Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Cartesian Coordinates for each Structure (angstroms)

1. Structure DATCE

	x	y	z
N	-1.33864176	0.06926695	-1.14312768
C	0.99088925	0.04023018	-1.31120181
C	-1.16956186	0.03552746	0.30082774
C	1.06715286	0.00649245	0.19109078
C	-0.01169499	0.76534992	0.95553982
C	-0.03304746	-0.75432605	0.92246419
H	1.49665296	0.91842294	-1.71849322
H	1.47209334	-0.83325911	-1.75658917
H	-2.12382007	0.03793455	0.80657989
H	2.06011534	-0.01692376	0.62685603
H	0.02480233	1.45217907	1.78253877
H	-0.01637538	-1.47721994	1.71879339
N	-0.36841473	0.07142519	-1.87093878

2. Structure DAP_1

	x	y	z
N	-1.24321604	0.12574799	-1.03812397
C	1.03742003	-0.21093599	-1.30370796
C	-1.25653994	-0.75852501	0.06709400
C	1.54057300	0.32737800	0.00317100
C	0.86407501	0.04521700	1.15865898
C	-0.38955301	-0.73746699	1.13297999
H	1.72502697	0.00448500	-2.11670709
H	0.88891202	-1.29329300	-1.24131298

H	-2.17757297	-1.32030404	0.13091099
H	2.43005109	0.94322199	0.02128800
H	1.24473500	0.38176200	2.11456299
H	-0.66945100	-1.29520500	2.01813602
N	-0.23882701	0.43701500	-1.64848804

3. Structure DAP_2

	x	y	z
N	-1.16779101	-0.64002001	-1.08525395
C	0.68300301	0.75432998	-1.25431597
C	-1.47904301	-0.10512900	0.18798700
C	1.48783505	0.28317201	-0.07852600
C	0.86488998	-0.00468100	1.10520506
C	-0.60514897	0.07661000	1.23283005
H	0.06928100	1.61709297	-0.97713298
H	1.32201004	1.03113604	-2.08814597
H	-2.54451108	-0.06943700	0.36536899
H	2.55957389	0.17099699	-0.17685100
H	1.44391096	-0.28888100	1.97464800
H	-1.02901101	0.24935301	2.21440911
N	-0.19210300	-0.32655400	-1.73923600

4. Structure NdisTS

	x	y	z
N	-1.30195343	0.01342211	-1.08620119
C	1.05292690	0.07258783	-1.29336417
C	-1.21845627	-0.64856392	0.12370900
C	1.28874016	-0.29430455	0.15287189
C	0.70504355	0.52046371	1.27374268

C	0.04811408	-0.79807019	0.92320359
H	1.64533305	0.94120276	-1.58244169
H	1.38154840	-0.75137752	-1.93326998
H	-2.17247462	-0.90840471	0.55546230
H	2.23382282	-0.78592616	0.35617012
H	1.14248049	0.83859372	2.20771027
H	0.11646657	-1.64245570	1.59758270
N	-0.31415167	0.37006265	-1.72467542

5. Structure CdisTS

	x	y	z
C	-1.23991597	0.00001755	-1.08678555
N	1.11064184	0.12755996	-1.17369318
C	-1.22954774	-0.88036704	0.12311003
C	1.20902181	-0.22120188	0.22741903
C	0.50301600	0.57922471	1.29399884
C	-0.00173660	-0.81041926	0.99546325
H	-2.17851353	-1.15399027	0.56738806
H	2.19879723	-0.58687681	0.46176511
H	0.89500433	1.00905406	2.20304942
H	0.16966029	-1.61051345	1.70529115
N	0.05061551	0.21945223	-1.75495827
H	-1.89900517	-0.40604001	-1.85402000
H	-1.62471807	1.00128031	-0.85891795

6. Structure NconTS1

	x	y	z
N	-1.29244304	0.07636036	-1.01047087
C	1.04163992	0.14488558	-1.26618493

C	-1.16634893	-0.75647867	0.13728587
C	1.26299679	-0.10212760	0.20811179
C	0.59815705	0.67613679	1.21299589
C	-0.12937532	-0.67258233	1.08854246
H	1.65934813	0.96744531	-1.62766850
H	1.31439888	-0.73823875	-1.84796941
H	-2.03141189	-1.38707054	0.28535643
H	1.98126447	-0.85941786	0.49409425
H	0.03639345	1.52687764	0.83496058
H	0.02891397	-1.46834338	1.80330479
N	-0.33586344	0.48483324	-1.64720857

7. Structure CconTS1

	x	y	z
C	-1.23598480	0.02076247	-1.07024336
N	1.11656094	0.21811867	-1.17233992
C	-1.21964467	-0.75743264	0.21374667
C	1.20177174	-0.11838255	0.21241990
C	0.55813766	0.68511385	1.23024774
C	-0.10755118	-0.71358263	1.08197474
H	-2.08826065	-1.36226428	0.44462928
H	2.03538108	-0.75830472	0.46382228
H	-0.02436638	1.51902115	0.84208316
H	0.09314413	-1.49601495	1.80005956
N	0.04187234	0.33545503	-1.72625780
H	-1.78527188	-0.54973620	-1.82126570
H	-1.76637816	0.97401685	-0.99474645

