Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Morita-Baylis-Hillman Reaction: How Do Optimal Enzyme Active Sites Compare With Organocatalysts

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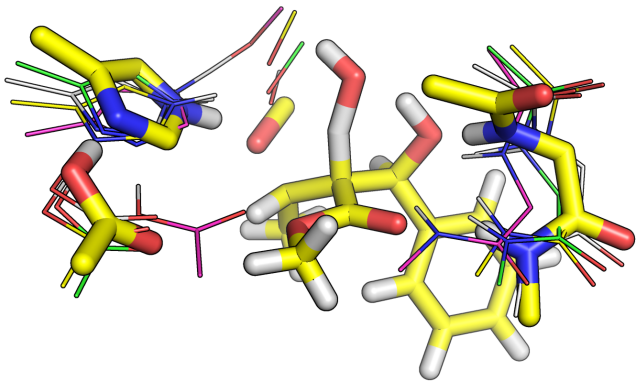
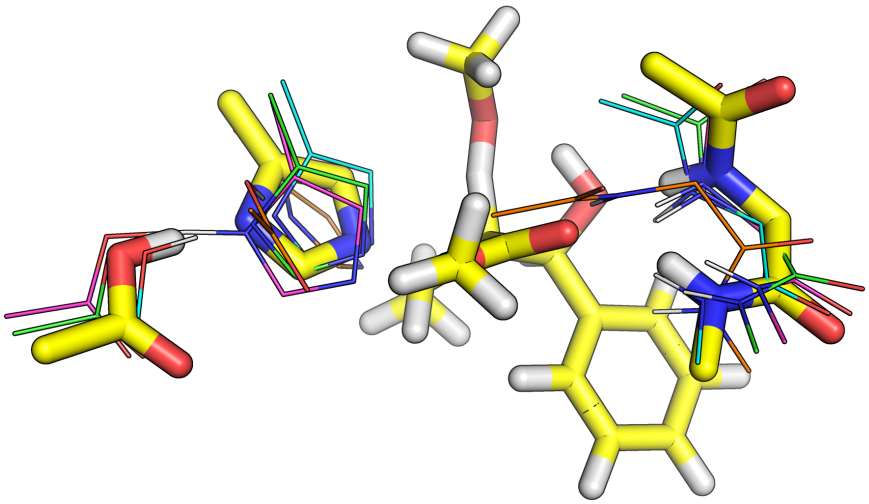
OVERLAY OF KEY STATIONARY POINTS ALONG THE REACTION PATHWAY

T3	
T7	

COORDINATES AND PROPERTIES OF OPTIMIZED STATIONARY POINTS

Optimized Molecular Properties for **Methyl Acrylate**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 1 positive frequencies below 100 cm^–1. Zero–point correction: 0.124102 hartree Enthalpy correction: 0.133228 hartree Free Energy correction: 0.091358 hartree Quasiharmonic Free Energy correction: 0.091479 hartree SCF Energy: –345.788392 hartree SCF Energy + ZPVE: –345.664290 hartree Enthalpy: –345.655164 hartree Free Energy: –345.697034 hartree Free Energy with quasiharmonic correction: –345.696913 hartree (correction: 0.08 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –345.902768366 A.U.
Cartesian Coordinates	15 spD3–substrate.out Energy: –217057.2625030 H –2.94777 –0.43494 0.89106 H –2.69654 –1.97114 –0.00264 C –2.51214 –0.89607 0.00023 O –1.08594 –0.74955 –0.00094 H 1.26132 –1.40978 0.00209 H 3.59931 –0.79183 0.87954 H –2.94981 –0.42969 –0.88682 C –0.63970 0.53251 –0.00024 C 1.67815 –0.40417 0.00058 O –1.38409 1.49408 0.00081 C 0.83493 0.63663 –0.00094 C 3.17121 –0.29214 0.00024 H 1.19775 1.66130 –0.00215 H 3.50269 0.75086 0.00026 H 3.59868 –0.79145 –0.87962

Optimized Molecular Properties for **Methyl Acrylate•DiGly** Complex

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6-31G(d)** There are 11 positive frequencies below 100 cm^-1. Zero-point correction: 0.284453 hartree Enthalpy correction: 0.306280 hartree Free Energy correction: 0.228945 hartree Quasiharmonic Free Energy correction: 0.236897 hartree SCF Energy: -802.334825 hartree SCF Energy + ZPVE: -802.050372 hartree Enthalpy: -802.028545 hartree Free Energy: -802.105880 hartree Free Energy with quasiharmonic correction: -802.097927 hartree (correction: 4.99 kcal/mol) **B3LYP-D3/6-311+G(d,p)** SCF Done: E(RB3LYP) = -802.612185248 A.U. **B3LYP/6-31G(d)(PCM)** There are 9 positive frequencies below 100 cm^-1. Zero-point correction: 0.284879 hartree Enthalpy correction: 0.306331 hartree Free Energy correction: 0.234683 hartree Quasiharmonic Free Energy correction: 0.240670 hartree SCF Energy: -802.352162 hartree SCF Energy + ZPVE: -802.067283 hartree Enthalpy: -802.045831 hartree Free Energy: -802.117479 hartree Free Energy with quasiharmonic correction: -802.111493 hartree (correction: 3.76 kcal/mol) **B3LYP-D3/6-311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = -802.630798909 A.U.
Cartesian Coordinates	34 spD3-substrate-diGly.out Energy: -503646.7461779 C -3.78175 -0.60761 1.10974 C -2.27054 0.72668 -0.35511 O -1.17874 0.88507 -0.88951 C -2.60646 -0.43404 0.48840 H -1.80499 -1.16244 0.57969 O -3.27397 1.61197 -0.49445

	C -2.98204 2.76724 -1.29931 H -3.89525 3.36236 -1.29291 H -2.72399 2.46864 -2.31853 H -2.15057 3.33214 -0.87046 H -4.55063 0.15330 0.98792 C -4.12379 -1.78104 1.97175 H -4.38211 -1.45157 2.98689 H -5.00749 -2.30258 1.58078 H -3.29878 -2.49633 2.03827 C 2.75595 0.48737 1.18651 O 3.09568 0.85069 2.30700 C 1.83347 -0.72746 1.01395 N 1.18117 -0.85284 -0.27653 H 2.43450 -1.63077 1.15799 H 1.10068 -0.67933 1.82663 H 0.41026 -0.22329 -0.49404 C 1.41264 -1.92707 -1.10175 O 2.23801 -2.79716 -0.85293 C 0.57609 -1.94996 -2.37386 H 0.04693 -2.90652 -2.42776 H 1.24643 -1.90508 -3.23852 H -0.14550 -1.13066 -2.43488 N 3.16550 1.07722 0.03133 H 2.82767 0.68099 -0.83450 C 4.09119 2.19191 0.00508 H 3.66233 3.04991 -0.52647 H 4.29014 2.47356 1.04047 H 5.03717 1.91633 -0.47746 (PCM) 34 spD3-opt-substrate-ox.out Energy: -503658.4264264 H -4.52688 2.19823 -1.16939 C -3.43925 2.08555 -1.13190 H -2.99103 3.01617 -0.78117 H -3.07282 1.87852 -2.14569 H -1.51111 -3.10170 -1.94406 N -3.08095 1.02712 -0.20367 H -3.50638 0.10636 -0.30074 O -3.19298 -1.90302 -0.22179 O -1.30345 2.11058 0.75271 C -2.01921 1.11143 0.63158 H 3.74574 -2.51357 -0.88486 C -1.96305 -2.04319 -0.13961 H -2.69038 -0.53239 1.88561 C -1.23570 -3.14576 -0.88608 H -0.14900 -3.08059 -0.78916 C -1.75772 -0.17265 1.43970 N -1.18898 -1.24162 0.62890 O 1.74287 -1.36443 0.40728 C 4.27148 -1.88340 -0.16328 H -0.17212 -1.32494 0.59169 H -1.57056 -4.11484 -0.50079 H 5.32364 -1.79150 -0.43156 C 2.44965 -0.40238 0.11347 H 4.16676 -2.31311 0.83590

	O	3.75143	−0.54174	−0.19211
	H	−1.05246	0.07467	2.23424
	H	0.91881	1.11672	0.33964
	C	1.96188	0.98462	0.06507
	C	2.70811	2.04212	−0.29017
	H	2.32469	3.86390	−1.35128
	H	3.75134	1.88739	−0.56028
	H	1.13487	3.49824	−0.07449
	C	2.19342	3.44551	−0.34439
	H	2.76588	4.09154	0.33477

Optimized Molecular Properties for **Methyl Acrylate•GlySer** Complex

Geometry	
Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 10 positive frequencies below 100 cm^–1. Zero–point correction: 0.318569 hartree Enthalpy correction: 0.342361 hartree Free Energy correction: 0.262606 hartree Quasiharmonic Free Energy correction: 0.269144 hartree SCF Energy: –916.863216 hartree SCF Energy + ZPVE: –916.544647 hartree Enthalpy: –916.520855 hartree Free Energy: –916.600610 hartree Free Energy with quasiharmonic correction: –916.594072 hartree (correction: 4.10 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –917.189874295 A.U.
Cartesian Coordinates	38 spD3–substrate–SerGly.out Energy: –575545.3309910 C –0.93359 1.25507 1.02270 O –1.68676 2.18814 0.72649 N –0.99177 0.03991 0.42025 C –1.82796 –0.22285 –0.75728 C –3.29548 –0.52858 –0.36177 O –3.77843 –1.65040 –0.49814 O 0.08167 –1.16092 –1.99516 N –3.97403 0.54899 0.10969 C –5.33753 0.45417 0.59573 H 0.67553 –1.43392 –1.27262 C 3.80440 1.24598 –0.89994 H –1.81177 0.68549 –1.37164 C 2.73787 –0.70684 0.20963 H –0.27646 –0.64120 0.64757 O 1.77646 –1.46530 0.33973 H –5.38652 0.56763 1.68664 C 2.77267 0.39971 –0.76013 H –3.43147 1.39585 0.27318 H –5.96604 1.22608 0.13721 H –5.72139 –0.53071 0.32550 C –1.25250 –1.39257 –1.56769 H –1.33886 –2.31821 –0.98464 H –1.86922 –1.52361 –2.46034 C 0.13012 1.41475 2.09692 H 0.60427 0.47077 2.38043

	H	−0.32577	1.87122	2.97958
	H	0.90119	2.10198	1.73191
	O	3.84641	−0.83122	0.95603
	C	3.85284	−1.91195	1.90600
	C	3.84942	2.37153	−1.88322
	H	3.98989	3.33041	−1.36662
	H	2.93675	2.42865	−2.48308
	H	4.70640	2.25637	−2.56023
	H	4.67718	1.11638	−0.26203
	H	4.83239	−1.87125	2.38207
	H	3.06025	−1.77648	2.64646
	H	3.70866	−2.86831	1.39786
	H	1.87914	0.47769	−1.37418

Optimized Molecular Properties for **Methyl Acrylate•Ser•Asn** Complex

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 10 positive frequencies below 100 cm^–1. Zero–point correction: 0.253473 hartree Enthalpy correction: 0.274110 hartree Free Energy correction: 0.198394 hartree Quasiharmonic Free Energy correction: 0.207379 hartree SCF Energy: –670.739356 hartree SCF Energy + ZPVE: –670.485883 hartree Enthalpy: –670.465246 hartree Free Energy: –670.540962 hartree Free Energy with quasiharmonic correction: –670.531977 hartree (correction: 5.64 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –670.984678740 A.U.
Cartesian Coordinates	30 spD3–substrate–SerAsn–A.out Energy: –421049.2394633 C –3.61223 0.24751 –0.69166 O –4.37833 –0.67010 –0.95702 N –2.29614 0.05653 –0.39578 O –0.47532 –2.04843 0.65016 H –0.15733 –1.18231 0.97609 C 3.46953 –0.35319 –0.94920 C 1.64530 0.67100 0.39404 H –1.70995 0.80321 –0.05289 O 0.57454 0.57019 0.98968 C 2.29572 –0.44808 –0.30735 C –0.92019 –2.82080 1.75714 H –0.11371 –3.00861 2.48163 H –1.26064 –3.78251 1.36424 C –4.08146 1.70048 –0.68308 H –3.27132 2.42701 –0.56144 H –4.80227 1.83614 0.13038 H –4.60683 1.90488 –1.62030 O 2.32101 1.83176 0.33496 C 1.72094 2.94696 1.01467 C 4.13485 –1.48250 –1.66951 H 4.28679 –1.22862 –2.72707 H 3.54957 –2.40490 –1.61432 H 5.13178 –1.67446 –1.25064 H 3.98538 0.60548 –0.95700 H 2.42013 3.77347 0.88776 H 0.75371 3.19264 0.56824 H 1.57906 2.71995 2.07415

	H	−1.93537	−0.88707	−0.27405
	H	−1.76142	−2.34683	2.28310
	H	1.73536	−1.37884	−0.27002

Optimized Molecular Properties for **Methyl Acrylate•Arg** Complex

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 5 positive frequencies below 100 cm^–1. Zero–point correction: 0.243390 hartree Enthalpy correction: 0.260669 hartree Free Energy correction: 0.201000 hartree Quasiharmonic Free Energy correction: 0.204145 hartree SCF Energy: –590.953635 hartree SCF Energy + ZPVE: –590.710245 hartree Enthalpy: –590.692966 hartree Free Energy: –590.752635 hartree Free Energy with quasiharmonic correction: –590.749491 hartree (correction: 1.97 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –591.158454188 A.U.
Cartesian Coordinates	(PCM) 28 spD3–MA.out Energy: –370957.5276824 H 1.07848 2.85773 0.86625 N –2.29196 1.27605 0.04859 H –4.73253 0.75852 –0.03923 H –1.27572 1.34233 0.04834 H 1.07345 2.82248 –0.92331 H –4.76810 –1.91216 –0.89079 C –2.84544 0.05464 –0.01396 C 1.69681 2.75274 –0.02875 N –4.17631 –0.08338 0.02066 H 2.47196 3.51753 –0.04469 O 0.43866 0.39504 –0.04402 N –2.04671 –1.01348 –0.10688 H –1.03770 –0.86047 –0.11787 C –4.87279 –1.36677 0.05418 H –5.93126 –1.16960 0.22125 O 2.40392 1.49733 –0.00502 C 1.67301 0.38034 –0.01797 H –4.50074 –1.98336 0.87786 C 2.45319 –0.86260 0.00146 H 1.85403 –1.76870 –0.00560 C 3.79488 –0.91069 0.02846 H 4.34965 0.02570 0.03474 C 4.60216 –2.16681 0.05136 H 3.97566 –3.06330 0.04629 H 5.27583 –2.20203 –0.81479 H 5.24431 –2.19006 0.94150

	H	−2.81895	2.05164	0.42331
	H	−2.40506	−1.90470	−0.41613

Optimized Molecular Properties for **Benzaldehyde**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 0 positive frequencies below 100 cm^–1. Zero–point correction: 0.110226 hartree Enthalpy correction: 0.117457 hartree Free Energy correction: 0.079708 hartree Quasiharmonic Free Energy correction: 0.079708 hartree SCF Energy: –345.573442 hartree SCF Energy + ZPVE: –345.463216 hartree Enthalpy: –345.455985 hartree Free Energy: –345.493734 hartree Free Energy with quasiharmonic correction: –345.493734 hartree (correction: 0.00 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –345.677065116 A.U.
Cartesian Coordinates	14 spD3–aldehyde.out Energy: –216915.6315764 C –1.99225 0.46872 0.00007 C –0.53401 0.21441 0.00006 H –2.27404 1.54570 0.00015 O –2.84766 –0.39585 –0.00012 C –0.04519 –1.10108 0.00006 C 0.36117 1.29212 0.00002 C 1.32635 –1.33123 0.00002 H –0.75893 –1.91939 0.00010 C 1.73590 1.06063 –0.00004 H –0.02501 2.30953 0.00004 C 2.21686 –0.25081 –0.00005 H 1.70780 –2.34858 0.00003 H 2.43024 1.89617 –0.00010 H 3.28826 –0.43329 –0.00009

Optimized Molecular Properties for **Benzaldehyde•H_2O** Complex

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 2 positive frequencies below 100 cm^–1. Zero–point correction: 0.134922 hartree Enthalpy correction: 0.145404 hartree Free Energy correction: 0.099453 hartree Quasiharmonic Free Energy correction: 0.100604 hartree SCF Energy: –421.994653 hartree SCF Energy + ZPVE: –421.859731 hartree Enthalpy: –421.849249 hartree Free Energy: –421.895200 hartree Free Energy with quasiharmonic correction: –421.894049 hartree (correction: 0.72 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –422.145624441 A.U.
Cartesian Coordinates	17 spD3–aldw.out Energy: –264900.3766336 O –4.34154 0.51018 –0.07001 H –3.72372 –0.24367 –0.13504 O –1.93998 –1.02615 –0.01792 H –1.77519 0.98337 –0.02521 C –1.26979 –0.00161 –0.01728 H 0.28891 2.18195 –0.01818 C 0.20305 0.02709 –0.00683 H 0.40506 –2.11090 0.00391 C 0.86822 1.26122 –0.00828 C 0.94180 –1.16721 0.00406 C 2.26122 1.30480 0.00125 C 2.33120 –1.12196 0.01372 H 2.77736 2.26054 –0.00051 C 2.99053 0.11350 0.01237 H 2.90623 –2.04365 0.02180 H 4.07681 0.14562 0.01955 H –4.66070 0.45952 0.84309

Optimized Molecular Properties for **Benzaldehyde•MeOH** Complex

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6-31G(d)** There are 4 positive frequencies below 100 cm^-1. Zero-point correction: 0.164141 hartree Enthalpy correction: 0.176010 hartree Free Energy correction: 0.125227 hartree Quasiharmonic Free Energy correction: 0.127664 hartree SCF Energy: -461.300068 hartree SCF Energy + ZPVE: -461.135927 hartree Enthalpy: -461.124058 hartree Free Energy: -461.174841 hartree Free Energy with quasiharmonic correction: -461.172403 hartree (correction: 1.53 kcal/mol) **B3LYP-D3/6-311+G(d,p)** SCF Done: E(RB3LYP) = -461.453760075 A.U. **B3LYP/6-31G(d)(PCM)** There are 4 positive frequencies below 100 cm^-1. Zero-point correction: 0.164121 hartree Enthalpy correction: 0.175970 hartree Free Energy correction: 0.128449 hartree Quasiharmonic Free Energy correction: 0.130657 hartree SCF Energy: -461.306922 hartree SCF Energy + ZPVE: -461.142801 hartree Enthalpy: -461.130952 hartree Free Energy: -461.178473 hartree Free Energy with quasiharmonic correction: -461.176264 hartree (correction: 1.39 kcal/mol) **B3LYP-D3/6-311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = -461.461855051 A.U.
Cartesian Coordinates	20 spD3-aldehyde-meoh.out Energy: -289566.6039527 H -5.19439 1.11498 0.66348 C -4.49841 0.27001 0.66656 H -5.08849 -0.65393 0.77729 H -3.85053 0.36675 1.55305 O -3.77621 0.31271 -0.54913 H -3.12064 -0.41065 -0.52644

	O -1.34453 -1.10355 -0.25684 H -1.22346 0.90734 -0.35680 C -0.70015 -0.06238 -0.24845 H 0.80183 2.16034 -0.21544 C 0.76357 0.00691 -0.10107 H 1.01133 -2.12176 0.04001 C 1.39787 1.25727 -0.10350 C 1.52431 -1.16497 0.04168 C 2.78208 1.33922 0.03609 C 2.90497 -1.08132 0.18074 H 3.27442 2.30741 0.03416 C 3.53340 0.17016 0.17805 H 3.49708 -1.98542 0.29112 H 4.61295 0.23226 0.28672 (PCM) 20 spD3-opt-aldehyde-meoh.out Energy: -289571.6836268 C -0.21351 1.80400 -0.03358 C 0.76517 0.70606 -0.02023 O -1.42142 1.69626 -0.21067 C 0.37712 -0.63183 -0.21830 C 2.11659 1.01947 0.19811 C 1.33920 -1.63621 -0.19683 C 3.07592 0.00950 0.21881 C 2.68550 -1.31766 0.02112 H 4.12085 0.25241 0.38721 H 3.43130 -2.10770 0.03625 H 1.04524 -2.67055 -0.34993 H -0.66935 -0.86937 -0.38802 H 2.40861 2.05598 0.35054 H 0.21771 2.81037 0.13679 O -3.02503 -0.64350 -0.59623 C -3.64425 -0.84332 0.66575 H -2.91644 -0.89160 1.49002 H -4.37741 -0.05684 0.90039 H -4.17381 -1.80008 0.62387 H -2.52557 0.19511 -0.54098

Optimized Molecular Properties for **Benzaldehyde•PhOH** Complex

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 5 positive frequencies below 100 cm^–1. Zero–point correction: 0.217093 hartree Enthalpy correction: 0.231523 hartree Free Energy correction: 0.172542 hartree Quasiharmonic Free Energy correction: 0.177799 hartree SCF Energy: –653.053009 hartree SCF Energy + ZPVE: –652.835916 hartree Enthalpy: –652.821486 hartree Free Energy: –652.880467 hartree Free Energy with quasiharmonic correction: –652.875210 hartree (correction: 3.30 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –653.256466152 A.U.
Cartesian Coordinates	27 spD3–aldph.out Energy: –409924.6181959 O –1.86005 –1.00035 1.24333 O 0.56760 0.36379 1.27310 H 0.66904 –1.23535 0.04289 C 1.17863 –0.36374 0.49779 H 2.59450 –1.89146 –1.19025 C 2.58235 –0.16913 0.10954 H 2.84576 1.58206 1.32720 C 3.17785 –1.06493 –0.79057 C 3.32710 0.90186 0.63146 C 4.50791 –0.89395 –1.16865 C 4.65376 1.07002 0.25280 H 4.97042 –1.58646 –1.86581 C 5.24343 0.17280 –0.64655 H 5.23388 1.89626 0.65367 H 6.28095 0.30753 –0.94034 H –1.11498 –0.37999 1.40034 C –2.81873 –0.39171 0.49127 C –4.85974 0.75677 –1.05516 C –2.69928 0.92908 0.03584 C –3.96295 –1.13482 0.17063 C –4.97234 –0.55935 –0.59739 C –3.71887 1.49294 –0.73227 H –1.81192 1.50534 0.28574 H –4.03975 –2.15539 0.53358 H –5.85605 –1.14481 –0.83945 H –3.61634 2.51857 –1.07869 H –5.65054 1.20111 –1.65278

Optimized Molecular Properties for **Ser•His•Asp** Complex

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 8 positive frequencies below 100 cm^–1. Zero–point correction: 0.201978 hartree Enthalpy correction: 0.218822 hartree Free Energy correction: 0.153150 hartree Quasiharmonic Free Energy correction: 0.159256 hartree SCF Energy: –609.826255 hartree SCF Energy + ZPVE: –609.624277 hartree Enthalpy: –609.607433 hartree Free Energy: –609.673105 hartree Free Energy with quasiharmonic correction: –609.666998 hartree (correction: 3.83 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –610.058895229 A.U.
Cartesian Coordinates	25 spD3–SerHisAsp.out Energy: –382817.7334039 O 4.31122 –1.14935 –0.53977 C –3.15525 –0.90297 0.01088 O –2.30639 –1.79806 –0.17756 O –2.94874 0.35158 0.13806 C 0.41505 1.86737 0.01255 C 1.72932 1.48759 –0.15287 N –0.31652 0.70428 –0.06828 C 0.55694 –0.30479 –0.27381 N 1.81528 0.12315 –0.33296 H 2.61352 2.11393 –0.15402 H –1.38342 0.57614 0.01509 H 3.40824 –0.72976 –0.55029 H 0.20867 –1.32346 –0.37012 C –4.64295 –1.31594 0.11191 H –5.04563 –1.02546 1.09091 H –5.23295 –0.78217 –0.64406 H –4.76435 –2.39488 –0.02482 C –0.21256 3.20582 0.23750 H –0.92949 3.46146 –0.55413 H –0.76184 3.24813 1.18759 H 0.55708 3.98560 0.25897 C 4.45199 –1.75896 0.71492 H 5.46328 –2.18479 0.77833 H 4.33532 –1.05430 1.55838 H 3.73614 –2.58446 0.88470

Optimized Molecular Properties for **Ser•His** Complex

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 3 positive frequencies below 100 cm^–1. Zero–point correction: 0.152634 hartree Enthalpy correction: 0.163704 hartree Free Energy correction: 0.117510 hartree Quasiharmonic Free Energy correction: 0.120499 hartree SCF Energy: –381.273591 hartree SCF Energy + ZPVE: –381.120957 hartree Enthalpy: –381.109887 hartree Free Energy: –381.156081 hartree Free Energy with quasiharmonic correction: –381.153092 hartree (correction: 1.88 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –381.409063251 A.U.
Cartesian Coordinates	18 spD3–HisSer.out Energy: –239337.7987524 O –3.12400 –0.04521 –0.65352 C 1.91326 –0.26033 0.01224 C 0.67565 –0.80427 –0.23342 N 1.67040 1.09502 0.15548 C 0.33577 1.30633 –0.00561 N –0.29881 0.17480 –0.24266 H 0.43230 –1.84410 –0.40442 H 2.36418 1.80595 0.34394 H –2.14429 0.01851 –0.55767 H –0.11398 2.28731 0.05755 C 3.27429 –0.86447 0.12546 H 3.96723 –0.45480 –0.62008 H 3.71619 –0.69624 1.11556 H 3.21345 –1.94444 –0.03356 C –3.63829 –0.40641 0.61064 H –3.40822 0.33360 1.39579 H –4.72887 –0.47184 0.52487 H –3.27122 –1.38613 0.96059

Optimized Molecular Properties for **His•Asp** Complex

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 5 positive frequencies below 100 cm^–1. Zero–point correction: 0.148911 hartree Enthalpy correction: 0.161094 hartree Free Energy correction: 0.109097 hartree Quasiharmonic Free Energy correction: 0.111742 hartree SCF Energy: –494.087328 hartree SCF Energy + ZPVE: –493.938417 hartree Enthalpy: –493.926234 hartree Free Energy: –493.978231 hartree Free Energy with quasiharmonic correction: –493.975585 hartree (correction: 1.66 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –494.268994031 A.U. **B3LYP/6–31G(d)(PCM)** There are 5 positive frequencies below 100 cm^–1. Zero–point correction: 0.149246 hartree Enthalpy correction: 0.161366 hartree Free Energy correction: 0.112803 hartree Quasiharmonic Free Energy correction: 0.115068 hartree SCF Energy: –494.151013 hartree SCF Energy + ZPVE: –494.001767 hartree Enthalpy: –493.989647 hartree Free Energy: –494.038210 hartree Free Energy with quasiharmonic correction: –494.035944 hartree (correction: 1.42 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –494.332809983 A.U.
Cartesian Coordinates	19 spD3–asphis.out Energy: –310158.4739876 C –2.48174 –0.03927 –0.00085 O –2.19514 –1.25441 –0.00059 O –1.68162 0.95408 –0.00110 C 2.02674 0.60394 0.00006 C 2.98741 –0.38756 0.00045 N 0.82247 –0.06093 –0.00021 C 1.10503 –1.38744 0.00007

	N 2.40903 −1.63866 0.00026 H 4.06561 −0.26148 0.00073 H −0.16143 0.35046 −0.00060 H 0.30300 −2.11311 −0.00013 C −3.98178 0.35318 0.00113 H −4.20959 0.95673 0.88954 H −4.20713 0.97914 −0.87214 H −4.62478 −0.53274 −0.01021 C 2.13298 2.09564 0.00009 H 1.65377 2.54554 −0.88046 H 1.65561 2.54548 0.88169 H 3.18664 2.39881 −0.00097 (PCM) 19 spD3-CAT.out Energy: −310198.5191017 H 4.48346 −0.11597 −0.87848 H −1.75890 2.54013 −0.88338 H 4.19128 1.40980 0.00127 C 4.00508 0.33179 0.00146 H −3.27927 2.34059 0.00269 C −2.21673 2.07612 0.00022 O 1.70094 0.99564 −0.00151 C 2.49626 0.00043 −0.00034 H 0.13231 0.39389 −0.00114 C −2.05802 0.58885 0.00014 O 2.18554 −1.21431 −0.00047 H −4.06383 −0.34536 0.00138 N −0.83140 −0.03906 −0.00052 C −2.98312 −0.43462 0.00069 H 4.48114 −0.11524 0.88302 H −1.75467 2.54030 0.88150 C −1.06638 −1.37584 −0.00037 N −2.36059 −1.66719 0.00036 H −0.24205 −2.07555 −0.00071

Optimized Molecular Properties for **T1-complex**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 14 positive frequencies below 100 cm^–1. Zero–point correction: 0.326707 hartree Enthalpy correction: 0.353876 hartree Free Energy correction: 0.258942 hartree Quasiharmonic Free Energy correction: 0.273283 hartree SCF Energy: –955.626206 hartree SCF Energy + ZPVE: –955.299499 hartree Enthalpy: –955.272330 hartree Free Energy: –955.367264 hartree Free Energy with quasiharmonic correction: –955.352923 hartree (correction: 9.00 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –955.975311554 A.U.
Cartesian Coordinates	40 spD3–complex–T1.out Energy: –599883.5601304 O –1.24506 –2.16247 –0.72010 C 5.74832 –0.33875 0.59733 O 5.01371 –1.33209 0.77228 O 5.41258 0.80342 0.13074 C 1.97195 1.60502 –0.92176 C 0.73805 0.99672 –0.99294 N 2.82212 0.65585 –0.40077 C 2.09506 –0.45830 –0.18158 N 0.81786 –0.30053 –0.52640 H –0.19652 1.41290 –1.34927 H 3.88147 0.73788 –0.18949 H –0.48850 –1.51865 –0.61047 H 2.55678 –1.34571 0.22785 C 7.24257 –0.45678 0.97513 H 7.86844 –0.24920 0.09787 H 7.49762 0.29639 1.73154 H 7.47489 –1.45382 1.36134 C 2.42351 2.98158 –1.29191 H 2.82799 3.52634 –0.42863 H 3.21400 2.96206 –2.05368 H 1.58386 3.56059 –1.69197 C –3.00545 –0.35260 1.25552 C –5.28292 0.56864 0.79991 O –6.27205 1.18286 1.16541 C –1.16356 –2.68494 –2.02191 H –1.99313 –3.39060 –2.16037

	H	−1.24911	−1.91170	−2.80601
	H	−0.22373	−3.23405	−2.20571
	C	−4.09683	0.33153	1.63661
	H	−4.17471	0.76946	2.62907
	O	−5.18301	0.03110	−0.44709
	C	−6.31481	0.24275	−1.29060
	H	−6.07050	−0.24167	−2.23767
	H	−6.49485	1.31138	−1.44480
	H	−7.21644	−0.20150	−0.85682
	C	−1.80576	−0.58747	2.11348
	H	−2.94676	−0.78700	0.25915
	H	−1.62523	−1.66568	2.21145
	H	−0.90833	−0.18781	1.62331
	H	−1.90717	−0.14364	3.10988

Optimized Molecular Properties for **T1-TS1**

Number of (–) Vibrational Frequencies	1 (–181.3747)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 11 positive frequencies below 100 cm^–1. Zero–point correction: 0.325894 hartree Enthalpy correction: 0.350820 hartree Free Energy correction: 0.265803 hartree Quasiharmonic Free Energy correction: 0.274938 hartree SCF Energy: –955.596970 hartree SCF Energy + ZPVE: –955.271076 hartree Enthalpy: –955.246150 hartree Free Energy: –955.331167 hartree Free Energy with quasiharmonic correction: –955.322032 hartree (correction: 5.73 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –955.946816531 A.U.
Cartesian Coordinates	40 spD3–TS1–T1.out Energy: –599865.6792336 O –1.51501 –1.51814 –0.30408 C 5.68118 –0.78608 –0.09746 O 4.91990 –1.74054 –0.15188 O 5.31998 0.48662 –0.05235 C 1.83928 1.82667 –0.05323 C 0.54262 1.36690 –0.08733 N 2.69087 0.73940 –0.08756 C 1.90755 –0.33555 –0.14113 N 0.60176 –0.00643 –0.14268 H –0.40469 1.88711 –0.07855 H 4.27774 0.57799 –0.06760 H –0.27174 –0.67083 –0.18381 H 2.28121 –1.34907 –0.17786 C 7.19494 –0.94457 –0.07322 H 7.64093 –0.41504 –0.92250 H 7.60390 –0.49482 0.83846 H 7.46016 –2.00256 –0.11524 C 2.34794 3.23354 0.00906 H 2.95594 3.40589 0.90716 H 2.98000 3.47466 –0.85600 H 1.51558 3.94529 0.02550 C –2.78246 –0.97471 1.05189 C –4.55293 0.57940 0.18376 O –5.07503 1.68413 0.02507 C –2.03313 –1.28874 –1.57392 H –2.64304 –2.13800 –1.93920 H –2.67869 –0.38969 –1.60448

	H	−1.22355	−1.12767	−2.31082
	C	−3.32490	0.29360	0.85560
	H	−2.80830	1.17113	1.23827
	O	−5.21031	−0.56503	−0.28584
	C	−6.44026	−0.30621	−0.93710
	H	−6.82576	−1.28133	−1.25220
	H	−6.30938	0.34098	−1.81289
	H	−7.16231	0.18048	−0.26952
	C	−1.83430	−1.22357	2.20061
	H	−3.43323	−1.81197	0.81544
	H	−2.40249	−1.35431	3.13276
	H	−1.23617	−2.12287	2.02818
	H	−1.15400	−0.37657	2.34400

Optimized Molecular Properties for **T1-INT1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 11 positive frequencies below 100 cm^–1. Zero–point correction: 0.329244 hartree Enthalpy correction: 0.354268 hartree Free Energy correction: 0.270498 hartree Quasiharmonic Free Energy correction: 0.277958 hartree SCF Energy: –955.602345 hartree SCF Energy + ZPVE: –955.273101 hartree Enthalpy: –955.248077 hartree Free Energy: –955.331847 hartree Free Energy with quasiharmonic correction: –955.324387 hartree (correction: 4.68 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –955.950850463 A.U.
Cartesian Coordinates	40 spD3–INT1–T1.out Energy: –599868.2105641 O 1.83224 –2.15442 0.31753 C –5.30205 –0.60704 0.24883 O –4.58068 –1.59021 0.33464 O –4.89250 0.63365 0.03786 C –1.33734 1.74633 –0.38226 C –0.07193 1.20852 –0.40169 N –2.25910 0.73285 –0.17744 C –1.55734 –0.38798 –0.07494 N –0.23525 –0.14709 –0.20617 H 0.91002 1.65073 –0.52935 H –3.85139 0.67229 –0.04801 H 0.53044 –0.83784 –0.15489 H –1.99117 –1.36362 0.09069 C –6.81624 –0.68803 0.37890 H –7.15449 –0.06122 1.21156 H –7.29160 –0.30212 –0.52972 H –7.12138 –1.72256 0.54637 C –1.75415 3.17460 –0.54657 H –2.41787 3.30629 –1.41161 H –2.29820 3.54179 0.33392 H –0.87739 3.81332 –0.69316 C 3.01724 –1.69989 –0.53669 C 3.43135 0.81614 –0.31633 O 3.25483 2.02369 –0.58170 C 1.98945 –1.80155 1.67494 H 2.84587 –2.32755 2.13133 H 2.15151 –0.72300 1.80575

	H	1.07627	−2.09826	2.20642
	C	2.92633	−0.30350	−0.97602
	H	2.32818	−0.09069	−1.85950
	O	4.25727	0.49520	0.80483
	C	4.79103	1.61977	1.46906
	H	5.34192	1.23114	2.33446
	H	4.00953	2.31096	1.80924
	H	5.47745	2.19410	0.83110
	C	3.00605	−2.71219	−1.68178
	H	3.89187	−1.86774	0.10466
	H	3.88904	−2.57109	−2.31494
	H	2.99154	−3.74375	−1.30944
	H	2.11664	−2.56583	−2.30746

Optimized Molecular Properties for **T1-TS2**

Number of (–) Vibrational Frequencies	1 (–116.7123)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 14 positive frequencies below 100 cm^–1. Zero–point correction: 0.442993 hartree Enthalpy correction: 0.474379 hartree Free Energy correction: 0.376180 hartree Quasiharmonic Free Energy correction: 0.385490 hartree SCF Energy: –1301.184052 hartree SCF Energy + ZPVE: –1300.741059 hartree Enthalpy: –1300.709673 hartree Free Energy: –1300.807872 hartree Free Energy with quasiharmonic correction: –1300.798561 hartree (correction: 5.84 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1301.64310444 A.U.
Cartesian Coordinates	54 spD3–TS2–T1.out Energy: –816793.3732947 O 0.24807 1.79651 –1.42791 C –6.90586 –0.01382 –0.33718 O –6.29063 0.97775 –0.70198 O –6.36334 –1.14162 0.09419 C –2.67340 –1.81168 0.42447 C –1.48029 –1.16422 0.20541 N –3.71914 –0.97351 0.07178 C –3.16312 0.15205 –0.35364 N –1.81594 0.07971 –0.28880 H –0.43905 –1.45461 0.32583 H –5.32227 –1.08004 0.08571 H –1.14204 0.80543 –0.55460 H –3.71984 1.01023 –0.70178 C –8.42576 –0.07995 –0.33231 H –8.76658 –0.90528 –0.96720 H –8.78848 –0.28158 0.68173 H –8.84134 0.86222 –0.69408 C –2.90955 –3.19266 0.95154 H –3.49871 –3.17819 1.87826 H –3.45987 –3.81214 0.23099 H –1.95671 –3.68750 1.16410 C 1.41826 0.93311 –1.28118 C 1.71190 1.64941 1.20907 O 2.36661 2.17157 2.10909 C 0.48422 3.18718 –1.41344 H –0.49523 3.67554 –1.45884 H 1.00095 3.51278 –0.50052

	H	1.07500	3.51590	−2.28250
	C	2.24769	1.11316	−0.03010
	H	3.23548	1.53618	−0.20408
	C	2.56079	−0.78243	0.53124
	C	4.03466	−0.94899	0.18568
	H	2.45753	−0.58733	1.62081
	O	1.71771	−1.56014	−0.02941
	C	4.40736	−1.86139	−0.80758
	C	5.03969	−0.24956	0.87045
	C	5.75289	−2.06105	−1.12454
	H	3.61051	−2.40938	−1.30263
	C	6.38399	−0.44998	0.55914
	H	4.75115	0.46588	1.63874
	C	6.74802	−1.35697	−0.44266
	H	6.02786	−2.77428	−1.90029
	H	7.15287	0.10159	1.09773
	H	7.79744	−1.51458	−0.68441
	O	0.36581	1.40820	1.37657
	C	−0.15949	1.75382	2.65404
	H	−0.06116	2.82796	2.84808
	H	−1.21356	1.46891	2.62664
	H	0.35784	1.21364	3.45358
	H	0.97113	−0.06933	−1.23007
	C	2.28439	0.98829	−2.54210
	H	3.03517	0.19262	−2.49609
	H	2.81685	1.94267	−2.64214
	H	1.66844	0.83517	−3.43592

Optimized Molecular Properties for **T1-INT2**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 15 positive frequencies below 100 cm^–1. Zero–point correction: 0.443779 hartree Enthalpy correction: 0.475509 hartree Free Energy correction: 0.376306 hartree Quasiharmonic Free Energy correction: 0.386283 hartree SCF Energy: –1301.184548 hartree SCF Energy + ZPVE: –1300.740769 hartree Enthalpy: –1300.709039 hartree Free Energy: –1300.808242 hartree Free Energy with quasiharmonic correction: –1300.798265 hartree (correction: 6.26 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1301.64371808 A.U.
Cartesian Coordinates	54 spD3–INT2–T1.out Energy: –816793.7583596 O 0.33504 1.75901 –1.42098 C –6.87205 –0.11557 –0.50257 O –6.26154 0.84366 –0.95264 O –6.32736 –1.17298 0.07719 C –2.64680 –1.71385 0.63919 C –1.45622 –1.06973 0.39682 N –3.69237 –0.94764 0.14623 C –3.14006 0.13323 –0.38513 N –1.79560 0.09965 –0.25442 H –0.40976 –1.31102 0.58964 H –5.28637 –1.08877 0.10539 H –1.12398 0.80483 –0.56917 H –3.69693 0.93139 –0.85478 C –8.38923 –0.21857 –0.55523 H –8.68385 –1.11118 –1.11829 H –8.79302 –0.32781 0.45737 H –8.80759 0.67189 –1.02786 C –2.88124 –3.02978 1.31326 H –3.51414 –2.92270 2.20453 H –3.38453 –3.74247 0.64633 H –1.92972 –3.47225 1.62403 C 1.47284 0.86989 –1.24126 C 1.66890 1.78490 1.18589 O 2.26222 2.54879 1.93603 C 0.61453 3.13963 –1.51731 H –0.35037 3.65548 –1.56553 H 1.17224 3.51627 –0.64843

	H	1.18389	3.38453	−2.42672
	C	2.28060	1.05897	0.04602
	H	3.24033	1.54525	−0.14049
	C	2.57974	−0.55829	0.66035
	C	4.01336	−0.91202	0.20263
	H	2.66279	−0.34665	1.75919
	O	1.65615	−1.40872	0.30400
	C	4.19585	−2.00947	−0.64438
	C	5.14489	−0.21245	0.64423
	C	5.47423	−2.38853	−1.06088
	H	3.29908	−2.54715	−0.94037
	C	6.42531	−0.58951	0.23636
	H	5.01534	0.63429	1.31763
	C	6.59589	−1.67973	−0.62333
	H	5.59898	−3.24492	−1.72244
	H	7.29343	−0.03512	0.59014
	H	7.59377	−1.97602	−0.94176
	O	0.36984	1.43919	1.41199
	C	−0.21577	1.98201	2.59367
	H	−0.23675	3.07673	2.55760
	H	−1.23071	1.58203	2.62775
	H	0.34465	1.67684	3.48290
	H	1.00999	−0.12035	−1.14660
	C	2.36652	0.87128	−2.48218
	H	3.09323	0.05657	−2.40286
	H	2.92922	1.80666	−2.59657
	H	1.76407	0.71346	−3.38475

