1.173429	5.375502	0.609033
6	1	0	-0.576883	5.432820	0.869819
7	6	0	0.475931	5.736952	3.220775
8	1	0	1.360264	6.343426	2.997989
9	1	0	-0.418535	6.326240	2.993206
10	1	0	0.478614	5.527545	4.295800
11	6	0	1.805274	3.691898	2.758550
12	1	0	2.673694	4.194938	2.318964
13	1	0	1.943761	3.692209	3.845387
14	1	0	1.819852	2.647812	2.435371
15	6	0	-0.754765	3.629520	-1.118555
16	6	0	-2.661274	3.465668	-3.174197
17	6	0	-0.722391	2.570626	-2.069946
18	6	0	-1.773077	4.610563	-1.249092
19	6	0	-2.709693	4.522775	-2.266133
20	6	0	-1.659279	2.495999	-3.081834
21	1	0	0.007675	1.771010	-2.007466
22	1	0	-1.833246	5.442394	-0.561203

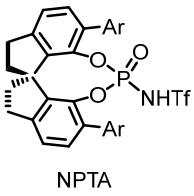
23	1	0	-3.491310	5.270942	-2.338836
24	1	0	-1.609227	1.664649	-3.777529
25	1	0	-3.412852	3.392557	-3.954875
26	6	0	1.348881	2.704084	-0.091987
27	1	0	2.248431	3.167387	0.312974
28	1	0	1.559939	2.359563	-1.101753
29	6	0	-2.432904	2.750928	1.248177
30	7	0	-2.668178	1.689601	0.455461
31	16	0	-3.432982	4.081565	1.474308
32	6	0	-3.681236	1.418359	-0.487260
33	6	0	-5.517434	0.624096	-2.441259
34	6	0	-3.352161	0.420871	-1.411162
35	6	0	-4.941496	2.019356	-0.535255
36	6	0	-5.843643	1.615705	-1.519592
37	6	0	-4.261091	0.022335	-2.379063
38	1	0	-2.367151	-0.035571	-1.361896
39	1	0	-5.213865	2.777117	0.184616
40	1	0	-6.822364	2.085419	-1.553704
41	1	0	-3.983064	-0.766104	-3.071707
42	1	0	-6.235786	0.320320	-3.196497
43	6	0	-0.723656	3.571766	2.855898
44	1	0	-0.460410	2.973867	3.736651
45	1	0	-1.562427	4.219922	3.113907
46	1	0	-0.739008	1.751430	1.775704
47	1	0	-1.935693	0.970373	0.474272
48	1	0	1.131822	1.815071	0.511029
49	6	0	2.405811	-3.851793	1.121917
50	6	0	3.366105	-4.075195	2.329746
51	6	0	2.499720	-4.749517	3.409593
52	1	0	3.700268	-3.095590	2.690580
53	1	0	4.252426	-4.653294	2.052308
54	1	0	2.488894	-5.840108	3.286657
55	1	0	2.849178	-4.542805	4.425392
56	6	0	2.347370	-5.126268	0.237898
57	1	0	1.465729	-5.054345	-0.409060
58	1	0	2.268962	-6.041751	0.832859

59	6	0	3.625784	-5.051789	-0.619949
60	1	0	3.506292	-5.533017	-1.594821
61	6	0	1.108906	-3.597938	1.856772
62	6	0	-1.158329	-3.532457	3.455809
63	6	0	1.132366	-4.169237	3.130898
64	6	0	-0.037115	-2.958721	1.420686
65	6	0	-1.203071	-2.930224	2.192790
66	6	0	0.002548	-4.135099	3.938210
67	1	0	0.016758	-4.575327	4.931151
68	1	0	-2.058081	-3.514774	4.064341
69	1	0	4.473843	-5.537140	-0.120521
70	6	0	3.020408	-2.869027	0.138887
71	6	0	4.764738	-1.489043	-1.515023
72	6	0	2.967834	-1.482324	0.075695
73	6	0	3.848355	-3.561332	-0.748703
74	6	0	4.712401	-2.876981	-1.590934
75	6	0	3.895128	-0.764193	-0.691635
76	1	0	5.353619	-3.412255	-2.284882
77	1	0	5.475843	-0.935995	-2.122053
78	8	0	-0.006868	-2.332329	0.182989
79	8	0	1.981199	-0.795381	0.777233
80	15	0	0.470031	-0.784421	0.155003
81	8	0	-0.315034	0.093070	1.074707
82	7	0	0.417905	-0.359323	-1.379674
83	16	0	0.579885	-1.157510	-2.735058
84	8	0	0.225610	-0.253395	-3.826179
85	8	0	1.798889	-1.951779	-2.849081
86	6	0	-0.759024	-2.450946	-2.765578
87	9	0	-0.342177	-3.584591	-2.218894
88	9	0	-1.847216	-2.032071	-2.120378
89	9	0	-1.085173	-2.686240	-4.032183
90	6	0	-2.470988	-2.345436	1.672305
91	6	0	-4.954199	-1.360617	0.771960
92	6	0	-3.039488	-1.211636	2.284745
93	6	0	-3.125929	-2.976558	0.593362
94	6	0	-4.377626	-2.453122	0.124961