8. Structure NconInt

	x	y	z
N	-1.17254436	-0.12935539	-1.03004634
C	1.14911330	0.52507800	-1.32641387
C	-1.20073497	-0.78021890	0.27967709
C	1.34310114	-0.15687630	-0.02968836
C	0.69569921	0.37333986	1.07144785
C	-0.48748320	-0.48004261	1.41496575
H	1.33888507	1.59884501	-1.31786120
H	1.69165754	0.09332362	-2.16674495
H	-2.09250116	-1.39012527	0.32793716
H	1.35121119	-1.23951328	-0.09737577
H	0.64599955	1.44558704	1.23436141
H	-0.81668174	-0.79587555	2.39674282
N	-0.30165136	0.40838382	-1.68327153

9. Structure CconInt

	x	y	z
C	-1.06391704	-0.29168245	-1.09964263
N	1.17967534	0.59556657	-1.25672734
C	-1.27702379	-0.75489688	0.35226682
C	1.28607547	-0.17518854	-0.05344008
C	0.69972783	0.31735843	1.08559728
C	-0.49822330	-0.51729470	1.45452821
H	-2.22556758	-1.27307343	0.47208774
H	1.33984542	-1.24352431	-0.22866115
H	0.64357913	1.39016211	1.23451269
H	-0.80712503	-0.80358273	2.45123553
N	0.04665386	0.53191787	-1.69741893
H	-1.08687139	-1.17469788	-1.74655640

H	-1.95164299	0.27860880	-1.37835872

10. Structure NconTS2

	x	y	z
N	-1.22473168	-0.45778599	-1.13910139
C	0.94505334	0.56573945	-1.36906683
C	-1.31874728	-0.57033855	0.28926978
C	1.41338336	0.01856516	-0.06715097
C	0.73123562	0.49870428	1.17475450
C	-0.57058573	-0.01180191	1.35865033
H	0.81215769	1.65091348	-1.34124863
H	1.63488150	0.34631550	-2.18331766
H	-2.27999783	-1.00280988	0.53255856
H	1.65092111	-1.04281521	-0.07590441
H	1.17330158	1.21783650	1.85320687
H	-1.07045138	0.05085879	2.31917119
N	-0.35554022	0.02986831	-1.83606148

11. Structure CconTS2

	x	y	z
C	-0.98741549	-0.43501547	-1.14645267
N	0.94523656	0.90839851	-1.08737504
C	-1.30527937	-0.63195413	0.32575455
C	1.41925013	-0.05428514	-0.13735721
C	0.86732721	0.10182675	1.24706852
C	-0.47469309	-0.34508145	1.42275000
H	-2.30822897	-0.98507929	0.53027695
H	1.53624642	-1.06233335	-0.52521968
H	1.40002048	0.63613701	2.02032113
H	-0.90457594	-0.39136788	2.41618919

N	-0.17153913	0.74174345	-1.53880131
H	-0.52493757	-1.32949257	-1.57737041
H	-1.92843127	-0.29718637	-1.67398417

12. Structure DATCA

	x	y	z
N	-1.42293572	0.19845748	-1.14382577
C	0.97666281	0.11770615	-1.38115907
C	-1.21422291	0.12395849	0.27996346
C	1.03657210	-0.02077130	0.13112727
C	0.00653699	0.74467486	0.95053643
C	-0.11138921	-0.77785206	0.80267608
H	1.23057044	1.14303195	-1.66671002
H	1.70794582	-0.53806341	-1.85897791
H	-2.14152622	0.14866386	0.84120041
H	2.02121615	-0.12557875	0.57551348
H	0.11214472	1.31699753	1.85691321
H	-0.11495087	-1.53014958	1.57237792
N	-0.33029807	-0.22865683	-1.92299938
H	-1.65234458	1.13811672	-1.41621232
H	-0.40628135	-1.22710514	-1.98618388

13. Structure $DHDAP_1$

	x	y	z
N	-1.39481902	0.23868400	-1.13966894
C	0.97603899	0.30155301	-1.36241305
C	-1.74704099	-0.15927500	0.15561500
C	1.39266598	0.20351399	0.08435500
C	0.60675901	-0.13192300	1.15226996

C	-0.86680102	-0.37098899	1.17894304
H	0.91113198	1.34645605	-1.66934705
H	1.75735795	-0.15404899	-1.97798204
H	-2.81018090	-0.26625401	0.33284000
H	2.44280696	0.39425400	0.28221199
H	1.09289396	-0.19347601	2.11922097
H	-1.28807199	-0.67126000	2.12922502
N	-0.26623699	-0.35127199	-1.72259498
H	-2.15979195	0.18431900	-1.78064704
H	-0.21916100	-1.32326603	-1.45930195