Optimized Molecular Properties for **T1-TS3**

Number of (–) Vibrational Frequencies	1 (–1536.2286)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 14 positive frequencies below 100 cm^–1. Zero–point correction: 0.439227 hartree Enthalpy correction: 0.470730 hartree Free Energy correction: 0.369631 hartree Quasiharmonic Free Energy correction: 0.382228 hartree SCF Energy: –1301.124063 hartree SCF Energy + ZPVE: –1300.684836 hartree Enthalpy: –1300.653333 hartree Free Energy: –1300.754432 hartree Free Energy with quasiharmonic correction: –1300.741834 hartree (correction: 7.90 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1301.58388694 A.U.
Cartesian Coordinates	54 spD3–TS3–T1.out Energy: –816756.2137527 O 0.16303 1.97962 0.61432 C –6.16650 –2.24378 0.35681 O –5.02101 –2.49445 0.69662 O –6.58007 –1.08419 –0.14246 C –4.33643 1.92694 –0.70893 C –3.01525 2.26885 –0.54545 N –4.51049 0.62036 –0.29365 C –3.31887 0.19479 0.10588 N –2.38423 1.15899 –0.03141 H –2.47288 3.18123 –0.74205 H –5.79202 –0.42515 –0.20332 H –1.37871 1.13430 0.20704 H –3.12835 –0.79352 0.49756 C –7.29999 –3.24975 0.46114 H –8.10018 –2.84877 1.09287 H –7.73047 –3.43204 –0.52972 H –6.92833 –4.18560 0.88141 C –5.47104 2.74951 –1.23458 H –5.91843 2.29391 –2.12724 H –6.27150 2.85227 –0.49074 H –5.13011 3.75466 –1.50419 C 1.30749 1.76812 –0.28767 C 1.72939 –0.72728 –0.01214 O 2.34255 –1.78065 0.07299 C 0.44718 2.07068 2.00310 H –0.42511 2.54892 2.46376 H 0.59586 1.08208 2.45496

	H	1.34132	2.67173	2.20031
	C	2.22767	0.63430	0.17171
	C	3.76288	0.94295	0.16116
	C	4.73072	−0.20481	−0.13055
	H	3.99219	1.69506	−0.62067
	O	3.87658	1.46913	1.46371
	C	5.55318	−0.68108	0.89329
	C	4.90713	−0.71914	−1.42204
	C	6.51535	−1.66074	0.64118
	H	5.41299	−0.23905	1.87488
	C	5.86573	−1.69778	−1.68072
	H	4.28050	−0.34968	−2.23313
	C	6.67661	−2.17611	−0.64670
	H	7.14723	−2.02129	1.45202
	H	5.98306	−2.08956	−2.69014
	H	7.42770	−2.93854	−0.84639
	H	2.61950	0.92579	1.39733
	O	0.34524	−0.76291	−0.22621
	C	−0.19371	−2.07747	−0.32991
	H	−1.25302	−1.95218	−0.56776
	H	−0.08263	−2.63069	0.60950
	H	0.30346	−2.65105	−1.11890
	H	0.78416	1.50391	−1.21460
	C	1.99441	3.12571	−0.48861
	H	2.56754	3.13505	−1.42204
	H	1.22825	3.90675	−0.55198
	H	2.68465	3.34017	0.33306

Optimized Molecular Properties for **T1-INT3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 14 positive frequencies below 100 cm^–1. Zero–point correction: 0.444779 hartree Enthalpy correction: 0.476301 hartree Free Energy correction: 0.377034 hartree Quasiharmonic Free Energy correction: 0.387696 hartree SCF Energy: –1301.194810 hartree SCF Energy + ZPVE: –1300.750031 hartree Enthalpy: –1300.718509 hartree Free Energy: –1300.817776 hartree Free Energy with quasiharmonic correction: –1300.807114 hartree (correction: 6.69 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1301.65585432 A.U.
Cartesian Coordinates	54 spD3–INT3–T1.out Energy: –816801.3739651 O –0.12788 –2.16999 0.84010 C 6.82691 0.01923 0.73838 O 6.12700 –0.74061 1.39106 O 6.40304 0.80658 –0.23970 C 2.84191 1.03727 –1.46788 C 1.61431 0.48485 –1.18870 N 3.78398 0.50713 –0.60250 C 3.13186 –0.34268 0.17849 N 1.81928 –0.38619 –0.13850 H 0.62581 0.62323 –1.61219 H 5.38101 0.69373 –0.38362 H 1.08954 –0.97801 0.29808 H 3.59459 –0.92338 0.96358 C 8.32261 0.16458 0.97181 H 8.87031 –0.07752 0.05433 H 8.56224 1.20282 1.22684 H 8.63969 –0.49796 1.77901 C 3.20528 2.04993 –2.50862 H 3.63095 2.95619 –2.05829 H 3.95327 1.65822 –3.21057 H 2.32156 2.34268 –3.08451 C –1.50225 –1.69085 1.26967 C –3.16474 –1.54930 –0.62594 O –3.69306 –1.03367 –1.64458 C –0.17852 –3.09843 –0.22570 H –0.72185 –4.00971 0.06768 H –0.67174 –2.67313 –1.10946

	H	0.85478	−3.36286	−0.47866
	C	−2.24654	−0.93904	0.23462
	C	−1.89885	0.49145	−0.11718
	C	−2.94591	1.55167	0.28718
	H	−0.97206	0.77034	0.40320
	O	−1.58599	0.66648	−1.51760
	C	−2.89361	2.83311	−0.28246
	C	−3.92795	1.30061	1.25102
	C	−3.78658	3.83157	0.10573
	H	−2.15083	3.02618	−1.05043
	C	−4.82722	2.29602	1.64237
	H	−3.98765	0.30074	1.67102
	C	−4.75962	3.56868	1.07429
	H	−3.72782	4.81777	−0.35216
	H	−5.58763	2.07269	2.38892
	H	−5.45932	4.34557	1.37676
	H	−2.32837	0.17787	−1.94798
	O	−3.51187	−2.87551	−0.30418
	C	−4.40069	−3.48853	−1.21873
	H	−4.56390	−4.50508	−0.84377
	H	−3.98345	−3.53200	−2.23269
	H	−5.35908	−2.95862	−1.27839
	H	−2.04385	−2.61508	1.50022
	C	−1.19656	−0.95638	2.57670
	H	−0.62617	−0.03698	2.40177
	H	−0.60710	−1.59282	3.24699
	H	−2.12865	−0.68008	3.08041

Optimized Molecular Properties for **T1-TS4**

Number of (–) Vibrational Frequencies	1 (–250.5422)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 14 positive frequencies below 100 cm^–1. Zero–point correction: 0.438356 hartree Enthalpy correction: 0.470151 hartree Free Energy correction: 0.369866 hartree Quasiharmonic Free Energy correction: 0.381074 hartree SCF Energy: –1301.182796 hartree SCF Energy + ZPVE: –1300.744440 hartree Enthalpy: –1300.712645 hartree Free Energy: –1300.812930 hartree Free Energy with quasiharmonic correction: –1300.801722 hartree (correction: 7.03 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1301.64874370 A.U.
Cartesian Coordinates	54 spD3–TS4–T1.out Energy: –816796.9119837 O –0.28788 2.46602 0.46648 C –6.92603 –0.20847 0.70906 O –6.38046 0.73441 1.26537 O –6.35598 –1.03730 –0.14673 C –2.85299 –1.01475 –1.33028 C –1.69211 –0.29261 –1.15987 N –3.84042 –0.44638 –0.54972 C –3.26372 0.58794 0.06373 N –1.96740 0.72245 –0.26979 H –0.70712 –0.41279 –1.59309 H –5.33778 –0.78812 –0.30285 H –1.20961 1.51874 0.09514 H –3.78721 1.23831 0.75082 C –8.39099 –0.55615 0.94480 H –8.94215 –0.51744 –0.00157 H –8.47677 –1.57976 1.32642 H –8.83122 0.14327 1.65819 C –3.10797 –2.21710 –2.18586 H –3.44048 –3.07806 –1.59010 H –3.88962 –2.02697 –2.93412 H –2.19701 –2.51010 –2.71889 C 1.46971 1.42100 1.28610 C 3.24436 1.58752 –0.41043 O 3.83766 1.19668 –1.42390 C 0.06758 3.14659 –0.68380 H 0.34748 4.20076 –0.48246 H 0.93302 2.68399 –1.20822

	H	−0.75411	3.17079	−1.42846
	C	2.22300	0.83641	0.29550
	C	2.01233	−0.58264	−0.21455
	C	3.12201	−1.56085	0.21124
	H	1.07548	−0.96242	0.20654
	O	1.81114	−0.63197	−1.63019
	C	3.45494	−2.64424	−0.61209
	C	3.77694	−1.43790	1.44337
	C	4.41601	−3.57594	−0.21753
	H	2.95229	−2.73557	−1.56926
	C	4.73661	−2.36989	1.84299
	H	3.54046	−0.59339	2.08453
	C	5.06176	−3.44465	1.01367
	H	4.66252	−4.40719	−0.87532
	H	5.23564	−2.25146	2.80277
	H	5.81190	−4.16981	1.32194
	H	2.54712	−0.09173	−1.98668
	O	3.55925	2.80089	0.14229
	C	4.49271	3.57818	−0.60110
	H	4.61540	4.50746	−0.03953
	H	4.11664	3.79357	−1.60681
	H	5.45399	3.06251	−0.69520
	H	1.77409	2.41199	1.59823
	C	0.58911	0.69557	2.26466
	H	0.04657	−0.13827	1.81130
	H	−0.14684	1.38895	2.67654
	H	1.19254	0.29220	3.09251

Optimized Molecular Properties for **T1-product**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 16 positive frequencies below 100 cm^–1. Zero–point correction: 0.442742 hartree Enthalpy correction: 0.476071 hartree Free Energy correction: 0.368780 hartree Quasiharmonic Free Energy correction: 0.384157 hartree SCF Energy: –1301.212243 hartree SCF Energy + ZPVE: –1300.769501 hartree Enthalpy: –1300.736172 hartree Free Energy: –1300.843463 hartree Free Energy with quasiharmonic correction: –1300.828086 hartree (correction: 9.65 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1301.67362745 A.U.
Cartesian Coordinates	54 spD3–product–T1.out Energy: –816812.5267725 O 1.59025 3.94565 –1.47531 C 3.92354 –3.06213 –0.34614 O 3.25243 –2.45291 –1.21467 O 4.46971 –2.56098 0.68665 C 3.92892 0.94804 1.72572 C 3.32889 2.10003 1.26741 N 3.74288 0.01673 0.72942 C 3.05797 0.61993 –0.26471 N 2.78334 1.89175 0.01663 H 3.26053 3.06122 1.76247 H 4.04988 –1.01009 0.71759 H 2.00446 3.17330 –0.99889 H 2.78448 0.07940 –1.15918 C 4.08312 –4.58823 –0.51241 H 4.98727 –4.94930 –0.01194 H 3.22131 –5.09355 –0.05546 H 4.10281 –4.86081 –1.57273 C 4.65321 0.64001 2.99686 H 4.17454 –0.17724 3.55189 H 5.69145 0.33390 2.81291 H 4.67221 1.52275 3.64535 C –0.95195 1.35013 –0.35918 C –1.59217 –0.82818 –1.30641 O –2.41390 –1.54796 –1.87389 C 2.37636 5.07629 –1.19857 H 1.96300 5.92530 –1.75830 H 2.38017 5.35584 –0.12888

	H	3.42864	4.95262	−1.50796
	C	−1.93164	0.51860	−0.76443
	C	−3.42375	0.83828	−0.74340
	C	−4.17108	0.09178	0.37511
	H	−3.54064	1.90952	−0.54800
	O	−4.02839	0.63387	−2.01511
	C	−5.47031	−0.37892	0.15312
	C	−3.60447	−0.07986	1.64498
	C	−6.18468	−1.01028	1.17240
	H	−5.90704	−0.24490	−0.83086
	C	−4.31829	−0.70837	2.66655
	H	−2.59262	0.26872	1.83242
	C	−5.61233	−1.17778	2.43454
	H	−7.19126	−1.37481	0.97829
	H	−3.85736	−0.83781	3.64312
	H	−6.16701	−1.67258	3.22848
	H	−3.75502	−0.27361	−2.26435
	O	−0.31750	−1.18401	−1.13268
	C	0.09393	−2.45096	−1.69233
	H	1.16877	−2.52264	−1.50569
	H	−0.12711	−2.47049	−2.76351
	H	−0.45577	−3.26218	−1.20517
	C	−1.06661	2.74205	0.17691
	H	0.07064	0.98527	−0.42336
	H	−0.71051	2.76436	1.21693
	H	−2.08186	3.14813	0.15431
	H	−0.39039	3.39828	−0.38802

Optimized Molecular Properties for **T2-complex/T3-complex/T4-complex/T5-complex**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.488701 hartree Enthalpy correction: 0.527900 hartree Free Energy correction: 0.405268 hartree Quasiharmonic Free Energy correction: 0.423911 hartree SCF Energy: –1412.193468 hartree SCF Energy + ZPVE: –1411.704767 hartree Enthalpy: –1411.665568 hartree Free Energy: –1411.788200 hartree Free Energy with quasiharmonic correction: –1411.769557 hartree (correction: 11.70 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1412.70783046 A.U.
Cartesian Coordinates	59 spD3–complex–T2.out Energy: –886487.5405441 O 3.80874 –3.52187 1.22908 C 1.12662 3.64412 0.74007 O 0.44494 2.58359 0.71901 O 2.36056 3.75590 0.47045 C 4.79540 1.09685 –0.17629 C 4.95360 –0.26572 –0.05722 N 3.49487 1.34889 0.20001 C 2.93357 0.16531 0.52626 N 3.78293 –0.84833 0.38344 H 5.83676 –0.85891 –0.25934 H 1.90788 0.10152 0.86032 C 0.39196 4.94346 1.11968 H 1.09039 5.77570 1.24419 H –0.33154 5.19988 0.33523 H –0.17786 4.79481 2.04390 C 5.73592 2.17684 –0.60550 H 6.72246 1.75389 –0.82323 H 5.38351 2.69297 –1.50818 H 5.85838 2.94245 0.17113 C 1.29190 –2.94214 –1.47120 C –0.46273 –1.17860 –1.54718 O –1.60652 –0.82671 –1.25848 C 3.37110 –3.50024 2.56720 H 3.98261 –2.83773 3.20262 H 2.31959 –3.18224 2.67479 H 3.45304 –4.51813 2.96864 C 0.00303 –2.57163 –1.42347

	H	−0.78657	−3.29276	−1.22595
	O	0.46599	−0.34063	−2.00944
	C	0.12671	1.06591	−2.07669
	H	0.86940	1.49916	−2.74808
	H	0.20743	1.52122	−1.08304
	H	−0.88026	1.18724	−2.48228
	H	2.04665	−2.17358	−1.62515
	C	1.79360	−4.33374	−1.26492
	H	2.38909	−4.66094	−2.12897
	H	2.46544	−4.34702	−0.39365
	H	0.97750	−5.04878	−1.11287
	C	−4.72785	1.32844	−0.20424
	O	−5.55273	2.23337	−0.32700
	C	−5.17967	−0.12756	−0.41837
	N	−4.24292	−1.17388	−0.06000
	H	−6.07611	−0.27668	0.18662
	H	−5.47507	−0.21758	−1.47222
	H	−3.36674	−1.24977	−0.57020
	C	−4.47579	−2.02622	0.98120
	O	−5.50392	−2.01833	1.65315
	C	−3.35912	−3.02900	1.24648
	H	−3.70422	−4.03273	0.97310
	H	−3.14751	−3.03763	2.31954
	H	−2.43910	−2.80492	0.69962
	N	−3.42636	1.53764	0.09572
	H	−2.77657	0.76360	0.07371
	C	−2.89240	2.87822	0.28896
	H	−3.04165	3.48921	−0.61019
	H	−3.41344	3.37557	1.11477
	H	−1.82377	2.80634	0.51400
	H	3.01275	2.30124	0.27066
	H	3.76624	−2.58413	0.89379

Optimized Molecular Properties for **T2-TS1/T3-TS1/T4-TS1/T5-TS1**

Number of (–) Vibrational Frequencies	1 (–254.4283)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 19 positive frequencies below 100 cm^–1. Zero–point correction: 0.484991 hartree Enthalpy correction: 0.522405 hartree Free Energy correction: 0.406828 hartree Quasiharmonic Free Energy correction: 0.421813 hartree SCF Energy: –1412.165896 hartree SCF Energy + ZPVE: –1411.680905 hartree Enthalpy: –1411.643491 hartree Free Energy: –1411.759068 hartree Free Energy with quasiharmonic correction: –1411.744083 hartree (correction: 9.40 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1412.68256798 A.U.
Cartesian Coordinates	59 spD3–TS1–T2.out Energy: –886471.6880987 O 1.97235 –3.39273 0.52607 C 2.11399 3.64983 0.44616 O 1.23651 2.79561 0.37632 O 3.41071 3.41116 0.47435 C 5.11683 0.11146 0.32751 C 4.78624 –1.22570 0.32495 N 3.94923 0.84560 0.39144 C 2.96208 –0.04975 0.42368 N 3.41507 –1.31485 0.38399 H 5.41160 –2.10698 0.28578 H 1.91611 0.21240 0.47632 C 1.80314 5.13699 0.50621 H 2.27749 5.58405 1.38633 H 2.21974 5.63804 –0.37501 H 0.72426 5.29615 0.54320 C 6.46509 0.76063 0.27409 H 7.25777 0.00506 0.23611 H 6.57264 1.40404 –0.60945 H 6.64640 1.39324 1.15323 C 0.67172 –3.47808 –1.15571 C –0.64820 –1.37431 –1.21154 O –1.67845 –0.71041 –0.99369 C 1.25255 –3.26762 1.70329 H 1.71667 –2.54354 2.40210 H 0.21625 –2.90421 1.52716 H 1.16550 –4.22749 2.25097 C –0.49284 –2.77557 –0.94659

	H	−1.36845	−3.26438	−0.52919
	O	0.43679	−0.78909	−1.78613
	C	0.32158	0.59378	−2.13908
	H	1.16868	0.79348	−2.79890
	H	0.39469	1.23557	−1.25720
	H	−0.62097	0.78489	−2.65979
	H	1.47125	−2.98086	−1.69243
	C	0.68769	−4.98140	−1.18335
	H	0.38720	−5.34303	−2.17920
	H	1.68447	−5.36281	−0.95554
	H	−0.01798	−5.39748	−0.45531
	C	−4.33934	1.91782	−0.47045
	O	−5.02590	2.92615	−0.63822
	C	−5.01926	0.53652	−0.44003
	N	−4.28140	−0.55031	0.16992
	H	−5.95021	0.65538	0.11655
	H	−5.28142	0.28458	−1.47734
	H	−3.40359	−0.84832	−0.25645
	C	−4.65618	−1.09291	1.36350
	O	−5.67671	−0.77447	1.97136
	C	−3.71905	−2.17333	1.89089
	H	−4.19924	−3.15282	1.78093
	H	−3.56207	−2.00501	2.96009
	H	−2.75135	−2.19386	1.38146
	N	−2.99158	1.94974	−0.33534
	H	−2.45579	1.08716	−0.36771
	C	−2.27021	3.20891	−0.40866
	H	−2.25877	3.61297	−1.43101
	H	−2.76229	3.94825	0.23017
	H	−1.24175	3.05807	−0.07149
	H	3.61813	2.37665	0.43406
	H	2.76825	−2.26374	0.41184

Optimized Molecular Properties for **T2-INT1/T3-INT1/T4-INT1/T5-INT1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 17 positive frequencies below 100 cm^–1. Zero–point correction: 0.491276 hartree Enthalpy correction: 0.528338 hartree Free Energy correction: 0.414852 hartree Quasiharmonic Free Energy correction: 0.428118 hartree SCF Energy: –1412.176328 hartree SCF Energy + ZPVE: –1411.685052 hartree Enthalpy: –1411.647990 hartree Free Energy: –1411.761476 hartree Free Energy with quasiharmonic correction: –1411.748210 hartree (correction: 8.32 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1412.68906810 A.U.
Cartesian Coordinates	59 spD3–INT1–T2.out Energy: –886475.7669855 O 1.51394 –3.55415 0.05722 C 2.42611 3.73047 0.27721 O 1.53227 2.93170 0.03970 O 3.68779 3.40353 0.53093 C 5.00471 –0.17319 0.59880 C 4.50771 –1.44374 0.43017 N 3.96938 0.73107 0.45400 C 2.88181 0.01341 0.20270 N 3.16026 –1.30635 0.17726 H 4.98574 –2.41165 0.46426 H 1.89739 0.42105 0.03523 C 2.20861 5.23201 0.31980 H 2.44916 5.61368 1.31824 H 2.88117 5.72869 –0.38792 H 1.17142 5.46596 0.07591 C 6.40583 0.26502 0.89089 H 7.07546 –0.59815 0.97077 H 6.79446 0.92202 0.10222 H 6.46373 0.82554 1.83276 C 0.43620 –3.58632 –1.01558 C –0.79549 –1.38674 –1.15736 O –1.78198 –0.59671 –1.07462 C 1.04266 –3.74263 1.37634 H 1.85113 –3.45585 2.05883 H 0.16218 –3.11673 1.57567 H 0.78168 –4.79483 1.57420 C –0.72689 –2.71637 –0.77393

	H	−1.62877	−3.14459	−0.34637
	O	0.38673	−0.88996	−1.72724
	C	0.28342	0.37033	−2.37725
	H	1.20493	0.48140	−2.95745
	H	0.21544	1.19820	−1.66302
	H	−0.58481	0.40977	−3.04367
	H	1.02256	−3.22464	−1.86461
	C	0.06986	−5.05648	−1.23421
	H	−0.51424	−5.15977	−2.15559
	H	0.96735	−5.68172	−1.31319
	H	−0.54599	−5.44168	−0.41201
	C	−4.17414	2.10299	−0.38459
	O	−4.82959	3.14391	−0.47218
	C	−4.90827	0.75836	−0.22830
	N	−4.16035	−0.33103	0.36401
	H	−5.78112	0.94498	0.39902
	H	−5.26870	0.47197	−1.22716
	H	−3.31635	−0.65948	−0.12357
	C	−4.46740	−0.82223	1.59370
	O	−5.43643	−0.46101	2.26383
	C	−3.52030	−1.90651	2.09814
	H	−4.04987	−2.86647	2.11486
	H	−3.24385	−1.67050	3.13054
	H	−2.61539	−2.00948	1.49260
	N	−2.82185	2.06450	−0.44960
	H	−2.33559	1.17092	−0.55153
	C	−2.06294	3.28372	−0.65956
	H	−2.09380	3.61338	−1.70898
	H	−2.49363	4.08453	−0.05202
	H	−1.02118	3.12214	−0.37057
	H	3.80390	2.38114	0.50317
	H	2.48257	−2.07818	0.02678

Optimized Molecular Properties for **T2-TS2**

Number of (–) Vibrational Frequencies	1 (–193.8038)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.604486 hartree Enthalpy correction: 0.648185 hartree Free Energy correction: 0.519520 hartree Quasiharmonic Free Energy correction: 0.535992 hartree SCF Energy: –1757.737397 hartree SCF Energy + ZPVE: –1757.132911 hartree Enthalpy: –1757.089212 hartree Free Energy: –1757.217877 hartree Free Energy with quasiharmonic correction: –1757.201405 hartree (correction: 10.34 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.36912287 A.U.
Cartesian Coordinates	73 spD3–TS2–T2.out Energy: –1103393.2745981 O 0.08512 –4.02433 0.12913 C 4.15661 1.98229 –1.18990 O 3.07141 1.54291 –1.54332 O 4.97797 1.37723 –0.34197 C 4.51692 –2.08434 1.06410 C 3.55690 –3.06107 1.17171 N 3.93911 –0.95052 0.52559 C 2.66316 –1.24243 0.31789 N 2.38483 –2.51023 0.69973 H 3.60381 –4.07757 1.53312 H 4.56536 0.49763 –0.01155 H 1.48444 –3.00616 0.59706 H 1.93098 –0.56410 –0.09756 C 4.70393 3.31736 –1.65916 H 4.54968 4.06363 –0.87090 H 5.77934 3.25252 –1.84825 H 4.17669 3.64208 –2.55785 C 5.96585 –2.13325 1.43585 H 6.23538 –3.12056 1.82560 H 6.60753 –1.92337 0.57090 H 6.20771 –1.38836 2.20431 C –0.52672 –3.33739 –1.00242 C –0.73304 –0.81752 –1.11337 O –0.63658 0.29578 –0.56432 C –0.82129 –4.65946 1.03280 H –0.32096 –4.70691 2.00651 H –1.76982 –4.11466 1.11219

	H	−1.03950	−5.68433	0.70051
	C	−1.20001	−2.03954	−0.51941
	C	−3.21142	−2.26492	−0.65681
	C	−3.75497	−0.90121	−0.28227
	H	−3.19156	−2.38435	−1.76241
	O	−3.50679	−3.26082	0.07083
	C	−4.29153	−0.70485	0.99607
	C	−3.81543	0.14928	−1.20609
	C	−4.86357	0.51680	1.34810
	H	−4.26407	−1.54415	1.68488
	C	−4.39523	1.37120	−0.86289
	H	−3.40898	0.00008	−2.20520
	C	−4.92199	1.55995	0.41818
	H	−5.27501	0.65708	2.34577
	H	−4.43734	2.17722	−1.59237
	H	−5.37898	2.50985	0.68681
	H	−1.20983	−1.95506	0.56466
	O	−0.44946	−0.94410	−2.45197
	C	0.03790	0.23045	−3.10688
	H	0.17445	−0.05564	−4.15275
	H	0.99041	0.55925	−2.68019
	H	−0.68611	1.04785	−3.03450
	H	0.34697	−3.07077	−1.60732
	C	−1.35967	−4.31160	−1.84181
	H	−1.61289	−3.83059	−2.79315
	H	−0.76557	−5.20757	−2.06108
	H	−2.28789	−4.58609	−1.33569
	C	−0.94965	4.06873	0.13311
	O	−1.19239	5.26127	−0.05781
	C	−1.58746	3.34579	1.33012
	N	−1.02583	2.06264	1.69651
	H	−1.48725	4.00743	2.19243
	H	−2.65632	3.23731	1.10766
	H	−1.11844	1.28072	1.05011
	C	−0.31320	1.88956	2.84515
	O	−0.13259	2.77519	3.67975
	C	0.25510	0.48911	3.03820
	H	−0.12638	0.07726	3.97845
	H	1.34370	0.56289	3.13077
	H	0.01493	−0.19292	2.21843
	N	−0.15174	3.32995	−0.67603
	H	−0.09527	2.32356	−0.55463
	C	0.46784	3.90752	−1.85256
	H	−0.20960	3.91029	−2.71980
	H	0.73515	4.94533	−1.63805
	H	1.36311	3.33048	−2.09627

Optimized Molecular Properties for **T2-INT2**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.605349 hartree Enthalpy correction: 0.649323 hartree Free Energy correction: 0.519142 hartree Quasiharmonic Free Energy correction: 0.536990 hartree SCF Energy: –1757.739890 hartree SCF Energy + ZPVE: –1757.134541 hartree Enthalpy: –1757.090567 hartree Free Energy: –1757.220748 hartree Free Energy with quasiharmonic correction: –1757.202900 hartree (correction: 11.20 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.37043472 A.U.
Cartesian Coordinates	73 spD3–INT2–T2.out Energy: –1103394.0977964 O 0.62231 –3.87625 0.19764 C 4.00201 2.38533 –1.19968 O 2.92479 1.85804 –1.44297 O 4.93064 1.87532 –0.40306 C 4.86047 –1.55535 1.14573 C 4.00984 –2.62522 1.28534 N 4.16169 –0.50216 0.58696 C 2.92254 –0.93269 0.39961 N 2.78229 –2.21294 0.81320 H 4.16700 –3.62187 1.67007 H 4.61741 0.97749 –0.01335 H 1.93900 –2.80351 0.71499 H 2.12114 –0.34385 –0.02405 C 4.41257 3.73252 –1.76419 H 4.29870 4.49721 –0.98682 H 5.46420 3.72226 –2.06517 H 3.77616 3.99344 –2.61151 C 6.30891 –1.44188 1.50496 H 6.68415 –2.38566 1.91439 H 6.91875 –1.18564 0.62958 H 6.47562 –0.65789 2.25426 C –0.00455 –3.28293 –0.96649 C –0.61406 –0.83241 –1.07978 O –0.52437 0.21858 –0.44061 C –0.22378 –4.69098 1.02464 H 0.15520 –4.60482 2.04953 H –1.27258 –4.36423 0.95061

	H	−0.15178	−5.74233	0.71111
	C	−0.99643	−2.15647	−0.53040
	C	−2.59440	−2.59272	−0.78935
	C	−3.49193	−1.38498	−0.43967
	H	−2.63424	−2.68424	−1.90872
	O	−2.86259	−3.68534	−0.10801
	C	−4.12414	−1.36107	0.80845
	C	−3.75253	−0.34314	−1.33854
	C	−4.97216	−0.31193	1.16267
	H	−3.94516	−2.21085	1.46131
	C	−4.61027	0.70584	−0.99669
	H	−3.29119	−0.36479	−2.32542
	C	−5.22109	0.72773	0.26027
	H	−5.45323	−0.30660	2.13934
	H	−4.80821	1.50241	−1.71166
	H	−5.89440	1.53943	0.52806
	H	−0.95075	−2.05922	0.55649
	O	−0.40194	−0.85565	−2.41913
	C	−0.03698	0.39553	−3.02347
	H	0.06309	0.18222	−4.08943
	H	0.90830	0.76564	−2.61673
	H	−0.81812	1.14257	−2.85764
	H	0.85103	−2.81688	−1.46850
	C	−0.55986	−4.35130	−1.90962
	H	−0.79952	−3.89064	−2.87445
	H	0.20215	−5.12226	−2.07638
	H	−1.47322	−4.78512	−1.49424
	C	−1.59330	3.95303	0.11166
	O	−2.01547	5.07267	−0.17720
	C	−2.26546	3.14702	1.23400
	N	−1.57197	1.96130	1.69081
	H	−2.37005	3.81767	2.08910
	H	−3.27016	2.88057	0.88475
	H	−1.51858	1.15426	1.07619
	C	−0.94769	1.90656	2.90331
	O	−0.94527	2.83474	3.70914
	C	−0.27268	0.57543	3.20833
	H	−0.91965	−0.01451	3.86834
	H	0.66026	0.77147	3.74320
	H	−0.06617	−0.01022	2.30831
	N	−0.55246	3.36501	−0.52776
	H	−0.32040	2.39739	−0.33526
	C	0.12790	4.03224	−1.62106
	H	−0.47631	4.03849	−2.53982
	H	0.32183	5.07429	−1.34969
	H	1.07054	3.51402	−1.80995

Optimized Molecular Properties for **T2-TS3**

Number of (–) Vibrational Frequencies	1 (–1531.0551)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.601075 hartree Enthalpy correction: 0.644596 hartree Free Energy correction: 0.515182 hartree Quasiharmonic Free Energy correction: 0.532796 hartree SCF Energy: –1757.698727 hartree SCF Energy + ZPVE: –1757.097652 hartree Enthalpy: –1757.054131 hartree Free Energy: –1757.183545 hartree Free Energy with quasiharmonic correction: –1757.165931 hartree (correction: 11.05 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.32767378 A.U.
Cartesian Coordinates	73 spD3–TS3–T2.out Energy: –1103367.2649017 O 1.71575 –3.25688 –0.33355 C 5.10136 3.05960 –0.99809 O 4.09512 2.48487 –1.38494 O 6.00279 2.53907 –0.17442 C 5.84729 –0.99065 1.21926 C 4.98859 –2.06353 1.22121 N 5.25936 0.04845 0.52315 C 4.07590 –0.39409 0.12180 N 3.86808 –1.66719 0.52333 H 5.07494 –3.04981 1.65246 H 5.72421 1.58727 0.09494 H 3.03819 –2.24345 0.30678 H 3.36125 0.17654 –0.45304 C 5.46088 4.47398 –1.41487 H 5.50615 5.12122 –0.53210 H 6.45298 4.48864 –1.87886 H 4.71605 4.85618 –2.11452 C 7.20481 –0.86279 1.83641 H 7.96617 –0.62288 1.08347 H 7.23012 –0.06224 2.58640 H 7.49866 –1.79567 2.32900 C 0.84419 –2.47152 –1.21021 C –0.39445 –0.29283 –0.74270 O –1.37728 0.41035 –0.49318 C 1.11085 –4.27153 0.46859 H 1.91677 –4.69382 1.07891 H 0.32641 –3.86293 1.11805

	H	0.69779	−5.07709	−0.15536
	C	−0.26517	−1.71981	−0.48154
	C	−1.52751	−2.49115	0.00760
	C	−2.91897	−2.08631	−0.46640
	H	−1.42441	−3.54241	−0.33790
	O	−1.32554	−2.38970	1.40293
	C	−3.95639	−2.00561	0.46938
	C	−3.23000	−1.90769	−1.82167
	C	−5.26831	−1.74401	0.06431
	H	−3.70093	−2.15224	1.51378
	C	−4.53648	−1.64089	−2.23021
	H	−2.43704	−1.96639	−2.56441
	C	−5.56518	−1.55803	−1.28737
	H	−6.06099	−1.68638	0.80790
	H	−4.75294	−1.49059	−3.28621
	H	−6.58428	−1.34739	−1.60400
	H	−0.21718	−1.78416	0.83680
	O	0.76020	0.29280	−1.21295
	C	0.73489	1.71903	−1.33656
	H	1.74818	2.01496	−1.60975
	H	0.44869	2.18647	−0.38950
	H	0.02144	2.02820	−2.10832
	H	1.54674	−1.73657	−1.60547
	C	0.39110	−3.34138	−2.39030
	H	−0.08798	−2.71065	−3.14797
	H	1.25616	−3.83582	−2.84809
	H	−0.33122	−4.10872	−2.09576
	C	−4.19018	2.97452	0.08377
	O	−5.08382	3.77896	−0.18231
	C	−4.41971	1.92218	1.17923
	N	−3.26500	1.19005	1.64856
	H	−4.84947	2.44233	2.03756
	H	−5.17486	1.22654	0.79037
	H	−2.82646	0.50801	1.03642
	C	−2.74544	1.37547	2.90040
	O	−3.22390	2.16410	3.71488
	C	−1.51041	0.53824	3.19448
	H	−1.50670	−0.42016	2.66094
	H	−1.45187	0.37382	4.27344
	H	−0.61705	1.09993	2.89159
	N	−2.99328	2.93010	−0.55768
	H	−2.35670	2.15860	−0.37557
	C	−2.70348	3.80020	−1.67734
	H	−2.62895	3.23466	−2.61625
	H	−3.52113	4.51873	−1.75975
	H	−1.76049	4.34045	−1.52424

Optimized Molecular Properties for **T2-INT3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 23 positive frequencies below 100 cm^–1. Zero–point correction: 0.606231 hartree Enthalpy correction: 0.650146 hartree Free Energy correction: 0.519299 hartree Quasiharmonic Free Energy correction: 0.537513 hartree SCF Energy: –1757.764828 hartree SCF Energy + ZPVE: –1757.158597 hartree Enthalpy: –1757.114682 hartree Free Energy: –1757.245529 hartree Free Energy with quasiharmonic correction: –1757.227315 hartree (correction: 11.43 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.39375312 A.U.
Cartesian Coordinates	73 spD3–INT3–T2.out Energy: –1103408.7303132 O 1.64745 –0.37039 2.31524 C 8.65106 –0.27016 0.15887 O 8.00891 –0.13402 1.18929 O 8.13295 –0.42340 –1.05287 C 4.41493 –0.55606 –1.80614 C 3.22427 –0.48004 –1.12394 N 5.45981 –0.40705 –0.91017 C 4.90653 –0.24338 0.28211 N 3.55727 –0.27822 0.20052 H 2.18889 –0.53849 –1.43571 H 7.10190 –0.41446 –1.00726 H 2.88370 –0.19604 0.97611 H 5.46454 –0.10349 1.19690 C 10.17024 –0.28188 0.12834 H 10.52891 –1.22394 –0.30066 H 10.53760 0.52622 –0.51375 H 10.56371 –0.16032 1.13888 C 4.65155 –0.76209 –3.26973 H 5.20130 0.07937 –3.71070 H 5.24301 –1.66730 –3.45848 H 3.70108 –0.86107 –3.80352 C 0.43654 0.49276 2.41445 C –1.60215 –0.41203 1.24570 O –2.29860 –0.71891 0.21285 C 1.34995 –1.75459 2.33159 H 0.86887 –2.04361 3.27852 H 0.68843 –2.03534 1.50188

	H	2.29955	−2.29095	2.23489
	C	−0.46998	0.37824	1.23471
	C	−0.07095	0.94012	−0.11607
	C	−0.93504	2.11104	−0.62219
	H	0.95680	1.32066	−0.04759
	O	0.00160	−0.07711	−1.13651
	C	−0.98741	2.39596	−1.99427
	C	−1.63424	2.95111	0.25284
	C	−1.71401	3.48525	−2.47583
	H	−0.46145	1.73800	−2.67844
	C	−2.36137	4.04465	−0.22445
	H	−1.62082	2.72593	1.31494
	C	−2.40458	4.31790	−1.59227
	H	−1.74532	3.68224	−3.54564
	H	−2.89976	4.68080	0.47542
	H	−2.97446	5.16562	−1.96611
	H	−0.85379	−0.54702	−1.02403
	O	−2.02243	−0.89172	2.48841
	C	−2.88728	−2.01805	2.46814
	H	−3.10192	−2.24685	3.51607
	H	−2.40586	−2.88914	2.00203
	H	−3.82359	−1.81437	1.94038
	H	−0.09693	0.14171	3.30477
	C	1.01198	1.87996	2.70182
	H	1.55895	2.28001	1.84083
	H	1.70463	1.83643	3.54982
	H	0.20547	2.57998	2.94212
	C	−5.22242	−2.22407	−1.58789
	O	−5.90626	−2.92524	−2.33475
	C	−5.58753	−0.74181	−1.41560
	N	−5.04361	−0.05108	−0.26484
	H	−6.67498	−0.68202	−1.34786
	H	−5.29177	−0.23877	−2.34871
	H	−4.02966	−0.03368	−0.12514
	C	−5.84521	0.59965	0.62675
	O	−7.07224	0.63709	0.54374
	C	−5.08954	1.32397	1.73547
	H	−4.22496	0.75694	2.09485
	H	−4.71717	2.28352	1.35670
	H	−5.77932	1.51710	2.55986
	N	−4.12217	−2.67067	−0.92763
	H	−3.52118	−2.01853	−0.41932
	C	−3.63915	−4.02529	−1.10518
	H	−4.40230	−4.58626	−1.64724
	H	−2.70436	−4.04818	−1.68185
	H	−3.45483	−4.50272	−0.13478

Optimized Molecular Properties for **T2-TS4**

Number of (–) Vibrational Frequencies	1 (–834.7400)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 23 positive frequencies below 100 cm^–1. Zero–point correction: 0.597277 hartree Enthalpy correction: 0.642227 hartree Free Energy correction: 0.507033 hartree Quasiharmonic Free Energy correction: 0.527643 hartree SCF Energy: –1757.740064 hartree SCF Energy + ZPVE: –1757.142787 hartree Enthalpy: –1757.097837 hartree Free Energy: –1757.233031 hartree Free Energy with quasiharmonic correction: –1757.212421 hartree (correction: 12.93 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.37610812 A.U.
Cartesian Coordinates	73 spD3–TS4–T2.out Energy: –1103397.6579087 O 2.03561 –1.28265 2.11037 C 8.69411 –0.04580 –0.16527 O 8.23118 –0.34168 0.92825 O 8.00334 0.13920 –1.27421 C 4.35996 –0.12609 –1.75303 C 3.22627 –0.42176 –1.02593 N 5.44788 –0.21087 –0.90914 C 4.94850 –0.55010 0.28316 N 3.61122 –0.69036 0.27063 H 2.18762 –0.46979 –1.32888 H 6.96026 –0.00477 –1.11151 H 2.82849 –0.97903 1.22295 H 5.56812 –0.69259 1.15850 C 10.18918 0.15224 –0.38782 H 10.55115 –0.55093 –1.14645 H 10.38170 1.16229 –0.76675 H 10.73081 –0.00195 0.54753 C 4.49812 0.23208 –3.20081 H 4.95797 1.22075 –3.33525 H 5.12842 –0.48718 –3.74166 H 3.51716 0.25024 –3.68842 C 0.62414 0.38636 2.31240 C –1.53009 –0.49440 1.55002 O –2.39952 –0.70116 0.67756 C 1.38509 –2.44014 1.69393 H 1.08096 –3.06402 2.55262 H 0.46965 –2.22310 1.10452

	H	2.03134	−3.05612	1.04388
	C	−0.35406	0.31642	1.34504
	C	−0.25498	0.97236	−0.02551
	C	−1.24926	2.12890	−0.21946
	H	0.75150	1.38816	−0.13296
	O	−0.35414	0.02355	−1.09149
	C	−1.82433	2.36262	−1.47539
	C	−1.55562	3.00925	0.82731
	C	−2.69145	3.43850	−1.67729
	H	−1.57879	1.68825	−2.28919
	C	−2.41484	4.09084	0.62630
	H	−1.12379	2.83698	1.80936
	C	−2.99058	4.30900	−0.62747
	H	−3.13241	3.59773	−2.65870
	H	−2.63844	4.76184	1.45282
	H	−3.66296	5.14907	−0.78440
	H	−1.15600	−0.49283	−0.88702
	O	−1.67036	−1.02931	2.79169
	C	−2.77521	−1.91176	2.98317
	H	−2.71741	−2.22735	4.02648
	H	−2.69987	−2.78451	2.32628
	H	−3.72756	−1.40717	2.79481
	H	0.39116	−0.07629	3.26310
	C	1.74891	1.38058	2.35578
	H	2.17501	1.58965	1.37198
	H	2.55013	1.00171	2.99334
	H	1.38907	2.33003	2.78043
	C	−4.88594	−2.18678	−1.91867
	O	−5.24236	−2.90845	−2.84793
	C	−5.33530	−0.71741	−1.89989
	N	−4.97521	0.07329	−0.74181
	H	−6.42563	−0.70975	−1.96358
	H	−4.94914	−0.26165	−2.82078
	H	−3.99788	0.26187	−0.54861
	C	−5.91740	0.57753	0.11482
	O	−7.12282	0.39636	−0.03064
	C	−5.35193	1.41955	1.24882
	H	−4.37942	1.05268	1.58922
	H	−5.21254	2.45173	0.90671
	H	−6.06614	1.42013	2.07499
	N	−4.09113	−2.59404	−0.89652
	H	−3.77695	−1.92237	−0.20377
	C	−3.54206	−3.93472	−0.84261
	H	−3.78991	−4.43679	−1.77947
	H	−2.45322	−3.89966	−0.72274
	H	−3.96668	−4.51173	−0.00990