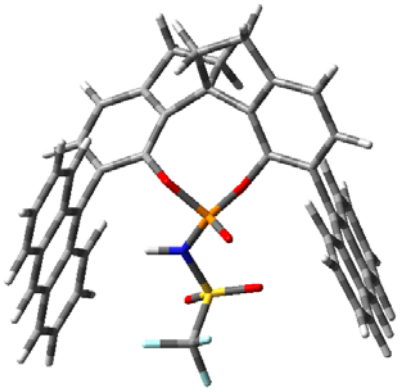
95	6	0	-4.319575	-0.734137	1.842832
96	1	0	-5.898008	-0.960647	0.404535
97	6	0	4.063333	0.716861	-0.604509
98	6	0	4.721144	3.466394	-0.531638
99	6	0	4.521274	1.300888	0.598527
100	6	0	3.882388	1.518302	-1.750873
101	6	0	4.210037	2.917350	-1.707233
102	6	0	4.865391	2.697245	0.624133
103	1	0	4.985560	4.522159	-0.505716
104	6	0	-2.596582	-4.133962	-0.065961
105	1	0	-1.666205	-4.564933	0.288524
106	6	0	-3.233726	-4.689017	-1.135903
107	1	0	-2.804784	-5.556669	-1.627865
108	6	0	-4.452721	-4.136125	-1.627151
109	1	0	-4.936372	-4.585169	-2.489160
110	6	0	-5.007583	-3.056326	-1.008846
111	1	0	-5.938496	-2.622261	-1.365143
112	6	0	-4.896589	0.411662	2.478513
113	1	0	-5.865087	0.757676	2.126838
114	6	0	-4.237922	1.069057	3.472603
115	1	0	-4.673870	1.950163	3.932187
116	6	0	-2.947188	0.620645	3.887904
117	1	0	-2.421203	1.166746	4.666435
118	6	0	-2.369939	-0.477509	3.319750
119	1	0	-1.379220	-0.798219	3.624173
120	6	0	3.948008	3.729312	-2.855806
121	1	0	4.211980	4.782983	-2.811084
122	6	0	3.354182	3.202449	-3.963949
123	1	0	3.135776	3.833906	-4.819729
124	6	0	3.013766	1.818010	-4.005697
125	1	0	2.516568	1.406577	-4.878015
126	6	0	3.293997	0.999573	-2.950178
127	1	0	3.044251	-0.054620	-2.999480
128	6	0	4.686104	0.554395	1.811311
129	1	0	4.456133	-0.505100	1.809677
130	6	0	5.127324	1.149934	2.956372

131	1	0	5.237365	0.561951	3.862192
132	6	0	5.460391	2.536082	2.977494
133	1	0	5.817821	2.989225	3.896973
134	6	0	5.341225	3.279697	1.842422
135	1	0	5.602025	4.335450	1.837339

NPTA



NPTA



E [RM06-2X /6-31G(d)] = -3240.531449 a.u.
Imaginary Freq = 0
Zero-point Energy Correction = 0.674186
Thermal Correction to Energy = 0.717845
Thermal Correction to Enthalpy = 0.718789
Thermal Correction to Free Energy = 0.59791
EE + Zero-point Energy = -3239.857263
EE + Thermal Energy Correction = -3239.813604
EE + Thermal Enthalpy Correction = -3239.812659
EE + Thermal Free Energy Correction = -3239.933538
Truhlar's quasiharmonic corrected Gibbs energy = -3239.922945

E_{sp} (RM06-2X/def2-TZVP) = -3241.621166
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -3241.677705

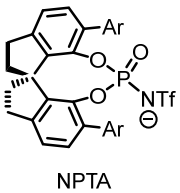
Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z

1	6	-0.000017895	0.001948790	-0.000276366
2	6	0.002074181	-0.002083067	-0.001670596
3	6	-0.001212297	-0.000233489	-0.001160953
4	1	0.000487613	-0.000802235	-0.000352097
5	1	0.000295303	-0.000326966	-0.000861844
6	1	-0.000146041	-0.001347183	-0.000105271
7	1	0.000044480	-0.001080859	-0.000922904
8	6	-0.002176945	-0.001491997	0.002334104
9	1	-0.000413647	-0.000610816	0.000565217
10	1	-0.000239058	0.000068427	0.000957499
11	6	0.001156648	0.000192070	0.001114359
12	1	-0.000059379	-0.000743848	0.001194795
13	6	0.000513982	0.000017770	0.000741690
14	6	-0.003106891	-0.000805507	-0.001701585
15	6	-0.000040323	-0.002285037	-0.001362822
16	6	-0.001218572	-0.003172483	-0.000267489
17	6	-0.001914672	0.002726711	0.000896028
18	6	-0.001637241	-0.001445811	-0.001459486
19	1	-0.000479553	-0.000267584	-0.000355937
20	1	0.000107100	-0.000570181	0.000082615
21	1	0.000114240	-0.001230040	0.000575170
22	6	-0.000699651	-0.000229759	-0.000930838
23	6	0.002915672	-0.000346921	0.002014193
24	6	0.001584751	-0.002770797	0.001230471
25	6	0.000056047	-0.001771092	0.002123829
26	6	0.001181152	-0.000980837	0.001829322
27	6	0.002119877	0.002064525	-0.001530618
28	1	0.000361900	-0.000215872	0.000451216
29	1	-0.000039280	-0.000660387	0.000215325
30	8	-0.001707873	0.000573163	0.005061058
31	8	0.002611899	-0.000979913	-0.003865618
32	15	0.002625074	0.000787227	0.002935466
33	8	-0.001786007	0.003444205	-0.010836034
34	7	0.005043813	-0.003605923	0.001147445
35	1	-0.002253244	0.000165453	-0.000596818