14. Structure $DHDAP_2$

	x	y	z
N	-1.36570203	-0.32421601	-1.11690795
C	0.93440503	0.44240099	-1.36343503
C	-1.52962899	-0.09297200	0.24612100
C	1.58951902	0.21596000	-0.02402100
C	0.88892901	-0.02088400	1.12418401
C	-0.59541303	-0.03583700	1.24591005
H	0.50688398	1.44633996	-1.42015803
H	1.68743205	0.38124600	-2.15160894
H	-2.57504106	-0.01370400	0.51987100
H	2.67274308	0.22763000	0.01977000
H	1.44114602	-0.16861600	2.04503012
H	-0.99180698	0.03722700	2.25064707
N	-0.12575100	-0.50236100	-1.71296000
H	-1.98272002	0.20465900	-1.69944596
H	0.17379400	-1.44221604	-1.52972806

15. Structure NdisTS’

	x	y	z
N	-1.42339540	-0.14606592	-1.16566598
C	0.93296069	0.25221679	-1.26147401
C	-1.40808904	-0.32721406	0.22840041
C	1.19161737	-0.16610871	0.18556029
C	0.84130841	0.81545776	1.26951730
C	-0.12877002	-0.34134027	1.01129293
H	0.80472010	1.33444512	-1.32227707
H	1.79706573	0.00164181	-1.87867403
H	-2.35516500	-0.18690881	0.72857887
H	2.00624251	-0.86340731	0.35096633
H	1.39543521	0.92786473	2.19372249
H	-0.11925846	-1.06822538	1.81810999
N	-0.23407100	-0.35943642	-1.87034750
H	-1.86182213	0.70168203	-1.47589076
H	-0.10957908	-1.35344136	-1.95132947

16. Structure NdisTS”

	x	y	z
N	-1.35345852	0.20459662	-1.05027461
C	1.04206014	0.13321534	-1.34365678
C	-1.22168159	0.42395344	0.33541670
C	1.28673506	-0.14588186	0.12525053
C	0.06758421	0.05781965	1.05366910
C	0.60426700	-1.32363117	0.78441113
H	1.15246558	1.20371866	-1.53755569
H	1.77541852	-0.38642454	-1.96429086
H	-2.15312290	0.39689919	0.89210719

H	2.25471497	0.14308731	0.52221948
H	0.21058591	0.51497751	2.02611446
H	0.94744480	-2.10143733	1.44823039
N	-0.27236584	-0.28958043	-1.79056585
H	-1.77515674	0.97728574	-1.53008449
H	-0.32491049	-1.29297805	-1.74940085

17. Structure CdisTS’

	x	y	z
N	-1.39562595	0.13293861	-1.09109366
C	0.99973285	0.19917566	-1.39172935
C	-1.28806067	0.19103202	0.34260291
C	1.29041827	0.19030157	0.08237755
C	0.11506672	0.24624294	1.03696835
C	-0.77405405	-0.98817056	1.11280930
H	1.01604879	1.23224723	-1.76587749
H	1.77840137	-0.33207700	-1.94385386
H	-2.09643722	0.75877380	0.78947771
H	2.25147820	0.55132854	0.42733517
H	0.23269734	0.84052205	1.93693876
H	-1.18028319	-1.48607981	1.98114049
N	-0.27926472	-0.37997854	-1.77376115
H	-1.58354163	1.04699314	-1.46162188
H	-0.27862626	-1.37567961	-1.64485288

18. Structure CdisTS”

	x	y	z
N	-1.33637977	0.31465718	-1.09704268
C	1.01107061	-0.03348709	-1.49189413

C	-1.25072801	0.00064490	0.30805078
C	1.25051641	-0.57820606	-0.11412560
C	-0.46861416	0.89247489	1.24482906
C	0.12283386	-0.45685077	0.88532895
H	1.23931909	1.03968787	-1.52898061
H	1.67403328	-0.51324832	-2.21523738
H	-2.13566422	-0.48302138	0.70886517
H	2.26258874	-0.67250121	0.26165459
H	-0.74728137	1.25632071	2.22391558
H	0.10247264	-1.20793450	1.66828823
N	-0.35648748	-0.20929363	-1.95280385
H	-1.39411724	1.30264926	-1.25304103
H	-0.55888206	-1.18373179	-2.08697677

19. Structure NconTS1’

	x	y	z
N	-1.43094933	0.00844477	-1.05635679
C	0.98796737	0.19592127	-1.31666112
C	-1.39533913	-0.48966303	0.27399421
C	1.13849020	-0.02605952	0.17835093
C	0.54325736	0.89400637	1.12329757
C	-0.24462490	-0.43452144	1.10718977
H	1.13207793	1.26165700	-1.51517606
H	1.75230050	-0.34002155	-1.88157892
H	-2.31300664	-0.94758868	0.62348062
H	1.86804652	-0.73859274	0.54489440
H	0.04017371	1.75133789	0.67512351
H	-0.11543095	-1.15248680	1.90509605
N	-0.30366421	-0.20636971	-1.86336851