Optimized Molecular Properties for **T2-product**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 25 positive frequencies below 100 cm^–1. Zero–point correction: 0.602455 hartree Enthalpy correction: 0.648494 hartree Free Energy correction: 0.508452 hartree Quasiharmonic Free Energy correction: 0.531358 hartree SCF Energy: –1757.756538 hartree SCF Energy + ZPVE: –1757.154083 hartree Enthalpy: –1757.108044 hartree Free Energy: –1757.248086 hartree Free Energy with quasiharmonic correction: –1757.225180 hartree (correction: 14.37 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.39277927 A.U.
Cartesian Coordinates	73 spD3–product–T2.out Energy: –1103408.1192132 O –2.59035 –1.29475 –2.17315 C –9.02705 1.39607 –0.13070 O –8.20103 1.56662 –1.05021 O –8.91065 0.62550 0.88386 C –5.93715 –1.46206 1.47713 C –4.72913 –1.73645 0.87499 N –6.55960 –0.54733 0.65813 C –5.73266 –0.30719 –0.37830 N –4.60222 –1.00851 –0.29191 H –3.94982 –2.41045 1.20973 H –7.53296 –0.07639 0.77485 H –3.32829 –1.16929 –1.50725 H –6.01514 0.38557 –1.15853 C –10.35520 2.18322 –0.18153 H –11.20266 1.48617 –0.19565 H –10.46286 2.79451 0.72338 H –10.39853 2.82762 –1.06460 C –6.55565 –1.97278 2.73909 H –6.75484 –1.16366 3.45393 H –7.51426 –2.47373 2.55096 H –5.88780 –2.69340 3.22368 C –0.57754 0.09069 –0.22930 C 1.54666 –0.98237 0.36110 O 2.58572 –1.02818 1.02753 C –2.96164 –2.35029 –3.02440 H –2.16373 –2.49119 –3.76496 H –3.09585 –3.30819 –2.49155

	H	−3.89638	−2.14705	−3.57406
	C	0.63544	0.18338	0.35848
	C	1.17597	1.42170	1.07748
	C	2.25771	2.13945	0.25343
	H	0.34746	2.12450	1.20449
	O	1.60928	1.12715	2.39942
	C	3.48234	2.49231	0.82829
	C	2.01694	2.49246	−1.08244
	C	4.45633	3.16254	0.08162
	H	3.66141	2.24425	1.86817
	C	2.98091	3.17258	−1.82765
	H	1.06995	2.22737	−1.54526
	C	4.21112	3.50394	−1.25053
	H	5.40326	3.42534	0.54738
	H	2.77168	3.44368	−2.85966
	H	4.96325	4.03418	−1.82954
	H	2.17100	0.33398	2.30598
	O	1.16351	−2.01097	−0.40902
	C	1.96019	−3.21065	−0.32970
	H	1.39894	−3.95637	−0.89311
	H	2.07459	−3.52056	0.71193
	H	2.94558	−3.05573	−0.77664
	H	−0.84804	−0.84173	−0.72173
	C	−1.64630	1.12753	−0.32332
	H	−1.40238	2.08480	0.14412
	H	−2.57284	0.73177	0.11371
	H	−1.88827	1.28785	−1.38169
	C	6.65258	−0.40081	1.16572
	O	7.69191	−0.21746	1.79664
	C	6.71336	−0.52713	−0.36389
	N	5.50476	−0.20763	−1.09992
	H	6.95995	−1.56487	−0.60951
	H	7.54642	0.10436	−0.69018
	H	5.19048	0.75484	−1.11493
	C	4.83011	−1.13675	−1.84573
	O	5.13488	−2.32768	−1.85313
	C	3.67858	−0.60126	−2.68012
	H	3.57021	0.48501	−2.63449
	H	3.84058	−0.90668	−3.71867
	H	2.74100	−1.05909	−2.35080
	N	5.42732	−0.53962	1.72585
	H	4.62206	−0.73056	1.13983
	C	5.22826	−0.52207	3.16199
	H	6.16301	−0.20333	3.62598
	H	4.42831	0.17652	3.43212
	H	4.96244	−1.51681	3.54171

Optimized Molecular Properties for **T3-TS2**

Number of (–) Vibrational Frequencies	1 (–55.3448)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 24 positive frequencies below 100 cm^–1. Zero–point correction: 0.627886 hartree Enthalpy correction: 0.675061 hartree Free Energy correction: 0.535388 hartree Quasiharmonic Free Energy correction: 0.556078 hartree SCF Energy: –1834.180059 hartree SCF Energy + ZPVE: –1833.552173 hartree Enthalpy: –1833.504998 hartree Free Energy: –1833.644671 hartree Free Energy with quasiharmonic correction: –1833.623981 hartree (correction: 12.98 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1834.86010943 A.U.
Cartesian Coordinates	76 spD3–TS2–T3.out Energy: –1151392.0929577 O –1.34441 –2.89847 –0.76038 C –5.89135 3.06922 –0.77378 O –4.69076 2.88101 –0.89143 O –6.80347 2.11397 –0.62222 C –5.92364 –1.60329 –0.35547 C –4.78604 –2.37413 –0.37969 N –5.57042 –0.28386 –0.56734 C –4.25249 –0.27033 –0.71274 N –3.73543 –1.51254 –0.60780 C –6.51862 4.45169 –0.78558 C –7.34585 –2.01824 –0.14264 C –0.30892 –2.74110 0.30181 C 0.65512 –0.48574 –0.38789 O 1.50164 0.27318 –0.89027 C –0.86738 –3.24052 –2.04883 C 0.83552 –1.85789 –0.06022 C 2.33812 –1.51109 1.76300 C 1.56228 –0.53023 2.57010 O 3.41927 –1.20268 1.21322 C 1.90399 0.83003 2.54227 C 0.52808 –0.95579 3.41620 C 1.21213 1.74456 3.33447 C –0.16389 –0.04117 4.20780 C 0.17521 1.31409 4.16772 H 1.69444 –2.32123 –0.53494 O –0.58918 0.01061 –0.03272 C –0.76638 1.41466 –0.21225

	C	0.11681	−4.14550	0.74015
	C	4.66977	2.66005	−0.36384
	O	5.27549	3.68535	−0.04909
	C	5.45012	1.34359	−0.51763
	N	4.73600	0.20768	−1.05632
	C	4.77222	−0.08738	−2.39617
	O	5.50054	0.50874	−3.18701
	C	3.85419	−1.22544	−2.80878
	N	3.32968	2.59863	−0.56760
	C	2.49103	3.77353	−0.45212
	H	−0.96625	−0.38345	4.85721
	H	−0.36272	2.02935	4.78536
	H	1.48633	2.79668	3.30762
	H	2.71456	1.14907	1.89655
	H	0.26948	−2.01227	3.45222
	H	0.66490	−4.10978	1.68783
	H	0.77730	−4.61479	0.00188
	H	−0.76302	−4.78416	0.87594
	H	−0.45077	−4.25862	−2.07628
	H	2.12437	−2.56449	2.00195
	H	−0.10040	−2.53895	−2.39938
	H	−1.72846	−3.19994	−2.72409
	H	−0.90956	−2.27823	1.09224
	H	−7.77879	−1.52824	0.73868
	H	−7.97493	−1.75035	−1.00100
	H	−7.41825	−3.10109	0.00396
	H	2.81371	−0.93017	−2.63392
	H	4.05132	−2.11740	−2.20227
	H	4.01470	−1.44371	−3.86644
	H	4.05272	−0.25266	−0.45658
	H	6.29412	1.55828	−1.17642
	H	5.84812	1.09433	0.47305
	H	2.87392	1.71164	−0.77517
	H	1.89093	3.91262	−1.35921
	H	1.80680	3.69620	0.40317
	H	−5.74476	5.20918	−0.91838
	H	−1.80799	1.62372	0.04141
	H	−0.10867	1.98364	0.45156
	H	−7.25324	4.52283	−1.59513
	H	−0.56454	1.71174	−1.24629
	H	−7.05403	4.62715	0.15397
	H	3.14303	4.63720	−0.30919
	O	4.99128	−3.09967	−0.12490
	H	4.39724	−2.53234	0.41838
	H	5.62317	−2.44894	−0.46669
	H	−2.74555	−1.79941	−0.66993
	H	−6.35071	1.19380	−0.60756
	H	−3.67057	0.62065	−0.89316
	H	−4.62999	−3.43514	−0.25461

Optimized Molecular Properties for **T3-INT2**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 25 positive frequencies below 100 cm^–1. Zero–point correction: 0.630434 hartree Enthalpy correction: 0.677271 hartree Free Energy correction: 0.539420 hartree Quasiharmonic Free Energy correction: 0.558809 hartree SCF Energy: –1834.190324 hartree SCF Energy + ZPVE: –1833.559890 hartree Enthalpy: –1833.513053 hartree Free Energy: –1833.650904 hartree Free Energy with quasiharmonic correction: –1833.631514 hartree (correction: 12.17 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1834.87132759 A.U.
Cartesian Coordinates	76 spD3–INT2–T3.out Energy: –1151399.1324593 O –1.18018 –2.65747 –0.05988 C –5.58770 2.81801 –0.88059 O –4.40501 2.51778 –0.83162 O –6.59545 1.95307 –0.81849 C –6.06332 –1.84240 –0.45542 C –4.99353 –2.69401 –0.31581 N –5.59220 –0.54615 –0.54978 C –4.27220 –0.62405 –0.46875 N –3.86366 –1.90339 –0.32735 C –6.07569 4.24746 –1.02139 C –7.52485 –2.16036 –0.50758 C –0.44693 –2.12322 1.08625 C 0.51243 –0.26012 –0.36321 O 1.27829 0.09543 –1.24582 C –0.49843 –3.58269 –0.89620 C 0.79920 –1.35632 0.62633 C 1.78360 –0.78839 1.81929 C 1.36348 0.62445 2.26038 O 3.07677 –0.88872 1.45400 C 2.15858 1.72174 1.91434 C 0.21918 0.85255 3.03638 C 1.80617 3.01538 2.30597 C –0.13795 2.14176 3.43425 C 0.65383 3.23210 3.06506 H 1.47161 –2.05986 0.13459 O –0.66883 0.36985 –0.14777 C –0.89358 1.55311 –0.93303

	C	−0.15275	−3.24912	2.08691
	C	5.00279	1.96993	−1.05730
	O	5.70793	2.97910	−1.01175
	C	5.57504	0.60799	−0.63341
	N	4.69782	−0.53042	−0.77753
	C	4.84017	−1.39281	−1.82450
	O	5.71450	−1.27763	−2.68644
	C	3.80989	−2.51260	−1.86164
	N	3.70615	1.96418	−1.45775
	C	3.00873	3.17543	−1.82813
	H	−1.03174	2.29517	4.03587
	H	0.37996	4.23828	3.37532
	H	2.44109	3.85392	2.02709
	H	3.06436	1.53115	1.35030
	H	−0.39892	0.00980	3.34321
	H	−0.03840	−2.84327	3.09628
	H	0.77164	−3.78701	1.85082
	H	−0.99774	−3.94778	2.10205
	H	−0.06975	−4.41374	−0.32311
	H	1.53751	−1.45175	2.67548
	H	0.30026	−3.10396	−1.47469
	H	−1.24646	−3.97758	−1.59069
	H	−1.17654	−1.43133	1.51507
	H	−8.07226	−1.65905	0.30040
	H	−7.97288	−1.83036	−1.45327
	H	−7.69320	−3.23813	−0.41183
	H	2.83065	−2.08840	−2.11596
	H	3.71245	−3.00893	−0.88849
	H	4.10197	−3.23211	−2.63009
	H	3.98463	−0.69218	−0.03849
	H	6.47058	0.43768	−1.23669
	H	5.88355	0.71202	0.41368
	H	3.17799	1.09898	−1.40196
	H	2.49215	3.04826	−2.78686
	H	2.26678	3.45968	−1.06956
	H	−5.22382	4.92700	−1.07223
	H	−1.89354	1.90436	−0.67706
	H	−0.14730	2.31202	−0.68283
	H	−6.68719	4.34701	−1.92478
	H	−0.82697	1.32491	−2.00028
	H	−6.71144	4.51036	−0.16894
	H	3.74973	3.97274	−1.91470
	O	3.29409	−3.51048	1.40488
	H	3.28988	−2.49367	1.45365
	H	4.19519	−3.74760	1.66961
	H	−2.88406	−2.21160	−0.24301
	H	−6.23566	1.00023	−0.72074
	H	−3.60379	0.22247	−0.50510
	H	−4.94080	−3.76759	−0.21127

Optimized Molecular Properties for **T3-TS3**

Number of (–) Vibrational Frequencies	1 (–833.6959)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.627426 hartree Enthalpy correction: 0.672902 hartree Free Energy correction: 0.540825 hartree Quasiharmonic Free Energy correction: 0.557365 hartree SCF Energy: –1834.159136 hartree SCF Energy + ZPVE: –1833.531710 hartree Enthalpy: –1833.486234 hartree Free Energy: –1833.618311 hartree Free Energy with quasiharmonic correction: –1833.601771 hartree (correction: 10.38 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1834.84115776 A.U.
Cartesian Coordinates	76 spD3–TS3–T3.out Energy: –1151380.2006053 O 1.50959 –3.02072 0.42151 C 5.57088 2.54547 –1.80538 O 4.48575 2.03108 –2.02763 O 6.44216 2.11803 –0.89889 C 5.95866 –0.97077 1.25286 C 4.98266 –1.89592 1.53445 N 5.44410 –0.03318 0.37757 C 4.18861 –0.38836 0.14516 N 3.86487 –1.50957 0.82597 C 6.07734 3.76858 –2.54783 C 7.36662 –0.89651 1.75496 C 0.66370 –2.39535 –0.60620 C –0.28782 –0.02065 –0.64523 O –1.17795 0.82098 –0.59506 C 0.86174 –3.78891 1.42434 C –0.32746 –1.36344 –0.04317 C –1.74618 –1.85970 0.34053 C –2.88039 –1.76295 –0.68476 O –2.21777 –1.27232 1.55673 C –4.19525 –1.96527 –0.23572 C –2.68159 –1.56878 –2.05580 C –5.26907 –1.98116 –1.12461 C –3.75308 –1.59224 –2.95267 C –5.05322 –1.80042 –2.49246 H 0.11228 –1.06971 1.15058 O 0.92155 0.29537 –1.22011 C 1.03920 1.64264 –1.69877

	C	0.11370	−3.50425	−1.51494
	C	−4.93255	1.99323	0.41986
	O	−6.12390	2.23407	0.21566
	C	−4.46186	1.62700	1.83774
	N	−3.03503	1.53279	2.04513
	C	−2.32396	2.58252	2.55643
	O	−2.85874	3.63043	2.92311
	C	−0.81863	2.38233	2.60754
	N	−3.97150	2.01582	−0.53500
	C	−4.27880	2.26714	−1.92635
	H	−3.56747	−1.43615	−4.01340
	H	−5.88898	−1.81080	−3.18822
	H	−6.27836	−2.12877	−0.74727
	H	−4.36357	−2.09852	0.82786
	H	−1.68281	−1.37952	−2.43423
	H	−0.26634	−3.07509	−2.44591
	H	−0.70686	−4.06979	−1.06323
	H	0.92035	−4.20361	−1.76370
	H	0.26170	−4.60181	0.99311
	H	−1.63369	−2.94338	0.52593
	H	0.23145	−3.16359	2.06528
	H	1.65655	−4.23806	2.03075
	H	1.41026	−1.85019	−1.18391
	H	2.96165	−2.00343	0.78270
	H	4.98678	−2.77262	2.16501
	H	8.08864	−0.92945	0.92930
	H	7.54699	0.03646	2.30349
	H	7.58523	−1.73169	2.42877
	H	3.50148	0.13570	−0.50259
	H	6.06435	1.29832	−0.40939
	H	−0.39137	2.73290	1.65932
	H	−0.51076	1.33772	2.73846
	H	−0.41547	3.00661	3.40981
	H	−2.57196	0.65972	1.78377
	H	−4.85933	2.39328	2.50710
	H	−4.93519	0.67130	2.09142
	H	−3.03644	1.69307	−0.30416
	H	−3.66337	3.08592	−2.32130
	H	−4.10454	1.37255	−2.53632
	H	5.35749	4.06334	−3.31288
	H	2.06449	1.74581	−2.05535
	H	0.32404	1.82878	−2.50669
	H	6.22658	4.59431	−1.84334
	H	0.84283	2.35578	−0.89332
	H	7.04812	3.55526	−3.00797
	H	−5.33275	2.54540	−1.98817
	O	0.10143	−0.77394	2.47262
	H	0.77046	−1.28547	2.95168
	H	−1.40603	−1.19081	2.15789

Optimized Molecular Properties for **T3-INT3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 23 positive frequencies below 100 cm^–1. Zero–point correction: 0.631005 hartree Enthalpy correction: 0.677772 hartree Free Energy correction: 0.542723 hartree Quasiharmonic Free Energy correction: 0.559581 hartree SCF Energy: –1834.180549 hartree SCF Energy + ZPVE: –1833.549544 hartree Enthalpy: –1833.502777 hartree Free Energy: –1833.637826 hartree Free Energy with quasiharmonic correction: –1833.620968 hartree (correction: 10.58 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1834.86371608 A.U.
Cartesian Coordinates	76 spD3–INT3–T3.out Energy: –1151394.3561647 O 1.57733 –2.37664 0.83421 C 5.74225 3.05246 –1.03892 O 4.57200 2.75030 –0.86899 O 6.77408 2.24294 –0.82082 C 6.42882 –1.34708 0.41202 C 5.43070 –2.22937 0.74942 N 5.85502 –0.14665 0.03845 C 4.54411 –0.30846 0.15151 N 4.24097 –1.55403 0.57998 C 6.18555 4.41798 –1.53071 C 7.91179 –1.54982 0.41358 C 0.85999 –2.01187 –0.51249 C –0.31445 0.17780 –0.29232 O –1.25050 0.98036 –0.08607 C 1.10035 –3.51193 1.54130 C –0.37297 –1.23050 –0.32787 C –1.66617 –1.90459 0.05100 C –2.85160 –1.74877 –0.90455 O –2.14265 –1.57043 1.38722 C –4.14573 –2.08847 –0.48205 C –2.66578 –1.38413 –2.24180 C –5.22267 –2.05109 –1.36888 C –3.74037 –1.34878 –3.13292 C –5.02507 –1.68078 –2.70096 O 0.96941 0.71199 –0.49070 C 1.02567 2.12978 –0.62795 C 0.79072 –3.28508 –1.35594

	C	−5.16048	1.68577	−0.18854
	O	−6.22305	2.00753	−0.72462
	C	−5.17743	1.01927	1.19886
	N	−3.90609	0.90365	1.88223
	C	−3.47159	1.89467	2.71385
	O	−4.16820	2.85270	3.04559
	C	−2.03431	1.73734	3.18958
	N	−3.94929	1.87224	−0.75574
	C	−3.83958	2.42851	−2.08803
	H	−3.57309	−1.05271	−4.16660
	H	−5.86497	−1.64418	−3.39057
	H	−6.22023	−2.30727	−1.01857
	H	−4.30080	−2.37764	0.55305
	H	−1.66497	−1.11786	−2.56897
	H	0.52533	−3.00968	−2.38187
	H	0.03582	−3.99668	−1.00642
	H	1.76042	−3.79810	−1.37868
	H	1.29191	−4.44889	0.99957
	H	−1.46887	−2.98977	0.06151
	H	0.02684	−3.43527	1.75453
	H	1.63512	−3.54538	2.49681
	H	1.62879	−1.36442	−0.93046
	H	8.33784	−1.39594	−0.58584
	H	8.41200	−0.84416	1.08873
	H	8.16639	−2.56471	0.73684
	H	−1.36912	1.89589	2.33186
	H	−1.84267	0.73509	3.58724
	H	−1.83167	2.48427	3.95926
	H	−3.26608	0.15118	1.61771
	H	−5.85023	1.61248	1.82137
	H	−5.61690	0.02426	1.07160
	H	−3.10295	1.48492	−0.33938
	H	−2.77837	2.54677	−2.31963
	H	−4.30083	1.77406	−2.83877
	H	5.31419	5.05274	−1.69799
	H	2.07763	2.37731	−0.78498
	H	0.42742	2.47161	−1.48094
	H	6.84970	4.88329	−0.79419
	H	0.65031	2.63654	0.26766
	H	6.75502	4.31374	−2.46072
	H	−4.33704	3.40347	−2.14153
	O	0.29268	−0.72001	2.76246
	H	3.28658	−1.92225	0.72988
	H	5.46462	−3.25406	1.08901
	H	3.80245	0.44506	−0.07181
	H	6.43537	1.33343	−0.49182
	H	0.83700	−1.11968	2.04786
	H	0.12792	0.17872	2.43747
	H	−1.34338	−1.34960	1.91394

Optimized Molecular Properties for **T3-TS4**

Number of (–) Vibrational Frequencies	1 (–208.6407)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.629438 hartree Enthalpy correction: 0.675734 hartree Free Energy correction: 0.542074 hartree Quasiharmonic Free Energy correction: 0.558272 hartree SCF Energy: –1834.179218 hartree SCF Energy + ZPVE: –1833.549780 hartree Enthalpy: –1833.503484 hartree Free Energy: –1833.637144 hartree Free Energy with quasiharmonic correction: –1833.620946 hartree (correction: 10.16 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1834.86221556 A.U.
Cartesian Coordinates	76 spD3–TS4–T3.out Energy: –1151393.4145742 O 1.63548 –2.42888 0.84964 C 5.68619 3.07273 –1.09612 O 4.51250 2.77115 –0.94608 O 6.71486 2.27423 –0.83609 C 6.40008 –1.27137 0.47769 C 5.41092 –2.16506 0.81395 N 5.81073 –0.09417 0.05873 C 4.50025 –0.28398 0.14569 N 4.21122 –1.52281 0.59869 C 6.13455 4.42852 –1.61139 C 7.88651 –1.44226 0.52202 C 0.80195 –1.95616 –0.66271 C –0.31122 0.21988 –0.30140 O –1.25234 1.00148 –0.08614 C 1.36179 –3.70521 1.38053 C –0.37930 –1.20215 –0.40516 C –1.68327 –1.88095 –0.04755 C –2.84875 –1.69989 –1.02076 O –2.16747 –1.55522 1.27543 C –4.15576 –2.00884 –0.61552 C –2.63685 –1.33286 –2.35364 C –5.22023 –1.93931 –1.51490 C –3.69899 –1.26755 –3.25805 C –4.99677 –1.56864 –2.84287 O 0.96417 0.74946 –0.46682 C 1.03547 2.17559 –0.50921 C 0.75955 –3.25511 –1.44484

	C	−5.18589	1.69691	−0.04247
	O	−6.26806	2.01043	−0.54231
	C	−5.15127	1.00999	1.33410
	N	−3.85279	0.85345	1.95422
	C	−3.38181	1.78176	2.83654
	O	−4.05223	2.72817	3.24655
	C	−1.93829	1.56454	3.27062
	N	−3.99432	1.91301	−0.64057
	C	−3.92999	2.48627	−1.96901
	H	−3.51127	−0.97202	−4.28831
	H	−5.82683	−1.50852	−3.54267
	H	−6.22823	−2.16991	−1.17755
	H	−4.32930	−2.29933	0.41601
	H	−1.62730	−1.08752	−2.67091
	H	0.45798	−3.03252	−2.47547
	H	0.04180	−3.97886	−1.04734
	H	1.74572	−3.73039	−1.47590
	H	1.76106	−4.52214	0.75724
	H	−1.48363	−2.96587	−0.05002
	H	0.28122	−3.87536	1.51084
	H	1.82467	−3.78415	2.37528
	H	1.62514	−1.32989	−0.99106
	H	8.33607	−1.30803	−0.47008
	H	8.35527	−0.70778	1.18916
	H	8.15326	−2.44210	0.88078
	H	−1.28504	1.70939	2.40174
	H	−1.77770	0.54939	3.64951
	H	−1.69070	2.29047	4.04718
	H	−3.23538	0.10161	1.63576
	H	−5.77782	1.60800	1.99922
	H	−5.62400	0.02909	1.21203
	H	−3.13539	1.53043	−0.25044
	H	−2.87821	2.63113	−2.22697
	H	−4.39545	1.83006	−2.71532
	H	5.26476	5.05601	−1.81150
	H	2.08227	2.41969	−0.69796
	H	0.40088	2.57859	−1.30591
	H	6.78231	4.91383	−0.87319
	H	0.70895	2.61852	0.43796
	H	6.72301	4.30436	−2.52707
	H	−4.44988	3.45033	−1.99760
	O	0.19837	−1.09183	2.75397
	H	3.25054	−1.91303	0.73682
	H	5.45891	−3.17933	1.18239
	H	3.74959	0.44861	−0.11337
	H	6.37501	1.36695	−0.49059
	H	0.79163	−1.47008	2.05107
	H	0.19873	−0.14117	2.56538
	H	−1.37199	−1.47765	1.85509

Optimized Molecular Properties for **T3-product**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 28 positive frequencies below 100 cm^–1. Zero–point correction: 0.628800 hartree Enthalpy correction: 0.676832 hartree Free Energy correction: 0.536382 hartree Quasiharmonic Free Energy correction: 0.555848 hartree SCF Energy: –1834.208989 hartree SCF Energy + ZPVE: –1833.580189 hartree Enthalpy: –1833.532157 hartree Free Energy: –1833.672607 hartree Free Energy with quasiharmonic correction: –1833.653140 hartree (correction: 12.22 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1834.89161548 A.U.
Cartesian Coordinates	76 spD3–product–T3.out Energy: –1151411.8633024 O 2.36929 –2.82289 1.96235 C 4.93034 3.14093 –1.09493 O 3.88035 2.70390 –0.56273 O 6.02824 2.51284 –1.22491 C 6.41487 –0.99923 –0.10604 C 5.65920 –1.98639 0.48601 N 5.58040 0.09046 –0.21149 C 4.38613 –0.26071 0.30431 N 4.38596 –1.51880 0.74213 C 4.89162 4.57249 –1.66301 C 7.83364 –0.98210 –0.57706 C 0.90281 –1.47992 –1.13998 C –0.41397 0.52660 –0.62222 O –1.48100 1.11746 –0.67894 C 2.89933 –3.44261 3.11934 C –0.25557 –0.95851 –0.69158 C –1.42913 –1.78821 –0.18789 C –2.63421 –1.84175 –1.12039 O –1.84415 –1.34830 1.10397 C –3.91799 –2.03558 –0.59671 C –2.47581 –1.79964 –2.51063 C –5.02097 –2.16512 –1.44191 C –3.57551 –1.94031 –3.35816 C –4.85395 –2.12075 –2.82736 O 0.76608 1.15754 –0.48180 C 0.76071 2.60269 –0.55996

	C	1.26198	−2.92915	−1.29255
	C	−5.46708	1.16961	0.24589
	O	−6.65044	1.08830	−0.08515
	C	−5.05183	0.80150	1.67866
	N	−3.64219	0.88579	1.99625
	C	−3.15879	1.85788	2.82946
	O	−3.87416	2.70201	3.36392
	C	−1.64949	1.83581	3.02496
	N	−4.48471	1.58971	−0.58311
	C	−4.76625	1.88130	−1.97550
	H	−3.43224	−1.89840	−4.43545
	H	−5.71323	−2.21971	−3.48601
	H	−6.01330	−2.28619	−1.01589
	H	−4.04568	−2.07799	0.47950
	H	−1.48661	−1.64332	−2.93171
	H	1.87580	−3.07357	−2.18900
	H	0.39498	−3.59120	−1.36202
	H	1.86576	−3.24347	−0.43033
	H	3.62448	−4.22991	2.86200
	H	−1.06579	−2.82172	−0.08852
	H	2.07311	−3.90718	3.66839
	H	3.39769	−2.72455	3.78794
	H	1.69367	−0.78039	−1.39957
	H	7.90454	−0.76845	−1.65133
	H	8.42580	−0.21631	−0.05976
	H	8.30521	−1.95357	−0.39439
	H	−1.15978	2.19573	2.11235
	H	−1.26702	0.83102	3.23231
	H	−1.39451	2.50388	3.84935
	H	−3.00637	0.17848	1.62445
	H	−5.57718	1.48253	2.35317
	H	−5.43347	−0.20951	1.86613
	H	−3.51489	1.48102	−0.30917
	H	−3.85817	2.27685	−2.43618
	H	−5.08224	0.98317	−2.52038
	H	4.21216	4.60563	−2.52440
	H	1.81601	2.88716	−0.58313
	H	0.23009	2.91999	−1.46203
	H	4.48977	5.26224	−0.91180
	H	0.24789	3.01784	0.31316
	H	5.88328	4.90731	−1.98027
	H	−5.56745	2.62343	−2.05081
	O	0.46838	−0.96023	2.47819
	H	3.12762	−2.32752	1.49537
	H	5.95506	−2.99665	0.74010
	H	3.56399	0.44039	0.32619
	H	5.79276	1.06374	−0.62169
	H	1.14487	−1.67501	2.31655
	H	0.82548	−0.19499	2.00023
	H	−1.02959	−1.30900	1.67453

Optimized Molecular Properties for **T4-TS2**

Number of (–) Vibrational Frequencies	1 (–44.6977)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 26 positive frequencies below 100 cm^–1. Zero–point correction: 0.656167 hartree Enthalpy correction: 0.705177 hartree Free Energy correction: 0.560662 hartree Quasiharmonic Free Energy correction: 0.581962 hartree SCF Energy: –1873.484741 hartree SCF Energy + ZPVE: –1872.828574 hartree Enthalpy: –1872.779564 hartree Free Energy: –1872.924079 hartree Free Energy with quasiharmonic correction: –1872.902778 hartree (correction: 13.37 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1874.16794735 A.U.
Cartesian Coordinates	79 spD3–TS2–T4.out Energy: –1176058.1334584 O –1.38373 –2.90776 –0.95000 C –6.01399 2.98549 –0.65238 O –4.80908 2.82337 –0.76442 O –6.91093 2.00909 –0.55586 C –5.97799 –1.69861 –0.44983 C –4.83148 –2.45413 –0.51139 N –5.64068 –0.36708 –0.60355 C –4.32316 –0.33188 –0.75144 N –3.79160 –1.57127 –0.70322 C –6.66512 4.35641 –0.60936 C –7.39462 –2.13938 –0.25212 C –0.32888 –2.75731 0.10153 C 0.54534 –0.41947 –0.39602 O 1.37186 0.41904 –0.80960 C –0.91522 –3.13327 –2.26664 C 0.76133 –1.80539 –0.23107 C 2.39178 –1.46971 1.68637 C 1.52423 –0.70074 2.61013 O 3.37530 –0.96133 1.11821 C 1.66634 0.69173 2.71350 C 0.60035 –1.35814 3.43540 C 0.88689 1.40969 3.61788 C –0.17812 –0.63898 4.33992 C –0.03761 0.74850 4.43246 H 1.65010 –2.19344 –0.71774 O –0.71694 0.00231 0.00548 C –0.93824 1.40938 –0.03008

	C	0.17233	−4.16228	0.44794
	C	4.12487	3.12893	−0.12016
	O	4.66116	4.15159	0.30916
	C	4.98678	1.89029	−0.41444
	N	4.36060	0.80864	−1.13685
	C	4.57236	0.60819	−2.47304
	O	5.36072	1.28025	−3.13688
	C	3.76133	−0.53732	−3.05944
	N	2.78936	3.00616	−0.33462
	C	1.88432	4.11020	−0.09066
	H	−0.89406	−1.15776	4.97296
	H	−0.64457	1.31145	5.13748
	H	1.00192	2.48848	3.69170
	H	2.38754	1.18900	2.07400
	H	0.49656	−2.43890	3.36422
	H	0.74197	−4.15093	1.38371
	H	0.83713	−4.55523	−0.32992
	H	−0.67167	−4.85103	0.56635
	H	−0.45191	−4.12585	−2.37358
	H	2.28943	−2.56417	1.74579
	H	−0.18682	−2.37270	−2.57378
	H	−1.78868	−3.08559	−2.92566
	H	−0.93621	−2.37192	0.92774
	H	−7.83046	−1.69539	0.65191
	H	−8.02979	−1.84006	−1.09551
	H	−7.45394	−3.22861	−0.15493
	H	3.99649	−0.63008	−4.12162
	H	2.69203	−0.34386	−2.92104
	H	3.99031	−1.47517	−2.53889
	H	3.65186	0.25614	−0.66078
	H	5.84130	2.23556	−0.99990
	H	5.36076	1.52740	0.55104
	H	2.38908	2.11306	−0.62026
	H	1.21088	4.25123	−0.94398
	H	1.27138	3.94643	0.80645
	H	−5.90205	5.13226	−0.68749
	H	−1.98473	1.55970	0.24490
	H	−0.29625	1.93181	0.68600
	H	−7.38267	4.45564	−1.43126
	H	−0.75385	1.81773	−1.02925
	H	−7.22434	4.47616	0.32500
	H	2.48445	5.01021	0.05585
	O	4.50553	−2.91350	−0.49003
	H	4.12633	−2.18482	0.05539
	H	−2.79794	−1.84415	−0.78295
	H	−6.44206	1.09651	−0.57934
	H	−3.75158	0.57261	−0.89338
	H	−4.66286	−3.51782	−0.43433
	C	5.90928	−2.83463	−0.36840
	H	6.34445	−3.62301	−0.99402
	H	6.25618	−2.99743	0.66698
	H	6.31263	−1.86848	−0.71050

Optimized Molecular Properties for **T4-INT2**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 26 positive frequencies below 100 cm^–1. Zero–point correction: 0.659052 hartree Enthalpy correction: 0.707511 hartree Free Energy correction: 0.562961 hartree Quasiharmonic Free Energy correction: 0.585743 hartree SCF Energy: –1873.496993 hartree SCF Energy + ZPVE: –1872.837941 hartree Enthalpy: –1872.789482 hartree Free Energy: –1872.934032 hartree Free Energy with quasiharmonic correction: –1872.911250 hartree (correction: 14.30 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1874.18004105 A.U.
Cartesian Coordinates	79 spD3–INT2–T4.out Energy: –1176065.7223697 O –1.19271 –2.55968 –0.43656 C –5.93387 2.74949 –0.62500 O –4.73420 2.52032 –0.62597 O –6.88649 1.82202 –0.62085 C –6.11131 –1.94757 –0.50668 C –4.98522 –2.73446 –0.46467 N –5.72611 –0.62151 –0.57485 C –4.40167 –0.61900 –0.57361 N –3.90803 –1.87426 –0.50993 C –6.51011 4.15280 –0.63161 C –7.55131 –2.35472 –0.48614 C –0.38952 –2.22093 0.73503 C 0.39530 –0.08515 –0.41056 O 1.08718 0.45876 –1.25705 C –0.54890 –3.26443 –1.48914 C 0.79177 –1.32033 0.35348 C 1.80406 –0.91641 1.58312 C 1.30922 0.34212 2.31466 O 3.07794 –0.83215 1.14549 C 1.94933 1.56744 2.09904 C 0.24543 0.29940 3.22546 C 1.52019 2.72460 2.75251 C –0.18618 1.45124 3.88550 C 0.44807 2.67259 3.64689 H 1.46692 –1.88803 –0.28789 O –0.79806 0.42921 –0.02412 C –1.12637 1.71696 –0.57151

	C	0.02330	−3.50283	1.47185
	C	4.67336	2.58018	−0.93549
	O	5.31244	3.61852	−0.76095
	C	5.35182	1.21362	−0.75225
	N	4.54587	0.05247	−1.04921
	C	4.70941	−0.63106	−2.21821
	O	5.52903	−0.31355	−3.08263
	C	3.77504	−1.82111	−2.38713
	N	3.35988	2.54240	−1.27747
	C	2.57048	3.74205	−1.44335
	H	−1.01372	1.39454	4.59000
	H	0.11639	3.57206	4.16117
	H	2.03368	3.66671	2.57172
	H	2.79787	1.58507	1.42453
	H	−0.24688	−0.65013	3.43160
	H	0.18786	−3.29808	2.53380
	H	0.95482	−3.92613	1.08075
	H	−0.78387	−4.24080	1.39524
	H	−0.07019	−4.18528	−1.13296
	H	1.66431	−1.75250	2.29997
	H	0.20207	−2.64914	−1.99852
	H	−1.33249	−3.52689	−2.20650
	H	−1.10385	−1.65912	1.34238
	H	−8.07571	−1.92665	0.37735
	H	−8.07740	−2.01074	−1.38542
	H	−7.64787	−3.44423	−0.43386
	H	4.06413	−2.36754	−3.28771
	H	2.74576	−1.45805	−2.49690
	H	3.80330	−2.48471	−1.51469
	H	3.89127	−0.28755	−0.31815
	H	6.23074	1.20525	−1.40220
	H	5.69648	1.17294	0.28795
	H	2.89882	1.64120	−1.35253
	H	2.08726	3.76264	−2.42811
	H	1.79028	3.81618	−0.67430
	H	−5.70220	4.88581	−0.62710
	H	−2.13832	1.94411	−0.23497
	H	−0.42463	2.46773	−0.19773
	H	−7.13686	4.29481	−1.51882
	H	−1.08123	1.69569	−1.66349
	H	−7.15099	4.29824	0.24469
	H	3.24439	4.59632	−1.35184
	O	3.53640	−3.35327	0.71567
	H	3.43703	−2.35066	0.89418
	H	−2.90952	−2.12626	−0.48296
	H	−6.46885	0.88787	−0.60992
	H	−3.79231	0.27069	−0.61435
	H	−4.86060	−3.80560	−0.40654
	C	4.61055	−3.82716	1.48548
	H	4.74394	−4.89881	1.28112
	H	4.44499	−3.71565	2.57251
	H	5.56429	−3.32430	1.24831

Optimized Molecular Properties for **T4-TS3**

Number of (–) Vibrational Frequencies	1 (–1105.4627)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 23 positive frequencies below 100 cm^–1. Zero–point correction: 0.656074 hartree Enthalpy correction: 0.703221 hartree Free Energy correction: 0.566628 hartree Quasiharmonic Free Energy correction: 0.583865 hartree SCF Energy: –1873.470212 hartree SCF Energy + ZPVE: –1872.814138 hartree Enthalpy: –1872.766991 hartree Free Energy: –1872.903584 hartree Free Energy with quasiharmonic correction: –1872.886346 hartree (correction: 10.82 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1874.15771546 A.U.
Cartesian Coordinates	79 spD3–TS3–T4.out Energy: –1176051.7128506 O 1.81942 –1.57467 1.44990 C 8.44556 –0.74271 –1.09112 O 7.66037 –1.62664 –0.78499 O 8.16804 0.55583 –1.10638 C 4.78189 2.03663 –0.20242 C 3.54326 1.59264 0.19524 N 5.61409 0.94488 –0.36815 C 4.88766 –0.12434 –0.07341 N 3.62771 0.21953 0.27100 C 9.88100 –1.01735 –1.50492 C 5.25293 3.43677 –0.44295 C 0.51931 –2.03540 0.96491 C –0.55433 –0.08276 –0.23841 O –1.47765 0.60207 –0.67448 C 1.97625 –1.42633 2.86097 C –0.55902 –0.92905 0.95612 C –1.98072 –1.29364 1.44538 C –2.92547 –1.99296 0.46796 O –2.67880 –0.15896 1.98196 C –4.29146 –2.07553 0.78121 C –2.47793 –2.63509 –0.69224 C –5.17918 –2.76793 –0.04162 C –3.36246 –3.33755 –1.51544 C –4.71812 –3.40518 –1.19586 H –0.28421 –0.06780 1.97245 O 0.67349 –0.04287 –0.86794 C 0.74096 0.79959 –2.01886

	C	0.14868	−3.34244	1.67666
	C	−5.36555	0.88450	−1.65750
	O	−6.36874	0.63802	−2.32874
	C	−5.52907	1.39950	−0.21741
	N	−4.32608	1.80646	0.47411
	C	−3.97186	3.12114	0.55746
	O	−4.64965	4.03743	0.09269
	C	−2.67154	3.38546	1.30197
	N	−4.09260	0.73135	−2.09281
	C	−3.79062	0.19633	−3.40246
	H	−2.98847	−3.82440	−2.41354
	H	−5.40980	−3.94042	−1.84155
	H	−6.23515	−2.80652	0.21552
	H	−4.64903	−1.58016	1.67852
	H	−1.42882	−2.57870	−0.96705
	H	−0.71256	−3.81463	1.19424
	H	−0.09682	−3.19681	2.73316
	H	0.99701	−4.03400	1.61759
	H	2.06779	−2.40322	3.35696
	H	−1.84051	−1.99973	2.27801
	H	1.15483	−0.84971	3.30217
	H	2.91572	−0.88253	3.00356
	H	0.77598	−2.29725	−0.06668
	H	2.86797	−0.41827	0.55724
	H	2.62979	2.11594	0.43421
	H	6.09464	3.69473	0.21219
	H	5.59560	3.57339	−1.47648
	H	4.44768	4.15469	−0.25656
	H	5.25850	−1.13868	−0.10771
	H	7.19186	0.71407	−0.82346
	H	−2.09344	2.47897	1.48758
	H	−2.89854	3.87002	2.25896
	H	−2.07143	4.08707	0.71491
	H	−3.71905	1.09666	0.89372
	H	−6.20017	2.26012	−0.26682
	H	−6.03450	0.60605	0.34502
	H	−3.32079	0.85983	−1.44398
	H	−3.12702	0.87171	−3.95768
	H	−3.30577	−0.78481	−3.32567
	H	10.06426	−0.61870	−2.50868
	H	1.77506	0.74436	−2.36379
	H	0.05784	0.45298	−2.80137
	H	10.57066	−0.50715	−0.82351
	H	0.47962	1.83218	−1.76843
	H	10.07299	−2.09138	−1.49097
	H	−4.73218	0.08901	−3.94453
	O	−0.38955	0.64549	3.03022
	H	−2.00559	0.31771	2.54356
	C	0.32026	1.83791	2.90464
	H	1.37458	1.73953	3.23297
	H	−0.12766	2.64006	3.51770
	H	0.34928	2.22139	1.86403