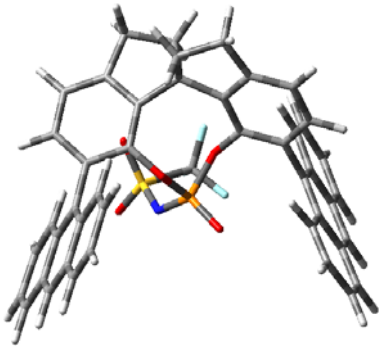
36	16	0.001408947	0.001104351	-0.002353904
37	8	0.005125024	0.004086484	0.014352383
38	8	-0.014481549	-0.000316366	-0.000685100
39	6	-0.000488095	-0.000595431	0.001233615
40	9	0.010511811	0.001328006	-0.001150258
41	9	-0.003391763	0.009723053	0.002236711
42	9	-0.003423597	-0.001081866	-0.010125818
43	6	0.000186527	-0.003357410	-0.000708141
44	6	-0.001471997	0.002070547	0.000495021
45	6	0.001469880	-0.002336494	-0.003871446
46	6	0.000872421	-0.003683570	0.002751052
47	6	-0.002686069	0.003358838	0.003142330
48	6	-0.002449311	0.004415981	-0.002299799
49	1	-0.000037975	-0.000055495	-0.000037177
50	6	-0.000379360	-0.003097434	0.001375293
51	6	0.001320487	0.002024653	-0.000924943
52	6	-0.000890496	-0.004355575	-0.001203434
53	6	-0.001672491	-0.000772398	0.004315652
54	6	0.002178657	0.004763089	0.000204066
55	6	0.002600001	0.001901487	-0.004214603
56	1	0.000018256	-0.000010733	0.000076408
57	6	-0.000860697	0.002938322	-0.003762303
58	1	-0.000292827	0.000271588	0.000167771
59	6	0.000942020	-0.003280422	0.004157352
60	1	-0.000253205	0.000077558	0.000818298
61	6	-0.001767139	0.001334401	0.004906770
62	1	-0.000000838	-0.000369277	0.000771809
63	6	0.000809603	-0.001491309	-0.004067099
64	1	-0.000511612	0.000634447	0.000263718
65	6	0.000816253	-0.002905230	0.003417392
66	1	-0.000725616	0.000890248	-0.000050985
67	6	-0.001197551	0.003281553	-0.004136003
68	1	0.000168603	-0.000074668	-0.000829718
69	6	0.001791025	-0.001325201	-0.005083700
70	1	-0.000063488	0.000438175	-0.000725982
71	6	-0.001425924	0.001025445	0.004681016

72	1	-0.000249227	0.000359001	-0.000128368
73	6	0.001708099	-0.000506675	-0.004333522
74	1	0.000243912	0.000345594	-0.000017939
75	6	-0.001807181	0.000180388	0.005183286
76	1	0.000021959	0.000600301	0.000560903
77	6	0.001451530	0.004673081	0.002800336
78	1	0.000124096	0.000224215	0.000649868
79	6	-0.000179044	-0.004154369	-0.001698771
80	1	0.000783476	0.000648530	-0.000188192
81	6	-0.001052683	0.000083380	0.004179061
82	1	0.000660297	0.000511999	-0.000554335
83	6	0.002108130	-0.000458698	-0.005082630
84	1	0.000007700	-0.000568201	-0.000579122
85	6	-0.000673653	-0.004690741	-0.002658067
86	1	0.000205446	-0.000174851	-0.000789225
87	6	0.000511487	0.004202702	0.002488182
88	1	0.000242573	0.000235262	-0.000180237

NPTA-anion



NPTA



E(RM06-2X/6-31G(d)) = -3240.027829
Imaginary Freq = 0
Zero-point Energy Correction = 0.661465
Thermal Correction to Energy = 0.704499
Thermal Correction to Enthalpy = 0.705443
Thermal Correction to Free Energy = 0.586638
EE + Zero-point Energy = -3239.366364

EE + Thermal Energy Correction = -3239.323330
EE + Thermal Enthalpy Correction = -3239.322386
EE + Thermal Free Energy Correction = -3239.44191
Truhlar's quasiharmonic corrected Gibbs energy = -3239.431646

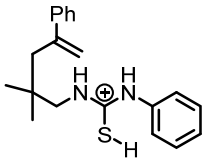
E_{sp} (RM06-2X/def2-TZVP) = -3241.122787
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -3241.227526

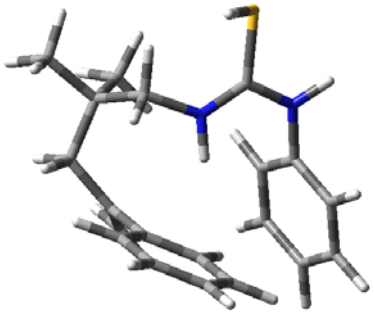
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.071666	-1.651335	2.863657
2	6	0	-0.497907	-3.089538	3.286939
3	6	0	0.812698	-3.892129	3.355337
4	1	0	-1.136275	-3.502102	2.497361
5	1	0	-1.068075	-3.095282	4.221225
6	1	0	1.286288	-3.794602	4.341524
7	1	0	0.669598	-4.961475	3.169772
8	6	0	0.328303	-0.817156	4.109416
9	1	0	0.867491	0.070739	3.759903
10	1	0	0.971267	-1.375073	4.799300
11	6	0	-1.019356	-0.387008	4.723348
12	1	0	-0.950224	0.565656	5.257061
13	6	0	1.109234	-1.973495	1.970940
14	6	0	3.382542	-2.888662	0.672822
15	6	0	1.650017	-3.220256	2.291718
16	6	0	1.692064	-1.203797	0.972909
17	6	0	2.849878	-1.644752	0.314956
18	6	0	2.787803	-3.687042	1.646862
19	1	0	3.206321	-4.659807	1.891099
20	1	0	4.275761	-3.230318	0.156596
21	1	0	-1.393439	-1.134633	5.435800
22	6	0	-1.283696	-0.863510	2.399440
23	6	0	-3.752613	0.363164	2.124130
24	6	0	-1.831759	-0.696949	1.134805