H	-1.77593493	0.94211507	-1.17049420
H	-0.29553342	-1.18461883	-2.08670139

20. Structure NconTS1$_a$”

	x	y	z
N	-1.33736515	0.32192284	-1.07347786
C	1.03748357	0.12912646	-1.38524425
C	-1.17192423	0.27935398	0.33617321
C	1.19287157	-0.22303137	0.07880460
C	0.08648123	0.24252611	1.06512630
C	0.36466718	-1.24542284	0.81046021
H	1.27329171	1.18689895	-1.54016256
H	1.73719871	-0.44634843	-1.99471390
H	-2.10495520	0.35779929	0.88236797
H	2.18828321	-0.10601499	0.49635628
H	0.26318210	0.73956609	2.01055074
H	-0.31991121	-2.01209474	0.47015148
N	-0.29615569	-0.13984543	-1.88805306
H	-1.60875452	1.24218035	-1.37538707
H	-0.42383334	-1.13234615	-1.97748208

21. Structure NconTS1$_b$”

	x	y	z
N	-1.37007999	0.21642189	-1.03387082
C	1.01358879	0.09395494	-1.36566508
C	-1.17764771	0.48460183	0.31954116
C	1.24384856	-0.23482305	0.09737201
C	-0.16166560	-0.02143468	1.13447988
C	0.62831956	-1.34321129	0.76988173

H	1.16087043	1.16113365	-1.54630864
H	1.72647870	-0.44072470	-1.99733388
H	-1.94308221	1.12372172	0.74224061
H	1.96049356	0.37644607	0.63625616
H	-0.03499719	0.42012647	2.11345911
H	0.05090978	-1.97989404	0.09782664
N	-0.32054877	-0.28873754	-1.81068313
H	-1.82399678	0.97171456	-1.50863016
H	-0.39848125	-1.28864574	-1.80960560

22. Structure CconTS1’

	x	y	z
N	-1.39204526	0.12252544	-1.07907808
C	1.00119078	0.18888251	-1.36349821
C	-1.23541296	0.07381579	0.34205797
C	1.20927906	0.34241784	0.12560329
C	0.12075529	0.46527982	1.06624746
C	-0.47619471	-0.97196239	1.05428267
H	1.14950013	1.18056560	-1.81362844
H	1.77378404	-0.44973451	-1.79583240
H	-2.08996129	0.46395597	0.88231999
H	2.22906733	0.50248492	0.46082073
H	0.16861869	1.06601584	1.96488047
H	0.02724839	-1.82898188	0.61913151
N	-0.28030020	-0.32539827	-1.80860305
H	-1.62760043	1.04729223	-1.39249980
H	-0.29082894	-1.32732880	-1.78085411

23. Structure CconTS1”

	x	y	z
N	-1.37918520	0.33643577	-1.15644407
C	1.00732672	-0.02059591	-1.45013666
C	-1.21840417	0.20094195	0.26702461
C	1.19852984	-0.57649338	-0.05059063
C	-0.36758199	1.05796087	1.07098007
C	0.20355304	-0.38456950	0.94631630
H	1.27565694	1.03581023	-1.52903795
H	1.67146790	-0.55035418	-2.13445640
H	-1.98380148	-0.37611693	0.77261817
H	2.07487488	-1.17643464	0.16400950
H	0.16595033	1.83800828	0.53014487
H	0.09975848	-1.07083881	1.77547991
N	-0.34726137	-0.19532865	-1.96000302
H	-1.46424091	1.30922759	-1.39181232
H	-0.53978330	-1.17438269	-2.07429242

24. Structure NconInt’

	x	y	z
N	-1.28932583	0.04634845	-0.94741422
C	1.05325341	0.43676457	-1.45664108
C	-1.46003604	-0.52121627	0.36293334
C	1.30981970	-0.01541957	-0.04763298
C	0.55006790	0.56903785	0.94047529
C	-0.60538483	-0.29326814	1.41034186
H	0.90941447	1.51290190	-1.53617311
H	1.79818821	0.12317528	-2.18886948
H	-2.40994430	-1.02145517	0.52036697
H	1.46781588	-1.08894932	0.03664571

H	0.32035694	1.62774205	0.85257143
H	-0.82317519	-0.63420898	2.41286302
N	-0.20619182	-0.24174021	-1.81216311
H	-2.12495565	-0.04916412	-1.48585749
H	-0.03512795	-1.23532736	-1.82547951

25. Structure NconInt$_a$"

	x	y	z
N	-1.37069941	0.21131562	-1.03988624
C	1.00963295	0.11624040	-1.33453441
C	-1.18363142	0.48190045	0.30083588
C	1.21398103	-0.23436050	0.12861913
C	-0.09080713	0.06123838	1.07631958
C	0.59785086	-1.38143158	0.78924429
H	1.15093708	1.18764114	-1.49759293
H	1.73718333	-0.40411642	-1.96020043
H	-1.99088168	1.04974210	0.74667197
H	2.04001880	0.25811371	0.63253444
H	0.03969629	0.49962756	2.05413985
H	-0.01792898	-1.97598946	0.10731504
N	-0.31133908	-0.26844308	-1.81672335
H	-1.88871181	0.91863626	-1.52220869
H	-0.37918606	-1.26993549	-1.82709599

26. Structure NconInt$_b$"

	x	y	z
N	-1.04582500	0.59907800	-0.92982298
C	1.12143099	-0.27352500	-1.59853399
C	-1.31762600	0.33106801	0.43827900