Optimized Molecular Properties for **T4-INT3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 26 positive frequencies below 100 cm^–1. Zero–point correction: 0.659015 hartree Enthalpy correction: 0.707739 hartree Free Energy correction: 0.566629 hartree Quasiharmonic Free Energy correction: 0.585013 hartree SCF Energy: –1873.480568 hartree SCF Energy + ZPVE: –1872.821553 hartree Enthalpy: –1872.772829 hartree Free Energy: –1872.913939 hartree Free Energy with quasiharmonic correction: –1872.895555 hartree (correction: 11.54 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1874.17230081 A.U.
Cartesian Coordinates	79 spD3–INT3–T4.out Energy: –1176060.8652958 O 1.57395 –2.85062 –0.04385 C 5.76204 2.99971 –1.20926 O 4.60592 2.64527 –1.37595 O 6.71155 2.25759 –0.64907 C 6.21788 –1.30852 0.55701 C 5.20803 –2.23317 0.67450 N 5.69054 –0.13556 0.05134 C 4.39512 –0.35546 –0.12686 N 4.05757 –1.61140 0.23920 C 6.28054 4.36397 –1.62660 C 7.67054 –1.44487 0.89080 C 0.56844 –2.22110 –0.97317 C –0.30047 0.07476 –0.38558 O –1.13606 0.94426 –0.06388 C 1.09295 –3.79311 0.89576 C –0.44473 –1.33044 –0.32655 C –1.75634 –1.89570 0.17735 C –2.99798 –1.75148 –0.71336 O –2.15576 –1.40863 1.48737 C –4.23464 –2.21908 –0.24032 C –2.93976 –1.23476 –2.01011 C –5.37699 –2.16634 –1.03918 C –4.08060 –1.18184 –2.81525 C –5.30457 –1.64565 –2.33389 H 0.59435 –1.12007 1.53049 O 0.96752 0.50842 –0.81142 C 1.08343 1.91381 –1.02752

	C	0.03195	−3.33325	−1.88516
	C	−4.95141	2.02239	−0.30181
	O	−5.95561	2.42921	−0.88989
	C	−5.09409	1.31481	1.05716
	N	−3.87386	1.06276	1.79195
	C	−3.40897	1.94998	2.71827
	O	−4.03044	2.95189	3.07026
	C	−2.04268	1.59170	3.28644
	N	−3.69783	2.14670	−0.79063
	C	−3.47606	2.71942	−2.10096
	H	−4.01265	−0.76670	−3.81842
	H	−6.19470	−1.59573	−2.95617
	H	−6.32624	−2.52949	−0.65074
	H	−4.29433	−2.61710	0.76904
	H	−1.98882	−0.86499	−2.38080
	H	−0.50851	−2.89154	−2.72822
	H	−0.66402	−4.00807	−1.37651
	H	0.86162	−3.93319	−2.27812
	H	0.67716	−4.68554	0.40550
	H	−1.61473	−2.98426	0.28326
	H	0.34116	−3.36505	1.56824
	H	1.95044	−4.10387	1.50297
	H	1.23629	−1.59609	−1.56639
	H	3.11494	−2.03243	0.17470
	H	5.20890	−3.25492	1.02428
	H	8.30210	−1.27046	0.01053
	H	7.97621	−0.71893	1.65480
	H	7.89086	−2.44794	1.27121
	H	3.68850	0.36089	−0.51848
	H	6.32604	1.34574	−0.37855
	H	−1.72948	2.37794	3.97602
	H	−1.32141	1.49065	2.46884
	H	−2.07585	0.63343	3.81802
	H	−3.28555	0.26524	1.54028
	H	−5.74248	1.94378	1.67107
	H	−5.61309	0.36847	0.86893
	H	−2.90790	1.68664	−0.33923
	H	−2.39810	2.79801	−2.26162
	H	−3.91362	2.09898	−2.89504
	H	5.48127	4.93575	−2.10041
	H	2.13425	2.10548	−1.25460
	H	0.45817	2.23866	−1.86930
	H	6.65420	4.90466	−0.75005
	H	0.77767	2.47977	−0.14286
	H	7.12104	4.25032	−2.31985
	H	−3.92977	3.71420	−2.16873
	O	0.58475	−1.05570	2.51422
	H	−1.33521	−1.21991	1.98479
	C	1.38362	0.05513	2.89657
	H	2.44367	−0.10210	2.64921
	H	1.29354	0.16441	3.98220
	H	1.05107	0.98902	2.42457

Optimized Molecular Properties for **T4-TS4**

Number of (–) Vibrational Frequencies	1 (–194.6013)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 24 positive frequencies below 100 cm^–1. Zero–point correction: 0.657747 hartree Enthalpy correction: 0.706006 hartree Free Energy correction: 0.566042 hartree Quasiharmonic Free Energy correction: 0.584344 hartree SCF Energy: –1873.480646 hartree SCF Energy + ZPVE: –1872.822899 hartree Enthalpy: –1872.774640 hartree Free Energy: –1872.914604 hartree Free Energy with quasiharmonic correction: –1872.896302 hartree (correction: 11.48 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1874.17069247 A.U.
Cartesian Coordinates	79 spD3–TS4–T4.out Energy: –1176059.8560472 O 1.62399 –2.49024 0.64473 C 5.69627 3.13997 –1.04852 O 4.52203 2.83978 –0.90197 O 6.72013 2.31442 –0.86171 C 6.38385 –1.31224 0.20201 C 5.39278 –2.21658 0.50145 N 5.79876 –0.10260 –0.11939 C 4.48871 –0.28336 –0.01244 N 4.19609 –1.54773 0.36189 C 6.15220 4.52465 –1.47174 C 7.86869 –1.50154 0.19450 C 0.74244 –1.94231 –0.76793 C –0.32777 0.24855 –0.32289 O –1.25783 1.04193 –0.10269 C 1.41935 –3.81033 1.10088 C –0.41078 –1.17054 –0.41864 C –1.69703 –1.84271 0.00737 C –2.89648 –1.73123 –0.93579 O –2.15255 –1.44667 1.32194 C –4.16539 –2.14333 –0.50030 C –2.75272 –1.31856 –2.26363 C –5.25864 –2.13327 –1.36712 C –3.84445 –1.30867 –3.13493 C –5.10303 –1.71484 –2.69088 O 0.95291 0.76669 –0.51050 C 1.02714 2.19122 –0.58687 C 0.60790 –3.19449 –1.61749

	C	−5.16525	1.77794	−0.34434
	O	−6.19731	2.10928	−0.93158
	C	−5.25524	1.08307	1.02533
	N	−4.01719	0.90553	1.75289
	C	−3.61776	1.80889	2.69472
	O	−4.30931	2.75847	3.06078
	C	−2.22790	1.54665	3.25625
	N	−3.92534	1.97850	−0.84099
	C	−3.74436	2.55177	−2.15783
	H	−3.71126	−0.97420	−4.16164
	H	−5.95614	−1.69818	−3.36471
	H	−6.23601	−2.44859	−1.00817
	H	−4.28745	−2.46568	0.52967
	H	−1.77229	−0.99528	−2.60123
	H	0.25710	−2.90180	−2.61396
	H	−0.11603	−3.91206	−1.21860
	H	1.57028	−3.70457	−1.73574
	H	1.82769	−4.56738	0.41253
	H	−1.48289	−2.92430	0.06126
	H	0.35285	−4.03309	1.25761
	H	1.92233	−3.92740	2.07121
	H	1.55074	−1.31482	−1.13116
	H	8.29352	−1.29969	−0.79698
	H	8.36367	−0.82260	0.90041
	H	8.13230	−2.52764	0.47220
	H	−1.48868	1.64048	2.45356
	H	−2.14647	0.53015	3.65718
	H	−2.02207	2.27221	4.04559
	H	−3.37440	0.15469	1.48888
	H	−5.92700	1.68626	1.63986
	H	−5.72964	0.11024	0.85545
	H	−3.10473	1.58586	−0.38278
	H	−2.67276	2.67851	−2.32945
	H	−4.16004	1.90450	−2.94118
	H	5.28621	5.17167	−1.61916
	H	2.08053	2.43183	−0.74110
	H	0.42663	2.57355	−1.42037
	H	6.81012	4.95171	−0.70694
	H	0.66188	2.65720	0.33376
	H	6.73201	4.46056	−2.39900
	H	−4.24373	3.52457	−2.22789
	O	0.34530	−1.31200	2.75023
	H	3.23768	−1.93823	0.49924
	H	5.43706	−3.25461	0.79693
	H	3.74001	0.47215	−0.20185
	H	6.37408	1.38972	−0.57666
	H	0.82313	−1.64263	1.94654
	H	−1.34591	−1.33392	1.87457
	C	1.01707	−0.13883	3.17874
	H	2.03694	−0.36066	3.53212
	H	0.45209	0.28749	4.01301
	H	1.08590	0.61549	2.38283

Optimized Molecular Properties for **T4-product**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 27 positive frequencies below 100 cm^–1. Zero–point correction: 0.653726 hartree Enthalpy correction: 0.702202 hartree Free Energy correction: 0.559195 hartree Quasiharmonic Free Energy correction: 0.580108 hartree SCF Energy: –1873.505647 hartree SCF Energy + ZPVE: –1872.851921 hartree Enthalpy: –1872.803445 hartree Free Energy: –1872.946452 hartree Free Energy with quasiharmonic correction: –1872.925539 hartree (correction: 13.12 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1874.19225730 A.U.
Cartesian Coordinates	79 spD3–product–T4.out Energy: –1176073.3881822 O –2.04537 3.48821 0.09698 C –4.79740 –3.07599 –1.57932 O –3.79865 –2.47526 –1.95394 O –5.67862 –2.61518 –0.70946 C –5.66535 0.59654 1.09459 C –4.93435 1.75377 1.23232 N –5.01004 –0.22924 0.20410 C –3.91729 0.43100 –0.17302 N –3.82653 1.63631 0.42339 C –5.15654 –4.46716 –2.07620 C –6.95202 0.19854 1.74878 C –0.20728 1.52241 –2.29783 C 0.71341 –0.58004 –1.42577 O 1.60370 –1.24857 –0.92303 C –2.59401 4.75850 0.23696 C 0.73803 0.90164 –1.56199 C 1.82812 1.63490 –0.78814 C 3.24660 1.33445 –1.26841 O 1.71649 1.39626 0.60983 C 4.31160 1.30060 –0.36215 C 3.52268 1.18115 –2.63330 C 5.62007 1.10079 –0.80656 C 4.82983 0.98888 –3.08106 C 5.88590 0.94491 –2.16836 O –0.41262 –1.14158 –1.91751 C –0.50647 –2.57233 –1.82843 C –0.40700 2.99055 –2.50168

	C	4.44074	−1.86240	1.89820
	O	5.60014	−2.08990	2.24676
	C	3.46581	−1.20211	2.88570
	N	2.13788	−0.90056	2.39636
	C	1.04211	−1.58267	2.84612
	O	1.10307	−2.48817	3.67609
	C	−0.28379	−1.14037	2.24433
	N	3.94413	−2.17927	0.68095
	C	4.79241	−2.74121	−0.35090
	H	5.02209	0.86779	−4.14492
	H	6.90497	0.78918	−2.51466
	H	6.43124	1.06098	−0.08374
	H	4.10209	1.42973	0.69361
	H	2.70487	1.20481	−3.34904
	H	−0.86617	3.18564	−3.47770
	H	0.51531	3.57479	−2.43102
	H	−1.09857	3.33854	−1.70783
	H	−2.41386	5.40199	−0.64857
	H	1.66738	2.70813	−0.95420
	H	−2.18506	5.31090	1.10706
	H	−3.69486	4.73275	0.37436
	H	−0.96204	0.88640	−2.75449
	H	−7.73548	−0.00753	1.00783
	H	−6.83457	−0.71124	2.35181
	H	−7.31439	0.99420	2.40883
	H	−0.19615	−0.26754	1.59344
	H	−0.98341	−0.92003	3.05650
	H	−0.70912	−1.97132	1.67130
	H	2.01202	−0.14075	1.72421
	H	3.35201	−1.88222	3.73422
	H	3.96012	−0.29401	3.25239
	H	3.02879	−1.83925	0.40656
	H	4.15855	−3.18281	−1.12421
	H	5.43335	−1.97914	−0.81374
	H	−4.45122	−4.78377	−2.84660
	H	−1.52961	−2.80953	−2.11742
	H	0.22182	−3.04099	−2.49907
	H	−5.13155	−5.17611	−1.24090
	H	−0.30483	−2.90360	−0.80651
	H	−6.17616	−4.47370	−2.47593
	H	5.43483	−3.51129	0.08474
	O	−0.02531	3.14775	1.55997
	H	−3.05292	2.40576	0.27459
	H	−5.10839	2.63613	1.83127
	H	−3.18367	0.04104	−0.86525
	H	−5.39376	−1.67009	−0.36278
	H	−0.84768	3.31110	0.92848
	H	1.03910	2.04514	0.97563
	C	−0.52691	2.81707	2.83708
	H	−0.84496	3.71430	3.39409
	H	0.26326	2.32553	3.41887
	H	−1.38747	2.13261	2.78393

Optimized Molecular Properties for **T5-INT2-1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 28 positive frequencies below 100 cm^–1. Zero–point correction: 0.711085 hartree Enthalpy correction: 0.762060 hartree Free Energy correction: 0.612110 hartree Quasiharmonic Free Energy correction: 0.635977 hartree SCF Energy: –2065.259284 hartree SCF Energy + ZPVE: –2064.548199 hartree Enthalpy: –2064.497224 hartree Free Energy: –2064.647174 hartree Free Energy with quasiharmonic correction: –2064.623307 hartree (correction: 14.98 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –2065.99292771 A.U.
Cartesian Coordinates	86 spD3–INT2–1–T5.out Energy: –1296430.1250251 O –1.33772 –2.19129 –1.27726 C –6.88099 1.68412 0.63053 O –5.67026 1.70408 0.47020 O –7.66047 0.63145 0.40337 C –6.27588 –2.74044 –0.86280 C –5.04015 –3.25666 –1.17199 N –6.12187 –1.42928 –0.45209 C –4.82480 –1.17007 –0.51566 N –4.12974 –2.24520 –0.94614 C –7.67316 2.88105 1.12033 C –7.61854 –3.39855 –0.92492 C –0.49001 –2.00645 –0.10477 C –0.29153 0.46441 –0.68823 O 0.16206 1.31648 –1.43488 C –0.69566 –2.47767 –2.51287 C 0.43793 –0.79671 –0.28925 C 1.45230 –0.49507 0.94280 C 0.80269 0.38299 2.01771 O 2.63209 0.00707 0.47321 C 1.11861 1.74390 2.09987 C –0.09505 –0.14897 2.95254 C 0.53274 2.55641 3.07280 C –0.68225 0.65752 3.92858 C –0.37315 2.01788 3.98952 H 1.13731 –1.02116 –1.09642 O –1.49529 0.59927 –0.08836 C –2.15962 1.85879 –0.29555

	C	0.25115	−3.30895	0.22120
	C	3.13710	4.17141	−0.67282
	O	3.52207	5.25509	−0.23344
	C	4.14471	3.04419	−0.94217
	N	3.60577	1.81510	−1.47768
	C	3.78741	1.48153	−2.78946
	O	4.38297	2.19744	−3.59511
	C	3.17179	0.14781	−3.18978
	N	1.83871	3.87857	−0.94309
	C	0.77222	4.82645	−0.70895
	H	−1.37526	0.22225	4.64551
	H	−0.82580	2.64907	4.75095
	H	0.79599	3.61081	3.12170
	H	1.84337	2.14757	1.40226
	H	−0.33036	−1.21191	2.92666
	H	0.53733	−3.33825	1.27609
	H	1.17109	−3.41957	−0.36209
	H	−0.40996	−4.16205	0.03010
	H	−0.05643	−3.36723	−2.44821
	H	1.59998	−1.48830	1.40888
	H	−0.09538	−1.63292	−2.87023
	H	−1.49501	−2.66820	−3.23506
	H	−1.22528	−1.79460	0.67575
	H	−3.10977	−2.27803	−1.07699
	H	−4.73834	−4.23215	−1.52348
	H	−8.10105	−3.41618	0.06023
	H	−8.29393	−2.86478	−1.60509
	H	−7.53110	−4.43169	−1.27699
	H	−4.37510	−0.22456	−0.25416
	H	−7.09952	−0.15843	0.07751
	H	2.08024	0.21363	−3.10912
	H	3.50896	−0.66234	−2.53350
	H	3.44883	−0.06829	−4.22368
	H	3.15540	1.15051	−0.82701
	H	4.87943	3.43419	−1.65152
	H	4.65970	2.85113	0.00637
	H	1.60245	2.94387	−1.25965
	H	0.16178	4.54296	0.15964
	H	1.22869	5.79908	−0.51432
	H	−8.43980	3.14875	0.38523
	H	−3.13071	1.77608	0.19245
	H	−1.57428	2.66480	0.15471
	H	−8.19125	2.62927	2.05208
	H	−2.28053	2.05691	−1.36380
	H	−7.00416	3.72674	1.28527
	H	0.11689	4.89634	−1.58488
	O	3.70136	−2.03334	−0.45188
	C	4.64652	−2.55263	0.34284
	C	6.63642	−3.72169	1.97618
	C	5.28026	−3.75299	−0.03666
	C	5.03173	−1.94397	1.55694
	C	6.01271	−2.52877	2.35479
	C	6.25968	−4.32465	0.77226
	H	4.98475	−4.21601	−0.97470
	H	6.73564	−5.25230	0.45782
	H	7.40190	−4.17066	2.60450

	H	6.29464	−2.04267	3.28734
	H	4.54512	−1.01532	1.84224
	H	3.29786	−1.11600	−0.04439

Optimized Molecular Properties for **T5-INT2-2**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 26 positive frequencies below 100 cm^–1. Zero–point correction: 0.713714 hartree Enthalpy correction: 0.764172 hartree Free Energy correction: 0.617705 hartree Quasiharmonic Free Energy correction: 0.639328 hartree SCF Energy: –2065.261399 hartree SCF Energy + ZPVE: –2064.547685 hartree Enthalpy: –2064.497227 hartree Free Energy: –2064.643694 hartree Free Energy with quasiharmonic correction: –2064.622070 hartree (correction: 13.57 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –2065.99606043 A.U.
Cartesian Coordinates	86 spD3–INT2–2–T5.out Energy: –1296432.0908365 O 1.05287 2.25301 –0.66010 C 6.83535 –1.61580 0.03006 O 5.61504 –1.66067 –0.01550 O 7.55959 –0.51129 –0.10924 C 5.99958 2.94714 –0.73006 C 4.73426 3.46936 –0.85465 N 5.90053 1.58624 –0.50723 C 4.60649 1.30415 –0.50044 N 3.86140 2.41181 –0.70720 C 7.70217 –2.83951 0.25656 C 7.32218 3.64336 –0.80562 C 0.56924 1.68405 0.58758 C 0.26141 –0.62114 –0.47569 O –0.30292 –1.35613 –1.26655 C 0.17068 3.15576 –1.33789 C –0.41027 0.54414 0.22861 C –1.38321 0.03512 1.38028 C –0.88494 –1.18771 2.13864 O –2.66448 –0.19758 0.85228 C –1.61537 –2.38026 2.13453 C 0.30239 –1.13329 2.88308 C –1.16382 –3.49711 2.84235 C 0.75446 –2.24450 3.59393 C 0.02286 –3.43463 3.57368 H –1.11207 0.96215 –0.49314 O 1.54889 –0.81159 –0.11405 C 2.18662 –1.97917 –0.66845

	C	0.00766	2.76778	1.51044
	C	-3.36162	-4.11709	-0.96066
	O	-3.80223	-5.20577	-0.59066
	C	-4.32115	-2.94207	-1.20128
	N	-3.71380	-1.67040	-1.52225
	C	-3.82165	-1.12225	-2.77402
	O	-4.42005	-1.67737	-3.69405
	C	-3.11051	0.20980	-2.94451
	N	-2.04931	-3.86537	-1.19518
	C	-1.02287	-4.85926	-0.96801
	H	1.67878	-2.18022	4.16327
	H	0.37460	-4.30277	4.12614
	H	-1.74717	-4.41429	2.82015
	H	-2.54445	-2.41936	1.58012
	H	0.88218	-0.21338	2.91095
	H	-0.06242	2.40263	2.54003
	H	-0.98903	3.09029	1.19616
	H	0.68845	3.62684	1.51553
	H	0.25933	4.17300	-0.93310
	H	-1.44511	0.86169	2.09984
	H	-0.87721	2.84516	-1.26442
	H	0.48050	3.16052	-2.38696
	H	1.47764	1.26940	1.03147
	H	2.83150	2.43627	-0.73690
	H	4.38941	4.47717	-1.03228
	H	7.88896	3.52674	0.12650
	H	7.94271	3.23601	-1.61349
	H	7.18934	4.71465	-0.98873
	H	4.19281	0.31953	-0.34438
	H	6.94776	0.29558	-0.26171
	H	-2.02947	0.03169	-3.00099
	H	-3.28867	0.89404	-2.10584
	H	-3.44509	0.66506	-3.87905
	H	-3.26132	-1.14220	-0.77318
	H	-4.96912	-3.21577	-2.03878
	H	-4.94908	-2.86173	-0.30587
	H	-1.76497	-2.91604	-1.41113
	H	-0.44745	-4.64318	-0.05765
	H	-1.51521	-5.82676	-0.85137
	H	8.38648	-2.97416	-0.58811
	H	3.21415	-1.96328	-0.30589
	H	1.66912	-2.88057	-0.33004
	H	8.31677	-2.70115	1.15262
	H	2.15977	-1.94223	-1.76060
	H	7.07403	-3.72416	0.37011
	H	-0.33197	-4.90001	-1.81804
	O	-3.04760	2.14097	-0.09643
	H	-2.97333	0.73072	0.51232
	C	-3.93987	2.99730	0.34179
	C	-5.85645	4.89602	1.29885
	C	-4.08825	4.28250	-0.25257
	C	-4.80331	2.70822	1.43701
	C	-5.73250	3.63688	1.89690
	C	-5.02134	5.20148	0.21798
	H	-3.44801	4.52599	-1.09841
	H	-5.10162	6.17406	-0.26802

	H	−6.58487	5.61716	1.66232
	H	−6.37363	3.37325	2.73806
	H	−4.71702	1.73152	1.90937

Optimized Molecular Properties for **T5-TS3**

Number of (–) Vibrational Frequencies	1 (–985.5740)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 26 positive frequencies below 100 cm^–1. Zero–point correction: 0.708375 hartree Enthalpy correction: 0.758847 hartree Free Energy correction: 0.611881 hartree Quasiharmonic Free Energy correction: 0.634095 hartree SCF Energy: –2065.228833 hartree SCF Energy + ZPVE: –2064.520458 hartree Enthalpy: –2064.469986 hartree Free Energy: –2064.616952 hartree Free Energy with quasiharmonic correction: –2064.594738 hartree (correction: 13.94 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –2065.96953581 A.U.
Cartesian Coordinates	86 spD3–TS3–T5.out Energy: –1296415.4463863 O –1.76268 0.89135 –2.22923 C –5.48429 –2.11244 2.99710 O –4.36938 –1.70268 2.71404 O –6.53651 –2.07796 2.18571 C –6.39504 –0.65502 –1.37326 C –5.45333 –0.08065 –2.19347 N –5.80285 –0.96324 –0.16297 C –4.53786 –0.58022 –0.26057 N –4.27994 –0.04014 –1.47077 C –5.82503 –2.72795 4.34149 C –7.83874 –0.94143 –1.64473 C –0.70039 –0.13293 –2.23861 C 0.43835 –0.17896 0.02022 O 1.38145 –0.26685 0.81015 C –1.59395 2.02942 –3.06416 C 0.50668 0.24253 –1.37071 C 1.90992 0.15162 –1.99385 C 2.60376 –1.21448 –2.01914 O 2.85958 1.06981 –1.41234 C 3.95128 –1.28461 –2.40757 C 1.93714 –2.41201 –1.74047 C 4.60973 –2.50975 –2.50728 C 2.59104 –3.64289 –1.84531 C 3.93092 –3.69796 –2.22657 H 0.47985 1.72340 –1.17633 O –0.84545 –0.41691 0.46895 C –0.95100 –0.72637 1.86510

	C	−0.41880	−0.55088	−3.68693
	C	4.98191	−1.84488	1.56124
	O	5.80121	−2.74910	1.73215
	C	5.46736	−0.46494	1.08551
	N	4.48878	0.59804	1.04909
	C	4.38874	1.50831	2.06304
	O	5.14049	1.51706	3.03715
	C	3.27962	2.53357	1.87613
	N	3.64755	−1.97150	1.75690
	C	3.04758	−3.23220	2.13482
	H	2.05049	−4.55887	−1.61738
	H	4.44431	−4.65361	−2.29621
	H	5.65703	−2.53758	−2.79929
	H	4.48143	−0.36124	−2.62012
	H	0.89841	−2.38587	−1.42518
	H	0.24443	−1.42022	−3.71350
	H	0.04908	0.24229	−4.27833
	H	−1.36110	−0.82364	−4.17680
	H	−1.75335	1.78845	−4.12593
	H	1.79837	0.44469	−3.04946
	H	−0.60754	2.48321	−2.92930
	H	−2.35061	2.75515	−2.75100
	H	−1.23290	−0.96197	−1.76387
	H	−3.36460	0.32693	−1.78122
	H	−5.51719	0.29517	−3.20396
	H	−8.05981	−2.01177	−1.54724
	H	−8.49164	−0.41245	−0.93907
	H	−8.11458	−0.63039	−2.65787
	H	−3.80041	−0.68611	0.52029
	H	−6.27469	−1.65718	1.28896
	H	3.13224	3.06944	2.81548
	H	2.34656	2.05329	1.56770
	H	3.55326	3.25813	1.09954
	H	3.83327	0.65162	0.26621
	H	6.27145	−0.16556	1.76168
	H	5.89848	−0.61214	0.08839
	H	3.02677	−1.21075	1.49270
	H	2.46512	−3.65968	1.30819
	H	3.85344	−3.92114	2.39531
	H	−6.62025	−2.15073	4.82576
	H	−2.00234	−0.94966	2.05289
	H	−0.33102	−1.59050	2.12090
	H	−6.20300	−3.74656	4.20167
	H	−0.62776	0.12402	2.47314
	H	−4.93882	−2.74450	4.97749
	H	2.38371	−3.10350	2.99871
	O	0.79430	2.85257	−1.15027
	H	2.38571	1.92006	−1.28964
	C	0.17086	3.61865	−0.23931
	C	−1.10465	5.31306	1.62936
	C	−1.01074	3.20963	0.41362
	C	0.69599	4.89217	0.05907
	C	0.06351	5.72358	0.98037
	C	−1.62962	4.05161	1.33712
	H	−1.42983	2.23450	0.18455
	H	−2.53796	3.71422	1.83273

	H	−1.59375	5.96227	2.35121
	H	0.48981	6.70184	1.19574
	H	1.60543	5.20499	−0.44720

Optimized Molecular Properties for **T5-INT3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 27 positive frequencies below 100 cm^–1. Zero–point correction: 0.711429 hartree Enthalpy correction: 0.762901 hartree Free Energy correction: 0.613908 hartree Quasiharmonic Free Energy correction: 0.636123 hartree SCF Energy: –2065.232789 hartree SCF Energy + ZPVE: –2064.521360 hartree Enthalpy: –2064.469888 hartree Free Energy: –2064.618881 hartree Free Energy with quasiharmonic correction: –2064.596666 hartree (correction: 13.94 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –2065.97628837 A.U.
Cartesian Coordinates	86 spD3–INT3–T5.out Energy: –1296419.6836816 O –1.49916 0.28550 –2.49169 C –5.25939 –2.31098 2.94701 O –4.12264 –2.01447 2.61507 O –6.33340 –2.18160 2.17454 C –6.23095 –0.75536 –1.36377 C –5.29765 –0.26198 –2.24386 N –5.58798 –1.14265 –0.20353 C –4.30053 –0.88495 –0.38714 N –4.07801 –0.35077 –1.60845 C –5.60565 –2.87735 4.31153 C –7.71174 –0.89299 –1.53249 C –0.53151 –0.79755 –2.09401 C 0.60278 –0.47696 0.13261 O 1.53998 –0.32154 0.93663 C –1.11516 1.14306 –3.54931 C 0.63352 –0.32168 –1.27832 C 1.97013 –0.03111 –1.93071 C 3.06036 –1.10848 –1.85580 O 2.61304 1.19421 –1.47975 C 4.35736 –0.80672 –2.30082 C 2.79562 –2.41299 –1.43054 C 5.35759 –1.77874 –2.31265 C 3.79267 –3.39172 –1.44640 C 5.07890 –3.07933 –1.88580 H –0.05909 1.58962 –0.97472 O –0.66306 –0.79453 0.64708 C –0.70686 –1.00438 2.05995

	C	−0.22520	−1.65021	−3.33205
	C	5.41602	−0.74423	1.72919
	O	6.43054	−1.37963	2.02377
	C	5.54424	0.66470	1.12432
	N	4.32378	1.42719	0.98010
	C	3.92232	2.31346	1.93870
	O	4.60644	2.60204	2.91982
	C	2.54977	2.92250	1.68941
	N	4.16249	−1.21899	1.89579
	C	3.94541	−2.56118	2.39268
	H	3.56349	−4.39827	−1.10331
	H	5.85883	−3.83681	−1.88828
	H	6.35832	−1.52024	−2.65185
	H	4.57805	0.20493	−2.62829
	H	1.79996	−2.65427	−1.07176
	H	0.28967	−2.56788	−3.03144
	H	0.41771	−1.14336	−4.05890
	H	−1.15648	−1.92834	−3.84056
	H	−1.10378	0.62822	−4.52185
	H	1.77595	0.10291	−3.00735
	H	−0.13219	1.59455	−3.37006
	H	−1.85364	1.95024	−3.58895
	H	−1.17752	−1.38665	−1.44268
	H	−3.15804	−0.06627	−1.98329
	H	−5.39536	0.13817	−3.24217
	H	−8.03040	−1.93874	−1.43767
	H	−8.25610	−0.32031	−0.77114
	H	−8.02757	−0.53136	−2.51673
	H	−3.52078	−1.07660	0.33580
	H	−6.06184	−1.79150	1.26642
	H	2.30722	3.59658	2.51279
	H	1.79843	2.12935	1.61570
	H	2.52899	3.48204	0.74702
	H	3.69127	1.21729	0.20544
	H	6.22221	1.22446	1.77234
	H	6.02671	0.54714	0.14709
	H	3.35607	−0.71264	1.53413
	H	4.36066	−3.31603	1.71245
	H	4.42178	−2.69463	3.37063
	H	−6.31617	−2.21687	4.82053
	H	−1.73558	−1.28694	2.29188
	H	−0.02125	−1.80367	2.36144
	H	−6.09214	−3.85245	4.19986
	H	−0.42910	−0.09586	2.60385
	H	−4.70022	−2.97999	4.91141
	H	2.86853	−2.71933	2.48845
	O	0.05636	2.58090	−0.98687
	H	1.91099	1.85439	−1.34379
	C	−0.94425	3.22303	−0.32329
	C	−2.97055	4.64279	0.99590
	C	−1.96699	2.53107	0.34046
	C	−0.93519	4.62438	−0.32264
	C	−1.94426	5.32425	0.33625
	C	−2.97110	3.24592	0.99293
	H	−1.95829	1.44512	0.34666
	H	−3.75973	2.69901	1.50406

	H	−3.75568	5.19249	1.50835
	H	−1.92680	6.41202	0.33338
	H	−0.13227	5.14240	−0.83914

Optimized Molecular Properties for **T5-TS4**

Number of (–) Vibrational Frequencies	1 (–160.4967)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 27 positive frequencies below 100 cm^–1. Zero–point correction: 0.710373 hartree Enthalpy correction: 0.761377 hartree Free Energy correction: 0.614576 hartree Quasiharmonic Free Energy correction: 0.635264 hartree SCF Energy: –2065.232524 hartree SCF Energy + ZPVE: –2064.522151 hartree Enthalpy: –2064.471147 hartree Free Energy: –2064.617948 hartree Free Energy with quasiharmonic correction: –2064.597260 hartree (correction: 12.98 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –2065.97533120 A.U.
Cartesian Coordinates	86 spD3–TS4–T5.out Energy: –1296419.0830484 O –1.45619 –0.09598 –2.50384 C –5.39129 –1.78958 3.20714 O –4.23282 –1.61214 2.86520 O –6.44337 –1.70049 2.39992 C –6.21593 –0.71482 –1.27422 C –5.24612 –0.38522 –2.19086 N –5.60631 –1.02354 –0.07335 C –4.30276 –0.87995 –0.26988 N –4.03736 –0.49502 –1.53807 C –5.79323 –2.14265 4.62731 C –7.70237 –0.76090 –1.44340 C –0.53418 –1.38235 –1.84567 C 0.54607 –0.64535 0.25912 O 1.47308 –0.30933 1.01368 C –1.29576 0.21145 –3.87662 C 0.62632 –0.91655 –1.13615 C 1.91640 –0.60159 –1.85439 C 3.11765 –1.50880 –1.57897 O 2.37582 0.76250 –1.66729 C 4.39969 –1.11567 –1.99266 C 2.96437 –2.77610 –1.00912 C 5.49627 –1.96263 –1.82992 C 4.05919 –3.62849 –0.84842 C 5.33108 –3.22532 –1.25604 O –0.73261 –0.78768 0.80059 C –0.81486 –0.62427 2.21793 C –0.39025 –2.38265 –2.98212

	C	5.37525	−0.32135	1.80698
	O	6.43062	−0.82116	2.20227
	C	5.40735	0.96524	0.96414
	N	4.13753	1.60190	0.69030
	C	3.67773	2.62605	1.46937
	O	4.34004	3.13468	2.37304
	C	2.27101	3.08952	1.12473
	N	4.15769	−0.84706	2.06204
	C	4.03167	−2.09407	2.78655
	H	3.91746	−4.60702	−0.39440
	H	6.18650	−3.88269	−1.12125
	H	6.48382	−1.63480	−2.14699
	H	4.52985	−0.13381	−2.43759
	H	1.97491	−3.08129	−0.68143
	H	0.00762	−3.31724	−2.57126
	H	0.30017	−2.05455	−3.76477
	H	−1.35767	−2.60406	−3.44655
	H	−1.70012	−0.57391	−4.53245
	H	1.71618	−0.71699	−2.93351
	H	−0.24061	0.37340	−4.14139
	H	−1.83442	1.14489	−4.08535
	H	−1.30715	−1.70776	−1.15584
	H	−8.09785	−1.76435	−1.24133
	H	−8.20537	−0.07172	−0.75346
	H	−7.98749	−0.48443	−2.46397
	H	1.56445	2.26436	1.26361
	H	2.20164	3.40623	0.07805
	H	2.00205	3.92564	1.77222
	H	3.52129	1.21193	−0.02509
	H	6.03376	1.67899	1.50362
	H	5.91038	0.71461	0.02335
	H	3.31994	−0.46799	1.62447
	H	2.96783	−2.31016	2.91031
	H	4.50690	−2.92347	2.24721
	H	−4.90495	−2.22032	5.25592
	H	−1.84173	−0.87527	2.49100
	H	−0.11378	−1.28890	2.73289
	H	−6.46560	−1.37545	5.02673
	H	−0.58492	0.40603	2.50937
	H	−6.34150	−3.09097	4.63682
	H	4.50584	−2.02006	3.77191
	O	−0.24599	2.19751	−1.79616
	H	−3.09325	−0.31614	−1.93512
	H	−5.31243	−0.08461	−3.22611
	H	−3.54151	−1.04674	0.47859
	H	−6.13522	−1.45015	1.45423
	H	−0.71278	1.31466	−1.84231
	H	1.57524	1.32266	−1.64838
	C	−0.90994	3.06266	−0.97995
	C	−2.22449	4.92617	0.65406
	C	−0.59159	4.42492	−1.06689
	C	−1.88274	2.63311	−0.06580
	C	−2.53461	3.56715	0.73937
	C	−1.24550	5.34576	−0.25063
	H	0.16549	4.73898	−1.77962
	H	−2.10174	1.57331	0.02292

	H	−3.28634	3.22225	1.44526
	H	−0.98815	6.40006	−0.32433
	H	−2.73276	5.64737	1.28856

Optimized Molecular Properties for **T5-product**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 27 positive frequencies below 100 cm^–1. Zero–point correction: 0.709167 hartree Enthalpy correction: 0.761500 hartree Free Energy correction: 0.608853 hartree Quasiharmonic Free Energy correction: 0.632624 hartree SCF Energy: –2065.270187 hartree SCF Energy + ZPVE: –2064.561020 hartree Enthalpy: –2064.508687 hartree Free Energy: –2064.661334 hartree Free Energy with quasiharmonic correction: –2064.637563 hartree (correction: 14.92 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –2066.00660423 A.U.
Cartesian Coordinates	86 spD3–product–T5.out Energy: –1296438.7071709 O –1.93490 2.62612 –1.57846 C –5.36560 –3.61434 0.32418 O –4.28140 –3.30066 –0.14707 O –6.32818 –2.75928 0.63707 C –6.13663 0.97751 0.33280 C –5.26131 1.96258 –0.05646 N –5.52223 –0.24921 0.17137 C –4.30826 0.00034 –0.30193 N –4.10625 1.32704 –0.45628 C –5.75582 –5.05005 0.62496 C –7.53231 1.10191 0.85890 C –0.32263 –0.52071 –2.70465 C 0.51158 –1.86134 –0.83184 O 1.41666 –2.31508 –0.15277 C –2.08209 3.81808 –2.32470 C 0.66350 –0.75171 –1.81694 C 1.94200 0.07680 –1.70674 C 3.21154 –0.71267 –2.02046 O 2.04216 0.69730 –0.43920 C 4.38127 –0.50009 –1.28424 C 3.25107 –1.60048 –3.10349 C 5.56070 –1.17089 –1.61429 C 4.42897 –2.26872 –3.43759 C 5.59081 –2.05809 –2.69182 O –0.75057 –2.34346 –0.75978 C –0.95139 –3.45992 0.12483 C –0.40843 0.54663 –3.75243

	C	4.22271	−1.53906	2.68449
	O	5.34507	−1.68112	3.17254
	C	3.38705	−0.30862	3.06306
	N	2.11844	−0.13635	2.38742
	C	0.94166	−0.09737	3.08775
	O	0.87411	−0.30747	4.29749
	C	−0.29290	0.20447	2.24901
	N	3.64624	−2.41388	1.82588
	C	4.34528	−3.57901	1.32585
	H	4.43751	−2.95805	−4.27918
	H	6.50947	−2.58107	−2.94739
	H	6.45687	−1.00039	−1.02259
	H	4.35374	0.19172	−0.45070
	H	2.34822	−1.77775	−3.68302
	H	−0.80372	0.13413	−4.68936
	H	0.54404	1.03680	−3.96629
	H	−1.11374	1.31010	−3.39735
	H	−3.09430	3.83793	−2.74719
	H	1.87268	0.86816	−2.46594
	H	−1.36589	3.86847	−3.15949
	H	−1.94305	4.71596	−1.70668
	H	−1.20011	−1.15992	−2.63863
	H	−8.25135	0.57429	0.21940
	H	−7.62073	0.67309	1.86494
	H	−7.83565	2.15274	0.91278
	H	−0.11936	0.99477	1.51076
	H	−1.10112	0.49724	2.92204
	H	−0.60774	−0.69460	1.70568
	H	2.11230	0.11998	1.39760
	H	3.17373	−0.37293	4.13361
	H	4.03625	0.56303	2.91020
	H	2.75923	−2.17442	1.39683
	H	3.73431	−4.48120	1.45204
	H	4.58824	−3.46785	0.26194
	H	−4.97960	−5.73032	0.27094
	H	−2.01452	−3.68857	0.05851
	H	−0.33741	−4.30855	−0.19247
	H	−5.89031	−5.17681	1.70509
	H	−0.67324	−3.18882	1.14701
	H	−6.71217	−5.28974	0.14858
	H	5.26924	−3.68352	1.89783
	O	0.36125	2.66686	−0.40162
	H	−3.25621	1.79484	−0.82809
	H	−5.35598	3.03816	−0.07692
	H	−3.56967	−0.75631	−0.52721
	H	−6.01565	−1.79373	0.45077
	H	−1.03665	2.64478	−1.08342
	H	1.40032	1.49066	−0.43008
	C	0.76837	3.82018	0.10212
	C	1.64027	6.31851	1.16275
	C	2.14499	4.15586	0.17357
	C	−0.15221	4.77919	0.59887
	C	0.27986	6.00021	1.11123
	C	2.56329	5.37784	0.69277
	H	2.86748	3.42689	−0.18554
	H	−1.21033	4.52701	0.58660

	H	−0.45702	6.71059	1.48463
	H	3.62895	5.60049	0.73150
	H	1.97383	7.27134	1.56655

Optimized Molecular Properties for **T6-complex**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 19 positive frequencies below 100 cm^–1. Zero–point correction: 0.438160 hartree Enthalpy correction: 0.471971 hartree Free Energy correction: 0.366132 hartree Quasiharmonic Free Energy correction: 0.381707 hartree SCF Energy: –1183.626992 hartree SCF Energy + ZPVE: –1183.188832 hartree Enthalpy: –1183.155021 hartree Free Energy: –1183.260860 hartree Free Energy with quasiharmonic correction: –1183.245285 hartree (correction: 9.77 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1184.04635895 A.U.
Cartesian Coordinates	(PCM) 52 spD3–complex–T6.out Energy: –743000.3019761 O –4.22035 –1.84287 –0.17202 C –2.55084 2.98013 –0.26345 C –2.25693 1.63652 –0.26435 N –3.93449 3.02645 –0.25656 C –4.40483 1.75002 –0.25331 N –3.41369 0.87982 –0.25772 H –1.27971 1.17350 –0.27606 H –3.84964 –0.93054 –0.25376 H –5.45931 1.51209 –0.24767 C –1.69494 4.20431 –0.27724 H –1.82739 4.77947 –1.20276 H –1.93474 4.87150 0.56038 H –0.63967 3.92916 –0.19628 C –1.37852 –3.10203 –1.24206 C 0.48502 –2.33338 0.21439 O 1.52972 –1.69929 0.36186 C –4.11309 –2.21212 1.18918 H –4.59096 –3.19048 1.31179 H –3.06717 –2.30343 1.52476 H –4.62231 –1.50242 1.86093 C –0.23172 –2.42644 –1.06349 H 0.23793 –1.88301 –1.87898 O –0.09317 –2.99978 1.22717 C 0.57767 –2.93838 2.49955 H –0.01760 –3.55777 3.16955 H 0.61316 –1.90835 2.86356