25	6	0	-1.908823	-0.280949	3.503957
26	6	0	-3.144701	0.334293	3.376137
27	6	0	-3.106928	-0.129051	0.985735
28	1	0	-3.629592	0.793776	4.233087
29	1	0	-4.734090	0.813905	2.003287
30	8	0	1.112102	-0.006269	0.644512
31	8	0	-1.123015	-1.074633	0.018204
32	15	0	0.002095	-0.019392	-0.585741
33	8	0	0.522529	-0.621269	-1.823386
34	7	0	-0.564234	1.477591	-0.584112
35	16	0	-0.470079	2.590898	0.522247
36	8	0	-0.972141	3.857827	0.001114
37	8	0	-0.920109	2.192387	1.859361
38	6	0	1.352203	2.925444	0.776943
39	9	0	1.539512	4.237454	0.934599
40	9	0	1.800569	2.322345	1.877759
41	9	0	2.074232	2.524110	-0.264938
42	6	0	3.539933	-0.817021	-0.715823
43	6	0	5.002011	0.658250	-2.622037
44	6	0	3.581156	-1.248262	-2.055342
45	6	0	4.215278	0.356610	-0.326684
46	6	0	4.940743	1.115177	-1.306559
47	6	0	4.346892	-0.506902	-3.016487
48	1	0	5.568149	1.226827	-3.357692
49	6	0	-3.786527	-0.078460	-0.340480
50	6	0	-5.207885	0.004485	-2.779739
51	6	0	-4.141572	-1.279706	-0.991285
52	6	0	-4.133188	1.162573	-0.912552
53	6	0	-4.859177	1.198678	-2.152244
54	6	0	-4.861633	-1.230077	-2.233119
55	1	0	-5.753816	0.036097	-3.721110
56	6	0	2.863396	-2.401661	-2.511197
57	1	0	2.211224	-2.913100	-1.812871
58	6	0	2.952703	-2.817932	-3.805489
59	1	0	2.386847	-3.684059	-4.134529
60	6	0	3.752323	-2.104778	-4.747527

61	1	0	3.807946	-2.452146	-5.775334
62	6	0	4.416625	-0.979346	-4.365806
63	1	0	5.008175	-0.409668	-5.078517
64	6	0	5.601571	2.319072	-0.906406
65	1	0	6.131738	2.888584	-1.665981
66	6	0	5.563365	2.744140	0.387047
67	1	0	6.060649	3.664989	0.677439
68	6	0	4.864201	1.981598	1.367425
69	1	0	4.828779	2.333685	2.393864
70	6	0	4.219295	0.830760	1.024324
71	1	0	3.673417	0.272074	1.776911
72	6	0	-3.752514	2.409065	-0.319942
73	1	0	-3.170844	2.400371	0.595014
74	6	0	-4.069710	3.595747	-0.910096
75	1	0	-3.711160	4.518210	-0.466264
76	6	0	-4.816186	3.627370	-2.123875
77	1	0	-5.061923	4.583528	-2.577432
78	6	0	-5.198250	2.465490	-2.724036
79	1	0	-5.752943	2.473456	-3.659430
80	6	0	-5.220537	-2.453195	-2.883450
81	1	0	-5.756715	-2.391129	-3.827566
82	6	0	-4.899749	-3.659818	-2.339791
83	1	0	-5.174704	-4.581478	-2.844627
84	6	0	-4.198973	-3.715712	-1.099436
85	1	0	-3.950101	-4.681626	-0.670014
86	6	0	-3.835646	-2.571959	-0.452149
87	1	0	-3.305455	-2.630297	0.492043

***S*-protonated alkenyl thiourea**





E(RM06-2X/6-31G(d)) = -1284.224690
Imaginary Freq = 0
Zero-point Energy Correction = 0.414107
Thermal Correction to Energy = 0.436113
Thermal Correction to Enthalpy = 0.437057
Thermal Correction to Free Energy = 0.36248
EE + Zero-point Energy = -1283.810582
EE + Thermal Energy Correction = -1283.788576
EE + Thermal Enthalpy Correction = -1283.787632
EE + Thermal Free Energy Correction = -1283.862210
Truhlar's quasiharmonic corrected Gibbs energy = -1283.857615

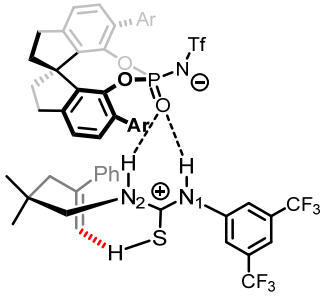
E_{sp} (RM06-2X/def2-TZVP) = -1284.587663
E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -1284.673147