C	1.33090401	-0.05010000	-0.12573899
C	-0.53163302	-0.34339300	1.34496295
C	0.71292698	-0.93837798	0.73650700
H	1.54193902	0.52914703	-2.20309305
H	1.50284600	-1.22447503	-1.97357702
H	-2.25413203	0.76937902	0.76498801
H	1.25982904	0.99320900	0.16193600
H	-0.89276499	-0.50508499	2.35211492
H	0.71693301	-2.00454593	0.51811498
N	-0.35087201	-0.30252901	-1.77176297
H	-1.85938799	0.91630900	-1.41344297
H	-0.65715700	-1.23778498	-1.55890298

27. Structure CconInt’

	x	y	z
N	-1.54577303	-0.25488600	-1.20525801
C	0.83828998	0.45557699	-1.26606703
C	-1.38421094	0.24584199	0.10359800
C	1.32028306	0.45265099	0.20247300
C	0.65373802	0.00839900	1.31776595
C	-0.70212299	-0.56299299	0.98760098
H	0.60008001	1.48591697	-1.54562104
H	1.70390201	0.18555000	-1.87536299
H	-1.32234395	1.32455599	0.22982199
H	2.33072495	0.83782601	0.31872499
H	1.13432896	-0.02192400	2.28807902
H	-0.78386301	-1.63970304	0.87174499
N	-0.23806199	-0.41413799	-1.76581800
H	-2.05685401	0.36631000	-1.80326200

H	0.01652400	-1.37323594	-1.61801803

28. Structure CconInt”

	x	y	z
N	-1.50680757	0.56806660	-1.30433857
C	0.90254611	-0.13684431	-1.34248567
C	-1.33901668	0.18480022	0.05263753
C	1.22509563	-0.68525136	0.07712884
C	-0.45107952	0.76213592	0.92525667
C	0.66651374	-0.21551019	1.24015796
H	1.28556395	0.88743246	-1.37062228
H	1.51083350	-0.69635767	-2.05396152
H	-1.55124116	-0.86979580	0.18505041
H	2.08378029	-1.34905469	0.12883927
H	-0.18387491	1.81044579	0.81894964
H	1.04705095	-0.47549337	2.22000599
N	-0.43426350	-0.10652254	-1.97062349
H	-1.36226058	1.55375171	-1.43762600
H	-0.75494838	-1.03908885	-2.15765285

29. Structure NconTS2’

	x	y	z
N	-1.29345250	-0.14148657	-1.06223071
C	0.98298764	0.52225679	-1.43695927
C	-1.43154299	-0.46441698	0.30293703
C	1.48590040	0.08770845	-0.08607526
C	0.72291613	0.46808505	1.14760506
C	-0.57767862	-0.12477954	1.35393023

H	0.63843900	1.55562139	-1.44227171
H	1.75030959	0.40812740	-2.20493650
H	-2.42516923	-0.81648183	0.55104113
H	1.81810308	-0.95227081	-0.08509157
H	1.10098279	1.20245564	1.84719050
H	-0.99238783	-0.19823252	2.35249138
N	-0.13304961	-0.33549953	-1.82581079
H	-2.07761145	-0.44912961	-1.59773958
H	0.16546376	-1.29778743	-1.75358987

30. Structure NconTS2”

	x	y	z
N	-0.95442176	0.70564193	-0.90830022
C	1.09275067	-0.32066563	-1.59886014
C	-1.29964244	0.34616992	0.40946886
C	1.53150833	-0.12862645	-0.17070051
C	-0.51763374	-0.47516546	1.24236357
C	0.80180967	-0.90327680	0.89841759
H	1.52177787	0.45718437	-2.23145628
H	1.41152573	-1.28543031	-2.00184107
H	-2.24236107	0.73953104	0.76580024
H	1.77199173	0.89397639	0.10826312
H	-0.98024762	-0.82737643	2.15669823
H	1.25232351	-1.75105810	1.39811301
N	-0.36664572	-0.28272822	-1.71884358
H	-1.72617841	1.10976660	-1.39820719
H	-0.73830664	-1.18157279	-1.45777547

31. Structure CconTS2’

	x	y	z
N	-1.48091173	-0.32316923	-1.22846985
C	0.79944986	0.56121582	-1.26692426
C	-1.60111916	0.18489447	0.07896924
C	1.31259978	0.44162902	0.16073807
C	0.61332721	-0.14667325	1.23267162
C	-0.76902974	-0.47871113	1.14310205
H	0.38076660	1.55287719	-1.45944369
H	1.66327238	0.47200024	-1.92983472
H	-1.80307865	1.24826133	0.20540553
H	2.34386492	0.73415506	0.32333699
H	1.16880322	-0.40741485	2.12682962
H	-1.21259475	-1.19246519	1.82513130
N	-0.16046345	-0.43579715	-1.72102416
H	-2.01503134	0.20841511	-1.88836086
H	0.16917495	-1.35795736	-1.50161695