	H	1.59417	−3.32971	2.41575
	C	−2.13455	−3.18451	−2.52577
	H	−1.81072	−3.62740	−0.39421
	H	−2.24123	−4.23043	−2.84325
	H	−3.14691	−2.79751	−2.35986
	H	−1.65358	−2.61979	−3.32996
	C	2.07924	2.15706	0.12532
	O	1.68531	3.32331	0.03431
	C	2.94497	1.56712	−0.99673
	N	3.41230	0.20997	−0.80955
	H	2.72949	−0.54022	−0.74582
	H	3.82621	2.20458	−1.10021
	H	2.36544	1.65698	−1.92358
	N	1.79268	1.35091	1.17150
	H	2.06602	0.37738	1.12921
	C	0.96312	1.79450	2.28029
	H	−0.10684	1.70871	2.05162
	H	1.18781	1.18788	3.16093
	H	1.18413	2.84174	2.49643
	C	4.73367	−0.08701	−0.62570
	O	5.62142	0.76470	−0.64218
	C	5.03864	−1.56329	−0.42808
	H	5.49930	−1.95895	−1.34039
	H	5.76869	−1.66660	0.37928
	H	4.15028	−2.15625	−0.19501
	H	−4.49743	3.86632	−0.25459

Optimized Molecular Properties for **T6-TS1**

Number of (–) Vibrational Frequencies	0 (–895.0805)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 13 positive frequencies below 100 cm^–1. Zero–point correction: 0.436348 hartree Enthalpy correction: 0.467313 hartree Free Energy correction: 0.373603 hartree Quasiharmonic Free Energy correction: 0.383067 hartree SCF Energy: –1183.591887 hartree SCF Energy + ZPVE: –1183.155539 hartree Enthalpy: –1183.124574 hartree Free Energy: –1183.218284 hartree Free Energy with quasiharmonic correction: –1183.208820 hartree (correction: 5.94 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1184.01513420 A.U.
Cartesian Coordinates	(PCM) 52 spD3–TS1–T6.out Energy: –742980.7081498 O 2.85349 2.10529 –0.10988 C 2.74194 –2.56397 –0.14970 C 2.20626 –1.31163 0.00998 N 4.05677 –2.33821 –0.53243 C 4.28129 –1.00960 –0.59458 N 3.17190 –0.36395 –0.27001 H 1.20665 –1.02057 0.29533 H 3.00645 0.88639 –0.21113 H 5.22376 –0.56012 –0.86798 C 2.15968 –3.92847 0.01218 H 2.20262 –4.49386 –0.92660 H 2.69963 –4.50489 0.77305 H 1.11353 –3.84860 0.32044 C 1.51423 2.54155 –1.05366 C –0.68651 2.21351 0.11497 O –1.76419 1.60043 0.36231 C 2.67876 2.41292 1.27258 H 2.71500 3.49814 1.41217 H 1.71916 2.03463 1.64358 H 3.49761 1.95016 1.83310 C 0.33352 1.79023 –0.74494 H 0.16584 0.84485 –1.25364 O –0.47622 3.43423 0.72621 C –1.53521 3.91296 1.55427 H –1.18436 4.86484 1.95896 H –1.75107 3.21756 2.37134

	H	−2.45407	4.07037	0.98025
	C	2.11075	2.36652	−2.43785
	H	1.46416	3.58646	−0.74792
	H	1.45060	2.83860	−3.17364
	H	3.09951	2.82883	−2.51205
	H	2.19678	1.30640	−2.70150
	C	−1.45298	−2.13652	0.73294
	O	−1.02877	−3.25343	1.05611
	C	−2.07309	−1.93558	−0.65730
	N	−2.85366	−0.73220	−0.85081
	H	−2.41981	0.17332	−0.64811
	H	−2.72629	−2.78887	−0.84880
	H	−1.24911	−1.98709	−1.38322
	N	−1.35957	−1.05704	1.53813
	H	−1.62546	−0.12955	1.20008
	C	−0.76706	−1.16382	2.86210
	H	0.31299	−1.35056	2.81086
	H	−0.93965	−0.22778	3.39722
	H	−1.22452	−1.98683	3.41876
	C	−4.19330	−0.77389	−1.09466
	O	−4.82372	−1.82061	−1.25996
	C	−4.86471	0.58842	−1.18396
	H	−5.13890	0.78665	−2.22639
	H	−5.79033	0.56325	−0.60153
	H	−4.22699	1.39947	−0.82255
	H	4.74205	−3.05439	−0.73662

Optimized Molecular Properties for **T6-INT1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 14 positive frequencies below 100 cm^–1. Zero–point correction: 0.441328 hartree Enthalpy correction: 0.472149 hartree Free Energy correction: 0.378896 hartree Quasiharmonic Free Energy correction: 0.388125 hartree SCF Energy: –1183.596706 hartree SCF Energy + ZPVE: –1183.155378 hartree Enthalpy: –1183.124557 hartree Free Energy: –1183.217810 hartree Free Energy with quasiharmonic correction: –1183.208581 hartree (correction: 5.79 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1184.01843606 A.U.
Cartesian Coordinates	(PCM) 52 spD3–INT1–T6.out Energy: –742982.7800982 O 2.92195 2.06882 –0.25275 C 2.46087 –2.74724 –0.13211 C 2.01693 –1.46160 0.03182 N 3.74113 –2.62210 –0.65948 C 4.05407 –1.32608 –0.80607 N 3.01704 –0.60828 –0.39130 H 1.07937 –1.07725 0.40271 H 2.96660 0.45744 –0.37413 H 4.98327 –0.94051 –1.19458 C 1.82274 –4.06582 0.14766 H 1.77963 –4.68204 –0.75775 H 2.38435 –4.62297 0.90682 H 0.80290 –3.91412 0.51220 C 1.68106 2.57194 –0.96508 C –0.52484 2.20264 0.24185 O –1.63650 1.62021 0.47802 C 2.92778 2.38447 1.13544 H 2.96811 3.47189 1.28100 H 2.03362 1.99682 1.63815 H 3.82381 1.93232 1.57203 C 0.45817 1.80719 –0.64705 H 0.23817 0.92567 –1.24514 O –0.25926 3.37480 0.94641 C –1.29149 3.83243 1.81267 H –0.91398 4.75575 2.25987 H –1.51231 3.10567 2.60216

	H	−2.21924	4.04007	1.26854
	C	2.07725	2.52818	−2.43869
	H	1.59054	3.61154	−0.63197
	H	1.30466	3.01279	−3.04382
	H	3.03088	3.03880	−2.61098
	H	2.17233	1.49252	−2.78863
	C	−1.57167	−2.06909	0.84136
	O	−1.26957	−3.21412	1.20715
	C	−2.08573	−1.85049	−0.58803
	N	−2.74459	−0.59030	−0.85552
	H	−2.28288	0.28258	−0.56832
	H	−2.79653	−2.65034	−0.80497
	H	−1.22547	−1.99700	−1.25829
	N	−1.42220	−0.98784	1.63329
	H	−1.59394	−0.03866	1.27840
	C	−0.94306	−1.13229	2.99918
	H	0.09198	−1.49397	3.03030
	H	−0.99331	−0.15715	3.48778
	H	−1.56282	−1.84462	3.55271
	C	−4.01841	−0.53224	−1.32911
	O	−4.68034	−1.52702	−1.63812
	C	−4.57356	0.87669	−1.47763
	H	−4.68529	1.10922	−2.54269
	H	−5.57116	0.91119	−1.02952
	H	−3.93629	1.63227	−1.01056
	H	4.35246	−3.39188	−0.90321

Optimized Molecular Properties for **T6-TS2**

Number of (–) Vibrational Frequencies	1 (–22.182)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 21 positive frequencies below 100 cm^–1. Zero–point correction: 0.607177 hartree Enthalpy correction: 0.649693 hartree Free Energy correction: 0.528799 hartree Quasiharmonic Free Energy correction: 0.542493 hartree SCF Energy: –1644.892367 hartree SCF Energy + ZPVE: –1644.285190 hartree Enthalpy: –1644.242674 hartree Free Energy: –1644.363568 hartree Free Energy with quasiharmonic correction: –1644.349874 hartree (correction: 8.59 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1645.48648611 A.U.
Cartesian Coordinates	(PCM) 72 spD3–TS2–T6.out Energy: –1032558.3511456 O 2.65024 –2.87572 –0.41539 C 5.04163 1.35067 –0.38572 C 4.14640 0.42871 0.08689 N 5.53787 0.81293 –1.56768 C 4.97148 –0.37897 –1.80173 N 4.12599 –0.62574 –0.80757 C 5.48034 2.67254 0.14757 C 1.30480 –2.76972 –0.99497 C –0.32418 –0.83835 –1.32641 O –0.75454 0.33335 –1.20324 C 2.73077 –3.13291 0.98920 C 0.62640 –1.49771 –0.53604 C –0.88064 –1.33412 1.68539 C –2.19012 –1.84373 1.23781 O –0.65782 –0.13429 1.93774 C –3.19715 –0.97084 0.79505 C –2.46476 –3.21829 1.32409 C –4.44542 –1.46908 0.42811 C –3.71577 –3.71480 0.96623 C –4.70852 –2.84010 0.51275 H 1.18004 –0.86683 0.14654 O –0.82697 –1.64792 –2.34928 C –1.79950 –1.05509 –3.20060 C 0.52342 –4.06872 –0.78154 C –3.41555 3.04804 –0.14121 O –4.48308 3.66831 –0.12300

	C	−2.47001	3.14671	1.06809
	N	−1.12237	2.65787	0.88393
	C	−0.14487	3.45437	0.36551
	O	−0.32078	4.64955	0.11742
	C	1.17522	2.74681	0.11941
	N	−3.02008	2.25443	−1.16221
	C	−3.84491	2.07919	−2.34436
	H	−3.91950	−4.77950	1.04121
	H	−5.68515	−3.22513	0.23170
	H	−5.21837	−0.78770	0.08272
	H	−2.98810	0.08953	0.73218
	H	−1.69245	−3.89573	1.68062
	H	−0.40761	−4.00124	−1.35024
	H	0.25775	−4.22345	0.26812
	H	1.09458	−4.93554	−1.13702
	H	2.25996	−4.08768	1.24419
	H	−0.16177	−2.10487	1.99989
	H	2.28278	−2.32721	1.58245
	H	3.79692	−3.19808	1.22574
	H	1.53304	−2.71834	−2.06937
	H	3.53079	−1.49060	−0.71275
	H	3.51299	0.43573	0.96743
	H	6.55633	2.68259	0.35575
	H	5.26505	3.48035	−0.56091
	H	4.95116	2.88808	1.07812
	H	5.16797	−1.01761	−2.64806
	H	1.52934	2.24064	1.02413
	H	1.91652	3.47596	−0.21319
	H	1.02739	1.97558	−0.64455
	H	−0.94462	1.66115	0.99572
	H	−2.43174	4.20289	1.34286
	H	−2.93914	2.60423	1.89682
	H	−2.17020	1.69278	−1.09136
	H	−3.20546	1.97573	−3.22534
	H	−4.48501	1.18953	−2.27141
	H	−1.99633	−1.78860	−3.98687
	H	−2.72933	−0.84066	−2.66323
	H	−1.43270	−0.12436	−3.64686
	H	−4.48633	2.95474	−2.45962
	O	2.02324	0.16167	2.50331
	C	2.16619	0.40086	3.89739
	H	3.23665	0.45884	4.11730
	H	1.73482	−0.40953	4.50254
	H	1.69964	1.34737	4.20538
	H	6.22016	1.25241	−2.17337
	H	1.05608	0.10565	2.30169

Optimized Molecular Properties for **T6-INT2-1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 19 positive frequencies below 100 cm^–1. Zero–point correction: 0.610290 hartree Enthalpy correction: 0.651551 hartree Free Energy correction: 0.534803 hartree Quasiharmonic Free Energy correction: 0.547012 hartree SCF Energy: –1644.902705 hartree SCF Energy + ZPVE: –1644.292415 hartree Enthalpy: –1644.251154 hartree Free Energy: –1644.367902 hartree Free Energy with quasiharmonic correction: –1644.355693 hartree (correction: 7.66 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1645.49919173 A.U.
Cartesian Coordinates	(PCM) 72 spD3–INT2–1–T6.out Energy: –1032566.3240424 O 2.65982 –2.74980 –0.01006 C 4.76989 1.64065 –0.29528 C 3.90146 0.68918 0.16938 N 5.35502 1.09024 –1.43020 C 4.86613 –0.13748 –1.64968 N 3.98408 –0.39406 –0.68920 C 5.10776 3.00263 0.20999 C 1.21248 –2.86008 –0.18835 C 0.28717 –0.68875 –1.20746 O –0.61373 0.09644 –1.42232 C 3.13300 –2.79508 1.34427 C 0.54310 –1.46598 0.07915 C –0.61838 –1.33331 1.13950 C –2.02023 –1.73670 0.64945 O –0.60513 –0.08413 1.72224 C –3.11093 –1.36437 1.45013 C –2.28463 –2.49745 –0.49674 C –4.41357 –1.74011 1.12379 C –3.58837 –2.87769 –0.83229 C –4.66044 –2.50202 –0.02227 H 1.32802 –0.88396 0.57122 O 1.25148 –0.92536 –2.13614 C 1.11740 –0.20655 –3.37650 C 0.66229 –4.05901 0.58511 C –4.00264 2.05308 –0.26961 O –5.20186 2.34315 –0.31842

	C	−3.16726	2.43581	0.96269
	N	−1.73424	2.27396	0.84956
	C	−0.96411	3.29206	0.39218
	O	−1.41514	4.39669	0.06515
	C	0.52163	2.98171	0.27940
	N	−3.34954	1.38655	−1.24573
	C	−4.03797	0.87343	−2.41478
	H	−3.76252	−3.46358	−1.73187
	H	−5.67464	−2.79509	−0.28095
	H	−5.23942	−1.43548	1.76222
	H	−2.91299	−0.76399	2.33239
	H	−1.47510	−2.79726	−1.15788
	H	−0.38700	−4.22057	0.32726
	H	0.71918	−3.94018	1.66937
	H	1.22638	−4.95518	0.30445
	H	2.97499	−3.78287	1.78706
	H	−0.35834	−2.10366	1.89704
	H	2.66327	−2.02433	1.96858
	H	4.20888	−2.60675	1.29418
	H	1.13272	−3.09326	−1.25134
	H	3.43530	−1.27573	−0.59461
	H	3.22711	0.69137	1.02474
	H	6.16647	3.07629	0.48313
	H	4.89738	3.77104	−0.54228
	H	4.51063	3.22322	1.09722
	H	5.14170	−0.79451	−2.45898
	H	0.84307	2.18696	0.95720
	H	1.08698	3.89682	0.47534
	H	0.73770	2.66442	−0.74812
	H	−1.30668	1.35299	1.10453
	H	−3.40181	3.47940	1.18738
	H	−3.53056	1.82132	1.79383
	H	−2.39524	1.08534	−1.07838
	H	−3.31443	0.72925	−3.22153
	H	−4.53288	−0.08481	−2.20916
	H	1.96303	−0.52022	−3.98906
	H	0.17557	−0.46193	−3.86760
	H	1.14809	0.87158	−3.20091
	H	−4.79660	1.59246	−2.73250
	O	1.77637	0.37637	2.47946
	C	1.82968	0.79063	3.82884
	H	2.87999	0.88506	4.13292
	H	1.34842	0.06731	4.50605
	H	1.34633	1.76819	3.98788
	H	6.04942	1.54248	−2.01250
	H	0.77520	0.20666	2.21795

Optimized Molecular Properties for **T6-INT2-2**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 20 positive frequencies below 100 cm^–1. Zero–point correction: 0.609520 hartree Enthalpy correction: 0.650946 hartree Free Energy correction: 0.533584 hartree Quasiharmonic Free Energy correction: 0.546315 hartree SCF Energy: –1644.901503 hartree SCF Energy + ZPVE: –1644.291983 hartree Enthalpy: –1644.250557 hartree Free Energy: –1644.367919 hartree Free Energy with quasiharmonic correction: –1644.355189 hartree (correction: 7.99 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1645.49700907 A.U.
Cartesian Coordinates	(PCM) 72 spD3–INT2–2–T6.out Energy: –1032564.9544026 O –2.66399 –2.74810 0.05908 C –4.75456 1.67562 0.28958 C –3.85420 0.73049 –0.12714 N –5.40477 1.12434 1.38972 C –4.92538 –0.10140 1.63807 N –3.98681 –0.35123 0.72968 C –5.07114 3.03598 –0.23531 C –1.21621 –2.87207 0.17631 C –0.29436 –0.66340 1.12348 O 0.58094 0.16439 1.28354 C –3.18756 –2.76629 –1.27833 C –0.54418 –1.48994 –0.12915 C 0.63279 –1.42592 –1.15284 C 2.02667 –1.79287 –0.65279 O 0.66810 –0.15471 –1.77234 C 3.12923 –1.45489 –1.45250 C 2.26394 –2.50835 0.52697 C 4.42449 –1.81667 –1.08337 C 3.55945 –2.88033 0.89823 C 4.64647 –2.53489 0.09484 H –1.31396 –0.92302 –0.67456 O –1.22650 –0.90249 2.07915 C –1.10431 –0.12354 3.28433 C –0.70515 –4.07869 –0.61303 C 4.05690 2.02033 0.26261 O 5.27229 2.22868 0.31335

	C	3.25798	2.45904	−0.97500
	N	1.81872	2.33252	−0.89853
	C	1.03865	3.38043	−0.51678
	O	1.49787	4.49199	−0.23633
	C	−0.44977	3.08485	−0.42732
	N	3.35536	1.41262	1.24362
	C	4.00230	0.87817	2.42763
	H	3.71541	−3.43449	1.82041
	H	5.65486	−2.81933	0.38313
	H	5.26264	−1.53790	−1.71674
	H	2.95817	−0.89782	−2.36791
	H	1.43912	−2.77851	1.18099
	H	0.34945	−4.25654	−0.38684
	H	−0.79660	−3.96165	−1.69557
	H	−1.27265	−4.96649	−0.31449
	H	−3.04202	−3.74292	−1.74996
	H	0.37725	−2.17235	−1.92296
	H	−2.74382	−1.97421	−1.89449
	H	−4.26157	−2.58575	−1.18306
	H	−1.09138	−3.09924	1.23637
	H	−3.43519	−1.22843	0.66189
	H	−3.10589	0.71900	−0.94157
	H	−6.11540	3.10742	−0.56083
	H	−4.89931	3.80875	0.52252
	H	−4.43161	3.25344	−1.09329
	H	−5.24744	−0.76002	2.42873
	H	−0.77907	2.26345	−1.07326
	H	−0.99959	3.99785	−0.67159
	H	−0.68877	2.81649	0.60943
	H	1.38881	1.42742	−1.12885
	H	3.51157	3.50600	−1.15754
	H	3.63147	1.87046	−1.82016
	H	2.38501	1.17051	1.07543
	H	3.26326	0.78677	3.22783
	H	4.44519	−0.10861	2.24076
	H	−1.92583	−0.44615	3.92411
	H	−0.14456	−0.31660	3.76903
	H	−1.18537	0.94290	3.06081
	H	4.79676	1.55793	2.74428
	O	−1.75971	0.38285	−2.17611
	H	−0.32362	0.09135	−2.04795
	C	−2.20280	0.56429	−3.48011
	H	−3.30053	0.72866	−3.53093
	H	−2.00079	−0.30249	−4.14540
	H	−1.74568	1.44262	−3.98287
	H	−6.13337	1.57336	1.93092

Optimized Molecular Properties for **T6-TS3**

Number of (–) Vibrational Frequencies	1 (–1189.8021)
Absolute Energies (Hartrees)	**B3LYP/6-31G(d)(PCM)** There are 18 positive frequencies below 100 cm^–1. Zero–point correction: 0.606193 hartree Enthalpy correction: 0.647133 hartree Free Energy correction: 0.531710 hartree Quasiharmonic Free Energy correction: 0.543459 hartree SCF Energy: –1644.879617 hartree SCF Energy + ZPVE: –1644.273424 hartree Enthalpy: –1644.232484 hartree Free Energy: –1644.347907 hartree Free Energy with quasiharmonic correction: –1644.336158 hartree (correction: 7.37 kcal/mol) **B3LYP-D3/6-311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1645.47839092 A.U.
Cartesian Coordinates	(PCM) 72 spD3–TS3–T6.out Energy: –1032553.2713372 O 2.87166 –2.08981 0.56582 C 5.69101 1.57695 –0.89348 C 4.55257 1.10097 –0.30149 N 6.30259 0.46247 –1.45419 C 5.56939 –0.63374 –1.20873 N 4.50288 –0.26201 –0.51160 C 6.26099 2.95172 –0.98677 C 1.46441 –2.34418 0.20107 C 0.44292 –0.13404 –0.47655 O –0.45600 0.68870 –0.64236 C 3.23400 –2.24464 1.94471 C 0.52761 –1.17148 0.55200 C –0.82909 –1.50370 1.21905 C –1.98636 –1.95506 0.32856 O –1.30988 –0.41896 2.03509 C –3.27022 –2.05805 0.88898 C –1.81725 –2.35004 –1.00304 C –4.34838 –2.52963 0.13988 C –2.89365 –2.82680 –1.75742 C –4.16496 –2.91661 –1.19052 H 1.05146 –0.51651 1.63089 O 1.56490 –0.07959 –1.28103 C 1.54396 0.92751 –2.29870 C 1.06117 –3.72893 0.71410 C –4.38401 1.42036 –0.94680

	O	−5.47732	1.42970	−1.52040
	C	−4.31898	1.58185	0.58052
	N	−3.01146	1.82934	1.14995
	C	−2.54140	3.09627	1.30332
	O	−3.19319	4.09873	0.99818
	C	−1.15530	3.20021	1.91829
	N	−3.20827	1.24984	−1.58500
	C	−3.16126	0.99213	−3.01200
	H	−2.73502	−3.12431	−2.79110
	H	−5.00364	−3.28280	−1.77647
	H	−5.33316	−2.59697	0.59550
	H	−3.41667	−1.76180	1.92316
	H	−0.83768	−2.28068	−1.46692
	H	0.09696	−4.02343	0.29017
	H	0.97669	−3.77706	1.80336
	H	1.81010	−4.46334	0.39816
	H	3.22588	−3.30123	2.23566
	H	−0.63112	−2.34335	1.90104
	H	2.57800	−1.65797	2.59652
	H	4.25991	−1.87315	2.03228
	H	1.55906	−2.41988	−0.88582
	H	3.75008	−0.91852	−0.16265
	H	3.78234	1.61526	0.25060
	H	7.25142	3.00482	−0.52111
	H	6.35858	3.27394	−2.02937
	H	5.60494	3.65749	−0.47296
	H	5.80593	−1.63692	−1.52600
	H	−0.62694	2.24573	1.93267
	H	−1.24564	3.57408	2.94488
	H	−0.57235	3.93289	1.35256
	H	−2.40833	1.03519	1.38537
	H	−4.98367	2.40951	0.83781
	H	−4.73279	0.66653	1.01658
	H	−2.35009	1.14277	−1.05080
	H	−2.11504	0.97661	−3.32484
	H	−3.62301	0.02905	−3.26270
	H	2.49618	0.83645	−2.82449
	H	0.71620	0.76566	−2.99522
	H	1.44554	1.92627	−1.86447
	H	−3.68983	1.77625	−3.56332
	O	1.19703	0.03051	2.77367
	H	−0.50913	−0.09276	2.52973
	C	1.96101	1.19342	2.66646
	H	3.04813	0.99573	2.75484
	H	1.70819	1.91637	3.46040
	H	1.80917	1.72427	1.70439
	H	7.17258	0.46727	−1.97282

Optimized Molecular Properties for **T6-INT3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 20 positive frequencies below 100 cm^–1. Zero–point correction: 0.609671 hartree Enthalpy correction: 0.651850 hartree Free Energy correction: 0.533915 hartree Quasiharmonic Free Energy correction: 0.545371 hartree SCF Energy: –1644.891936 hartree SCF Energy + ZPVE: –1644.282265 hartree Enthalpy: –1644.240086 hartree Free Energy: –1644.358021 hartree Free Energy with quasiharmonic correction: –1644.346565 hartree (correction: 7.19 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1645.49380273 A.U.
Cartesian Coordinates	(PCM) 72 spD3–INT3–T6.out Energy: –1032562.9423939 O 2.83959 2.18417 –0.49936 C 5.85723 –1.35567 0.72960 C 4.63086 –0.75613 0.62689 N 6.75545 –0.44267 0.19027 C 6.10268 0.65536 –0.21904 N 4.81244 0.48006 0.03974 C 6.27445 –2.67993 1.27440 C 1.62087 2.12001 0.39360 C 0.45011 –0.09250 0.70026 O –0.46197 –0.94103 0.62668 C 2.64511 2.55971 –1.85833 C 0.57665 1.12234 –0.00420 C –0.55089 1.55282 –0.92968 C –1.85906 2.04032 –0.29408 O –0.94755 0.55236 –1.90554 C –2.85007 2.57586 –1.13289 C –2.10133 2.01196 1.08193 C –4.04826 3.06495 –0.61179 C –3.30062 2.49919 1.61056 C –4.27875 3.02702 0.76711 H 1.61756 –0.14693 –1.40075 O 1.54348 –0.38660 1.55428 C 1.31045 –1.44420 2.48284 C 1.15176 3.56312 0.61216 C –4.33045 –1.30340 1.00572 O –5.40288 –1.34930 1.61704

	C	−4.31434	−0.94858	−0.48978
	N	−3.15243	−1.37026	−1.24646
	C	−3.07970	−2.62298	−1.76479
	O	−3.97788	−3.45943	−1.63340
	C	−1.81710	−2.93782	−2.55211
	N	−3.13345	−1.51445	1.59123
	C	−3.04303	−1.76152	3.01782
	H	−3.47013	2.46281	2.68383
	H	−5.21072	3.40646	1.17775
	H	−4.80092	3.47739	−1.27937
	H	−2.67618	2.60387	−2.20569
	H	−1.34061	1.60912	1.74273
	H	0.41679	3.59029	1.42236
	H	0.67478	3.99930	−0.27063
	H	2.00030	4.19817	0.88989
	H	2.22914	3.57113	−1.93733
	H	−0.17675	2.41355	−1.50569
	H	1.99811	1.85466	−2.39086
	H	3.63109	2.55362	−2.33388
	H	2.08942	1.77646	1.31580
	H	4.02927	1.16329	−0.18385
	H	3.64471	−1.07702	0.92646
	H	6.76693	−3.28928	0.50831
	H	6.96830	−2.56662	2.11486
	H	5.39725	−3.22508	1.62945
	H	6.55282	1.52164	−0.67712
	H	−1.10254	−2.11260	−2.57068
	H	−2.09609	−3.19491	−3.57951
	H	−1.33677	−3.81869	−2.11406
	H	−2.36418	−0.72791	−1.35785
	H	−5.20980	−1.40162	−0.92080
	H	−4.40779	0.13934	−0.57066
	H	−2.26802	−1.32858	1.08315
	H	−1.99989	−1.96664	3.26770
	H	−3.38849	−0.89980	3.60401
	H	2.25538	−1.59367	3.01271
	H	0.53237	−1.17452	3.20700
	H	1.01067	−2.36681	1.97911
	H	−3.65530	−2.62400	3.30076
	O	1.65517	−0.64869	−2.24856
	H	−0.13136	0.09486	−2.19538
	C	1.85215	−2.02873	−1.94056
	H	2.87068	−2.21721	−1.57095
	H	1.71286	−2.59383	−2.86634
	H	1.13067	−2.38144	−1.19466
	H	7.75637	−0.57672	0.11382

Optimized Molecular Properties for **T6-TS4**

Number of (–) Vibrational Frequencies	1 (–137.5699)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 19 positive frequencies below 100 cm^–1. Zero–point correction: 0.607974 hartree Enthalpy correction: 0.649855 hartree Free Energy correction: 0.532316 hartree Quasiharmonic Free Energy correction: 0.543808 hartree SCF Energy: –1644.892265 hartree SCF Energy + ZPVE: –1644.284291 hartree Enthalpy: –1644.242410 hartree Free Energy: –1644.359949 hartree Free Energy with quasiharmonic correction: –1644.348457 hartree (correction: 7.21 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1645.49201142 A.U.
Cartesian Coordinates	(PCM) 72 spD3–TS4–T6.out Energy: –1032561.8183299 O 2.72686 1.64597 –0.96700 C 5.88051 –1.21139 1.11207 C 4.65281 –0.68981 0.80495 N 6.79526 –0.40779 0.44236 C 6.14969 0.55297 –0.23643 N 4.84846 0.39592 –0.02610 C 6.28500 –2.37119 1.95813 C 1.62742 1.92295 0.27637 C 0.30938 –0.11706 0.81115 O –0.67873 –0.87300 0.84626 C 2.89080 2.61991 –1.99566 C 0.43883 1.11101 0.12470 C –0.66595 1.52863 –0.82317 C –1.98903 1.98885 –0.20601 O –0.99619 0.52444 –1.81489 C –3.10652 2.18798 –1.03257 C –2.10359 2.30830 1.15053 C –4.30569 2.67829 –0.51329 C –3.30152 2.80245 1.67456 C –4.40949 2.98620 0.84604 H 1.99396 0.33690 –1.94558 O 1.44795 –0.50742 1.54787 C 1.22805 –1.58962 2.45273 C 1.49810 3.43499 0.38657 C –4.60499 –1.25140 0.61830 O –5.76264 –1.23593 1.05029

	C	−4.35961	−1.31611	−0.89813
	N	−3.01282	−1.62910	−1.32624
	C	−2.60479	−2.91967	−1.46741
	O	−3.36042	−3.88453	−1.32509
	C	−1.13281	−3.08108	−1.81080
	N	−3.51300	−1.19235	1.40645
	C	−3.63854	−1.03667	2.84319
	H	−3.36871	3.03986	2.73373
	H	−5.34306	3.36598	1.25270
	H	−5.16013	2.82159	−1.17045
	H	−3.03013	1.95101	−2.08964
	H	−1.24311	2.15954	1.79611
	H	0.93589	3.66289	1.29836
	H	0.95685	3.88619	−0.44981
	H	2.47602	3.92108	0.46804
	H	3.34177	3.54790	−1.62288
	H	−0.29051	2.40382	−1.37975
	H	1.93411	2.85990	−2.47479
	H	3.55101	2.19064	−2.75809
	H	2.24952	1.54563	1.08427
	H	4.04866	0.98618	−0.43206
	H	3.65525	−0.97573	1.10391
	H	6.83365	−3.11906	1.37465
	H	6.92357	−2.05565	2.79089
	H	5.39629	−2.85076	2.37421
	H	6.61425	1.31283	−0.84448
	H	−0.92075	−4.13510	−1.99822
	H	−0.52724	−2.71912	−0.97315
	H	−0.86424	−2.49020	−2.69312
	H	−2.31900	−0.87886	−1.39726
	H	−5.04329	−2.07046	−1.29367
	H	−4.65057	−0.34492	−1.31158
	H	−2.58352	−1.08753	1.00048
	H	−2.65106	−1.16739	3.29149
	H	−4.02276	−0.04421	3.11226
	H	2.18824	−1.76928	2.94440
	H	0.47641	−1.33342	3.20729
	H	0.89981	−2.49324	1.93177
	H	−4.32357	−1.78658	3.25027
	O	1.61833	−0.25514	−2.64106
	H	−0.14150	0.16129	−2.13986
	C	2.17348	−1.55035	−2.45584
	H	3.26534	−1.54714	−2.59241
	H	1.73737	−2.21102	−3.20992
	H	1.94773	−1.96257	−1.46249
	H	7.80144	−0.52196	0.45811

Optimized Molecular Properties for **T6-product**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 25 positive frequencies below 100 cm^–1. Zero–point correction: 0.607249 hartree Enthalpy correction: 0.651604 hartree Free Energy correction: 0.522844 hartree Quasiharmonic Free Energy correction: 0.540913 hartree SCF Energy: –1644.947845 hartree SCF Energy + ZPVE: –1644.340596 hartree Enthalpy: –1644.296241 hartree Free Energy: –1644.425001 hartree Free Energy with quasiharmonic correction: –1644.406932 hartree (correction: 11.34 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1645.54204861 A.U.
Cartesian Coordinates	(PCM) 72 spD3–product–T6.out Energy: –1032593.2171404 O 3.57900 –2.30052 1.22430 C 4.67366 1.75262 –1.43845 C 3.95928 0.62690 –1.10600 N 5.68370 1.81276 –0.49413 C 5.54411 0.75517 0.34765 N 4.50710 0.01393 0.00549 C 4.51329 2.76012 –2.52877 C 0.86984 –2.46525 –1.44864 C –0.31640 –0.33042 –1.71777 O –1.20084 0.46383 –1.44409 C 4.66062 –2.88912 1.93754 C –0.10107 –1.63114 –1.02331 C –1.00225 –1.90609 0.17614 C –2.48760 –1.99367 –0.16511 O –0.78668 –0.94178 1.20743 C –3.45394 –1.56324 0.75086 C –2.91155 –2.59159 –1.35945 C –4.81458 –1.70763 0.47017 C –4.27049 –2.74036 –1.63993 C –5.22922 –2.29520 –0.72695 H 2.14553 –1.99172 2.11718 O 0.56991 –0.08957 –2.71342 C 0.36328 1.12848 –3.45086 C 1.27656 –3.79402 –0.89130 C –3.77202 2.43359 0.98030 O –4.89001 2.82937 1.32161

	C	−2.64175	2.39003	2.01977
	N	−1.34612	1.92762	1.56745
	C	−0.30389	2.78494	1.37866
	O	−0.38881	4.00243	1.55245
	C	0.99952	2.13475	0.94218
	N	−3.46204	2.03691	−0.27151
	C	−4.46809	1.95612	−1.31558
	H	−4.57946	−3.20288	−2.57394
	H	−6.28794	−2.40809	−0.94478
	H	−5.55083	−1.36019	1.19034
	H	−3.13317	−1.11498	1.68452
	H	−2.17485	−2.94086	−2.07827
	H	1.42664	−4.51307	−1.70552
	H	0.56201	−4.21966	−0.18355
	H	2.23969	−3.67875	−0.37498
	H	5.47501	−3.18008	1.26044
	H	−0.71588	−2.88556	0.57752
	H	4.28403	−3.78845	2.43233
	H	5.06733	−2.21490	2.70506
	H	1.46377	−2.13365	−2.29699
	H	3.91024	−1.47060	0.77669
	H	3.08163	0.22912	−1.59710
	H	4.35846	3.77057	−2.13122
	H	5.39026	2.79305	−3.18706
	H	3.64459	2.50566	−3.14172
	H	6.21180	0.57366	1.17789
	H	1.79014	2.42986	1.63946
	H	1.27914	2.51929	−0.04411
	H	0.94443	1.04506	0.89659
	H	−1.20080	0.92932	1.40656
	H	−2.51856	3.40535	2.40433
	H	−2.99835	1.76416	2.84608
	H	−2.56093	1.60760	−0.45053
	H	−3.97106	1.96955	−2.28850
	H	−5.06348	1.03738	−1.23592
	H	1.14836	1.14575	−4.20695
	H	−0.62187	1.12665	−3.92373
	H	0.44344	1.99685	−2.79249
	H	−5.14129	2.81287	−1.23873
	O	1.32526	−1.81877	2.64970
	H	0.00454	−1.23626	1.73143
	C	1.68262	−1.00897	3.76471
	H	2.38174	−1.53265	4.43096
	H	0.76902	−0.79300	4.32517
	H	2.13672	−0.05602	3.45840
	H	6.39912	2.52509	−0.43468

Optimized Molecular Properties for **T7-complex**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 19 positive frequencies below 100 cm^–1. Zero–point correction: 0.433834 hartree Enthalpy correction: 0.469163 hartree Free Energy correction: 0.350344 hartree Quasiharmonic Free Energy correction: 0.372445 hartree SCF Energy: –1296.442074 hartree SCF Energy + ZPVE: –1296.008240 hartree Enthalpy: –1295.972911 hartree Free Energy: –1296.091730 hartree Free Energy with quasiharmonic correction: –1296.069630 hartree (correction: 13.87 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1296.90269197 A.U.
Cartesian Coordinates	53 complex–T7.out Energy: –813529.6777086 C –7.68283 –1.53929 –0.58987 O –6.58824 –2.05173 –0.90425 O –7.88077 –0.42606 0.00390 C –5.09556 1.83434 0.99432 C –3.71732 1.84914 0.93556 N –5.47090 0.63326 0.43836 C –4.33690 –0.00886 0.07770 N –3.24049 0.68975 0.36002 C –8.97665 –2.31122 –0.94148 C –6.07930 2.83125 1.51844 C –0.54341 –0.09233 –1.19328 C 1.55196 0.09424 0.12656 O 2.78512 0.10380 0.18619 C 0.79904 –0.12709 –1.10827 H 1.42319 –0.32129 –1.97773 O 0.78892 0.29461 1.21270 C 1.47175 0.53734 2.44619 C –1.30828 –0.31351 –2.45550 C 6.32191 –1.52315 0.52487 O 7.14895 –2.38496 0.81164 C 6.26936 –0.98230 –0.91241 N 5.37358 0.12562 –1.17024 C 5.84114 1.36427 –1.51903 O 7.03069 1.61450 –1.68660 C 4.76095 2.41823 –1.72344 N 5.41956 –1.01228 1.40516 C 5.32639 –1.49639 2.76791

	H	−1.96588	−1.18595	−2.34399
	H	−0.66390	−0.46099	−3.32895
	H	−1.98108	0.53498	−2.63035
	H	−1.16843	0.12140	−0.32139
	H	−3.04676	2.63042	1.27676
	H	−6.77675	3.16966	0.74042
	H	−6.69001	2.41901	2.33304
	H	−5.55507	3.71244	1.90545
	H	−4.39240	−0.98409	−0.38655
	H	5.11256	3.36334	−1.30127
	H	3.80495	2.14473	−1.26867
	H	4.60911	2.57430	−2.79784
	H	4.37679	0.00926	−1.00870
	H	7.27661	−0.64769	−1.17004
	H	6.03285	−1.83742	−1.55908
	H	4.69998	−0.38331	1.06987
	H	5.40608	−0.67063	3.48557
	H	4.37799	−2.02153	2.94272
	H	−9.62139	−1.69188	−1.57807
	H	0.68530	0.71532	3.17977
	H	2.07097	−0.33148	2.73547
	H	−8.75048	−3.25043	−1.45555
	H	2.12466	1.41122	2.36407
	H	−9.54526	−2.52382	−0.02708
	H	6.15095	−2.19297	2.92785
	H	−6.45773	0.23371	0.28272

Optimized Molecular Properties for **T7-TS1**

Number of (–) Vibrational Frequencies	1 (–166.8481)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 16 positive frequencies below 100 cm^–1. Zero–point correction: 0.434440 hartree Enthalpy correction: 0.467790 hartree Free Energy correction: 0.359848 hartree Quasiharmonic Free Energy correction: 0.375141 hartree SCF Energy: –1296.431497 hartree SCF Energy + ZPVE: –1295.997057 hartree Enthalpy: –1295.963707 hartree Free Energy: –1296.071649 hartree Free Energy with quasiharmonic correction: –1296.056355 hartree (correction: 9.60 kcal/mol **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1296.89498873 A.U.
Cartesian Coordinates	53 spD3–TS1–T7.out Energy: –813813.8857267 C –7.32641 –0.36012 –0.12438 O –6.64286 –1.35412 –0.44269 O –6.89809 0.80863 0.17851 C –3.31906 1.65820 0.19105 C –2.12143 1.02586 –0.06043 N –4.29925 0.70974 –0.00600 C –3.69060 –0.43566 –0.36106 N –2.36828 –0.27837 –0.40701 C –8.86056 –0.50599 –0.07478 C –3.62559 3.06489 0.59546 C –0.84296 –1.57725 –0.77364 C 1.10733 –0.77480 0.54124 O 2.21447 –0.20579 0.67081 C 0.38346 –0.92638 –0.66904 H 0.82968 –0.45993 –1.54257 O 0.50909 –1.33097 1.64159 C 1.20692 –1.18775 2.87379 C –1.31972 –2.06909 –2.11826 C 5.76458 –0.88601 –0.62589 O 6.75565 –1.49041 –1.03344 C 5.30476 0.38094 –1.36489 N 4.27927 1.18129 –0.73101 C 4.53360 2.44409 –0.27582 O 5.60437 3.02505 –0.43901 C 3.35623 3.10843 0.42733 N 5.01914 –1.28165 0.43977 C 5.31610 –2.50353 1.15936

	H	−0.75957	−2.97543	−2.38732
	H	−1.14054	−1.32096	−2.89729
	H	−2.38435	−2.31512	−2.11402
	H	−1.14759	−2.17733	0.07723
	H	−1.11031	1.40940	−0.01896
	H	−4.25479	3.57408	−0.14589
	H	−4.16189	3.10508	1.55220
	H	−2.69922	3.63861	0.70311
	H	−4.26416	−1.32843	−0.56772
	H	3.73753	3.68652	1.27343
	H	2.61159	2.38658	0.77410
	H	2.87350	3.81137	−0.26208
	H	3.38819	0.74741	−0.48615
	H	6.18251	1.01808	−1.49118
	H	4.98800	0.05863	−2.36644
	H	4.14646	−0.80585	0.65431
	H	5.45658	−2.30706	2.22998
	H	4.50953	−3.23965	1.04487
	H	−9.32742	0.21829	−0.75372
	H	0.54993	−1.61555	3.63431
	H	2.16056	−1.72803	2.86063
	H	−9.16847	−1.51832	−0.35163
	H	1.40811	−0.13582	3.09865
	H	−9.22490	−0.27577	0.93417
	H	6.23754	−2.91686	0.74572
	H	−5.39373	0.79509	0.08547