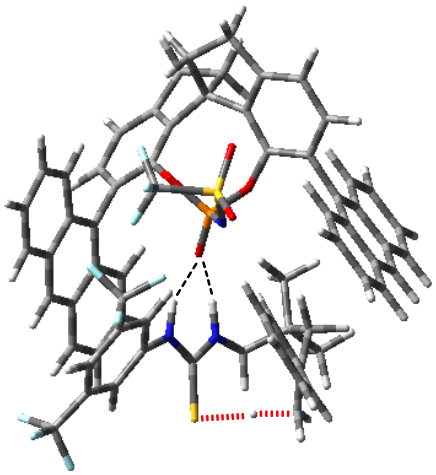
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.633569	1.732782	1.349740
2	6	0	-2.139189	1.570453	1.330882
3	6	0	-2.694474	0.228125	0.789710
4	7	0	-0.836184	-0.705296	-0.661940
5	1	0	-2.514807	1.679251	2.353935
6	1	0	-2.598493	2.381699	0.755303
7	6	0	-4.217129	0.376754	0.660435
8	1	0	-4.645272	0.717616	1.607495
9	1	0	-4.483182	1.109892	-0.109384

10	1	0	-4.686772	-0.578743	0.403627
11	6	0	-2.371456	-0.917807	1.749720
12	1	0	-2.687390	-1.883832	1.337054
13	1	0	-1.300364	-0.962060	1.969696
14	1	0	-2.899721	-0.772990	2.697073
15	6	0	0.063311	2.174463	0.104208
16	6	0	1.409903	2.964486	-2.244614
17	6	0	1.373076	1.742573	-0.163577
18	6	0	-0.554949	3.010970	-0.837508
19	6	0	0.113087	3.405977	-1.992999
20	6	0	2.037463	2.130814	-1.323194
21	1	0	1.876659	1.091645	0.546525
22	1	0	-1.555491	3.391492	-0.658544
23	1	0	-0.381073	4.068667	-2.696237
24	1	0	3.050045	1.780684	-1.500835
25	1	0	1.926622	3.272253	-3.147648
26	6	0	0.056667	1.487060	2.470668
27	1	0	-0.447364	1.170879	3.379830
28	1	0	1.129643	1.640225	2.533021
29	6	0	-0.511691	-1.938812	-0.972520
30	7	0	0.713016	-2.418928	-0.751998
31	6	0	1.744773	-1.762315	0.006436
32	6	0	3.785374	-0.610383	1.477876
33	6	0	2.903979	-1.348636	-0.645836
34	6	0	1.588861	-1.608308	1.382564
35	6	0	2.616663	-1.022280	2.116520
36	6	0	3.929793	-0.776053	0.100537
37	1	0	2.998685	-1.477465	-1.719786
38	1	0	0.689531	-1.971550	1.870551
39	1	0	2.508469	-0.904080	3.189585
40	1	0	4.842790	-0.461531	-0.394056
41	1	0	4.589210	-0.166301	2.055514
42	16	0	-1.631173	-3.122485	-1.659045
43	1	0	-2.233913	-2.264995	-2.496324
44	6	0	-2.179269	-0.107365	-0.628842
45	1	0	-2.869233	-0.822425	-1.078328

46	1	0	-2.153507	0.786058	-1.260596
47	1	0	-0.066412	-0.090652	-0.376729
48	1	0	0.944952	-3.299411	-1.199686

$TS^{NPTA}_{C1\_s}$ of real system





E(RM06-2X/6-31G(d)) = -5198.294294
Imaginary Freq = 1: -700.20 cm-1
Zero-point Energy Correction = 1.086961
Thermal Correction to Energy = 1.158513
Thermal Correction to Enthalpy = 1.159457
Thermal Correction to Free Energy = 0.984042
EE + Zero-point Energy = -5197.207333
EE + Thermal Energy Correction = -5197.135781
EE + Thermal Enthalpy Correction = -5197.134837
EE + Thermal Free Energy Correction = -5197.310252
Truhlar's quasiharmonic corrected Gibbs energy =
-5197.296427 (at 298.15 K)
-5197.283395 (at 273.15 K)

E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -5200.105198

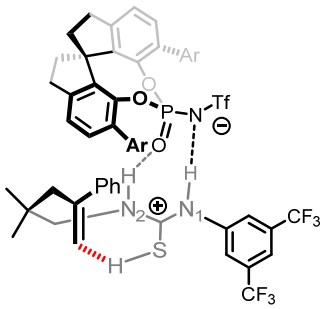
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.406203	4.533460	0.565887
2	6	0	1.558114	3.856153	1.245907
3	6	0	1.524481	3.561029	2.773494
4	7	0	-0.551794	2.330242	2.347893
5	1	0	2.423179	4.510656	1.053189
6	1	0	1.798243	2.936485	0.702895
7	6	0	2.421823	2.331252	2.990879
8	1	0	3.432100	2.534688	2.624008
9	1	0	2.055220	1.446681	2.455861
10	1	0	2.489795	2.091594	4.058178
11	6	0	2.091368	4.717108	3.605395
12	1	0	3.142436	4.881503	3.344751
13	1	0	2.046482	4.474413	4.672876
14	1	0	1.551477	5.657166	3.456062
15	6	0	0.024024	4.110737	-0.778936
16	6	0	-0.873776	3.303167	-3.301214
17	6	0	-0.478531	5.053314	-1.698607
18	6	0	0.085844	2.755778	-1.161358
19	6	0	-0.374208	2.355891	-2.409658
20	6	0	-0.912549	4.653018	-2.952131
21	1	0	-0.481662	6.108282	-1.443327
22	1	0	0.434915	1.994189	-0.469060
23	1	0	-0.314726	1.309946	-2.693903
24	1	0	-1.278413	5.391954	-3.657820
25	1	0	-1.218157	2.983486	-4.280406
26	6	0	-0.352147	5.526199	1.195420
27	1	0	0.030551	5.986432	2.101984
28	1	0	-0.958498	6.178620	0.568133
29	6	0	-1.766421	2.404337	1.796337
30	7	0	-2.084528	1.333270	1.051525
31	6	0	-3.191496	1.087825	0.221354
32	6	0	-5.293482	0.278565	-1.431462
33	6	0	-4.500782	1.395939	0.573407