32. Structure CconTS2”

	x	y	z
N	-1.37026465	0.73302871	-1.28783345
C	0.87258899	-0.26980808	-1.42273438
C	-1.54870033	0.32182592	0.05344129
C	1.16283774	-0.62507212	0.03527457
C	-0.60129660	0.69691128	1.16412342
C	0.62601334	-0.01556111	1.19647968
H	1.41744506	0.66357487	-1.60980988
H	1.35420501	-1.01914442	-2.05298281
H	-1.88953984	-0.70950902	0.10131884
H	2.09415388	-1.16732562	0.16407259

H	-0.87284940	1.39373589	1.94623566
H	1.21124625	-0.05525590	2.10910273
N	-0.46208549	-0.09558035	-1.98351347
H	-1.05760002	1.68298090	-1.36993039
H	-0.91536391	-0.98043090	-2.11986423

33. Structure TATCE

	x	y	z
N	-1.24102449	0.06335469	-1.16420841
N	0.98353422	0.21775147	-1.21458483
C	-1.14219677	0.04522111	0.28056934
C	1.06271446	0.05945647	0.20733991
C	-0.01450774	0.76942956	0.99471682
C	-0.01210226	-0.75345653	0.91220111
H	1.68854368	-0.22541514	-1.76783109
H	-2.11477113	0.01972986	0.74835366
H	2.07657313	0.05117608	0.58292556
H	0.00053438	1.46258247	1.81677806
H	0.00012857	-1.53649640	1.64929664
N	-0.22080594	0.09270635	-1.82924676

34. Structure TAP_1

	x	y	z
N	-1.25923800	-0.01367800	-1.06760204
N	0.93691301	-0.49631900	-1.11592805
C	-1.35856998	-0.51352400	0.25779101
C	1.45615697	0.30840701	-0.06771700
C	0.78232801	0.44971099	1.10806799
C	-0.52416301	-0.21822999	1.29869795

H	1.59358597	-0.54096001	-1.87049699
H	-2.30729604	-1.00040996	0.43006501
H	2.40791202	0.79541701	-0.23728800
H	1.21059501	1.04139698	1.90509200
H	-0.83647400	-0.48687300	2.29989004
N	-0.23817199	0.03142600	-1.70864499

35. Structure TAP_2

	x	y	z
N	-1.25038016	0.06708711	-1.03472793
N	0.98191047	0.30544290	-1.13496149
C	-1.23415029	0.39496627	0.34649506
C	1.43981278	-0.69842780	-0.24118215
C	-0.40244716	-0.13646780	1.29148936
C	0.79877442	-0.92553216	0.93960589
H	1.61059022	0.38616386	-1.91021681
H	-2.10653996	0.96405649	0.63256407
H	2.31400514	-1.26715899	-0.53131658
H	-0.63691020	0.02892942	2.33540797
H	1.17717683	-1.67305398	1.62283337
N	-0.26755595	-0.00521927	-1.73074698

36. Structure $N1disTS_2$

	x	y	z
N	-1.33099222	-0.33006421	-1.14672804
N	0.86660159	0.12573440	-1.16036201
C	-1.35058701	-0.19655491	0.22691783
C	1.15805352	-0.20634329	0.20225337
C	0.83608705	0.80457932	1.27590036

C	-0.11088291	-0.36102125	1.06437349
H	1.62620080	0.04583286	-1.80154109
H	-2.33074379	-0.20847273	0.67531455
H	1.98558068	-0.89060324	0.34683317
H	1.40113795	1.02322769	2.17011189
H	-0.13698517	-1.13811433	1.81993032
N	-0.28204060	-0.21620022	-1.78218412

37. Structure N1disTS_1

	x	y	z
N	-1.30169976	0.19081797	-1.04405200
N	0.94327176	0.05109686	-1.23695779
C	-1.21334004	0.30604666	0.32166755
C	1.23439634	-0.20356037	0.14254661
C	0.04350619	-0.00710853	1.08998549
C	0.64197320	-1.38673258	0.87150085
H	1.56055403	-0.38587660	-1.89167881
H	-2.15111351	0.45885873	0.83115613
H	2.20896363	0.16127288	0.43982437
H	0.18502170	0.49485105	2.03912592
H	1.08914125	-2.05898929	1.58883250
N	-0.30465758	0.03788886	-1.75479543

38. Structure N3disTS_2

	x	y	z
N	-1.26098287	-0.11335032	-1.09756756
N	0.96018976	0.19475992	-1.23826563
C	-1.22259617	0.11114339	0.32740036

C	1.29074740	0.03986797	0.11038735
C	0.13311155	0.19243215	1.06727517
C	-0.78314894	-1.00025153	1.24457669
H	1.67388237	0.02211608	-1.91340268
H	-2.04474854	0.73682499	0.64738613
H	2.26751041	0.41516444	0.37965891
H	0.24753155	0.89269352	1.88646662
H	-1.26557875	-1.35765290	2.14206529
N	-0.25107780	-0.07207775	-1.77588069

39. Structure N3disTS$_1$

	x	y	z
N	-1.33402169	0.07713960	-1.10628259
N	0.89154190	-0.10330334	-1.31662345
C	-1.22622192	-0.08966351	0.32074741
C	1.18516088	-0.70151305	-0.08374879
C	-0.40124962	0.85500580	1.16130280
C	0.10227987	-0.54994255	0.95930445
H	1.54356277	-0.24694774	-2.05811739
H	-2.15559125	-0.44409946	0.74359560
H	2.22735739	-0.62521011	0.20406279
H	-0.66284949	1.39568162	2.05771351
H	0.08753270	-1.26916194	1.76845801
N	-0.35202155	0.05420474	-1.82448196