Optimized Molecular Properties for **T7-INT1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 16 positive frequencies below 100 cm^–1. Zero–point correction: 0.436918 hartree Enthalpy correction: 0.470053 hartree Free Energy correction: 0.363384 hartree Quasiharmonic Free Energy correction: 0.378197 hartree SCF Energy: –1296.447425 hartree SCF Energy + ZPVE: –1296.010507 hartree Enthalpy: –1295.977372 hartree Free Energy: –1296.084041 hartree Free Energy with quasiharmonic correction: –1296.069229 hartree (correction: 9.30 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1296.90856334 A.U.
Cartesian Coordinates	53 spD3–INT1–T7.out Energy: –813822.4039230 C –7.20539 –0.64826 –0.29990 O –6.44510 –1.57715 –0.52889 O –6.83850 0.59318 –0.01525 C –3.26816 1.81397 0.17566 C –2.00043 1.30223 0.02911 N –4.18290 0.79826 –0.02113 C –3.46919 –0.29100 –0.27987 N –2.14015 –0.03564 –0.26393 C –8.71815 –0.80117 –0.31163 C –3.69000 3.21435 0.49575 C –1.01158 –1.03472 –0.49765 C 1.11229 –0.53556 0.78757 O 2.29513 –0.09497 0.97482 C 0.33971 –0.43885 –0.34807 H 0.77808 0.06886 –1.20267 O 0.50556 –1.20470 1.85960 C 1.30115 –1.35629 3.01967 C –1.22279 –1.66077 –1.88556 C 5.38656 –1.10252 –0.88995 O 6.27789 –1.75463 –1.43800 C 4.98049 0.25443 –1.48979 N 4.19702 1.13613 –0.65156 C 4.67096 2.34574 –0.24498 O 5.73186 2.83980 –0.62960 C 3.74899 3.08155 0.72231 N 4.70585 –1.52148 0.20676 C 4.96465 –2.81893 0.79544

	H	−0.49263	−2.46348	−2.02941
	H	−1.06326	−0.91123	−2.66990
	H	−2.22871	−2.07783	−2.01509
	H	−1.16066	−1.79634	0.27302
	H	−1.01885	1.74037	0.11711
	H	−4.31318	3.64195	−0.30076
	H	−4.27833	3.25713	1.42166
	H	−2.81586	3.86153	0.62280
	H	−3.90464	−1.26044	−0.47494
	H	4.36115	3.54070	1.50428
	H	3.00238	2.42039	1.17143
	H	3.23649	3.89133	0.18892
	H	3.34180	0.77254	−0.20902
	H	5.90039	0.77931	−1.75453
	H	4.44993	0.03252	−2.42746
	H	3.88890	−1.00323	0.54724
	H	5.04613	−2.73607	1.88611
	H	4.16593	−3.53795	0.56422
	H	−9.15814	−0.11800	−1.04647
	H	0.64442	−1.79810	3.77621
	H	2.15700	−2.02472	2.85197
	H	−8.98658	−1.83069	−0.55463
	H	1.68992	−0.39725	3.37863
	H	−9.12898	−0.53087	0.66744
	H	5.90370	−3.19625	0.38636
	H	−5.80450	0.67746	−0.01353

Optimized Molecular Properties for **T7-TS2-conformer**

Number of (–) Vibrational Frequencies	1 (–114.6451)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.603422 hartree Enthalpy correction: 0.647844 hartree Free Energy correction: 0.515013 hartree Quasiharmonic Free Energy correction: 0.533819 hartree SCF Energy: –1757.757746 hartree SCF Energy + ZPVE: –1757.154324 hartree Enthalpy: –1757.109902 hartree Free Energy: –1757.242733 hartree Free Energy with quasiharmonic correction: –1757.223927 hartree (correction: 11.80 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.38737524 A.U.
Cartesian Coordinates	73 spD3–TS2–T7–conf.out Energy: –1103404.7281332 C 7.11002 –0.13890 1.01391 O 6.33350 0.77747 1.23147 O 6.87067 –1.17154 0.21326 C 3.70384 –1.63350 –1.81813 C 2.48637 –1.01962 –1.98676 N 4.42304 –0.93999 –0.86538 C 3.64658 0.06221 –0.47531 N 2.46176 0.05825 –1.12500 C 8.48843 –0.22455 1.64736 C 4.24949 –2.85249 –2.49401 C 1.36849 1.06438 –0.98431 C –0.20141 –0.58920 0.14462 O –1.20298 –1.33662 0.20964 C 0.00413 0.44990 –0.81357 C –1.05386 1.98707 0.33977 C –1.69816 2.78212 –0.76449 O –0.20567 2.53981 1.09925 C –1.30292 4.10771 –0.98633 C –2.74999 2.25368 –1.52558 C –1.92693 4.87961 –1.96714 C –3.37691 3.02326 –2.50379 C –2.96391 4.33992 –2.73183 O 0.76679 –0.64640 1.09615 C 0.55928 –1.52131 2.21052 C 1.43721 2.01902 –2.18403 C –4.93400 –1.19771 1.14867 O –6.01279 –0.83900 1.62125

	C	−4.90639	−1.76598	−0.28101
	N	−3.67834	−2.39101	−0.72779
	C	−3.63127	−3.70563	−1.09163
	O	−4.61932	−4.43544	−1.15055
	C	−2.24077	−4.20760	−1.46352
	N	−3.75000	−1.07862	1.79618
	C	−3.66160	−0.47809	3.11765
	H	−4.19208	2.59959	−3.08600
	H	−3.45419	4.94199	−3.49345
	H	−1.61027	5.90780	−2.12999
	H	−0.51006	4.51090	−0.36330
	H	−3.07486	1.23140	−1.34265
	H	0.71722	2.83123	−2.06521
	H	1.20551	1.49097	−3.11711
	H	2.44036	2.44956	−2.27604
	H	1.60863	1.62002	−0.06784
	H	1.64138	−1.26042	−2.61362
	H	5.17958	−2.63097	−3.03312
	H	4.47832	−3.64400	−1.76916
	H	3.52873	−3.25371	−3.21419
	H	3.92107	0.79270	0.27230
	H	−2.11952	−5.21886	−1.06539
	H	−1.44419	−3.56122	−1.08524
	H	−2.16016	−4.27240	−2.55539
	H	−2.79967	−1.87769	−0.65687
	H	−5.69468	−2.51821	−0.34915
	H	−5.19163	−0.93838	−0.94645
	H	−2.88114	−1.34310	1.33997
	H	−3.73342	−1.23582	3.91096
	H	−2.70942	0.05217	3.21567
	H	9.25751	−0.27473	0.86880
	H	1.55294	−1.70811	2.62403
	H	−0.06144	−1.02055	2.95837
	H	8.65929	0.64514	2.28387
	H	0.09659	−2.45756	1.88995
	H	8.56942	−1.14129	2.24185
	H	−4.49305	0.21970	3.24177
	O	−0.55540	1.28998	3.46429
	C	−0.82458	2.36133	4.33804
	H	−1.22339	1.94819	5.27268
	H	−1.56999	3.06432	3.93216
	H	0.08014	2.94283	4.58700
	H	5.93152	−1.08819	−0.19968
	H	−0.60554	0.34735	−1.70722
	H	−1.73162	1.21756	0.74592
	H	−0.28826	1.69144	2.59302

Optimized Molecular Properties for **INT2-T7**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 21 positive frequencies below 100 cm^–1. Zero–point correction: 0.605491 hartree Enthalpy correction: 0.649348 hartree Free Energy correction: 0.520287 hartree Quasiharmonic Free Energy correction: 0.536509 hartree SCF Energy: –1757.770199 hartree SCF Energy + ZPVE: –1757.164708 hartree Enthalpy: –1757.120851 hartree Free Energy: –1757.249912 hartree Free Energy with quasiharmonic correction: –1757.233691 hartree (correction: 10.18 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.40514569 A.U.
Cartesian Coordinates	73 spD3–INT2–T7.out Energy: –1103415.8792588 C –6.72511 0.99432 –1.08360 O –5.95016 1.66443 –0.41882 O –6.56506 –0.29063 –1.37997 C –3.58271 –2.38328 –0.22912 C –2.43395 –2.20192 0.50127 N –4.26842 –1.18522 –0.29072 C –3.54369 –0.30841 0.38661 N –2.41904 –0.87255 0.88783 C –8.00681 1.55381 –1.67532 C –4.09212 –3.62467 –0.89157 C –1.38941 –0.20359 1.71656 C –0.07076 0.45689 –0.36391 O 0.62933 0.17274 –1.32064 C –0.03312 –0.22803 0.97647 C 1.27113 0.27470 1.82822 C 1.45866 1.79706 1.71155 O 2.36243 –0.44479 1.49039 C 2.52092 2.30984 0.96002 C 0.61422 2.70138 2.37016 C 2.71863 3.68773 0.84481 C 0.80696 4.07952 2.26177 C 1.86023 4.57957 1.49219 H 0.22184 –1.27183 0.78772 O –0.94852 1.49044 –0.40261 C –0.97104 2.24424 –1.62064 C –1.34430 –0.87492 3.10083 C 4.73532 0.42062 –1.94806

	O	5.74894	1.03584	−2.28172
	C	4.84757	−0.84967	−1.09112
	N	3.60845	−1.51892	−0.76967
	C	3.25061	−2.67110	−1.40734
	O	3.93991	−3.20746	−2.27732
	C	1.90808	−3.24181	−0.97260
	N	3.47340	0.79280	−2.28247
	C	3.19715	1.99575	−3.03479
	H	0.13999	4.76273	2.78412
	H	2.01678	5.65299	1.40888
	H	3.55400	4.06379	0.25782
	H	3.19390	1.60335	0.48815
	H	−0.19884	2.32479	2.98932
	H	−0.88584	−0.20916	3.83697
	H	−0.74910	−1.79417	3.07754
	H	−2.36155	−1.10255	3.43715
	H	0.96410	0.09588	2.87959
	H	−1.74097	0.82598	1.81690
	H	−1.64019	−2.88232	0.77131
	H	−5.08096	−3.90599	−0.50778
	H	−4.19311	−3.48557	−1.97513
	H	−3.41009	−4.46366	−0.72149
	H	−3.80701	0.73115	0.51758
	H	1.78496	−4.22831	−1.42528
	H	1.10382	−2.58177	−1.31927
	H	1.83275	−3.31318	0.11881
	H	3.02911	−1.13133	−0.00069
	H	5.48620	−1.54882	−1.63753
	H	5.36969	−0.55971	−0.17146
	H	2.69255	0.26136	−1.91098
	H	2.55896	1.77882	−3.90024
	H	2.69516	2.74946	−2.41296
	H	−8.86888	0.99011	−1.30226
	H	−1.77494	2.97170	−1.49964
	H	−0.01482	2.75290	−1.77121
	H	−8.10928	2.60742	−1.41086
	H	−1.16837	1.59167	−2.47527
	H	−7.99485	1.44287	−2.76509
	H	4.15210	2.39798	−3.37934
	O	1.62328	−2.74291	2.45510
	H	2.00039	−1.86509	2.08720
	C	2.52111	−3.23709	3.41555
	H	2.13556	−4.19208	3.79873
	H	2.64410	−2.55873	4.27900
	H	3.52733	−3.42765	3.00387
	H	−5.69171	−0.64255	−0.97183

Table S63. Optimized Molecular Properties for **T7-TS3**

Number of (–) Vibrational Frequencies	1 (–1109.2168)
Absolute Energies (Hartrees)	**B3LYP/6-31G(d)** There are 21 positive frequencies below 100 cm^-1. Zero-point correction: 0.601349 hartree Enthalpy correction: 0.644633 hartree Free Energy correction: 0.518182 hartree Quasiharmonic Free Energy correction: 0.532891 hartree SCF Energy: –1757.742604 hartree SCF Energy + ZPVE: –1757.141255 hartree Enthalpy: –1757.097971 hartree Free Energy: –1757.224422 hartree Free Energy with quasiharmonic correction: –1757.209714 hartree (correction: 9.23 kcal/mol) **B3LYP-D3/6-311+G(d,p)** SCF Done: E(RB3LYP) = –1758.38102468 A.U.
Cartesian Coordinates	73 spD3-TS3-T7.out Energy: –1103400.7430966 C –6.85631 –1.54834 1.39785 O –5.87045 –2.24439 1.20696 O –6.99571 –0.28997 1.00254 C –4.36846 1.68084 –0.89496 C –3.09026 1.49932 –1.36439 N –4.78897 0.52239 –0.26715 C –3.77958 –0.32986 –0.35707 N –2.72428 0.21337 –1.00693 C –8.08705 –2.04695 2.13728 C –5.24039 2.89402 –0.98698 C –1.47709 –0.50596 –1.37845 C 0.07003 0.01981 0.56183 O 1.12718 0.24133 1.15334 C –0.20423 0.20713 –0.86302 C 1.05902 0.12677 –1.75621 C 1.91063 –1.13939 –1.69280 O 1.92712 1.25084 –1.55959 C 3.19143 –1.12680 –2.26801 C 1.43871 –2.34654 –1.16474 C 3.97573 –2.27868 –2.30526 C 2.21886 –3.50601 –1.20722 C 3.49196 –3.47707 –1.77473 H –0.39012 1.54532 –1.05712 O –1.02903 –0.40627 1.26963 C –0.85904 –0.48769 2.68380 C –1.52200 –0.75867 –2.89556

	C	5.03909	−0.72986	1.22039
	O	6.00733	−1.48439	1.32367
	C	5.19199	0.59587	0.45566
	N	4.07096	1.50769	0.49203
	C	4.02835	2.53716	1.38810
	O	4.94450	2.79226	2.16903
	C	2.74321	3.35017	1.34261
	N	3.81178	−0.98185	1.73626
	C	3.50863	−2.22467	2.41163
	H	1.82972	−4.43036	−0.78591
	H	4.10496	−4.37460	−1.79707
	H	4.97017	−2.24078	−2.74377
	H	3.56561	−0.19443	−2.67902
	H	0.45750	−2.38612	−0.70160
	H	−0.71810	−1.43363	−3.20496
	H	−1.43250	0.17396	−3.46178
	H	−2.47883	−1.22416	−3.15601
	H	0.69830	0.18892	−2.79325
	H	−1.59749	−1.47783	−0.88527
	H	−2.38340	2.15927	−1.84964
	H	−6.17071	2.68249	−1.53044
	H	−5.52504	3.26002	0.00782
	H	−4.71995	3.70412	−1.50778
	H	−3.78948	−1.33140	0.04790
	H	2.58935	3.79051	0.35103
	H	2.80078	4.14482	2.08876
	H	1.88450	2.70210	1.54536
	H	3.27198	1.35058	−0.12965
	H	6.06029	1.10366	0.88181
	H	5.42713	0.33376	−0.58210
	H	3.03914	−0.35847	1.51806
	H	3.04045	−2.03485	3.38576
	H	2.83162	−2.84739	1.81292
	H	−8.97287	−1.95136	1.49992
	H	−1.82543	−0.80959	3.07738
	H	−0.08074	−1.21043	2.94929
	H	−7.94912	−3.08939	2.42911
	H	−0.58371	0.48523	3.10288
	H	−8.26147	−1.43242	3.02744
	H	4.44786	−2.76123	2.55933
	O	−0.27050	2.73362	−1.50729
	H	1.31128	2.03722	−1.59234
	C	−0.52116	3.67081	−0.50150
	H	−1.57755	4.00399	−0.49062
	H	0.09677	4.57663	−0.63487
	H	−0.30731	3.28704	0.51397
	H	−6.14585	0.03096	0.50912

Optimized Molecular Properties for **T7-INT3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.605309 hartree Enthalpy correction: 0.649812 hartree Free Energy correction: 0.520030 hartree Quasiharmonic Free Energy correction: 0.535799 hartree SCF Energy: –1757.746841 hartree SCF Energy + ZPVE: –1757.141532 hartree Enthalpy: –1757.097029 hartree Free Energy: –1757.226811 hartree Free Energy with quasiharmonic correction: –1757.211042 hartree (correction: 9.90 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.39131062 A.U.
Cartesian Coordinates	73 spD3–INT3–T7.out Energy: –1103407.1976214 C –4.97854 1.97009 0.85646 O –4.17083 1.64698 1.70993 O –5.35385 1.19859 –0.16596 C –3.87039 –2.21260 –0.96868 C –2.73493 –2.93238 –0.65545 N –3.92515 –1.10111 –0.15063 C –2.84865 –1.16336 0.62670 N –2.09731 –2.25551 0.36322 C –5.67379 3.31841 0.82976 C –4.94730 –2.52710 –1.96277 C –0.75654 –2.56359 1.05636 C 0.59574 –0.54242 1.67528 O 1.47534 0.33986 1.61314 C 0.32446 –1.57455 0.76498 C 1.08855 –1.61396 –0.52839 C 2.60987 –1.78417 –0.42187 O 0.87038 –0.47848 –1.41585 C 3.44741 –1.40069 –1.47874 C 3.19039 –2.41830 0.68290 C 4.82144 –1.64308 –1.43148 C 4.56240 –2.66849 0.73196 C 5.38700 –2.28298 –0.32687 H –2.32272 –1.09065 –2.21695 O –0.25975 –0.53178 2.80166 C 0.08009 0.41514 3.80155 C –0.42292 –4.03894 0.79025 C 3.78756 2.60023 –0.66630

	O	4.88097	3.03291	−1.04165
	C	2.52894	2.91352	−1.49280
	N	1.27556	2.38686	−0.99919
	C	0.34754	3.19334	−0.40775
	O	0.44964	4.41967	−0.35097
	C	−0.84217	2.46467	0.19723
	N	3.61696	1.85415	0.44324
	C	4.75438	1.45053	1.24440
	H	4.98977	−3.15715	1.60564
	H	6.45788	−2.47138	−0.28851
	H	5.45225	−1.32505	−2.25886
	H	3.00880	−0.89985	−2.33467
	H	2.54836	−2.69581	1.51354
	H	0.44087	−4.31111	1.40272
	H	−0.15317	−4.23196	−0.25404
	H	−1.25742	−4.70104	1.05515
	H	0.74283	−2.50044	−1.08771
	H	−1.00978	−2.47062	2.11276
	H	−2.35274	−3.85581	−1.06153
	H	−5.89502	−2.76670	−1.46318
	H	−5.14306	−1.67810	−2.62911
	H	−4.66790	−3.38596	−2.58216
	H	−2.58192	−0.43019	1.37447
	H	−0.72020	2.43335	1.28452
	H	−0.93941	1.43481	−0.15402
	H	−1.75611	3.02519	−0.01707
	H	1.14221	1.37118	−0.99236
	H	2.43226	4.00095	−1.54145
	H	2.72535	2.55030	−2.50941
	H	2.71667	1.43202	0.67395
	H	5.23954	2.31760	1.71093
	H	4.39277	0.77267	2.01993
	H	−5.37236	3.87133	−0.06694
	H	−0.69383	0.32792	4.57046
	H	1.06373	0.20633	4.24143
	H	−6.75979	3.18523	0.78061
	H	0.09860	1.43645	3.40837
	H	−5.40387	3.89095	1.71826
	H	5.50387	0.93368	0.63400
	O	−1.68999	−0.48801	−2.64594
	H	−0.05215	−0.52513	−1.74296
	C	−2.32997	0.76810	−2.85820
	H	−2.98080	0.73962	−3.74560
	H	−1.54162	1.50624	−3.02678
	H	−2.92650	1.07891	−1.99287
	H	−4.85443	0.30904	−0.12324

Optimized Molecular Properties for **T7-TS4**

Number of (–) Vibrational Frequencies	1 (–232.2431)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 21 positive frequencies below 100 cm^–1. Zero–point correction: 0.603601 hartree Enthalpy correction: 0.647795 hartree Free Energy correction: 0.519753 hartree Quasiharmonic Free Energy correction: 0.533962 hartree SCF Energy: –1757.739971 hartree SCF Energy + ZPVE: –1757.136370 hartree Enthalpy: –1757.092175 hartree Free Energy: –1757.220217 hartree Free Energy with quasiharmonic correction: –1757.206009 hartree (correction: 8.92 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1758.38389107 A.U.
Cartesian Coordinates	73 spD3–TS4–T7.out Energy: –1103402.5417835 C –4.64523 2.27728 0.93750 O –3.80177 1.90761 1.73931 O –5.19400 1.51545 –0.00276 C –4.22042 –2.01647 –0.83325 C –3.16039 –2.86960 –0.56860 N –4.08306 –0.90241 –0.03496 C –2.96661 –1.11055 0.67668 N –2.37393 –2.28183 0.39828 C –5.18385 3.69785 0.90105 C –5.38262 –2.19952 –1.76296 C –0.63452 –2.71266 1.07698 C 0.54228 –0.62419 1.66188 O 1.37340 0.28282 1.54171 C 0.33754 –1.73043 0.77416 C 1.10555 –1.72293 –0.52812 C 2.62702 –1.83008 –0.39814 O 0.82078 –0.59008 –1.37824 C 3.46870 –1.31513 –1.39253 C 3.20910 –2.53571 0.66238 C 4.85201 –1.49064 –1.32328 C 4.59026 –2.72171 0.73037 C 5.42076 –2.19866 –0.26295 H –2.32082 –1.40186 –2.07712 O –0.29333 –0.62500 2.76931 C –0.10869 0.46446 3.66802 C –0.53154 –4.13358 0.55594 C 3.89403 2.48717 –0.60563

	O	5.01815	2.87642	−0.93105
	C	2.69910	2.75647	−1.53440
	N	1.40414	2.28825	−1.09193
	C	0.44511	3.15631	−0.65561
	O	0.58981	4.37913	−0.65068
	C	−0.84604	2.50604	−0.18395
	N	3.63378	1.82408	0.54027
	C	4.70649	1.45245	1.44021
	H	5.01912	−3.26915	1.56745
	H	6.49848	−2.33562	−0.20831
	H	5.48653	−1.06642	−2.09798
	H	3.02679	−0.76856	−2.21819
	H	2.56459	−2.92535	1.44537
	H	0.36378	−4.60915	0.97502
	H	−0.44709	−4.18107	−0.53420
	H	−1.40424	−4.72277	0.85465
	H	0.80087	−2.61865	−1.09108
	H	−0.97750	−2.67474	2.10529
	H	−2.93819	−3.84603	−0.97826
	H	−6.32880	−2.28908	−1.21238
	H	−5.49400	−1.35049	−2.44953
	H	−5.26088	−3.10652	−2.36574
	H	−2.57659	−0.39746	1.38913
	H	−1.01134	2.74541	0.87082
	H	−0.85255	1.42016	−0.29912
	H	−1.68233	2.93908	−0.74260
	H	1.22005	1.28230	−1.06834
	H	2.62772	3.83903	−1.66648
	H	2.95545	2.31813	−2.50722
	H	2.71620	1.41992	0.71330
	H	5.20016	2.34109	1.85234
	H	4.27617	0.86423	2.25339
	H	−4.89157	4.17866	−0.03936
	H	−0.84128	0.31521	4.46502
	H	0.90530	0.47311	4.08278
	H	−6.27851	3.69120	0.93685
	H	−0.28868	1.42323	3.17282
	H	−4.78234	4.26858	1.73990
	H	5.46626	0.85216	0.92609
	O	−1.69756	−0.85036	−2.58968
	H	−0.09069	−0.69889	−1.73117
	C	−2.36477	0.35276	−2.96007
	H	−3.08655	0.17606	−3.77222
	H	−1.60055	1.04650	−3.32139
	H	−2.89032	0.80982	−2.11401
	H	−4.79272	0.55966	0.02539

Optimized Molecular Properties for **T7-product**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6-31G(d)** There are 25 positive frequencies below 100 cm^-1. Zero-point correction: 0.603818 hartree Enthalpy correction: 0.649054 hartree Free Energy correction: 0.515993 hartree Quasiharmonic Free Energy correction: 0.533387 hartree SCF Energy: -1757.779382 hartree SCF Energy + ZPVE: -1757.175564 hartree Enthalpy: -1757.130328 hartree Free Energy: -1757.263389 hartree Free Energy with quasiharmonic correction: -1757.245995 hartree (correction: 10.92 kcal/mol) **B3LYP-D3/6-311+G(d,p)** SCF Done: E(RB3LYP) = -1758.41724937 A.U.
Cartesian Coordinates	73 spD3-product-T7.out Energy: -1103423.4744326 C 3.83951 2.57813 -1.52439 O 2.74004 2.02463 -1.26222 O 4.99754 2.12450 -1.26573 C 5.51423 -1.04636 0.65495 C 4.71831 -1.99365 1.26028 N 4.64361 -0.16424 0.05399 C 3.39255 -0.59205 0.31019 N 3.38553 -1.70544 1.04102 C 3.78633 3.93769 -2.24658 C 6.99997 -0.89379 0.58927 C 0.70104 -2.36257 -1.52135 C -0.49968 -0.22631 -1.64702 O -1.21898 0.61766 -1.13846 C -0.35005 -1.61969 -1.12239 C -1.35689 -2.05952 -0.06376 C -2.80688 -1.94184 -0.52076 O -1.17189 -1.36213 1.16212 C -3.80145 -1.48392 0.34819 C -3.17811 -2.36439 -1.80423 C -5.13471 -1.42459 -0.06251 C -4.51088 -2.31744 -2.21365 C -5.49582 -1.84258 -1.34452 H 1.92733 -2.24282 1.75652 O 0.23700 0.00393 -2.74750 C 0.32354 1.37659 -3.19067 C 1.11981 -3.72759 -1.06692 C -3.98739 2.09164 1.30773

	O	−5.16795	2.25423	1.62232
	C	−2.93338	1.87777	2.40412
	N	−1.60434	1.50891	1.97191
	C	−0.53134	2.34094	2.16648
	O	−0.63669	3.45057	2.68610
	C	0.80034	1.79133	1.68738
	N	−3.52195	2.11670	0.03617
	C	−4.40724	2.23760	−1.10315
	H	−4.77808	−2.64602	−3.21560
	H	−6.53378	−1.79470	−1.66521
	H	−5.88561	−1.03346	0.61904
	H	−3.52100	−1.16836	1.34611
	H	−2.41527	−2.72469	−2.49059
	H	1.24681	−4.39306	−1.93189
	H	0.42959	−4.19750	−0.36342
	H	2.09729	−3.64741	−0.57413
	H	−1.17985	−3.12780	0.12291
	H	1.37121	−1.90460	−2.24474
	H	5.02513	−2.85738	1.83709
	H	7.37059	−0.93088	−0.44353
	H	7.33041	0.06312	1.01339
	H	7.48804	−1.69766	1.15064
	H	2.53794	−0.04733	−0.06178
	H	1.07940	2.22353	0.71900
	H	0.79020	0.70320	1.57777
	H	1.57433	2.07794	2.40461
	H	−1.45005	0.58177	1.57595
	H	−2.83851	2.81710	2.95723
	H	−3.34931	1.13017	3.09135
	H	−2.56682	1.82119	−0.13620
	H	−5.38412	2.55706	−0.73532
	H	−4.02234	2.98174	−1.81060
	H	3.10876	4.61497	−1.71446
	H	0.69921	1.31892	−4.21442
	H	−0.66462	1.84171	−3.16987
	H	4.77844	4.39133	−2.32397
	H	1.03390	1.90997	−2.54955
	H	3.37692	3.80206	−3.25611
	H	−4.51757	1.27924	−1.62578
	O	1.05565	−2.47164	2.21593
	H	−0.33272	−1.71303	1.56535
	C	1.22500	−2.25819	3.60542
	H	1.90347	−3.00242	4.05109
	H	0.24592	−2.35796	4.08639
	H	1.61998	−1.25675	3.82939
	H	4.84611	0.73986	−0.49134

Optimized Molecular Properties for **T8-complex**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 17 positive frequencies below 100 cm^–1. Zero–point correction: 0.469409 hartree Enthalpy correction: 0.506003 hartree Free Energy correction: 0.391355 hartree Quasiharmonic Free Energy correction: 0.406950 hartree SCF Energy: –1410.980080 hartree SCF Energy + ZPVE: –1410.510671 hartree Enthalpy: –1410.474077 hartree Free Energy: –1410.588725 hartree Free Energy with quasiharmonic correction: –1410.573130 hartree (correction: 9.79 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1411.48892998 A.U.
Cartesian Coordinates	57 spD3–complex–T8.out Energy: –885722.6689511 C 4.90961 2.73462 –0.35858 O 3.74739 2.28736 –0.18744 O 5.94521 2.06782 –0.65806 C 5.92860 –1.69927 –0.71535 C 5.02539 –2.72774 –0.54211 N 5.18260 –0.54597 –0.62857 C 3.89831 –0.91808 –0.41226 N 3.75029 –2.23764 –0.35196 C 5.10112 4.25756 –0.18331 C 7.40467 –1.69865 –0.95369 C 0.92505 –1.90189 1.47112 C –0.27292 0.27024 1.42980 O –1.33424 0.90928 1.50028 C –0.21782 –1.19725 1.52304 H –1.18832 –1.67703 1.62706 O 0.90328 0.85535 1.24215 C 0.94031 2.29555 1.09776 C 1.03053 –3.38917 1.50647 H 1.63895 –3.70633 0.65089 H 0.05443 –3.88542 1.49422 H 1.57842 –3.70980 2.40387 H 1.86964 –1.37480 1.36882 H 5.22839 –3.79316 –0.54629 H 7.66851 –1.23092 –1.91201 H 7.94758 –1.14941 –0.17277 H 7.78487 –2.72626 –0.96738 H 3.12572 –0.17015 –0.30084

	H	6.12874	4.56422	−0.39984
	H	1.95003	2.51919	0.74055
	H	0.18043	2.61254	0.37872
	H	4.41073	4.79764	−0.84297
	H	0.72712	2.75921	2.06618
	H	4.84859	4.54464	0.84555
	H	5.50907	0.46226	−0.67270
	C	−3.21114	−0.62979	−1.49973
	O	−3.98672	−1.38169	−2.10582
	N	−3.56337	0.03415	−0.36927
	C	−4.79271	−0.26318	0.37614
	C	−6.02637	0.45761	−0.22407
	O	−6.63883	1.32654	0.39494
	O	−3.55527	−0.56190	2.47979
	N	−6.37297	0.01367	−1.46106
	C	−7.44847	0.61229	−2.22415
	H	−2.73755	−0.05967	2.28818
	H	−4.96121	−1.34569	0.30880
	H	−2.83337	0.53508	0.13210
	H	−7.06859	1.17299	−3.08900
	H	−5.72934	−0.64397	−1.90421
	H	−8.14324	−0.15458	−2.58820
	H	−7.98395	1.29895	−1.56600
	C	−4.62193	0.12510	1.85349
	H	−4.50885	1.21483	1.93026
	H	−5.54551	−0.13439	2.37868
	C	−1.78724	−0.40792	−1.97814
	H	−1.39529	0.57259	−1.69231
	H	−1.75745	−0.51287	−3.06451
	H	−1.13090	−1.17134	−1.54407

Optimized Molecular Properties for **T8-TS1**

Number of (–) Vibrational Frequencies	1 (–149.2073)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 16 positive frequencies below 100 cm^–1. Zero–point correction: 0.468207 hartree Enthalpy correction: 0.503648 hartree Free Energy correction: 0.391049 hartree Quasiharmonic Free Energy correction: 0.407082 hartree SCF Energy: –1410.960427 hartree SCF Energy + ZPVE: –1410.492220 hartree Enthalpy: –1410.456779 hartree Free Energy: –1410.569378 hartree Free Energy with quasiharmonic correction: –1410.553345 hartree (correction: 10.06 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1411.47260017 A.U.
Cartesian Coordinates	57 spD3–TS1–T8.out Energy: –885712.4218407 C –7.87446 –0.63154 –0.13770 O –7.08534 –1.59764 –0.10066 O –7.57522 0.61090 –0.21537 C –4.08341 1.79340 –0.37124 C –2.82221 1.23874 –0.37026 N –4.96304 0.73599 –0.28636 C –4.23518 –0.39464 –0.23861 N –2.93153 –0.12692 –0.29085 C –9.38957 –0.91777 –0.09200 C –4.53420 3.21725 –0.44615 C –1.24789 –1.34269 –0.15272 C 0.45781 0.01455 1.03902 O 1.50247 0.70429 1.09094 C –0.09762 –0.56429 –0.13610 H 0.40750 –0.30733 –1.06312 O –0.22260 –0.24862 2.19180 C 0.32036 0.32151 3.38098 C –1.55666 –2.21724 –1.34115 H –0.92090 –3.11323 –1.30393 H –1.34461 –1.69528 –2.27960 H –2.60019 –2.53989 –1.35220 H –1.61292 –1.69887 0.80429 H –1.85453 1.72107 –0.42247 H –5.16631 3.39877 –1.32495 H –5.12111 3.50567 0.43545 H –3.66877 3.88502 –0.50916 H –4.71593 –1.36037 –0.16667

	H	−9.86660	−0.54544	−1.00738
	H	−0.36412	0.03324	4.18144
	H	1.32447	−0.06500	3.58558
	H	−9.58483	−1.98923	0.00933
	H	0.37745	1.41152	3.30667
	H	−9.84803	−0.37899	0.74636
	H	−6.05984	0.73250	−0.25857
	C	4.13226	−1.73229	−0.23019
	O	4.99325	−2.21343	−0.98134
	N	4.02226	−0.40479	0.01853
	C	4.72780	0.61284	−0.77031
	C	6.18196	0.82091	−0.28051
	O	6.56003	1.87727	0.22403
	O	2.63730	1.81598	−1.22783
	N	6.99074	−0.25223	−0.49426
	C	8.36313	−0.28787	−0.03506
	H	2.08217	1.48812	−0.48859
	H	4.76332	0.25680	−1.80811
	H	3.20606	−0.08563	0.54383
	H	8.49377	−0.98281	0.80618
	H	6.53522	−1.10346	−0.82771
	H	9.03844	−0.59510	−0.84324
	H	8.63120	0.71764	0.29467
	C	3.95091	1.93993	−0.72520
	H	3.96430	2.32895	0.30194
	H	4.48665	2.66443	−1.34614
	C	3.12282	−2.61267	0.48988
	H	3.15027	−2.43484	1.57103
	H	3.36072	−3.65829	0.28829
	H	2.10410	−2.39298	0.14871

Optimized Molecular Properties for **T8-INT1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 15 positive frequencies below 100 cm^–1. Zero–point correction: 0.470684 hartree Enthalpy correction: 0.505713 hartree Free Energy correction: 0.395650 hartree Quasiharmonic Free Energy correction: 0.410118 hartree SCF Energy: –1410.977806 hartree SCF Energy + ZPVE: –1410.507122 hartree Enthalpy: –1410.472093 hartree Free Energy: –1410.582156 hartree Free Energy with quasiharmonic correction: –1410.567688 hartree (correction: 9.08 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1411.48723457 A.U.
Cartesian Coordinates	57 spD3–INT1–T8.out Energy: –885721.6050653 C –7.78447 –0.83622 0.20429 O –6.96872 –1.73655 0.33596 O –7.49793 0.42455 –0.08731 C –4.01726 1.78421 –0.65795 C –2.72226 1.32233 –0.64030 N –4.86667 0.73872 –0.35282 C –4.08865 –0.31957 –0.16029 N –2.78029 –0.01703 –0.32607 C –9.28102 –1.05227 0.36456 C –4.52318 3.16446 –0.94127 C –1.60155 –0.97152 –0.18139 C 0.41022 0.19059 0.83020 O 1.54557 0.77174 0.84581 C –0.28164 –0.29407 –0.26077 H 0.16031 –0.12732 –1.23893 O –0.22066 –0.00130 2.06197 C 0.50696 0.43704 3.19655 C –1.75911 –2.06990 –1.24473 H –0.99585 –2.83839 –1.08604 H –1.61725 –1.65145 –2.24824 H –2.74618 –2.54618 –1.21240 H –1.73279 –1.40544 0.81436 H –1.77192 1.80710 –0.79867 H –5.19977 3.17802 –1.80591 H –5.08262 3.57197 –0.08909 H –3.69157 3.84431 –1.15367 H –4.46139 –1.29941 0.10196

	H	−9.80265	−0.75986	−0.55336
	H	−0.14971	0.26348	4.05503
	H	1.44009	−0.12505	3.33052
	H	−9.48399	−2.10069	0.58957
	H	0.76231	1.50013	3.13203
	H	−9.66575	−0.41806	1.17094
	H	−6.47364	0.55271	−0.19126
	C	3.96614	−1.70171	−0.57881
	O	4.88981	−2.15122	−1.28081
	N	3.91458	−0.42464	−0.14330
	C	4.79738	0.62863	−0.65814
	C	6.18548	0.62335	0.02795
	O	6.59279	1.56793	0.70408
	O	2.87774	2.07312	−1.16074
	N	6.91507	−0.49904	−0.22136
	C	8.20500	−0.73060	0.39027
	H	2.21941	1.65538	−0.55395
	H	4.95089	0.43406	−1.72830
	H	3.05489	−0.10496	0.32873
	H	8.16624	−1.54100	1.13208
	H	6.43382	−1.24878	−0.72443
	H	8.95812	−0.99288	−0.36412
	H	8.50583	0.19134	0.89197
	C	4.11733	2.00112	−0.49442
	H	4.02126	2.22480	0.57681
	H	4.78386	2.75819	−0.92101
	C	2.82545	−2.59513	−0.11591
	H	2.99399	−2.90356	0.92361
	H	2.81109	−3.48993	−0.74196
	H	1.85625	−2.08509	−0.16216

Optimized Molecular Properties for **T8-INT2**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 21 positive frequencies below 100 cm^–1. Zero–point correction: 0.639950 hartree Enthalpy correction: 0.685530 hartree Free Energy correction: 0.554755 hartree Quasiharmonic Free Energy correction: 0.569222 hartree SCF Energy: –1872.297699 hartree SCF Energy + ZPVE: –1871.657749 hartree Enthalpy: –1871.612169 hartree Free Energy: –1871.742944 hartree Free Energy with quasiharmonic correction: –1871.728477 hartree (correction: 9.08 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1872.97813800 A.U.
Cartesian Coordinates	77 spD3–INT2–T8.out Energy: –1175311.5168250 C –6.79722 –0.48959 –1.69340 C 3.74426 –0.44348 –2.22165 O –6.26071 0.58506 –1.46909 O 4.84795 –0.93167 –2.51772 N 3.05350 –0.79887 –1.11562 O –6.38482 –1.66359 –1.23327 C –3.33043 –2.13873 0.99195 C 3.60019 –1.69400 –0.09068 C –2.36438 –1.35756 1.57740 C 3.41326 –3.17639 –0.49612 N –4.18797 –1.33022 0.26779 O 2.65489 –3.94172 0.09482 C –3.74258 –0.09241 0.41555 O 3.44647 –0.16890 1.78676 N –2.63903 –0.05334 1.20021 N 4.19056 –3.54529 –1.55568 C –8.04223 –0.62704 –2.55327 C 4.08224 –4.85119 –2.16917 C –3.50792 –3.62298 1.06159 H 2.66486 0.42491 2.00424 C –1.87627 1.14908 1.60155 H 4.67606 –1.48984 –0.03782 C –0.46542 1.11975 –0.50878 H 2.13893 –0.38014 –0.95352 O 0.33058 0.53346 –1.22704 H 3.58746 –4.80509 –3.14999 C –0.45395 1.07081 0.99262

	H	4.68807	−2.79227	−2.03354
	C	0.62309	2.11429	1.66735
	H	5.07250	−5.30424	−2.30492
	C	1.33232	2.99109	0.61486
	H	3.48626	−5.48154	−1.50620
	C	2.99238	−1.40531	1.28788
	O	1.45613	1.44582	2.49167
	C	2.66559	2.76267	0.25450
	H	1.89674	−1.45752	1.23534
	C	0.66988	4.09023	0.04852
	H	3.29993	−2.22554	1.95180
	C	3.30880	3.60399	−0.65731
	C	3.09947	0.61738	−3.09720
	C	1.30671	4.92848	−0.86828
	H	2.03019	0.72863	−2.90632
	C	2.63554	4.68773	−1.22540
	H	3.27712	0.36114	−4.14550
	H	−0.02328	0.10185	1.24506
	H	3.58045	1.58162	−2.89790
	O	−1.42402	1.92623	−1.02324
	C	−1.41311	2.08129	−2.44886
	C	−1.93857	1.28892	3.13058
	H	0.77189	5.77791	−1.28939
	H	3.14256	5.34354	−1.93016
	H	4.34844	3.41456	−0.91745
	H	3.19680	1.92462	0.69259
	H	−0.35947	4.29677	0.33731
	H	−1.53647	2.25519	3.44559
	H	−1.36284	0.50471	3.62929
	H	−2.98528	1.23425	3.45075
	H	−0.02757	2.83552	2.21081
	H	−2.40951	1.98822	1.14644
	H	−1.52117	−1.59383	2.21272
	H	−4.47921	−3.89137	1.49686
	H	−3.46332	−4.07745	0.06398
	H	−2.72275	−4.07712	1.67369
	H	−4.19417	0.77872	−0.03696
	H	−8.84826	−1.09050	−1.97391
	H	−2.29234	2.68307	−2.68362
	H	−0.50082	2.59470	−2.76483
	H	−8.35836	0.35455	−2.91009
	H	−1.47232	1.10820	−2.94254
	H	−7.83733	−1.28459	−3.40524
	O	0.50464	−0.72880	3.61501
	H	0.83920	0.15569	3.24892
	C	1.43718	−1.17060	4.57651
	H	1.25086	−2.23254	4.78346
	H	1.35147	−0.62347	5.53301
	H	2.47208	−1.06479	4.22031
	H	−5.53851	−1.54815	−0.65653