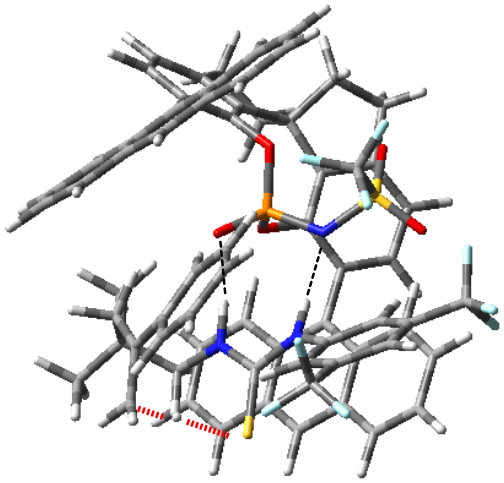
34	6	0	-2.925017	0.388002	-0.958874
35	6	0	-3.973179	0.000943	-1.779350
36	6	0	-5.537441	0.972106	-0.253584
37	1	0	-4.715324	1.917629	1.498404
38	1	0	-1.895611	0.155800	-1.223134
39	1	0	-6.111906	-0.031304	-2.071694
40	16	0	-2.775050	3.792113	1.964387
41	1	0	-1.358336	4.784207	1.585968
42	6	0	0.098144	3.240099	3.265526
43	1	0	-0.519344	4.129486	3.388399
44	1	0	0.170552	2.759949	4.251096
45	1	0	-0.037598	1.464790	2.146228
46	6	0	3.490976	-3.587949	0.884598
47	6	0	4.618470	-3.685016	1.957043
48	6	0	3.991040	-4.461935	3.128016
49	1	0	4.869402	-2.670010	2.286026
50	1	0	5.527539	-4.146312	1.560303
51	1	0	4.096691	-5.545396	2.988292
52	1	0	4.441989	-4.215251	4.093655
53	6	0	3.482699	-4.859813	-0.005874
54	1	0	2.528048	-4.894586	-0.543237
55	1	0	3.589103	-5.778900	0.579265
56	6	0	4.629649	-4.627200	-1.009931
57	1	0	4.455416	-5.125780	-1.967528
58	6	0	2.274524	-3.497199	1.784982
59	6	0	0.258505	-3.685670	3.689004
60	6	0	2.539072	-4.053974	3.038869
61	6	0	1.007729	-3.005856	1.518142
62	6	0	-0.032401	-3.097694	2.452273
63	6	0	1.536111	-4.151218	3.994846
64	1	0	1.740510	-4.583381	4.970232
65	1	0	-0.540882	-3.764608	4.420487
66	1	0	5.586712	-4.996435	-0.620096
67	6	0	3.849481	-2.539538	-0.156023
68	6	0	5.100244	-0.953473	-2.063722
69	6	0	3.587361	-1.179727	-0.217460

70	6	0	4.637190	-3.121457	-1.153038
71	6	0	5.259205	-2.336444	-2.112939
72	6	0	4.252860	-0.350807	-1.129338
73	1	0	5.866501	-2.789036	-2.891204
74	1	0	5.613615	-0.318150	-2.780005
75	8	0	0.786161	-2.400503	0.290722
76	8	0	2.623068	-0.624124	0.616256
77	15	0	1.062650	-0.807391	0.181051
78	8	0	0.313315	-0.017513	1.207889
79	7	0	0.739117	-0.430359	-1.334101
80	1	0	-1.342710	0.619543	0.987754
81	16	0	0.814849	-1.358632	-2.627188
82	8	0	0.372231	-0.579230	-3.776648
83	8	0	2.036148	-2.148017	-2.743097
84	6	0	-0.529293	-2.637034	-2.404070
85	9	0	-1.105921	-2.872190	-3.574114
86	9	0	-0.013618	-3.772004	-1.950605
87	9	0	-1.456729	-2.201787	-1.549044
88	6	0	-1.415502	-2.632423	2.140174
89	6	0	-4.072838	-1.837361	1.608087
90	6	0	-1.985336	-1.559592	2.854758
91	6	0	-2.170133	-3.310211	1.159642
92	6	0	-3.505152	-2.869749	0.861861
93	6	0	-3.351913	-1.189576	2.609829
94	1	0	-5.093418	-1.520398	1.397819
95	6	0	4.131516	1.136649	-1.068382
96	6	0	4.085520	3.960153	-1.012842
97	6	0	4.722548	1.830500	0.012474
98	6	0	3.526825	1.851741	-2.120823
99	6	0	3.489586	3.289498	-2.078614
100	6	0	4.706356	3.266937	0.027628
101	1	0	4.077935	5.049336	-0.997849
102	6	0	-1.246451	-0.788075	3.812961
103	1	0	-0.198306	-1.021902	3.969269
104	6	0	-1.835242	0.234106	4.498843
105	1	0	-1.256980	0.804169	5.221000