Imaginary Frequencies for Transition State

3,4-diazatricyclo[4.1.0.0^{2,7}]hept-3-ene (DATCE)

Transition State	Imaginary Frequencies
NdisTS	403.3i

CdisTS	441.3i
NconTS1	326.8i
CconTS1	235.6i
NconTS2	708.1i
CconTS2	774.7i

3,4-diazatricyclo[4.1.0.$0^{2,7}$]heptane (DATCA)

Transition State	Imaginary Frequencies
NdisTS’	439.8i
NdisTS”	329.4i
CdisTS’	462.0i
CdisTS”	364.3i
NconTS1’	422.7i
$NconTS1_a$”	330.1i **488.5i**
$NconTS1_b$”	305.2i **460.6i**
CconTS1’	200.0i
CconTS1”	313.2i
NconTS2’	909.8i
NconTS2”	872.4i
CconTS2’	769.4i
CconTS2”	648.8i

Bold values are obtained at CCSD/ cc-pVDZ//CCSD/cc-pVDZ level.

3,4,5-triazatricyclo[4.1.0.$0^{2,7}$] hept-3-ene (TATCE)

Transition State	Imaginary Frequencies
$N1disTS_1$	433.4i
$N1disTS_2$	358.4i
$N3disTS_2$	433.1i
$N3disTS_1$	367.5i

$N3disTS_2$	433.1i

Calculated Energies (Hartree) for Each Structure

3,4-diazatricyclo[4.1.0.$0^{2,7}$]hept-3-ene (DATCE)

Structure	MCSCF	ZPE	MRMP2	PBEPBE-D3
DATCE	-301.7236903001	0.109598	-302.5916366963	-303.154923914
DAP_1	-301.7852845205	0.109653	-302.6411678211	-303.200469402
DAP_2	-301.7852845205	0.109653	-302.6411678211	-303.200469402
NdisTS	-301.6377758015	0.104762	-302.5165611764	-303.084220255
CdisTS	-301.6297400607	0.104782	-302.4971132792	-303.070595746
NconTS1	-301.6548840380	0.105993	-302.5306600574	-303.096217765
CconTS1	-301.6541621627	0.105710	-302.5275531027	-303.092147066
NconTS2	-301.6716130840	0.104074	-302.5408009928	-303.102330698
CconTS2	-301.6753745419	0.104256	-302.5406569291	-303.071244272
NconInt	-301.7029804905	0.107762	-302.5669236398	-303.129153587
CconInt	-301.7068060498	0.107480	-302.5684475418	-303.120216093

3,4-diazatricyclo[4.1.0.$0^{2,7}$]heptane(DATCA)

Structure	MCSCF	ZPE	MRMP2	PBEPBE-D3	CCSD(T)
DATCA	-302.9014682620	0.136254	-303.7919340517	-304.358283994	**-304.2159678**
$DHDAP_1$	-302.9699715730	0.136015	-303.8422778172	-304.405386697	**-304.2646917**
$DHDAP_2$	-302.9670840146	0.135608	-303.8400754340	-304.405322061	**-304.264046**
NdisTS’	-302.8103316983	0.130948	-303.7036413285	-304.264818910	
NdisTS”	-302.8142990640	0.131305	-303.7083851669	-304.271767750	
CdisTS’	-302.8084016120	0.131051	-303.6966586044	-304.238467370	
CdisTS”	-302.8088782722	0.131338	-303.6960771353	-304.244315176	
NconTS1’	-302.8258076723	0.131611	-303.7186204701	-304.283595573	
$NconTS1_a$”	-302.8318041029	0.132247	-303.7277955740	-304.293443717	**-304.1477485**
$NconTS1_b$”	-302.8387148631	0.133087	-303.7336127380	-304.307086151	**-304.1565024**

CconTS1’	-302.8342550094	0.132362	-303.7286637027	-304.292573920	
CconTS1”	-302.8266871968	0.132188	-303.7191381912	-304.280327288	
NconTS2’	-302.8579700341	0.130918	-303.7471642280	-304.294975744	
NconTS2”	-302.8679603487	0.131180	-303.7567059467	-304.299523558	
CconTS2’	-302.8647380936	0.130944	-303.7527406669	-304.295483333	
CconTS2”	-302.8535195921	0.130730	-303.7403459915	-304.283278600	
NconInt’	-302.8946024660	0.134561	-303.7760106639	-304.334280565	
$NconInt_a$”	-302.8392140314	0.133210	-303.7365206912	-304.310168129	**-304.1625306**
$NconInt_b$”	-302.8979780559	0.134985	-303.7803967063	-304.339154227	
CconInt’	-302.8978176085	0.134888	-303.7790600561	-304.335552596	
CconInt”	-302.8890279445	0.134556	-303.7700277060	-304.326755513	

Bold values are obtained at CCSD(T)/aug- cc-pVTZ//CCSD/cc-pVDZ level.