Optimized Molecular Properties for **T8-TS3**

Number of (–) Vibrational Frequencies	2 (–1112.2814)
Absolute Energies (Hartrees)	**B3LYP/6-31G(d)** There are 20 positive frequencies below 100 cm^-1. Zero-point correction: 0.635351 hartree Enthalpy correction: 0.680595 hartree Free Energy correction: 0.549258 hartree Quasiharmonic Free Energy correction: 0.565255 hartree SCF Energy: –1872.271313 hartree SCF Energy + ZPVE: –1871.635962 hartree Enthalpy: –1871.590718 hartree Free Energy: –1871.722055 hartree Free Energy with quasiharmonic correction: –1871.706058 hartree (correction: 10.04 kcal/mol) **B3LYP-D3/6-311+G(d,p)** SCF Done: E(RB3LYP) = –1872.95342301 A.U.
Cartesian Coordinates	77 spD3-TS3-T8.out Energy: –1175296.0079347 C –7.09962 –0.75950 –2.23093 C 4.28394 0.10307 –1.80143 O –6.31162 0.14644 –2.45751 O 5.47750 0.02052 –2.14046 N 3.78908 –0.48887 –0.69236 O –7.05780 –1.56861 –1.18104 C –4.49675 –1.36312 1.60512 C 4.63782 –1.15779 0.29591 C –3.39113 –0.61591 1.93190 C 5.00096 –2.59874 –0.14109 N –4.99680 –0.92691 0.39149 O 4.60746 –3.59356 0.46572 C –4.20240 0.05758 0.00133 O 3.81825 0.14080 2.19585 N –3.21104 0.28301 0.89444 N 5.81496 –2.64660 –1.23253 C –8.26469 –1.08794 –3.15015 C 6.18980 –3.89618 –1.85843 C –5.12717 –2.48910 2.36355 H 2.88592 0.43305 2.09282 C –2.21578 1.38519 0.80910 H 5.56771 –0.57951 0.36496 C –0.27096 0.12893 –0.23311 H 2.80002 –0.36678 –0.47247 O 0.89583 –0.19860 –0.45773 H 5.69510 –4.03165 –2.83069

	C	−0.76177	0.87092	0.92630
	H	5.98663	−1.75755	−1.70691
	C	0.30120	1.84017	1.52326
	H	7.27480	−3.94679	−2.01525
	C	1.02720	2.75699	0.53972
	H	5.88480	−4.70670	−1.19362
	C	3.96288	−1.16281	1.67455
	O	1.26502	1.14809	2.31863
	C	2.40863	2.97606	0.62214
	H	3.00310	−1.69213	1.60951
	C	0.30115	3.48061	−0.41896
	H	4.59840	−1.74763	2.34977
	C	3.03993	3.88777	−0.22787
	C	3.28871	0.89731	−2.62752
	C	0.92891	4.39279	−1.26724
	H	2.25331	0.67982	−2.35692
	C	2.30600	4.60446	−1.17415
	H	3.46082	0.68311	−3.68657
	H	−0.76128	−0.00310	1.97386
	H	3.46625	1.96601	−2.46587
	O	−1.26143	−0.25477	−1.09852
	C	−0.85901	−1.10191	−2.17430
	C	−2.61738	2.44718	1.84885
	H	0.33996	4.93698	−2.00247
	H	2.79949	5.31549	−1.83289
	H	4.11473	4.03423	−0.14687
	H	2.99568	2.42086	1.34270
	H	−0.77099	3.33008	−0.51059
	H	−2.07967	3.38688	1.68953
	H	−2.41680	2.10116	2.86817
	H	−3.68951	2.65262	1.75997
	H	−0.24175	2.51082	2.20332
	H	−2.40211	1.80707	−0.18665
	H	−2.68903	−0.65810	2.75546
	H	−6.17142	−2.26791	2.62075
	H	−5.12991	−3.41686	1.77702
	H	−4.58197	−2.68020	3.29335
	H	−4.32148	0.60801	−0.92076
	H	−9.20890	−1.01482	−2.59937
	H	−1.78310	−1.39797	−2.67502
	H	−0.20657	−0.56936	−2.87448
	H	−8.27522	−0.40114	−3.99817
	H	−0.32633	−1.98200	−1.80282
	H	−8.17867	−2.11972	−3.50840
	O	−0.55963	−0.54664	3.11211
	H	0.73278	0.48502	2.85265
	C	−0.18658	−1.88527	2.92675
	H	−1.05516	−2.53653	2.71050
	H	0.29648	−2.28438	3.83454
	H	0.52750	−2.02085	2.09372
	H	−6.25919	−1.32792	−0.56936

Optimized Molecular Properties for **T8-INT3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 21 positive frequencies below 100 cm^–1. Zero–point correction: 0.639571 hartree Enthalpy correction: 0.685896 hartree Free Energy correction: 0.553292 hartree Quasiharmonic Free Energy correction: 0.568104 hartree SCF Energy: –1872.281822 hartree SCF Energy + ZPVE: –1871.642251 hartree Enthalpy: –1871.595926 hartree Free Energy: –1871.728530 hartree Free Energy with quasiharmonic correction: –1871.713718 hartree (correction: 9.29 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1872.96849509 A.U.
Cartesian Coordinates	77 spD3–INT3–T8.out Energy: –1175305.4658077 C 7.98815 –0.80116 0.75955 C –4.73541 0.25829 0.91626 O 7.34732 –0.07234 1.50186 O –5.95511 0.01863 0.85311 N –3.82066 –0.39746 0.16485 O 7.53192 –1.35142 –0.35763 C 4.04702 –0.82082 –1.75384 C –4.22702 –1.33046 –0.88782 C 2.89572 –0.15168 –1.40999 C –4.51845 –2.73672 –0.31136 N 4.99437 –0.61745 –0.77033 O –3.80503 –3.71560 –0.53738 C 4.41699 0.15623 0.13956 O –3.01337 –0.16327 –2.66184 N 3.14254 0.46260 –0.19669 N –5.64933 –2.78184 0.44564 C 9.43431 –1.18460 1.02723 C –6.03737 –3.96561 1.18225 C 4.31901 –1.66370 –2.96041 H –2.18400 0.22036 –2.30595 C 2.22401 1.38444 0.57966 H –5.16319 –0.93670 –1.30067 C 0.01722 0.43764 1.36680 H –2.82863 –0.19346 0.31817 O –1.20883 0.16429 1.35196 H –5.90074 –3.83529 2.26501 C 0.76191 1.10021 0.38474

	H	−6.08095	−1.87807	0.65375
	C	0.04342	1.58404	−0.84561
	H	−7.08927	−4.21690	0.99620
	C	−1.06107	2.63554	−0.64646
	H	−5.40620	−4.79012	0.84501
	C	−3.19707	−1.40877	−2.02324
	O	−0.48154	0.50004	−1.68027
	C	−1.96281	2.92164	−1.68255
	H	−2.25169	−1.81377	−1.64492
	C	−1.12841	3.41197	0.51601
	H	−3.57541	−2.13243	−2.75618
	C	−2.90833	3.93975	−1.55331
	C	−4.18959	1.33411	1.83433
	C	−2.06752	4.43690	0.64745
	H	−3.14088	1.16057	2.08672
	C	−2.96530	4.70577	−0.38704
	H	−4.80997	1.37647	2.73389
	H	0.91277	−1.54509	−0.05120
	H	−4.25797	2.30261	1.32501
	O	0.76606	0.02009	2.48091
	C	0.01228	−0.50454	3.56176
	C	2.66487	2.83042	0.27684
	H	−2.10184	5.02068	1.56520
	H	−3.70078	5.50094	−0.28613
	H	−3.60313	4.13253	−2.36765
	H	−1.92934	2.34233	−2.59912
	H	−0.43880	3.19345	1.32519
	H	2.08925	3.52888	0.89265
	H	2.50445	3.09270	−0.77436
	H	3.73059	2.97041	0.49398
	H	0.78636	2.07814	−1.48832
	H	2.46436	1.17054	1.62246
	H	1.93488	−0.08395	−1.89781
	H	5.15592	−1.26620	−3.54930
	H	4.58087	−2.69180	−2.67991
	H	3.43757	−1.70600	−3.60779
	H	4.90432	0.49490	1.04324
	H	10.06585	−0.87459	0.18742
	H	0.74435	−0.77157	4.33014
	H	−0.69054	0.23458	3.96589
	H	9.78075	−0.71088	1.94724
	H	−0.56066	−1.39268	3.27463
	H	9.52247	−2.27323	1.11330
	O	0.29966	−2.07413	−0.59046
	H	−0.33018	−0.34182	−1.20166
	C	−0.44244	−2.92159	0.29218
	H	0.20752	−3.68128	0.75156
	H	−1.20817	−3.42385	−0.30255
	H	−0.94088	−2.33855	1.07405
	H	6.54923	−1.07680	−0.52137

Optimized Molecular Properties for **T8-TS4**

Number of (–) Vibrational Frequencies	1 (–214.4171)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.637265 hartree Enthalpy correction: 0.683599 hartree Free Energy correction: 0.548960 hartree Quasiharmonic Free Energy correction: 0.565982 hartree SCF Energy: –1872.269772 hartree SCF Energy + ZPVE: –1871.632507 hartree Enthalpy: –1871.586173 hartree Free Energy: –1871.720812 hartree Free Energy with quasiharmonic correction: –1871.703790 hartree (correction: 10.68 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1872.95462092 A.U.
Cartesian Coordinates	77 spD3–TS4–T8.out Energy: –1175296.7596346 C 5.49686 2.92212 –1.13577 C –4.59630 0.69122 –0.37147 O 4.67932 2.48109 –1.92889 O –5.66734 1.16701 0.04499 N –3.38466 1.12527 0.03513 O 5.92345 2.30268 –0.04440 C 4.89866 –1.10263 1.12919 C –3.19458 2.10551 1.10493 C 4.00041 –2.09786 0.77493 C –3.40278 3.55498 0.59922 N 4.74441 –0.05534 0.25037 O –2.49324 4.38248 0.56793 C 3.77811 –0.44158 –0.59567 O –1.68186 0.74790 2.47896 N 3.29805 –1.66582 –0.32857 N –4.68616 3.82183 0.22853 C 6.14888 4.28706 –1.30056 C –5.06845 5.08596 –0.36289 C 5.92209 –1.08544 2.22466 H –1.38304 0.01369 1.89869 C 1.71366 –2.40583 –1.21820 H –3.94898 1.90204 1.87534 C 0.00282 –0.64512 –1.36690 H –2.54946 0.68168 –0.35167 O –1.08142 –0.09516 –1.12948 H –5.30445 4.98262 –1.43150 C 0.49431 –1.85439 –0.77642

	H	−5.32658	3.02497	0.20530
	C	−0.28665	−2.42000	0.39150
	H	−5.94641	5.50702	0.14341
	C	−1.67652	−2.96810	0.05992
	H	−4.22718	5.77323	−0.25403
	C	−1.80190	1.94176	1.73180
	O	−0.43167	−1.51558	1.49730
	C	−2.69004	−2.97739	1.02782
	H	−1.03782	2.01731	0.94635
	C	−1.93110	−3.57837	−1.17491
	H	−1.64343	2.78214	2.41401
	C	−3.91975	−3.58618	0.76834
	C	−4.57968	−0.43262	−1.39137
	C	−3.15756	−4.19091	−1.43554
	H	−3.57623	−0.65217	−1.76279
	C	−4.15885	−4.20226	−0.46204
	H	−5.24004	−0.16411	−2.22240
	H	2.73047	−1.02425	2.22063
	H	−4.97992	−1.33908	−0.92629
	O	0.84935	−0.08376	−2.30067
	C	0.38630	1.12107	−2.90607
	C	2.05183	−3.87270	−1.04295
	H	−3.33242	−4.65638	−2.40344
	H	−5.11569	−4.67947	−0.66230
	H	−4.69404	−3.57787	1.53258
	H	−2.50446	−2.49681	1.98173
	H	−1.15753	−3.55664	−1.93764
	H	1.35231	−4.48327	−1.62847
	H	1.97785	−4.20394	−0.00241
	H	3.06806	−4.07792	−1.39061
	H	0.27771	−3.28955	0.76395
	H	2.05793	−2.00670	−2.16589
	H	3.84978	−3.07987	1.20561
	H	6.94383	−1.06087	1.82218
	H	5.81210	−0.20358	2.86858
	H	5.83326	−1.97642	2.85635
	H	3.41537	0.18293	−1.39998
	H	5.88671	4.92880	−0.45186
	H	1.20317	1.45966	−3.54672
	H	−0.51677	0.94576	−3.50178
	H	7.23981	4.18675	−1.30565
	H	0.16137	1.88200	−2.15319
	H	5.81202	4.75082	−2.22935
	O	1.92534	−0.77946	2.71882
	H	0.46224	−1.32977	1.87238
	C	1.83374	0.64673	2.76054
	H	2.54237	1.06846	3.48806
	H	0.81249	0.88762	3.06537
	H	2.02943	1.09544	1.77912
	H	5.45800	1.37653	0.06124

Optimized Molecular Properties for **T8-product**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.637817 hartree Enthalpy correction: 0.685008 hartree Free Energy correction: 0.548103 hartree Quasiharmonic Free Energy correction: 0.565715 hartree SCF Energy: –1872.306716 hartree SCF Energy + ZPVE: –1871.668899 hartree Enthalpy: –1871.621708 hartree Free Energy: –1871.758613 hartree Free Energy with quasiharmonic correction: –1871.741001 hartree (correction: 11.05 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1872.98841635 A.U.
Cartesian Coordinates	77 spD3–product–T8.out Energy: –1175317.9665869 C –5.01743 –2.44958 –2.18892 C 4.63135 –0.53280 –0.88188 O –3.83942 –2.15945 –1.87011 O 5.81588 –0.79989 –0.62181 N 3.59996 –0.90777 –0.09129 O –6.07767 –2.08645 –1.58704 C –6.03556 0.09800 1.40714 C 3.78017 –1.56767 1.20433 C –5.12248 0.74257 2.21223 C 4.04394 –3.08566 1.03706 N –5.28749 –0.57499 0.46723 O 3.24695 –3.93889 1.42232 C –3.98855 –0.32362 0.72700 O 2.46968 0.01077 2.55294 N –3.83790 0.47720 1.78122 N 5.24182 –3.36963 0.45487 C –5.21120 –3.35179 –3.42442 C 5.63351 –4.72283 0.12060 C –7.52966 0.05295 1.43777 H 1.87519 0.51692 1.96052 C –1.94216 2.11374 –0.85374 H 4.66043 –1.11651 1.67824 C –0.17958 0.42539 –1.10019 H 2.65736 –0.63701 –0.36338 O 0.98782 0.06047 –1.03965 H 5.64845 –4.88494 –0.96603 C –0.67730 1.73547 –0.58187

	H	5.76834	−2.57494	0.08819
	C	0.27578	2.50118	0.32656
	H	6.63058	−4.95254	0.51704
	C	1.53666	3.01940	−0.35769
	H	4.90443	−5.40088	0.56807
	C	2.56456	−1.32955	2.11198
	O	0.62231	1.72451	1.46020
	C	2.77931	2.96478	0.28358
	H	1.65187	−1.66165	1.59817
	C	1.44608	3.66167	−1.59977
	H	2.68022	−1.96992	2.99145
	C	3.90522	3.54320	−0.30722
	C	4.25944	0.24058	−2.13407
	C	2.57014	4.23937	−2.18963
	H	3.18156	0.28996	−2.30175
	C	3.80690	4.18589	−1.54259
	H	4.75182	−0.22755	−2.99236
	H	−2.35949	0.95757	2.52896
	H	4.64274	1.26179	−2.04469
	O	−1.14956	−0.32377	−1.63365
	C	−0.80401	−1.62877	−2.14103
	C	−2.67953	3.33230	−0.38976
	H	2.47929	4.73136	−3.15543
	H	4.68470	4.63789	−1.99846
	H	4.86387	3.48766	0.20315
	H	2.86311	2.45953	1.23862
	H	0.48662	3.70453	−2.10980
	H	−3.15637	3.83598	−1.24079
	H	−2.05936	4.06132	0.13706
	H	−3.48543	3.01354	0.28481
	H	−0.26206	3.39361	0.67730
	H	−2.53673	1.43389	−1.45851
	H	−5.31249	1.37300	3.07206
	H	−7.96966	0.43488	0.50741
	H	−7.90432	−0.97023	1.57065
	H	−7.90970	0.66122	2.26555
	H	−3.20617	−0.74189	0.11078
	H	−4.79728	−4.34700	−3.21778
	H	−1.76785	−2.09877	−2.34537
	H	−0.18887	−1.52326	−3.04098
	H	−6.26749	−3.45312	−3.68993
	H	−0.23907	−2.18350	−1.38716
	H	−4.65308	−2.94442	−4.27577
	O	−1.48183	1.16405	2.98285
	H	−0.20762	1.55509	1.99536
	C	−1.10007	0.02335	3.74027
	H	−1.53996	0.04728	4.74919
	H	−0.00872	0.01935	3.83420
	H	−1.41146	−0.91121	3.25378
	H	−5.62853	−1.18709	−0.34958

Optimized Molecular Properties for **T9-complex**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 19 positive frequencies below 100 cm^–1. Zero–point correction: 0.403054 hartree Enthalpy correction: 0.437073 hartree Free Energy correction: 0.322137 hartree Quasiharmonic Free Energy correction: 0.342722 hartree SCF Energy: –1164.844402 hartree SCF Energy + ZPVE: –1164.441348 hartree Enthalpy: –1164.407329 hartree Free Energy: –1164.522265 hartree Free Energy with quasiharmonic correction: –1164.501679 hartree (correction: 12.92 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1165.27390926 A.U.
Cartesian Coordinates	49 spD3–complex–T9.out Energy: –731220.4120393 C 6.51118 0.67910 1.82586 O 5.39082 1.19180 2.02817 O 6.82443 –0.18554 0.93963 C 4.36954 –1.53932 –1.49844 C 3.03012 –1.40134 –1.79841 N 4.59081 –0.70418 –0.42799 C 3.41006 –0.11370 –0.13405 N 2.42697 –0.50573 –0.93993 C 7.68680 1.11459 2.73280 C 5.44612 –2.37326 –2.11638 C –0.27661 1.20792 –1.29144 C –2.38494 0.18004 –0.49378 O –3.60802 0.24824 –0.30282 C –1.61160 1.24881 –1.12386 H –2.21319 2.09630 –1.44398 O –1.66937 –0.89170 –0.13104 C –2.35998 –1.95112 0.54189 C 0.51943 2.29994 –1.92419 H 1.27365 2.66529 –1.21506 H –0.09703 3.13880 –2.26412 H 1.09081 1.89616 –2.76965 H 0.32015 0.35145 –0.96664 H 2.47089 –1.89987 –2.58285 H 6.27567 –1.76071 –2.49445 H 5.87935 –3.08467 –1.40030 H 5.04286 –2.94816 –2.95781 H 3.34511 0.59110 0.68366

	H	8.49283	1.54122	2.12204
	H	−1.60894	−2.72464	0.70202
	H	−2.75584	−1.60391	1.50095
	H	7.36337	1.85136	3.47454
	H	−3.18356	−2.33454	−0.06617
	H	8.10759	0.24034	3.24586
	H	5.50514	−0.51588	0.10613
	C	−6.75394	−1.47305	1.11357
	O	−7.82753	−2.05104	1.24108
	N	−6.05658	−1.45085	−0.05753
	O	−4.66017	2.75919	−1.17422
	H	−4.40202	1.85166	−0.91532
	H	−5.22462	−0.88180	−0.18783
	C	−4.73729	3.52209	0.01287
	H	−5.53039	3.17070	0.69385
	H	−4.97356	4.55275	−0.27287
	C	−6.08319	−0.74733	2.27483
	H	−5.81343	−1.48111	3.04229
	H	−6.80734	−0.06067	2.72336
	H	−5.18886	−0.19165	1.97974
	H	−6.50308	−1.85746	−0.86784
	H	−3.78944	3.53554	0.57456

Optimized Molecular Properties for **T9-TS1**

Number of (–) Vibrational Frequencies	1 (–165.3629)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** Zero–point correction: 0.403409 hartree Enthalpy correction: 0.435571 hartree Free Energy correction: 0.330211 hartree Quasiharmonic Free Energy correction: 0.345015 hartree SCF Energy: –1164.833124 hartree SCF Energy + ZPVE: –1164.429715 hartree Enthalpy: –1164.397553 hartree Free Energy: –1164.502913 hartree Free Energy with quasiharmonic correction: –1164.488109 hartree (correction: 9.29 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1165.26628323 A.U.
Cartesian Coordinates	49 spD3–TS1–T9.out Energy: –731215.6266333 C –6.59155 –0.32700 –0.47099 O –5.98920 0.60874 –1.03537 O –6.09639 –1.19579 0.32910 C –2.54067 –1.19512 1.29034 C –1.41258 –0.45276 1.01919 N –3.55909 –0.62047 0.56084 C –3.03921 0.42223 –0.11098 N –1.73883 0.55446 0.14698 C –8.10151 –0.49635 –0.73572 C –2.74831 –2.38771 2.16829 C –0.31962 1.81898 –0.58364 C 1.82641 0.57245 –0.55763 O 2.97581 0.33594 –0.11105 C 0.92384 1.52853 –0.02787 H 1.25328 2.02239 0.88117 O 1.37395 –0.10459 –1.65587 C 2.28127 –1.01712 –2.26610 C –1.01053 3.11466 –0.23515 H –0.51742 3.93859 –0.76966 H –0.93912 3.32119 0.83739 H –2.06619 3.10872 –0.51763 H –0.50506 1.44543 –1.58522 H –0.40061 –0.56634 1.38543 H –3.48513 –2.18954 2.95734 H –3.11261 –3.25324 1.60006 H –1.80668 –2.67167 2.64954 H –3.65676 1.03013 –0.75731 H –8.65542 –0.43769 0.20948 H 1.73171 –1.46148 –3.09885

	H	3.17334	−0.50295	−2.64093
	H	−8.46908	0.27112	−1.42294
	H	2.59869	−1.79946	−1.57035
	H	−8.29781	−1.49002	−1.15734
	H	−4.62006	−0.89900	0.49107
	C	6.02040	−1.86349	−0.10069
	O	6.86874	−2.72707	0.10609
	N	4.75899	−1.92019	0.40395
	O	3.69958	2.18361	1.87039
	H	3.46430	1.45933	1.24831
	H	4.08136	−1.16737	0.27908
	C	4.17661	3.25015	1.08251
	H	5.11331	3.00674	0.55072
	H	4.38454	4.09354	1.75195
	C	6.30794	−0.63931	−0.96411
	H	6.61391	−0.97401	−1.96112
	H	7.15463	−0.09743	−0.52999
	H	5.45199	0.03521	−1.04916
	H	4.54556	−2.68094	1.03379
	H	3.44296	3.58670	0.33166

Optimized Molecular Properties for **T9-INT1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 16 positive frequencies below 100 cm^–1. Zero–point correction: 0.405890 hartree Enthalpy correction: 0.437653 hartree Free Energy correction: 0.334447 hartree Quasiharmonic Free Energy correction: 0.348067 hartree SCF Energy: –1164.848687 hartree SCF Energy + ZPVE: –1164.442797 hartree Enthalpy: –1164.411034 hartree Free Energy: –1164.514240 hartree Free Energy with quasiharmonic correction: –1164.500620 hartree (correction: 8.55 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1165.27935220 A.U.
Cartesian Coordinates	49 spD3–INT1–T9.out Energy: –731223.8275357 C 6.49866 –0.25846 0.69807 O 5.85302 0.60311 1.27631 O 6.02614 –1.08598 –0.22267 C 2.47324 –1.13568 –1.49261 C 1.29201 –0.47010 –1.26350 N 3.44401 –0.61824 –0.65752 C 2.84753 0.33463 0.04922 N 1.54257 0.46344 –0.28356 C 7.97535 –0.50026 0.96963 C 2.76075 –2.24591 –2.45503 C 0.54051 1.44732 0.31103 C –1.80971 0.53709 0.52159 O –3.04159 0.39813 0.20706 C –0.84717 1.23656 –0.17124 H –1.15812 1.70228 –1.10137 O –1.37020 –0.07060 1.70195 C –2.37882 –0.59581 2.54725 C 1.05368 2.86588 0.01475 H 0.41702 3.59178 0.53060 H 1.00113 3.07192 –1.06083 H 2.09045 3.01659 0.33957 H 0.58685 1.25776 1.38743 H 0.30122 –0.57192 –1.67733 H 3.53611 –1.96340 –3.17941 H 3.11723 –3.14639 –1.93798 H 1.85907 –2.51466 –3.01523 H 3.34881 0.92794 0.80055

	H	8.55119	−0.37883	0.04552
	H	−1.85451	−0.99063	3.42364
	H	−3.09050	0.17652	2.86690
	H	8.33476	0.19996	1.72569
	H	−2.94537	−1.40215	2.06868
	H	8.12872	−1.52931	1.31306
	H	5.01733	−0.90714	−0.39419
	C	−5.87918	−1.89543	0.13584
	O	−6.67084	−2.82231	−0.03649
	N	−4.57116	−1.94953	−0.21982
	O	−3.75275	2.18742	−1.74304
	H	−3.51344	1.46844	−1.10381
	H	−3.93440	−1.14633	−0.11618
	C	−3.85862	3.36468	−0.98151
	H	−4.70440	3.34590	−0.26959
	H	−4.02822	4.20284	−1.67094
	C	−6.30342	−0.57910	0.78041
	H	−6.77449	−0.79428	1.74558
	H	−7.06197	−0.10723	0.14614
	H	−5.46763	0.11178	0.91675
	H	−4.25927	−2.78139	−0.70156
	H	−2.94455	3.57950	−0.40377

Optimized Molecular Properties for **T9-INT2**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 21 positive frequencies below 100 cm^–1. Zero–point correction: 0.575323 hartree Enthalpy correction: 0.617702 hartree Free Energy correction: 0.491690 hartree Quasiharmonic Free Energy correction: 0.507577 hartree SCF Energy: –1626.169136 hartree SCF Energy + ZPVE: –1625.593813 hartree Enthalpy: –1625.551434 hartree Free Energy: –1625.677446 hartree Free Energy with quasiharmonic correction: –1625.661559 hartree (correction: 9.97 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1626.76853502 A.U.
Cartesian Coordinates	69 spD3–INT2–T9.out Energy: –1020812.6595963 C 6.09018 1.54399 –0.71902 C –2.02130 4.34596 2.24608 O 5.22411 1.52132 –1.58038 O –2.06996 5.35915 2.93888 N –0.90425 3.57600 2.13841 O 6.08472 0.81866 0.39242 C 3.31929 –1.62003 1.34431 C 2.12452 –2.06199 0.83035 N 3.87030 –0.69356 0.47785 C 3.02162 –0.58316 –0.53255 O –3.71304 –2.57452 1.60921 N 1.94686 –1.39123 –0.36783 C 7.31986 2.43173 –0.80678 C 3.99609 –2.01142 2.62059 H –3.23463 –2.57284 0.72819 C 0.80097 –1.54685 –1.29189 C –0.40817 0.48877 –0.40069 H –0.88557 2.69497 1.62951 O –0.84539 1.06399 0.58422 C –0.47999 –0.99801 –0.61174 C –1.85655 –1.50333 –1.34683 C –2.86695 –0.35169 –1.53290 C –2.87000 –1.91114 2.52842 O –2.33725 –2.58943 –0.70833 C –3.95937 –0.18285 –0.67295 H –1.91436 –2.43822 2.67179 C –2.73361 0.53139 –2.61498

	H	−3.38848	−1.86734	3.49526
	C	−4.87141	0.85558	−0.87755
	C	−3.21183	3.87140	1.42172
	C	−3.64135	1.57204	−2.82114
	H	−3.04381	2.92001	0.91073
	C	−4.71712	1.74109	−1.94654
	H	−3.45625	4.63871	0.67897
	H	−0.57286	−1.42361	0.38756
	H	−4.07805	3.77576	2.08402
	O	0.15263	1.15725	−1.43878
	C	0.13552	2.58847	−1.35441
	C	0.74619	−3.00336	−1.77623
	H	−3.51746	2.23969	−3.67200
	H	−5.43275	2.54536	−2.10413
	H	−5.71381	0.96825	−0.19797
	H	−4.10730	−0.88016	0.14539
	H	−1.90678	0.39605	−3.31010
	H	−0.02016	−3.12324	−2.54548
	H	0.51439	−3.69209	−0.96096
	H	1.71697	−3.26690	−2.21233
	H	−1.52166	−1.72701	−2.38713
	H	1.03683	−0.90526	−2.14516
	H	1.39226	−2.77430	1.18775
	H	4.98877	−2.44082	2.43361
	H	4.13775	−1.14601	3.28039
	H	3.40126	−2.75446	3.16102
	H	3.16116	0.07207	−1.38053
	H	8.22817	1.82183	−0.75259
	H	0.68600	2.93886	−2.22882
	H	−0.89444	2.95495	−1.37893
	H	7.30537	2.99624	−1.74050
	H	0.62037	2.93330	−0.43800
	H	7.34245	3.12192	0.04380
	O	−0.73996	−4.02581	0.83870
	H	−1.32990	−3.50366	0.20158
	C	−1.48376	−5.13424	1.29889
	H	−0.92342	−5.61330	2.11294
	H	−1.64094	−5.89314	0.51159
	H	−2.46804	−4.83064	1.68149
	H	5.23888	0.23228	0.43415
	H	−0.11557	3.82202	2.72017
	H	−2.63865	−0.87681	2.22336

Optimized Molecular Properties for **T9-TS3**

Number of (–) Vibrational Frequencies	1 (–1102.6361)
Absolute Energies (Hartrees)	**B3LYP/6-31G(d)** There are 22 positive frequencies below 100 cm^–1. Zero–point correction: 0.570448 hartree Enthalpy correction: 0.612656 hartree Free Energy correction: 0.486814 hartree Quasiharmonic Free Energy correction: 0.502634 hartree SCF Energy: –1626.141501 hartree SCF Energy + ZPVE: –1625.571053 hartree Enthalpy: –1625.528845 hartree Free Energy: –1625.654687 hartree Free Energy with quasiharmonic correction: –1625.638866 hartree (correction: 9.93 kcal/mol) **B3LYP-D3/6-311+G(d,p)** SCF Done: E(RB3LYP) = –1626.74314329 A.U.
Cartesian Coordinates	69 spD3–TS3–T9.out Energy: –1020796.7260453 C –6.34553 1.88738 0.67137 C 3.78149 3.44207 –1.81031 O –5.43929 1.91038 1.49047 O 4.37418 4.27875 –2.48801 N 2.86365 2.58251 –2.32684 O –6.40111 1.09328 –0.38940 C –3.76687 –1.45048 –1.33618 C –2.54374 –1.88692 –0.88804 N –4.22745 –0.45278 –0.49649 C –3.29569 –0.29631 0.43146 O 4.86629 –2.06767 –1.16835 N –2.25305 –1.13623 0.23789 C –7.56276 2.79323 0.76240 C –4.54913 –1.90814 –2.52750 H 4.01969 –2.25141 –0.70656 C –1.08383 –1.28829 1.14547 C 0.52582 0.19931 –0.13786 H 2.39391 1.86513 –1.77251 O 1.57262 0.55763 –0.68369 C 0.25054 –1.13865 0.38179 C 1.50893 –1.81582 1.01458 C 2.31924 –0.91682 1.94514 C 4.55415 –1.21943 –2.25701 O 2.36171 –2.39439 0.02706 C 3.63259 –0.52179 1.66462 H 3.99369 –1.74238 –3.05118

	C	1.73706	−0.47734	3.14463
	H	5.50006	−0.87163	−2.68958
	C	4.33482	0.29372	2.55661
	C	4.01499	3.30353	−0.31030
	C	2.43482	0.33950	4.03343
	H	3.47084	2.46908	0.13931
	C	3.74304	0.73162	3.74163
	H	3.72083	4.23749	0.18161
	H	0.15852	−1.96113	−0.72158
	H	5.08727	3.16990	−0.13580
	O	−0.52533	1.06920	−0.01342
	C	−0.36390	2.35303	−0.61263
	C	−1.26199	−2.62695	1.88763
	H	1.95730	0.66588	4.95499
	H	4.29361	1.36731	4.43159
	H	5.35494	0.58634	2.31775
	H	4.11467	−0.86256	0.75674
	H	0.72096	−0.77812	3.39064
	H	−0.60038	−2.70210	2.75563
	H	−1.05842	−3.47527	1.22544
	H	−2.29395	−2.70748	2.24559
	H	1.13501	−2.63651	1.64041
	H	−1.22058	−0.47714	1.87244
	H	−1.83645	−2.61431	−1.26646
	H	−5.53376	−2.29861	−2.23843
	H	−4.72414	−1.08621	−3.23372
	H	−4.01298	−2.70082	−3.05914
	H	−3.35100	0.42225	1.23637
	H	−8.47676	2.19070	0.80437
	H	−1.29823	2.88478	−0.42176
	H	0.47753	2.89529	−0.17062
	H	−7.49209	3.42378	1.65027
	H	−0.19550	2.26863	−1.69099
	H	−7.62961	3.41983	−0.13386
	O	0.31095	−2.89816	−1.54907
	H	1.74725	−2.77945	−0.66202
	C	0.47717	−2.36190	−2.83407
	H	−0.45787	−1.91999	−3.22977
	H	0.78275	−3.14974	−3.54387
	H	1.24736	−1.57122	−2.87105
	H	−5.56105	0.49113	−0.43432
	H	2.70933	2.61636	−3.32477
	H	3.96775	−0.34183	−1.95324

Optimized Molecular Properties for **T9-INT3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 21 positive frequencies below 100 cm^–1. Zero–point correction: 0.574644 hartree Enthalpy correction: 0.617771 hartree Free Energy correction: 0.489983 hartree Quasiharmonic Free Energy correction: 0.505837 hartree SCF Energy: –1626.154329 hartree SCF Energy + ZPVE: –1625.579685 hartree Enthalpy: –1625.536558 hartree Free Energy: –1625.664346 hartree Free Energy with quasiharmonic correction: –1625.648492 hartree (correction: 9.95 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1626.76120734 A.U.
Cartesian Coordinates	69 spD3–INT3–T9.out Energy: –1020808.0614077 C 7.23900 1.08920 –0.59854 C –5.23620 2.45325 0.11124 O 6.39403 1.54472 –1.35442 O –6.42722 2.64569 –0.13630 N –4.53685 1.38154 –0.32794 O 7.02457 0.16047 0.32327 C 3.70609 –1.55760 0.93087 C 2.41944 –1.50436 0.44927 N 4.46805 –0.60688 0.28028 C 3.64861 –0.00040 –0.56863 O –2.94231 –2.09204 2.80277 N 2.39409 –0.50237 –0.50104 C 8.69017 1.54171 –0.61628 C 4.27758 –2.44668 1.99064 H –2.33339 –2.05760 2.03396 C 1.23962 –0.10694 –1.39933 C –0.63004 1.02968 –0.15963 H –3.54073 1.24406 –0.13526 O –1.75046 1.20495 0.38309 C –0.11237 –0.12994 –0.74216 C –0.88100 –1.41517 –0.59419 C –2.28381 –1.46465 –1.21473 C –3.99118 –1.17176 2.55358 O –0.94689 –1.90214 0.78236 C –3.25880 –2.35095 –0.73466 H –3.62348 –0.19185 2.22185 C –2.58048 –0.71777 –2.36210

	H	−4.54452	−1.04008	3.49131
	C	−4.49541	−2.47196	−1.37213
	C	−4.42764	3.43338	0.95885
	C	−3.81250	−0.84054	−3.00678
	H	−3.38853	3.12052	1.08847
	C	−4.78039	−1.71921	−2.51379
	H	−4.90745	3.53022	1.93889
	H	0.68387	0.50078	1.99091
	H	−4.45953	4.42061	0.48462
	O	0.27444	2.11405	−0.15534
	C	−0.28083	3.37271	0.19010
	C	1.36660	−0.93978	−2.68976
	H	−4.02098	−0.23872	−3.88883
	H	−5.74330	−1.81402	−3.01058
	H	−5.23947	−3.15786	−0.97270
	H	−3.05382	−2.93591	0.15515
	H	−1.83610	−0.01770	−2.72984
	H	0.59662	−0.63643	−3.40662
	H	1.25093	−2.01174	−2.49850
	H	2.35077	−0.79253	−3.15001
	H	−0.32104	−2.19436	−1.13205
	H	1.46573	0.93181	−1.64701
	H	1.52830	−2.04818	0.72392
	H	5.09703	−3.06470	1.60065
	H	4.68318	−1.86333	2.82705
	H	3.50789	−3.11493	2.38941
	H	3.94552	0.79996	−1.23188
	H	8.96629	1.95054	0.36196
	H	0.53797	4.09336	0.10151
	H	−1.09625	3.65911	−0.48540
	H	9.34731	0.68590	−0.80604
	H	−0.67018	3.38424	1.21425
	H	8.83452	2.29924	−1.38847
	O	0.34413	−0.16870	2.60685
	H	−0.49014	−1.23951	1.34784
	C	−0.66513	0.43496	3.42418
	H	−0.21487	1.00669	4.24999
	H	−1.26504	−0.38278	3.83029
	H	−1.31500	1.08415	2.82892
	H	6.03314	−0.13652	0.31631
	H	−5.01464	0.69645	−0.89778
	H	−4.69784	−1.53398	1.79023

Optimized Molecular Properties for **T9-TS4**

Number of (–) Vibrational Frequencies	1 (–223.2375)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 21 positive frequencies below 100 cm^–1. Zero–point correction: 0.572715 hartree Enthalpy correction: 0.615548 hartree Free Energy correction: 0.489044 hartree Quasiharmonic Free Energy correction: 0.504377 hartree SCF Energy: –1626.142066 hartree SCF Energy + ZPVE: –1625.569351 hartree Enthalpy: –1625.526518 hartree Free Energy: –1625.653022 hartree Free Energy with quasiharmonic correction: –1625.637689 hartree (correction: 9.62 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1626.74916246 A.U.
Cartesian Coordinates	69 spD3–TS4–T9.out Energy: –1020800.5031315 C 5.43955 2.46643 –0.35522 C –4.62056 2.98712 –0.27799 O 4.39902 2.57503 –0.98791 O –5.78376 3.34890 –0.45444 N –4.23584 1.68992 –0.22539 O 5.91175 1.34652 0.16957 C 4.19672 –2.01041 0.10157 C 3.01468 –2.52912 –0.40454 N 4.27209 –0.68461 –0.26225 C 3.15674 –0.44677 –0.96662 O –1.78263 –0.14576 3.45950 N 2.36594 –1.52380 –1.08748 C 6.35705 3.64874 –0.07958 C 5.27937 –2.69098 0.88365 H –1.57927 –0.56779 2.59590 C 0.56597 –1.39898 –1.81668 C –0.53528 0.47456 –0.66437 H –3.26389 1.39854 –0.12144 O –1.39122 1.03669 0.03474 C –0.41009 –0.93425 –0.90714 C –1.26590 –1.86610 –0.07494 C –2.77482 –1.73523 –0.29583 C –2.27808 1.15547 3.20793 O –1.03113 –1.79384 1.33869 C –3.68038 –1.81500 0.77032 H –1.54820 1.79470 2.68994 C –3.28563 –1.62421 –1.59628

	H	−2.51101	1.60976	4.17921
	C	−5.05799	−1.78178	0.53802
	C	−3.48943	3.99500	−0.08954
	C	−4.66003	−1.59831	−1.83132
	H	−2.51233	3.51966	0.02763
	C	−5.55720	−1.67955	−0.76233
	H	−3.70481	4.60557	0.79410
	H	2.24395	−1.85835	1.55449
	H	−3.47011	4.66946	−0.95237
	O	0.43664	1.22895	−1.29048
	C	0.40761	2.63419	−1.05811
	C	0.49790	−2.77792	−2.44432
	H	−5.03165	−1.50432	−2.84940
	H	−6.62977	−1.65614	−0.94109
	H	−5.74352	−1.83204	1.38113
	H	−3.29909	−1.87854	1.78285
	H	−2.59013	−1.53389	−2.42648
	H	−0.40764	−2.86503	−3.05856
	H	0.46457	−3.57950	−1.69985
	H	1.36885	−2.94977	−3.08265
	H	−1.02180	−2.89323	−0.39001
	H	0.91172	−0.64111	−2.51138
	H	2.62228	−3.53701	−0.35235
	H	6.22547	−2.71639	0.32621
	H	5.48085	−2.17528	1.83134
	H	5.00056	−3.72461	1.11688
	H	2.91223	0.52545	−1.36785
	H	6.44931	3.80481	1.00109
	H	1.37790	3.00842	−1.39199
	H	−0.40008	3.11402	−1.62459
	H	7.36226	3.44232	−0.46327
	H	0.26549	2.85312	0.00355
	H	5.95687	4.54901	−0.54927
	O	1.56404	−1.71020	2.24032
	H	−0.06223	−1.85302	1.51574
	C	1.64219	−0.34955	2.67386
	H	2.53673	−0.18194	3.29083
	H	0.74619	−0.15747	3.26960
	H	1.66317	0.34625	1.82621
	H	5.26867	0.54145	−0.00680
	H	−4.93601	0.97213	−0.35727
	H	−3.19687	1.14973	2.60232

Optimized Molecular Properties for **T9-product**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)** There are 24 positive frequencies below 100 cm^–1. Zero–point correction: 0.572855 hartree Enthalpy correction: 0.616929 hartree Free Energy correction: 0.485195 hartree Quasiharmonic Free Energy correction: 0.503410 hartree SCF Energy: –1626.179289 hartree SCF Energy + ZPVE: –1625.606434 hartree Enthalpy: –1625.562360 hartree Free Energy: –1625.694094 hartree Free Energy with quasiharmonic correction: –1625.675879 hartree (correction: 11.43 kcal/mol) **B3LYP–D3/6–311+G(d,p)** SCF Done: E(RB3LYP) = –1626.78174933
Cartesian Coordinates	69 spD3–product–T9.out Energy: –1020820.9517010 C 4.67325 3.03789 –0.27921 C –4.87950 2.91981 0.38976 O 3.53068 2.66569 0.08184 O –6.02535 3.34298 0.25398 N –4.50514 1.65815 0.05818 O 5.68465 2.29405 –0.48133 C 5.54384 –1.40081 –0.09574 C 4.62196 –2.37447 0.21996 N 4.85777 –0.20867 –0.02874 C 3.58482 –0.49208 0.31383 O –2.51263 –1.60273 3.11473 N 3.39220 –1.80073 0.47409 C 4.87885 4.54757 –0.51718 C 6.99404 –1.48382 –0.44974 H –2.10572 –1.67778 2.22629 C 0.70639 –0.87335 –1.81727 C –0.58332 0.56890 –0.31235 H –3.54651 1.32879 0.11701 O –1.62681 0.89980 0.23511 C –0.37029 –0.73271 –1.01869 C –1.34652 –1.85437 –0.68783 C –2.79275 –1.59104 –1.09529 C –2.82140 –0.23848 3.33024 O –1.28684 –2.18336 0.68842 C –3.85522 –1.91251 –0.24283 H –1.93420 0.41178 3.27800 C –3.07991 –1.11120 –2.38048