106	6	0	-3.207785	0.567074	4.286536
107	1	0	-3.658321	1.376823	4.852191
108	6	0	-3.939659	-0.128674	3.371646
109	1	0	-4.985091	0.109278	3.188521
110	6	0	-4.234895	-3.509448	-0.187785
111	1	0	-5.225502	-3.131233	-0.427424
112	6	0	-3.700853	-4.559092	-0.871798
113	1	0	-4.258754	-5.032581	-1.673424
114	6	0	-2.403138	-5.041356	-0.535415
115	1	0	-1.991491	-5.886624	-1.078139
116	6	0	-1.664105	-4.439465	0.439772
117	1	0	-0.669954	-4.808351	0.669071
118	6	0	2.942631	1.195920	-3.252017
119	1	0	2.970327	0.112988	-3.301980
120	6	0	2.355474	1.910617	-4.252789
121	1	0	1.889914	1.381715	-5.078008
122	6	0	2.315192	3.336026	-4.203404
123	1	0	1.835542	3.886114	-5.007804
124	6	0	2.860026	4.002723	-3.148436
125	1	0	2.831773	5.088340	-3.096778
126	6	0	5.333526	3.962579	1.110313
127	1	0	5.312427	5.050421	1.102039
128	6	0	5.963107	3.284433	2.112653
129	1	0	6.446193	3.823297	2.922095
130	6	0	5.996604	1.859110	2.093833
131	1	0	6.507132	1.327395	2.890654
132	6	0	5.396313	1.160677	1.086222
133	1	0	5.437275	0.076584	1.080648
134	6	0	-6.940571	1.187981	0.233298
135	6	0	-3.684964	-0.737738	-3.059321
136	9	0	-7.138735	2.444098	0.651665
137	9	0	-7.200111	0.386111	1.286416
138	9	0	-7.854014	0.917756	-0.705269
139	9	0	-4.539010	-0.364464	-4.027295
140	9	0	-2.444080	-0.497783	-3.494104
141	9	0	-3.818671	-2.062717	-2.916530

$TS^{NPTA}_{C1\_R}$ of real system





E(RM06-2X/6-31G(d)) = -5198.292963
Imaginary Freq = 1: -397.56 cm-1
Zero-point Energy Correction = 1.087305
Thermal Correction to Energy = 1.158897
Thermal Correction to Enthalpy = 1.159841
Thermal Correction to Free Energy = 0.983039
EE + Zero-point Energy = -5197.205658
EE + Thermal Energy Correction = -5197.134066
EE + Thermal Enthalpy Correction = -5197.133122
EE + Thermal Free Energy Correction = -5197.309923
Truhlar's quasiharmonic corrected Gibbs energy =
-5197.29459 (at 298.15 K)
-5197.281568 (at 273.15 K)

E_{sp} (RM06-2X/def2-TZVP/SMD (CH_2Cl_2)) = -5200.102136

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

1	6	0	1.900334	1.352083	3.737178
2	6	0	0.416675	1.380048	3.954273
3	6	0	-0.326731	0.092844	4.421108
4	7	0	0.697333	-0.939007	2.389442
5	1	0	0.254318	2.159760	4.717238
6	1	0	-0.076649	1.763356	3.056729
7	6	0	-1.803780	0.266103	4.024234
8	1	0	-2.220540	1.161339	4.498881
9	1	0	-1.923411	0.369801	2.942213
10	1	0	-2.381246	-0.602924	4.358738
11	6	0	-0.298079	-0.131386	5.940077
12	1	0	-0.758856	0.714037	6.461559
13	1	0	-0.879327	-1.028719	6.181662
14	1	0	0.704784	-0.279706	6.347629
15	6	0	2.491402	2.037668	2.589626
16	6	0	3.727759	3.122051	0.317632
17	6	0	3.815239	2.527722	2.650105
18	6	0	1.789980	2.143597	1.371671
19	6	0	2.416013	2.660764	0.242870
20	6	0	4.419857	3.074790	1.530102
21	1	0	4.359946	2.513056	3.588129
22	1	0	0.775308	1.769209	1.271989
23	1	0	1.873318	2.684211	-0.696937
24	1	0	5.439389	3.439944	1.589033
25	1	0	4.221339	3.509324	-0.568070
26	6	0	2.746048	0.614349	4.588039
27	1	0	2.355858	0.305663	5.552225
28	1	0	3.804199	0.872095	4.596807
29	6	0	1.871330	-1.274814	1.849161
30	7	0	1.959272	-1.095148	0.511443
31	6	0	3.125924	-0.891192	-0.257006
32	6	0	5.332310	-0.410850	-1.917406
33	6	0	3.094837	-1.279020	-1.592427
34	6	0	4.245166	-0.218026	0.243161
35	6	0	5.331914	0.008090	-0.587254
36	6	0	4.200255	-1.043482	-2.406056