3,4,5-triazatricyclo[4.1.0.$0^{2,7}$] hept-3-ene (TATCE)

Structure	MCSCF	ZPE	MRMP2	PBEPBE-D3
TATCE	-317.7018181259	0.097622	-318.5983668777	-319.184536393
TAP_1	-317.7612944617	0.097650	-318.6421572698	-319.220672449
TAP_2	-317.7612944617	0.097650	-318.6421572698	-319.220672449
$N1disTS_1$	-317.6174718748	0.092727	-318.5263960453	-319.115340267
$N1disTS_2$	-317.6157311962	0.092735	-318.5229665412	-319.112267448
$N3disTS_1$	-317.6175024882	0.093715	-318.5191920020	-319.112849315
$N3disTS_2$	-317.6147485780	0.093452	-318.5162733931	-319.109702140

Natural Orbital Occupation Numbers for active space orbitals

3,4-diazatricyclo[4.1.0.$0^{2,7}$]hept-3-ene (DATCE)

MOs	21	22	23	24	25	26	27	28	29	30
NdisTS	1.984	1.979	1.969	1.968	1.122	0.879	0.037	0.022	0.021	0.018
CdisTS	1.984	1.979	1.969	1.969	1.089	0.912	0.037	0.022	0.021	0.018
NconTS1	1.983	1.980	1.969	1.951	1.815	0.195	0.042	0.027	0.020	0.017

CconTS1	1.983	1.980	1.969	1.957	1.801	0.207	0.038	0.026	0.020	0.017
NconTS2	1.984	1.979	1.977	1.911	1.259	0.741	0.089	0.022	0.021	0.017
CconTS2	1.984	1.979	1.977	1.911	1.184	0.817	0.089	0.023	0.021	0.017
NconInt	1.984	1.980	1.975	1.923	1.880	0.123	0.075	0.021	0.020	0.018
CconInt	1.984	1.981	1.975	1.924	1.879	0.124	0.074	0.021	0.020	0.018
DATCE	1.984	1.976	1.972	1.967	1.961	0.049	0.029	0.022	0.021	0.020
DAP_1	1.984	1.981	1.977	1.936	1.914	0.090	0.059	0.022	0.020	0.016
DAP_2	1.984	1.981	1.977	1.936	1.914	0.090	0.059	0.022	0.020	0.016

3,4-diazatricyclo[4.1.0.$0^{2,7}$]heptane(DATCA)

MOs	22	23	24	25	26	27	28	29	30	31
NdisTS’	1.983	1.979	1.968	1.967	1.170	0.833	0.038	0.024	0.021	0.018
NdisTS”	1.984	1.979	1.969	1.969	1.231	0.770	0.037	0.023	0.021	0.019
CdisTS’	1.984	1.979	1.968	1.967	1.059	0.943	0.037	0.024	0.021	0.018
CdisTS”	1.983	1.979	1.968	1.968	1.004	0.997	0.038	0.023	0.021	0.018
NconTS1’	1.983	1.980	1.970	1.954	1.774	0.234	0.041	0.027	0.020	0.017
$NconTS1_a$”	1.984	1.978	1.969	1.967	1.786	0.216	0.037	0.022	0.021	0.019
$NconTS1_b$”	1.983	1.981	1.970	1.952	1.886	0.122	0.039	0.029	0.021	0.017
CconTS1’	1.984	1.979	1.969	1.965	1.766	0.237	0.036	0.024	0.020	0.019
CconTS1”	1.983	1.980	1.969	1.956	1.760	0.247	0.040	0.027	0.020	0.018
NconTS2’	1.983	1.978	1.976	1.915	1.241	0.759	0.086	0.024	0.021	0.017
NconTS2”	1.983	1.979	1.976	1.915	1.164	0.835	0.085	0.023	0.021	0.017
CconTS2’	1.983	1.979	1.976	1.910	1.171	0.829	0.090	0.023	0.021	0.017
CconTS2”	1.983	1.979	1.976	1.906	1.215	0.785	0.094	0.022	0.021	0.017
NconInt’	1.984	1.981	1.975	1.923	1.878	0.124	0.076	0.021	0.020	0.018
$NconInt_a$”	1.983	1.981	1.971	1.961	1.874	0.130	0.036	0.026	0.020	0.018
$NconInt_b$”	1.984	1.980	1.975	1.930	1.867	0.135	0.069	0.022	0.020	0.018
CconInt’	1.984	1.981	1.975	1.924	1.877	0.126	0.074	0.021	0.020	0.018
CconInt”	1.984	1.981	1.974	1.920	1.889	0.114	0.079	0.022	0.020	0.018

DATCA	1.984	1.976	1.972	1.966	1.960	0.050	0.028	0.023	0.021	0.021
$DHDAP_1$	1.984	1.981	1.977	1.939	1.908	0.094	0.058	0.023	0.020	0.015
$DHDAP_2$	1.984	1.981	1.978	1.940	1.911	0.091	0.058	0.023	0.020	0.015

Intrinsic Reaction Coordinates for the Four Disrotatory Channels for DATCA Isomerization