	H	−3.24720	−0.15352	4.33694
	C	−5.17629	−1.75449	−0.67086
	C	−3.76495	3.78766	0.96626
	C	−4.39771	−0.95257	−2.80719
	H	−2.79413	3.28552	0.98065
	C	−5.45539	−1.27748	−1.95331
	H	−4.03607	4.07818	1.98692
	H	1.95504	−2.51712	1.12157
	H	−3.69321	4.70686	0.37576
	O	0.50797	1.34434	−0.32983
	C	0.43762	2.63883	0.30050
	C	1.17056	−2.08107	−2.57211
	H	−4.59936	−0.57166	−3.80553
	H	−6.48421	−1.15707	−2.28403
	H	−5.98982	−2.00449	0.00608
	H	−3.64661	−2.26749	0.75980
	H	−2.26162	−0.85083	−3.04771
	H	1.36656	−1.82310	−3.62115
	H	0.47400	−2.92237	−2.55018
	H	2.12511	−2.41181	−2.14136
	H	−1.03113	−2.73490	−1.26658
	H	1.36254	−0.01175	−1.90781
	H	4.77149	−3.44527	0.28249
	H	7.19571	−1.07623	−1.44896
	H	7.61935	−0.92155	0.25579
	H	7.32708	−2.52717	−0.43767
	H	2.84944	0.29127	0.42418
	H	4.53519	5.11274	0.35725
	H	1.46058	3.01830	0.25239
	H	−0.26837	3.27698	−0.24134
	H	5.92651	4.78590	−0.72230
	H	0.09803	2.52964	1.33436
	H	4.26493	4.87082	−1.36763
	O	1.12340	−2.85700	1.57909
	H	−0.35136	−2.45366	0.92371
	C	1.14419	−2.39028	2.92217
	H	1.70516	−3.07687	3.57482
	H	0.11305	−2.32638	3.28632
	H	1.60309	−1.39509	2.99936
	H	5.21994	0.78702	−0.20946
	H	−5.19141	1.04266	−0.35640
	H	−3.56004	0.14865	2.61183

Optimized Molecular Properties for **TArg-Int1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 20 positive frequencies below 100 cm^–1. Zero–point correction: 0.560791 hartree Enthalpy correction: 0.601910 hartree Free Energy correction: 0.480874 hartree Quasiharmonic Free Energy correction: 0.497583 hartree SCF Energy: –1546.445654 hartree SCF Energy + ZPVE: –1545.884863 hartree Enthalpy: –1545.843744 hartree Free Energy: –1545.964780 hartree Free Energy with quasiharmonic correction: –1545.948071 hartree (correction: 10.49 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1546.99857596 A.U.
Cartesian Coordinates	(PCM) 67 spD3–R–TS2–Targ.out Energy: –970756.2549444 C 6.79119 0.11935 0.18681 O 5.97547 0.98698 –0.09495 O 6.52475 –1.18292 0.21205 C 3.13819 –2.72580 –0.57192 C 1.87415 –2.30773 –0.91466 N 3.95190 –1.61615 –0.44031 C 3.18500 –0.56496 –0.70179 N 1.91851 –0.93016 –0.99531 C 8.23210 0.41592 0.54888 C 3.64665 –4.11655 –0.35072 C 0.78849 –0.00856 –1.36237 C –0.52072 0.07306 0.80331 O –1.48678 –0.15845 1.60434 C –0.44429 –0.23342 –0.54651 C –2.39237 1.91380 –1.14253 C –1.64832 2.98863 –0.46507 O –3.45325 1.44839 –0.71541 C –2.06013 3.45145 0.79552 C –0.55210 3.59017 –1.10235 C –1.37701 4.49668 1.40989 C 0.12864 4.63872 –0.48676 C –0.28273 5.09135 0.77023 H –1.24682 –0.82714 –0.97159 O 0.59300 0.72260 1.30548 C 0.55961 1.06838 2.68691 C 0.53342 –0.13901 –2.87094

	N	−3.80296	−1.36897	0.73753
	N	−2.52619	−2.70005	2.11006
	H	0.97659	5.10233	−0.98263
	H	0.24787	5.90831	1.25162
	H	−1.69442	4.85378	2.38578
	H	−2.91121	2.97773	1.27344
	H	−0.23967	3.23569	−2.08190
	H	−0.18789	0.61668	−3.19884
	H	0.11954	−1.12462	−3.11382
	H	1.45793	−0.00592	−3.44238
	H	−2.00459	1.61261	−2.12921
	H	1.20564	0.98406	−1.15673
	H	0.96022	−2.85545	−1.08717
	H	4.46096	−4.36123	−1.04407
	H	4.03974	−4.24295	0.66573
	H	2.84790	−4.85040	−0.49746
	H	3.52401	0.46068	−0.67411
	H	−3.07148	−0.65541	0.90442
	H	−1.89009	−1.88991	2.14104
	H	8.41243	1.49141	0.51889
	H	1.50852	1.57183	2.88624
	H	−0.27180	1.74164	2.91566
	H	8.45315	0.03135	1.55028
	H	0.47548	0.18007	3.32290
	H	8.90576	−0.09183	−0.14968
	O	−5.29044	−0.43067	−1.49602
	H	−4.58942	0.26040	−1.43745
	C	−6.54619	0.22475	−1.33569
	H	−7.32122	−0.54660	−1.32288
	H	−6.75257	0.90868	−2.17014
	H	−6.59966	0.79203	−0.39654
	H	5.54161	−1.35042	−0.03687
	H	−4.51234	−1.19329	0.01884
	H	−2.12461	−3.61611	2.25458
	C	−3.54494	−2.57211	1.23097
	N	−4.28484	−3.65098	0.90637
	H	−4.16251	−4.47157	1.48326
	C	−5.48740	−3.58934	0.08203
	H	−5.77453	−4.60989	−0.17486
	H	−5.28640	−3.04305	−0.84276
	H	−6.32056	−3.10553	0.60683

Optimized Molecular Properties for **TArg-TS2**

Number of (–) Vibrational Frequencies	1 (–130.1561)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 20 positive frequencies below 100 cm^–1. Zero–point correction: 0.560791 hartree Enthalpy correction: 0.601910 hartree Free Energy correction: 0.480874 hartree Quasiharmonic Free Energy correction: 0.497583 hartree SCF Energy: –1546.445654 hartree SCF Energy + ZPVE: –1545.884863 hartree Enthalpy: –1545.843744 hartree Free Energy: –1545.964780 hartree Free Energy with quasiharmonic correction: –1545.948071 hartree (correction: 10.49 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1546.99834953 A.U.
Cartesian Coordinates	(PCM) 67 spD3–TS2–Targ.out Energy: –970756.1128574 C –6.58254 –0.15921 –0.34375 O –5.82960 0.76869 –0.08095 O –6.24357 –1.44371 –0.27375 C –2.82458 –2.72744 0.80981 C –1.60797 –2.21521 1.19151 N –3.68022 –1.67824 0.53023 C –2.98627 –0.56870 0.74185 N –1.72467 –0.83788 1.14593 C –8.01778 0.02968 –0.78913 C –3.25182 –4.15684 0.68589 C –0.66961 0.16502 1.48093 C 0.46551 0.07816 –0.79202 O 1.34338 –0.28001 –1.61286 C 0.56675 0.01956 0.62590 C 2.02178 1.70335 0.93041 C 1.26114 2.85330 0.35607 O 3.11133 1.33301 0.40491 C 1.54049 3.30071 –0.94397 C 0.30589 3.53889 1.12004 C 0.86260 4.39674 –1.47429 C –0.37238 4.63783 0.59033 C –0.09814 5.06792 –0.71020 H 1.31162 –0.68607 0.98430 O –0.67768 0.66787 –1.24619 C –0.79627 0.82938 –2.66305 C –0.37153 0.06995 2.98401

	N	3.87899	−1.25814	−0.79842
	N	2.67256	−2.74290	−2.08491
	H	−1.10844	5.16224	1.19415
	H	−0.62328	5.92510	−1.12324
	H	1.08674	4.73559	−2.48283
	H	2.29611	2.77584	−1.51940
	H	0.10457	3.22034	2.14073
	H	0.29551	0.87785	3.29836
	H	0.11615	−0.88033	3.22934
	H	−1.29530	0.14179	3.56675
	H	1.86897	1.56848	2.01260
	H	−1.14927	1.12720	1.27191
	H	−0.68806	−2.70040	1.48080
	H	−4.09847	−4.37999	1.34670
	H	−3.57042	−4.39195	−0.33718
	H	−2.43201	−4.83261	0.94872
	H	−3.37096	0.43108	0.60149
	H	3.11483	−0.58620	−0.94239
	H	1.95322	−2.01539	−2.12090
	H	−8.25823	1.09253	−0.83727
	H	−1.76754	1.30017	−2.82190
	H	−0.00014	1.46824	−3.05338
	H	−8.16798	−0.42893	−1.77233
	H	−0.76116	−0.13796	−3.17322
	H	−8.69557	−0.47182	−0.09008
	O	5.12625	−0.07972	1.42151
	H	4.32685	0.48404	1.21671
	C	6.27210	0.75348	1.29479
	H	7.15920	0.13182	1.45072
	H	6.27656	1.55300	2.04909
	H	6.34216	1.21714	0.30043
	H	−5.26922	−1.53559	0.03141
	H	4.56427	−1.01353	−0.07399
	H	2.37032	−3.69794	−2.21578
	C	3.69885	−2.49385	−1.24130
	N	4.53581	−3.49206	−0.89896
	H	4.45830	−4.35338	−1.42129
	C	5.75127	−3.29083	−0.11594
	H	6.15724	−4.27121	0.13529
	H	5.52337	−2.76172	0.81304
	H	6.50681	−2.72353	−0.67293

Optimized Molecular Properties for **TArg-Int2-1**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 18 positive frequencies below 100 cm^–1. Zero–point correction: 0.563626 hartree Enthalpy correction: 0.603314 hartree Free Energy correction: 0.485202 hartree Quasiharmonic Free Energy correction: 0.498997 hartree SCF Energy: –1546.461078 hartree SCF Energy + ZPVE: –1545.897452 hartree Enthalpy: –1545.857764 hartree Free Energy: –1545.975876 hartree Free Energy with quasiharmonic correction: –1545.962081 hartree (correction: 8.66 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1547.01835635 A.U.
Cartesian Coordinates	(PCM) 67 spD3–R–TS3–meoh–Targ.out Energy: –970768.6673264 C –6.42871 1.15177 –1.01980 O –5.51655 1.81452 –0.54471 O –6.43069 –0.17695 –1.09363 C –3.58838 –2.40511 0.16921 C –2.36622 –2.25820 0.77794 N –4.13999 –1.15280 –0.03196 C –3.26700 –0.28044 0.44460 N –2.17006 –0.89645 0.94763 C –7.69222 1.75764 –1.59335 C –4.29007 –3.65979 –0.24669 C –1.01334 –0.23366 1.58420 C 0.17028 –0.31949 –0.68123 O 0.73766 –0.97589 –1.53760 C 0.28621 –0.56014 0.81090 C 1.61020 0.14988 1.36094 C 1.59089 1.67074 1.16548 O 2.70893 –0.46154 0.79881 C 1.04630 2.52032 2.13804 C 2.14310 2.25270 0.01589 C 1.03046 3.90652 1.96145 C 2.13083 3.63589 –0.16675 C 1.57080 4.47021 0.80466 H 0.51209 –1.62322 0.93556 O –0.59885 0.74828 –0.97645 C –0.72397 1.07632 –2.37068 C –0.96096 –0.63840 3.06498

	N	5.17823	0.04032	0.03011
	N	3.84981	−0.90042	−1.58547
	H	2.56492	4.06567	−1.06657
	H	1.56472	5.54811	0.66522
	H	0.60515	4.54422	2.73245
	H	0.64262	2.09792	3.05583
	H	2.59563	1.60922	−0.73185
	H	−0.22620	−0.04466	3.61348
	H	−0.69060	−1.69362	3.17909
	H	−1.93999	−0.47936	3.52757
	H	1.57574	−0.02489	2.45234
	H	−1.22000	0.83665	1.50765
	H	−1.63778	−2.98791	1.09716
	H	−5.26016	−3.75909	0.25536
	H	−4.48134	−3.67006	−1.32663
	H	−3.68956	−4.54074	−0.00088
	H	−3.39884	0.79165	0.43007
	H	4.30146	0.01075	0.61233
	H	3.08493	−0.81568	−0.88104
	H	−7.81038	1.45708	−2.63982
	H	−1.42399	1.91039	−2.41231
	H	0.24580	1.37153	−2.77969
	H	−8.56598	1.38506	−1.04809
	H	−1.11004	0.22224	−2.93195
	H	−7.65094	2.84538	−1.52379
	O	2.51866	−2.99856	1.63134
	H	2.66931	−2.05433	1.32977
	C	2.62951	−3.82585	0.49230
	H	2.33655	−4.84398	0.77654
	H	3.65981	−3.87574	0.09823
	H	1.97530	−3.50220	−0.33268
	H	−5.56694	−0.55198	−0.69574
	H	3.62810	−1.02006	−2.56293
	H	6.08835	0.12312	0.45763
	C	5.05319	−0.45464	−1.20396
	N	6.09746	−0.48792	−2.05672
	H	5.98412	−1.03247	−2.89973
	C	7.43778	−0.02601	−1.72220
	H	8.02651	0.00635	−2.63979
	H	7.94137	−0.69038	−1.00860
	H	7.39690	0.98552	−1.30709

Optimized Molecular Properties for **TArg-Int2-2**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 19 positive frequencies below 100 cm^–1. Zero–point correction: 0.564857 hartree Enthalpy correction: 0.604672 hartree Free Energy correction: 0.487994 hartree Quasiharmonic Free Energy correction: 0.502831 hartree SCF Energy: –1546.466962 hartree SCF Energy + ZPVE: –1545.902105 hartree Enthalpy: –1545.862290 hartree Free Energy: –1545.978968 hartree Free Energy with quasiharmonic correction: –1545.964131 hartree (correction: 9.31 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1547.02309325 A.U.
Cartesian Coordinates	(PCM) 67 spD3–opt–INT2–2–Targ.out Energy: –970771.6397760 C –6.05921 0.05763 –0.82241 O –5.17330 0.88750 –0.66584 O –5.99964 –1.19575 –0.37724 C –2.77632 –2.68207 1.13375 C –1.53638 –2.21117 1.48815 N –3.58742 –1.60809 0.81119 C –2.84995 –0.52346 0.97037 N –1.59408 –0.82852 1.38281 C –7.35682 0.34464 –1.54626 C –3.26721 –4.09433 1.07540 C –0.50871 0.13945 1.62102 C –0.02175 –0.07536 –0.88220 O 0.34507 –0.87105 –1.73035 C 0.57520 0.02339 0.51592 C 1.68470 1.14267 0.57638 C 1.17841 2.57200 0.45161 O 2.63387 0.90979 –0.44922 C 1.05866 3.18249 –0.80472 C 0.84991 3.31655 1.59170 C 0.60085 4.49500 –0.91677 C 0.38375 4.62898 1.48215 C 0.25503 5.22161 0.22570 H 1.11584 –0.91802 0.66104 O –1.00531 0.80972 –1.08422 C –1.67458 0.76852 –2.36303 C 0.05110 –0.05499 3.03620

	N	3.72993	−1.51565	−0.22817
	N	2.55999	−2.95578	−1.62339
	H	0.13585	5.18934	2.37966
	H	−0.10071	6.24459	0.13703
	H	0.51797	4.95375	−1.89867
	H	1.34612	2.62765	−1.69132
	H	0.97476	2.87916	2.57921
	H	0.76962	0.72779	3.28900
	H	0.56032	−1.01939	3.13663
	H	−0.76269	−0.01694	3.76636
	H	2.15819	1.03521	1.56345
	H	−0.97960	1.12274	1.54968
	H	−0.64289	−2.72846	1.80253
	H	−4.11445	−4.24939	1.75421
	H	−3.60835	−4.35465	0.06619
	H	−2.47465	−4.79406	1.35702
	H	−3.18372	0.48318	0.76707
	H	2.93184	−0.06185	−0.41938
	H	1.83426	−2.24001	−1.63944
	H	−8.20450	0.17294	−0.87440
	H	−2.59285	1.33834	−2.22741
	H	−1.04077	1.22551	−3.12695
	H	−7.36879	1.37685	−1.89843
	H	−1.89823	−0.26320	−2.63896
	H	−7.47158	−0.33839	−2.39456
	O	5.33030	1.21315	0.35780
	H	4.38826	1.27736	0.09005
	C	6.10428	1.39688	−0.81580
	H	7.15873	1.29984	−0.53654
	H	5.96265	2.39331	−1.26289
	H	5.88395	0.64233	−1.58670
	H	−5.10843	−1.36310	0.08718
	H	4.62180	−1.36328	0.23687
	H	2.19660	−3.90054	−1.59326
	C	3.61355	−2.68765	−0.77513
	N	4.47499	−3.74835	−0.58829
	H	4.49807	−4.41130	−1.35290
	C	5.72839	−3.58312	0.13123
	H	6.22353	−4.55451	0.19048
	H	5.53231	−3.24156	1.15252
	H	6.41237	−2.86940	−0.35048

Optimized Molecular Properties for **TArg-TS3-1**

Number of (–) Vibrational Frequencies	0 (–1227.5912)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 18 positive frequencies below 100 cm^–1. Zero–point correction: 0.558959 hartree Enthalpy correction: 0.598288 hartree Free Energy correction: 0.482736 hartree Quasiharmonic Free Energy correction: 0.497789 hartree SCF Energy: –1546.422087 hartree SCF Energy + ZPVE: –1545.863128 hartree Enthalpy: –1545.823799 hartree Free Energy: –1545.939351 hartree Free Energy with quasiharmonic correction: –1545.924298 hartree (correction: 9.45 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1546.97975040 A.U.
Cartesian Coordinates	(PCM) 67 spD3–TS3–meoh–Targ.out Energy: –970744.4417273 C 6.79934 0.81068 1.13739 O 5.88474 1.62419 1.12891 O 6.72512 –0.40951 0.61603 C 3.66395 –1.83800 –1.13562 C 2.38732 –1.44322 –1.45671 N 4.29565 –0.80998 –0.45825 C 3.41228 0.17338 –0.37643 N 2.23807 –0.15923 –0.95981 C 8.15577 1.08857 1.75246 C 4.34724 –3.13913 –1.42145 C 1.07683 0.75292 –1.12806 C –0.33763 0.03579 0.85098 O –1.34408 –0.25633 1.51021 C –0.23328 0.12051 –0.60279 C –1.53979 0.54955 –1.31001 C –2.22679 1.83468 –0.85093 O –2.52307 –0.51022 –1.30331 C –3.49798 2.14658 –1.36106 C –1.61141 2.76440 –0.00479 C –4.13790 3.33872 –1.02417 C –2.24708 3.96303 0.33280 C –3.51387 4.25460 –0.17241 H –0.28224 –1.20059 –1.02589 O 0.83803 0.26804 1.50222 C 0.82942 0.07519 2.92173 C 1.04789 1.21474 –2.59518

	N	−4.95392	−1.01456	−0.13772
	N	−3.80872	−1.43376	1.82034
	H	−1.74822	4.66635	0.99474
	H	−4.00897	5.18583	0.09020
	H	−5.12245	3.55648	−1.43108
	H	−3.98385	1.44405	−2.03182
	H	−0.62753	2.55711	0.40393
	H	0.34674	2.04322	−2.73389
	H	0.76809	0.40189	−3.27374
	H	2.04408	1.56763	−2.88040
	H	−1.27932	0.70798	−2.36351
	H	1.35255	1.62409	−0.52231
	H	1.56624	−1.95635	−1.93759
	H	5.24705	−2.99431	−2.03248
	H	4.66217	−3.63907	−0.49693
	H	3.67869	−3.81709	−1.96088
	H	3.59729	1.12344	0.10339
	H	−4.05797	−0.73611	−0.58196
	H	−2.95505	−0.99024	1.44757
	H	8.36214	0.36240	2.54605
	H	1.85061	0.27532	3.24871
	H	0.13356	0.76553	3.40681
	H	8.94019	0.97453	0.99673
	H	0.54606	−0.95064	3.17390
	H	8.18209	2.09930	2.16207
	O	−0.64894	−2.28005	−1.56315
	H	−2.00055	−1.34849	−1.50704
	C	−0.64004	−3.29901	−0.59432
	H	0.37247	−3.47989	−0.19233
	H	−0.98666	−4.24868	−1.03342
	H	−1.29602	−3.07902	0.26724
	H	5.79506	−0.56757	0.20589
	H	−3.84139	−1.54567	2.82380
	H	−5.75164	−1.18612	−0.73064
	C	−4.95210	−1.44002	1.12510
	N	−6.08764	−1.87198	1.70580
	H	−6.01180	−2.27859	2.62684
	C	−7.37684	−1.94717	1.03071
	H	−8.12747	−2.23709	1.76617
	H	−7.37592	−2.69199	0.22544
	H	−7.65845	−0.97070	0.62313

Optimized Molecular Properties for **TArg-TS3-2**

Number of (–) Vibrational Frequencies	0 (–1280.874)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 17 positive frequencies below 100 cm^–1. Zero–point correction: 0.560951 hartree Enthalpy correction: 0.599793 hartree Free Energy correction: 0.487770 hartree Quasiharmonic Free Energy correction: 0.500269 hartree SCF Energy: –1546.427312 hartree SCF Energy + ZPVE: –1545.866361 hartree Enthalpy: –1545.827519 hartree Free Energy: –1545.939542 hartree **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1546.98665916 A.U.
Cartesian Coordinates	(PCM) 67 spD3–TS3–arg–Targ.out Energy: –970748.7770396 C 5.69135 –1.22862 –1.21286 O 4.64456 –1.82969 –1.41686 O 5.87922 –0.36129 –0.22183 C 3.07262 0.78027 2.15989 C 1.73892 0.49299 2.32929 N 3.59006 –0.06484 1.19646 C 2.58718 –0.83509 0.80330 N 1.43786 –0.53984 1.45400 C 6.92903 –1.39421 –2.06864 C 3.91580 1.79805 2.86292 C 0.11897 –1.20983 1.24230 C –0.47270 –0.73980 –1.19146 O –1.15378 –0.32060 –2.15599 C –0.75591 –0.47096 0.20355 C –2.25901 –0.34438 0.52065 C –3.08238 –1.64172 0.52825 O –2.91008 0.57720 –0.38314 C –2.65917 –2.83343 –0.07110 C –4.34973 –1.61627 1.13251 C –3.47892 –3.96657 –0.07208 C –5.17021 –2.74267 1.13632 C –4.73609 –3.92582 0.53026 H –0.27214 0.93454 0.13609 O 0.69093 –1.39448 –1.42628 C 1.14335 –1.46909 –2.78959 C –0.53041 –1.42560 2.61721 N 0.14151 2.11822 0.08037 N –1.12235 2.77671 –1.76776 H –6.14635 –2.70032 1.61290

	H	−5.37151	−4.80746	0.53272
	H	−3.12952	−4.88154	−0.54356
	H	−1.68012	−2.88986	−0.53734
	H	−4.69466	−0.69641	1.60000
	H	−0.83579	−0.48616	3.08913
	H	0.17747	−1.92595	3.28495
	H	−1.41643	−2.05672	2.52299
	H	−2.37105	0.11641	1.50678
	H	0.39565	−2.19735	0.85925
	H	1.00634	0.91167	3.00196
	H	4.74120	1.32329	3.40723
	H	4.36215	2.50586	2.15387
	H	3.32092	2.36810	3.58332
	H	2.66174	−1.59425	0.04194
	H	−2.57815	0.31017	−1.27089
	H	−1.06795	1.79229	−2.02543
	H	7.21279	−0.43091	−2.50578
	H	2.17013	−1.83174	−2.73185
	H	0.52056	−2.16094	−3.36347
	H	7.76863	−1.73044	−1.45110
	H	1.11177	−0.48385	−3.25999
	H	6.74119	−2.11827	−2.86242
	O	−3.89651	3.09592	−0.98713
	H	−3.62613	2.24351	−0.57920
	C	−5.09706	2.86278	−1.71460
	H	−5.37689	3.80372	−2.19706
	H	−5.92075	2.55490	−1.05513
	H	−4.97297	2.09730	−2.49402
	H	5.02558	−0.25382	0.33044
	H	0.73606	2.41627	0.84604
	H	−2.08194	3.13237	−1.81415
	C	−0.48289	3.06336	−0.59087
	N	−0.52159	4.35882	−0.19826
	H	−0.80992	5.03234	−0.89395
	C	0.05908	4.85387	1.03777
	H	−0.28008	5.87946	1.19208
	H	1.15701	4.85020	1.01614
	H	−0.28081	4.24992	1.88552

Optimized Molecular Properties for **TArg-Int3**

Number of (–) Vibrational Frequencies	0
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 17 positive frequencies below 100 cm^–1. Zero–point correction: 0.563954 hartree Enthalpy correction: 0.603248 hartree Free Energy correction: 0.491800 hartree Quasiharmonic Free Energy correction: 0.502644 hartree SCF Energy: –1546.446460 hartree SCF Energy + ZPVE: –1545.882506 hartree Enthalpy: –1545.843212 hartree Free Energy: –1545.954660 hartree Free Energy with quasiharmonic correction: –1545.943816 hartree (correction: 6.80 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1547.01074846 A.U.
Cartesian Coordinates	(PCM) 67 spD3–R–TS4–Targ.out Energy: –970763.8933034 C –4.65478 0.72592 –0.39378 O –3.64922 1.25861 –0.95261 O –4.65874 –0.37110 0.23849 C –2.31958 –3.08253 0.38021 C –1.01254 –3.40403 0.66013 N –2.44988 –1.73296 0.65500 C –1.27304 –1.26640 1.07885 N –0.37347 –2.25265 1.09294 C –5.97855 1.48672 –0.46851 C –3.46405 –3.92386 –0.08638 C 1.11443 –2.02311 1.51579 C 1.63243 0.42915 1.59300 O 2.05187 1.54812 1.19981 C 1.68067 –0.78700 0.90478 C 2.12403 –0.77762 –0.53367 C 3.49785 –0.16082 –0.81007 O 1.15973 –0.14596 –1.43799 C 3.76178 0.51736 –2.00645 C 4.55675 –0.35878 0.08657 C 5.04347 0.99531 –2.29264 C 5.83928 0.10967 –0.19895 C 6.09039 0.79208 –1.39241 H –1.05322 –2.59030 –1.75267 O 1.03301 0.35591 2.86234 C 1.11221 1.53820 3.65143 C 1.87029 –3.33234 1.26852

	N	−0.91052	1.53399	−0.49914
	N	0.25964	3.40884	0.18629
	H	6.64324	−0.05270	0.51546
	H	7.08825	1.16196	−1.61509
	H	5.22263	1.52646	−3.22491
	H	2.95039	0.67362	−2.70815
	H	4.35973	−0.87126	1.02397
	H	2.90128	−3.19717	1.60544
	H	1.89813	−3.61596	0.21142
	H	1.44001	−4.16507	1.83607
	H	2.20183	−1.82133	−0.86973
	H	1.03534	−1.87382	2.59307
	H	−0.50764	−4.35347	0.59308
	H	−4.22130	−4.02857	0.69902
	H	−3.95609	−3.47983	−0.95839
	H	−3.11436	−4.92320	−0.35728
	H	−1.06194	−0.24450	1.34650
	H	−0.04432	1.02585	−0.73618
	H	1.01330	2.78322	0.53076
	H	−5.96693	2.30212	0.26590
	H	0.63399	1.29271	4.60314
	H	2.15073	1.83864	3.82750
	H	−6.10513	1.93771	−1.45718
	H	0.58615	2.37675	3.18262
	H	−6.82446	0.83355	−0.24232
	O	−0.64941	−2.03923	−2.44401
	H	0.55527	−0.84785	−1.76527
	C	−1.69700	−1.42182	−3.20300
	H	−2.31664	−2.17439	−3.70656
	H	−1.20983	−0.80510	−3.96119
	H	−2.33639	−0.78134	−2.58271
	H	−3.33381	−1.12925	0.47717
	H	−1.82187	1.14334	−0.76259
	H	0.25803	4.36632	0.50451
	C	−0.89336	2.83413	−0.18842
	N	−2.04215	3.52698	−0.26449
	H	−2.85415	2.98620	−0.57511
	C	−2.21007	4.89356	0.19942
	H	−1.61048	5.59831	−0.38943
	H	−1.94675	5.00063	1.25940
	H	−3.25994	5.16466	0.08061

Optimized Molecular Properties for **TArg-TS4**

Number of (–) Vibrational Frequencies	0 (–266.7866)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 18 positive frequencies below 100 cm^–1. Zero–point correction: 0.563170 hartree Enthalpy correction: 0.602292 hartree Free Energy correction: 0.491403 hartree Quasiharmonic Free Energy correction: 0.501820 hartree SCF Energy: –1546.443548 hartree SCF Energy + ZPVE: –1545.880378 hartree Enthalpy: –1545.841256 hartree Free Energy: –1545.952145 hartree Free Energy with quasiharmonic correction: –1545.941728 hartree (correction: 6.54 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1547.00661396 A.U.
Cartesian Coordinates	(PCM) 67 spD3–TS4–Targ.out Energy: –970761.2988655 C –4.64981 0.90419 –0.28861 O –3.61373 1.38963 –0.84159 O –4.71961 –0.20556 0.30934 C –2.50142 –3.07003 0.21353 C –1.20709 –3.47526 0.45861 N –2.56257 –1.74868 0.61463 C –1.35225 –1.39254 1.07515 N –0.50557 –2.41172 0.99592 C –5.92036 1.75467 –0.33987 C –3.68558 –3.80682 –0.32589 C 1.25120 –2.17986 1.39520 C 1.65552 0.25067 1.62966 O 2.03879 1.38476 1.28201 C 1.74182 –0.94291 0.86416 C 2.17551 –0.81254 –0.57714 C 3.53372 –0.14524 –0.80071 O 1.19013 –0.13312 –1.40642 C 3.76309 0.68700 –1.90280 C 4.61099 –0.43966 0.04641 C 5.03154 1.22141 –2.14400 C 5.88007 0.08638 –0.19565 C 6.09735 0.92303 –1.29376 H –1.10047 –2.47551 –1.75387 O 1.09034 0.09010 2.88802 C 1.09003 1.25056 3.71919 C 1.83247 –3.51186 0.95311

	N	−0.87348	1.52826	−0.38094
	N	0.38105	3.38621	0.19215
	H	6.69985	−0.15358	0.47752
	H	7.08478	1.33690	−1.48239
	H	5.18557	1.87180	−3.00212
	H	2.93680	0.91609	−2.56608
	H	4.44281	−1.07625	0.91097
	H	2.89267	−3.53700	1.22670
	H	1.76327	−3.67310	−0.12665
	H	1.33865	−4.34782	1.45818
	H	2.27429	−1.82559	−0.98958
	H	1.11475	−2.14378	2.47224
	H	−0.75523	−4.44259	0.30054
	H	−4.45946	−3.92869	0.44095
	H	−4.14107	−3.27417	−1.16790
	H	−3.38788	−4.80147	−0.66798
	H	−1.09672	−0.40734	1.43102
	H	−0.02744	0.99986	−0.64021
	H	1.11008	2.74661	0.53812
	H	−5.82226	2.59483	0.35919
	H	0.62475	0.94102	4.65741
	H	2.10781	1.60666	3.90756
	H	−6.05428	2.17814	−1.34021
	H	0.51352	2.06521	3.26970
	H	−6.80062	1.17149	−0.06011
	O	−0.68798	−1.92097	−2.43930
	H	0.56299	−0.81238	−1.74378
	C	−1.72475	−1.25003	−3.16599
	H	−2.37605	−1.96873	−3.67925
	H	−1.22944	−0.62971	−3.91619
	H	−2.33490	−0.60620	−2.52022
	H	−3.40096	−1.09491	0.49690
	H	−1.80274	1.16482	−0.62431
	H	0.42215	4.34870	0.49188
	C	−0.80526	2.83825	−0.12374
	N	−1.92784	3.56944	−0.19123
	H	−2.76465	3.05085	−0.48024
	C	−2.02795	4.96236	0.20949
	H	−1.41892	5.61370	−0.42912
	H	−1.72978	5.10846	1.25545
	H	−3.06951	5.26973	0.10752

Optimized Molecular Properties for **TArgHis-TS3-1**

Number of (–) Vibrational Frequencies	1 (–1197.114)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 13 positive frequencies below 100 cm^–1. Zero–point correction: 0.510809 hartree Enthalpy correction: 0.543856 hartree Free Energy correction: 0.447769 hartree Quasiharmonic Free Energy correction: 0.455825 hartree SCF Energy: –1317.773791 hartree SCF Energy + ZPVE: –1317.262982 hartree Enthalpy: –1317.229935 hartree Free Energy: –1317.326022 hartree Free Energy with quasiharmonic correction: –1317.317966 hartree (correction: 5.06 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1318.23873771 A.U.
Cartesian Coordinates	(PCM) 60 spD3–TS3–meoh–TArgHis.out Energy: –827207.2903156 C 4.92734 –1.05794 –0.40868 C 3.67825 –0.70269 –0.83796 N 5.30049 –0.07755 0.50105 C 4.31954 0.82790 0.62023 N 3.32267 0.46803 –0.18319 C 5.79805 –2.21702 –0.75987 C 2.06504 1.27083 –0.39398 C 0.51043 0.06811 1.20051 O –0.52321 –0.44813 1.62910 C 0.81767 0.39300 –0.19480 C –0.41427 0.74647 –1.06302 C –1.34035 1.86448 –0.59156 O –1.21433 –0.42655 –1.31613 C –2.51676 2.11405 –1.31759 C –1.03850 2.70587 0.48474 C –3.37090 3.15850 –0.96783 C –1.88987 3.75772 0.83689 C –3.06067 3.98630 0.11505 H 1.03652 –0.82049 –0.78470 O 1.53995 0.33448 2.06042 C 1.33843 –0.06347 3.42559 C 2.19888 1.96366 –1.75781 N –3.78994 –1.32637 –0.86842 N –2.86842 –1.87116 1.17569 H –1.63514 4.39545 1.67932 H –3.72343 4.80277 0.38863

	H	−4.27620	3.33124	−1.54415
	H	−2.75783	1.48247	−2.16791
	H	−0.13398	2.54609	1.06331
	H	1.40515	2.70440	−1.88516
	H	2.14934	1.25130	−2.58712
	H	3.15817	2.48763	−1.81212
	H	−0.02247	1.06410	−2.03710
	H	2.13675	2.04185	0.38040
	H	2.97728	−1.20514	−1.49599
	H	6.74092	−1.88711	−1.21035
	H	6.03749	−2.81971	0.12342
	H	5.28353	−2.85741	−1.47956
	H	4.33460	1.69360	1.26246
	H	−2.89050	−0.89067	−1.12506
	H	−2.04258	−1.28617	0.99650
	H	2.24796	0.22771	3.95260
	H	0.47195	0.44530	3.85503
	H	1.18910	−1.14422	3.49598
	O	0.96665	−1.84293	−1.54599
	H	−0.55217	−1.13348	−1.58476
	C	0.94741	−3.01351	−0.76458
	H	1.88495	−3.15242	−0.19553
	H	0.82737	−3.90079	−1.40595
	H	0.12084	−3.02384	−0.03259
	H	−3.00944	−2.13980	2.13915
	H	−4.48162	−1.48202	−1.58555
	C	−3.89942	−1.91633	0.32257
	N	−5.03019	−2.55528	0.67000
	H	−5.03925	−3.03582	1.55770
	C	−6.19849	−2.69292	−0.19135
	H	−6.97860	−3.19794	0.37840
	H	−5.97899	−3.29398	−1.08166
	H	−6.57789	−1.71213	−0.49678
	H	6.17270	−0.04749	1.01482

Optimized Molecular Properties for **TArgHis-TS3-2**

Number of (–) Vibrational Frequencies	1 (–1099.3385)
Absolute Energies (Hartrees)	**B3LYP/6–31G(d)(PCM)** There are 13 positive frequencies below 100 cm^–1. Zero–point correction: 0.512228 hartree Enthalpy correction: 0.544985 hartree Free Energy correction: 0.450025 hartree Quasiharmonic Free Energy correction: 0.457771 hartree SCF Energy: –1317.772984 hartree SCF Energy + ZPVE: –1317.260756 hartree Enthalpy: –1317.227999 hartree Free Energy: –1317.322959 hartree Free Energy with quasiharmonic correction: –1317.315213 hartree (correction: 4.86 kcal/mol) **B3LYP–D3/6–311+G(d,p)(PCM)** SCF Done: E(RB3LYP) = –1318.24029925 A.U.
Cartesian Coordinates	(PCM) 60 spD3–TS3–arg–TArgHis.out Energy: –827208.2701968 C 4.47011 –0.80100 –0.31851 C 3.11833 –0.78485 –0.52737 N 4.84811 0.53158 –0.25912 C 3.77461 1.31639 –0.41995 N 2.70910 0.53805 –0.58710 C 5.43474 –1.92772 –0.16328 C 1.32548 1.06561 –0.83632 C 0.45818 0.32453 1.43602 O –0.36226 –0.13822 2.26025 C 0.27247 0.32256 –0.00335 C –1.18702 0.62131 –0.46042 C –1.58177 2.10160 –0.46193 O –2.14761 –0.12631 0.30657 C –1.39709 2.92271 0.66095 C –2.19205 2.65398 –1.59573 C –1.80709 4.25604 0.64554 C –2.60047 3.99001 –1.61780 C –2.40766 4.79594 –0.49545 H 0.29891 –1.17678 –0.32571 O 1.65060 0.79353 1.87969 C 1.90663 0.65811 3.29033 C 1.08879 1.02092 –2.35487 N 0.17423 –2.34504 –0.66378 N –1.11946 –2.89503 1.19260 H –3.07072 4.39694 –2.50901 H –2.72383 5.83537 –0.50654

	H	−1.65887	4.87499	1.52650
	H	−0.94312	2.51883	1.56150
	H	−2.35740	2.02897	−2.47131
	H	0.98372	−0.00602	−2.71938
	H	1.92786	1.48756	−2.87997
	H	0.18651	1.57759	−2.61447
	H	−1.30219	0.25649	−1.48618
	H	1.40027	2.11917	−0.53648
	H	2.42264	−1.60562	−0.60187
	H	6.18053	−1.92829	−0.96599
	H	5.96614	−1.86619	0.79295
	H	4.89991	−2.87942	−0.19448
	H	3.77611	2.39462	−0.40948
	H	−1.80174	−0.13229	1.22808
	H	−0.65917	−2.12005	1.66632
	H	2.89950	1.08138	3.44488
	H	1.16358	1.20721	3.87253
	H	1.88997	−0.39346	3.58713
	O	−3.86112	−2.37059	0.58212
	H	−3.41840	−1.53849	0.30909
	C	−5.12187	−2.04689	1.16439
	H	−5.57824	−2.98405	1.49305
	H	−5.79236	−1.56836	0.43816
	H	−5.01595	−1.38542	2.03466
	H	0.28325	−2.49002	−1.66295
	H	−2.11041	−2.96134	1.42825
	C	−0.85981	−3.00255	−0.13665
	N	−1.64606	−3.83658	−0.85137
	H	−2.52529	−4.08251	−0.41135
	C	−1.58853	−3.94769	−2.30241
	H	−2.33918	−4.67429	−2.61542
	H	−0.61012	−4.31857	−2.62393
	H	−1.79638	−2.99304	−2.80298
	H	5.79022	0.87298	−0.11244

POTENTIAL ENERGY SURFACE SCAN RESULTS FOR C-C BOND FORMATION STEP

T3		**T4**		**T5**		**T7**		**T8**		**T9**	
$d_{C\text{-}C}$ (Å)	$\Delta\Delta E$ (kcal/mol)	$d_{C\text{-}C}$ (Å)	$\Delta\Delta E$ (kcal/mol)	$d_{C\text{-}C}$ (Å)	$\Delta\Delta E$ (kcal/mol)	$d_{C\text{-}C}$ (Å)	$\Delta\Delta E$ (kcal/mol)	$d_{C\text{-}C}$ (Å)	$\Delta\Delta E$ (kcal/mol)	$d_{C\text{-}C}$ (Å)	$\Delta\Delta E$ (kcal/mol)
3.15	3.02	3.14	7.69	3.12	12.56	3.14	9.59	3.14	11.45	-	-
3.05	3.13	3.04	7.48	3.02	12.23	3.04	9.33	3.04	10.94	-	-
2.95	4.48	2.94	7.33	2.92	11.94	2.94	9.10	2.94	10.47	2.99	9.35
2.85	4.52	2.84	7.28	2.82	11.73	2.84	8.94	2.84	10.06	2.89	9.11
2.75	4.68	2.74	7.32	2.72	11.59	2.74	8.90	2.74	9.67	2.79	8.96
2.65	4.96	2.64	7.48	2.62	11.52	2.64	9.04	2.64	9.34	2.69	8.91
2.55	5.38	2.54	7.76	2.52	11.44	2.54	9.00	2.54	9.06	2.59	8.93
2.45	5.87	2.44	7.60	2.42	11.06	2.44	8.76	2.44	8.79	2.49	8.83
2.35	6.44	2.34	7.46	2.32	10.55	2.34	8.46	2.34	8.48	2.39	8.52
2.25	6.30	2.24	7.10	2.22	9.82	2.24	8.02	2.24	8.02	2.29	8.10
2.15	5.94	2.14	6.50	2.12	8.78	2.14	7.32	2.14	7.30	2.19	7.48
2.05	5.16	2.04	5.56	2.02	7.31	2.04	6.13	2.04	6.18	2.09	6.52
1.95	3.95	1.94	4.20	1.92	5.39	1.94	4.56	1.94	4.61	1.99	5.16
1.85	2.39	1.84	2.52	1.82	3.14	1.84	2.70	1.84	2.72	1.89	3.43
1.75	0.82	1.74	0.84	1.72	1.03	1.74	0.90	1.74	0.90	1.79	1.52
1.65	0.00	1.64	0.00	1.62	0.00	1.64	0.00	1.64	0.00	1.69	0.00