37	1	0	2.207345	-1.752659	-2.003036
38	1	0	4.262884	0.136043	1.265978
39	1	0	6.194278	-0.242487	-2.553256
40	16	0	3.182000	-1.869517	2.796420
41	1	0	2.863864	-0.449760	3.920978
42	6	0	0.237124	-1.180534	3.746421
43	1	0	1.061113	-1.616815	4.314020
44	1	0	-0.567337	-1.921050	3.718033
45	1	0	0.031338	-0.427573	1.787361
46	6	0	-5.098600	-0.596370	-1.330067
47	6	0	-7.138150	0.297587	-0.291110
48	1	0	-7.789070	0.550083	-1.137921
49	1	0	-7.768586	0.261240	0.602121
50	6	0	-5.403309	-0.520824	-2.850062
51	1	0	-4.587306	0.024507	-3.336330
52	1	0	-6.347880	-0.008937	-3.060228
53	6	0	-5.382113	-1.993131	-3.311989
54	1	0	-5.070086	-2.097358	-4.354906
55	6	0	-4.835461	0.761018	-0.705224
56	6	0	-4.848502	3.312534	0.410197
57	6	0	-6.011427	1.296327	-0.170818
58	6	0	-3.668309	1.504485	-0.635134
59	6	0	-3.646431	2.791390	-0.080939
60	6	0	-6.027644	2.571301	0.379918
61	1	0	-6.945177	2.986446	0.786883
62	1	0	-4.842267	4.313498	0.832651
63	1	0	-6.370044	-2.461348	-3.218148
64	6	0	-4.094966	-1.736344	-1.319328
65	6	0	-2.797492	-4.185498	-1.477258
66	6	0	-3.056602	-2.035564	-0.452394
67	6	0	-4.381727	-2.618309	-2.365174
68	6	0	-3.741752	-3.846859	-2.445423
69	6	0	-2.411342	-3.279533	-0.482700
70	1	0	-3.964725	-4.537050	-3.253697
71	1	0	-2.305660	-5.153415	-1.511739
72	8	0	-2.503308	0.966813	-1.155725

73	8	0	-2.588659	-1.058158	0.419525
74	15	0	-1.570707	0.038702	-0.226882
75	8	0	-0.975115	0.755147	0.941010
76	7	0	-0.507886	-0.690127	-1.196851
77	1	0	1.081194	-1.035815	-0.027458
78	16	0	-0.501959	-0.632292	-2.793391
79	8	0	0.432638	-1.618277	-3.320405
80	8	0	-1.812209	-0.510403	-3.413465
81	6	0	0.348206	0.989287	-3.098423
82	9	0	0.046590	1.452892	-4.301938
83	9	0	-0.023765	1.884675	-2.180293
84	9	0	1.667701	0.841182	-3.006039
85	6	0	-2.380508	3.575051	-0.032462
86	6	0	0.050063	5.001030	0.040479
87	6	0	-1.804805	3.915596	1.209486
88	6	0	-1.761582	3.968196	-1.235598
89	6	0	-0.512357	4.675231	-1.192281
90	6	0	-0.572606	4.652372	1.238480
91	1	0	0.996811	5.537261	0.070410
92	6	0	-1.355874	-3.643193	0.509592
93	6	0	0.602112	-4.492363	2.367139
94	6	0	-0.050953	-3.957077	0.070833
95	6	0	-1.680799	-3.749455	1.881270
96	6	0	-0.690239	-4.217418	2.812226
97	6	0	0.946550	-4.363369	1.023095
98	1	0	1.358127	-4.810879	3.081886
99	6	0	-6.378572	-1.015378	-0.544065
100	1	0	-6.964764	-1.766578	-1.080994
101	1	0	-6.070056	-1.448653	0.414270
102	6	0	0.136664	5.024819	-2.419472
103	1	0	1.087693	5.548974	-2.365561
104	6	0	-0.422101	4.709197	-3.620385
105	1	0	0.080557	4.970566	-4.546319
106	6	0	-1.681043	4.039681	-3.668518
107	1	0	-2.120290	3.801674	-4.631922
108	6	0	-2.327570	3.686714	-2.522408

109	1	0	-3.282448	3.175061	-2.576809
110	6	0	-2.392278	3.550181	2.465645
111	1	0	-3.296868	2.951475	2.466300
112	6	0	-1.835673	3.946523	3.647285
113	1	0	-2.313242	3.678088	4.585793
114	6	0	-0.619097	4.691186	3.669642
115	1	0	-0.188571	4.991110	4.620813
116	6	0	0.002035	5.010509	2.499471
117	1	0	0.940829	5.559005	2.496327
118	6	0	-1.035832	-4.361786	4.194572
119	1	0	-0.270897	-4.726208	4.875962
120	6	0	-2.279322	-4.035359	4.646689
121	1	0	-2.530632	-4.144853	5.697322
122	6	0	-3.263296	-3.558513	3.730096
123	1	0	-4.254632	-3.307911	4.095203
124	6	0	-2.978267	-3.430098	2.401436
125	1	0	-3.747236	-3.086694	1.718137
126	6	0	0.340833	-3.868202	-1.303845
127	1	0	-0.378034	-3.537652	-2.041651
128	6	0	1.615459	-4.152719	-1.695365
129	1	0	1.886634	-4.044478	-2.741027
130	6	0	2.608049	-4.528134	-0.742507
131	1	0	3.623622	-4.718936	-1.076094
132	6	0	2.281446	-4.626617	0.576412
133	1	0	3.023867	-4.902713	1.320314
134	6	0	4.127569	-1.506914	-3.834714
135	6	0	6.513459	0.781268	-0.078353
136	9	0	5.294833	-1.332867	-4.473681
137	9	0	3.189118	-0.852914	-4.522843
138	9	0	3.827600	-2.815508	-3.901382
139	9	0	7.670685	0.245316	-0.487956
140	9	0	6.545734	0.846146	1.260459
141	9	0	6.504039	2.053545	-0.527794
